ORGANIZING

Latin American Congress on Industrial and Applied Mathematics 2023

FGV SCHOOL OF APPLIED MATHEMATICS

JBMAC

JANUARY 30<sup>TH</sup> -FEBRUARY 3<sup>RD</sup> 2023 FGV, RIO DE JANEIRO, BRAZIL

#### **Plenary speakers**

Alberto Paccanaro -FGV EMAp - Brazil Álvaro José Riascos Villegas -Universidad de los Andes & Quantil -Colombia André Luiz Diniz - CEPEL - Brazil Claudia D'Ambrosio -Ecole Polytechnique & CNRS - France

#### José Luis Aragón Vera -

UNAM - Mexico Juan Carlos De Los Reyes -MODEMAT - Escuela Politécnica Nacional - Ecuador Maya Stein -CMM - Universidad de Chile - Chile

#### Ruben Spies -

IMAL & CONICET - Argentina Soledad Villar -Johns Hopkins University - USA Susana Gómez Gómez -UNAM - Mexico Wil Schilders -TU Eindhoven - The Netherlands

#### **Minicourses**

Graph Coloring - Theory and Application Ana Shirley Ferreira da Silva - Universidade Federal do Ceará - Brazil

Numerical solution of coupled problems in the cardiovascular field Christian Vergara - LABS - Politecnico di Milano - Italy

# BRAZILIAN ORGANIZING COMMITTEE:

Chair: María Soledad Aronna - FGV EMAp Co-chair: Pablo Martín Rodríguez - UFPE Liliane Basso Barichello - UFRGS Sandra Augusta Santos - UNICAMP José Alberto Cuminato - USP & CeMEAI

#### SCIENTIFIC COMMITTEE:

María Esteban - CNRS & Université Paris Dauphine, France Celina Herrera de Figueiredo - UFRJ, Brazil Volker Mehrmann - TU Berlin, Germany Héctor Ramírez Cabrera - CMM - U. de Chile, Chile Claudia Sagastizábal - UNICAMP, Brazil Domingo Alberto Tarzia - Universidad Austral, Rosario, Argentina

#### LOCAL COMMITTEE:

Dayse Haime Pastore - Cefet/RJ Hugo de la Cruz Cancino - FGV EMAp María Soledad Aronna - FGV EMAp Yuri Fahham Saporito - FGV EMAp



MORE INFORMATION AT eventos.fgv.br/laciam-2023







# Proceedings of the

# Latin American Congress on Industrial and Applied Mathematics

January 30th — February 3rd, 2023

Rio de Janeiro, Brazil

Last update on January 30th, 2023

Sponsorship



Center for Center for Mathematical en Area Des pare il Desarrito





Organization



APLICADA



# Committees

#### **Brazilian Organizing Committee**

- ◊ Chair: María Soledad Aronna, FGV EMAp
- ◊ Co-chair: Pablo Martín Rodriguez, UFPE and President of SBMAC
- ◊ Liliane Basso Barichello, UFRGS and ICIAM officer-at-large
- ◊ Sandra Augusta Santos, UNICAMP
- ◊ José Alberto Cuminato, USP and Director of the CeMEAI

### **Scientific Committee**

- ◊ Maria Esteban, CNRS & Université Paris Dauphine, France
- ◊ Celina Herrera de Figueiredo, UFRJ, Brazil
- ◊ Volker Mehrmann, TU Berlin, Germany
- ◊ Héctor Ramírez Cabrera, Center for Mathematical Modeling (CMM) U. de Chile, Chile
- ◊ Claudia Sagastizábal, UNICAMP, Brazil
- Obmingo Alberto Tarzia, Universidad Austral, Rosario, Argentina

## Local Committee

- ◊ Dayse Haime Pastore, Cefet/RJ
- ◊ Hugo de la Cruz Cancino, FGV EMAp
- ◊ María Soledad Aronna, FGV EMAp
- ◊ Yuri Fahham Saporito, FGV EMAp
- ◊ Lucas Machado Moschen, FGV EMAp

# **Practical Information**

The conference will take place at **FGV EMAp** - **5th floor**, **Praia de Botafogo 190**, **Botafogo borough**, **Rio de Janeiro**. FGV EMAp is easily accessible by taxi, bus or metro from Copacabana and the beach area<sup>1</sup>, the lagoon area<sup>2</sup>, the bay area<sup>3</sup> and downtown<sup>4</sup>.

# FGV has a strict dress code on its premises, with no entry allowed when wearing shorts, mini skirts and/or sandals.

During the conference, room 306 will be available as a working office from 8 am to 6 pm.

## **Arriving at FGV EMAp**

Flamengo metro station is the closest to FGV. There are two way outs, A and B. The first one is open between 5h and 0h from Monday to Saturday, and between 5h and 23h on Sundays and holidays. The second one is open between 7h and 20h from Monday to Friday, but it is closer to FGV's back door entrance.



#### **Transport Information**

- Metro's ticket costs R\$6.50 and bus' R\$4.05. Moreover, metro ticket can be paid by contactless card (such as Visa and Mastercard), RioCard and Giro card, such that the last two can be found at the metro stations. Consult more information here.
- Moovit app is helpful for bus and metro schedules and line options, arrival times, and other informations.
- Website with transport information in English.
- Private transport apps (Uber, 99 or InDriver) are usual choices to move around Rio.

<sup>&</sup>lt;sup>1</sup>ex.: Leme, Copacabana, Arpoador, Ipanema, Leblon, Jardim Oceânico.

<sup>&</sup>lt;sup>2</sup>ex.: Jardim Botânico, Gávea.

<sup>&</sup>lt;sup>3</sup>ex.: Botafogo, Flamengo, Catete, Glória.

<sup>&</sup>lt;sup>4</sup>ex.: Cinelância, Carioca, São Cristóvão.

# **Touristic Information**

Information about Rio can be found at the City Official Guide. Also check TripAdvisor, What to do.

#### Transport at the Galeão and Santos Dumont airports

We suggest to take **an accredited taxi** or use the **Uber app**. You can take a taxi at the exit of the terminal. Aerocoop/Aerotaxi company has a counter, the ride to Rio's main areas is about R\$ 60.00 to R\$ 120.00 and it can be payed by card at the counter or by cash to the driver. If you prefer to ride with Uber, you need to follow the signs that start already in the baggage claim. Uber has a dedicated parking area. Further information can be found in the website: https://www.riogaleao. com/passageiros/page/taxis-e-aplicativos, https://www.uber.com/global/en/airports/sdu/.

#### Restaurants

- TripAdvisor, Where to eat
- The 33 Essential Rio de Janeiro Restaurants

#### **Hotel options**

- Yoo2
- Hotel Argentina
- Novotel RJ Praia de Botafogo
- Hotel IBIS Style de Janeiro Botafogo
- Hotel IBIS Rio de Janeiro Botafogo
- Hotel Scorial
- Hostel & Suites Villa 25

#### **Useful Telephone Numbers**

- FGV EMAp: +55 21 3799-5917
- FGV Reception: +55 21 3799–5938
- Police: 190
- Public Ambulance: 192
- Fire Office: 193

#### **Useful E-mails**

- FGV EMAp: emap@fgv.br
- LACIAM: laciam2023@fgv.br

# **Restaurants near FGV**

Restaurant	Address	Comments	
Salsalito	Centro Empresarial Rio, Praia de Botafogo 228, Stores 117 to 119 — Botafogo Link to Google maps	Good self-service restaurant	
Broz	Marquês de Abrantes Street, 216 — Flamengo Link to Google maps	Nice Brazilian barbecue	
Garagem	Jorn. Orlando Dantas Street, 43 — Botafogo Link to Google maps	Usually, there's a waiting line before 1 pm, but the service is quick	
Miako	Farani Street, 20 — Botafogo Link to Google maps	Traditional Japanese food	
Arte SESC Bistrô	R. Marquês de Abrantes, 99 — Flamengo Link to Google maps	Gourmet restaurant at an affordable price	
Mizu	Farani Street, 16 — Botafogo Link to Google maps	Mexican and Japanese food	
Verde Vício	Visconde de Ouro Preto Street, 47 — Botafogo Link to Google maps	Health food restaurant	
Food Court at Botafogo Praia mall	Praia de Botafogo, 400 — Botafogo Link to Google maps	Several options from fast food to Japanese cuisine	
Port's Self Lanchonete	Marquês de Abrantes Street, 214 — Botafogo Link to Google maps	Cheaper self-service option	

	January 30st, 2023	January 31st, 2023				
		January 5130, 2025	February 1st, 2023	February 2nd, 2023		February 3rd, 2023
	Monday					
::30 - 8:10 ::10 - 8:30	Registration Opening (Cultural Center)	Tuesday	Wednesday	Thursday		Friday
	Susana Gómez Gómez Complex Applications of Industry and Environment for Global Optimization Cultural Center	André Luiz Diniz Modelling of nonlinear/nonconvex aspects in SDDP algorithms: experience in the official models applied to the energy planning of the large-scale Brazilian system Cultural Center	Alberto Paccanaro Machine learning algorithms for making inferences on networks and answering questions in biology, medicine and pharmacology Cultural Center	Claudia d'Ambrosio Mathematical Optimization for Urban Air Mobility Cultural Center	08:30-10:10	Thematic Session: IM (317) -> 08:30 CFM 2 (308) -> 08:55
9:15 - 10:00	Juan Carlos De Los Reyes Bilevel learning for inverse problems Cultural Center	Ruben Daniel Spies Diffusion in inverse problems and inverse problems in diffusion Cultural Center	Maya Stein Graph theory: Forbidden subgraphs, Colourings and Applications Cultural Center	José Luis Aragón Vera Pattern formation in Turing systems with space varying diffusion Cultural Center		BIO 5 (307) -> 09:20
0:00 - 10:30	Coffee Break Cultural Center	Coffee Break Cultural Center	10:00 - 10:50: Coffee Break Poster Session 1 Cultural Center	Coffee Break Cultural Center	10:10 - 11:00	Coffee Break Poster Session 2 Cultural Center
):30 - 12:10	Thematic Sessions: BIO 1 (307) CPDE 1 (308) MFG 1 (317) NR 1 (318)	Minicourse Christian Vergara Numerical solution of coupled problems in the cardiovascular field Cultural Center Thematic Sessions: MFG 2 (307) SP 1 (308)	10:50 - 12:30 Thematic Sessions: BIO 3 (307) CFM 1 (308) CPDE 2 (317) NR 2 (318)	Minicourse Christian Vergara Numerical solution of coupled problems in the cardiovascular field Cultural Center Thematic Sessions: MFG 3 (307) SP 2 (308)	11:00 - 11:45	Soledad Villar Machine learning that obeys physical law Cultural Center
2:10 - 13:40	Lunch	Lunch	12:30 - 13:15 Quick lunch (offered by FGV) Cultural Center	Lunch	11:45 - 13:00	Alvaro Riascos Villega Mathematical Models of Crin Prediction, Discrimination, Interpretability and Equilibrit Poster awards & Closu Cultural Center
8:40 - 15:20	Thematic Sessions: ML 1 (307) OC 1 (308) SDE 1 (317)	Thematic Sessions: ML 2 (307) OC 2 (308) SDE 2 (317)	13:15 - 14:00: Wil Schilders Mathematics: key enabling technology for scientific machine learning Cultural Center	Thematic Sessions: FM 2 (307) OC 3 (308) RC 2 (317)		
5:20 - 15:50	Coffee Break Cultural Center	Coffee Break Cultural Center		Coffee Break Cultural Center		
5:50 - 17:30	Thematic Sessions: FM 1 (307) IP (308) RC 1 (317)	Minicourse Ana da Silva Graph Coloring Theory and Application Cultural Center Thematic Sessions: BIO 2 (307) NPDEOPT (308)		Minicourse Ana da Silva Graph Coloring Theory and Application Cultural Center Thematic Session: BIO 4 (307)		
/:40 - 18:40	Panel discussion: New Challenges in the Modern Industrial Mathematics Cultural Center	Panel discussion: Policies focusing on Gender Equality in Applied Math across LATAM Countries Cultural Center				
3:40 - 20:40	Cocktail Cultural Center			19:30: Social Dinner		

Latin American Congress on Industrial and Applied Mathematics, Rio de Janeiro, Brazil, January 30th – February 3rd, 2023

# **Time Schedule**

Monday, January 30th

Hour	Event	Location
7:30 — 8:10	Registration	Main Entrance
8:10 — 8:30	Opening	Cultural Center
8:30 — 9:15	Susana Gómez Gómez Complex Applications of Industry and Environment for Global Optimization <i>Chair: Sandra Santos</i>	Cultural Center
9:15 — 10:00	Juan Carlos De Los Reyes Bilevel learning for inverse problems Chair: María Soledad Aronna	Cultural Center
10:00 — 10:30	Coffee Break	Cultural Center
10:30 — 12:10	Thematic Sessions: BIO 1 / CPDE 1 / MFG 1 / NR 1	Rooms 307 / 308 / 317 / 318
12:10 — 13:40	Lunch	_
13:40 — 15:20	Thematic Sessions: ML 1 / OC 1 / SDE 1	Rooms 307 / 308 / 317
15:20 - 15:50	Coffee Break	Cultural Center
15:50 — 17:30	Thematic Sessions: FM 1 / IP / RC 1	Rooms 307 / 308 / 317
17:40 — 18:40	Panel discussion: New Challenges in the Modern Industrial Mathematics	Cultural Center
18:40 - 20:40	Cocktail	Cultural Center

## Tuesday, January 31st

Hour	Event	Location
8:30 — 9:15	André Luiz Diniz Modeling of nonlinear/nonconvex aspects in SDDP algorithms: experience in the official models applied to the energy planning of the large-scale Brazilian system	Cultural Center
	Chair: Claudia Sagastizábal	

9:15 — 10:00	Ruben Daniel Spies Diffusion in inverse problems and inverse problems in diffusion <i>Chair: Domingo Tarzia</i>	Cultural Center
10:00 - 10:30	Coffee Break	Cultural Center
10:30 — 12:10	Christian Vergara Minicourse: Numerical solution of coupled problems in the cardiovascular field <i>Chair: Sônia Gomes</i>	Cultural Center
	Thematic sessions: MFG 2 / SP 1	307 / 308
12:10 — 13:40	Lunch	
13:40 — 15:20	Thematic Sessions: ML 2 / OC 2 / SDE 2	Rooms 307 / 308 / 317
15:20 - 15:50	Coffee Break	Cultural Center
15:50 — 17:30	Ana da Silva Minicourse: Graph Coloring — Theory and Application <i>Chair: Celina de Figueiredo</i> Thematic Sessions: BIO 2 / NPDEOPT	Cultural Center Rooms 307 / 308
17:40 — 18:40	Panel discussion: Policies focusing on Gender Equality in Applied Math across LATAM Countries	Cultural Center

#### Wednesday, February 1st

Hour	Event	Location	
8:30 — 9:15	Alberto Paccanaro Machine learning algorithms for making inferences on networks and answering questions in biology, medicine and pharmacology <i>Chair: María Soledad Aronna</i>	Cultural Center	
9:15 — 10:00	Maya Stein Graph theory: Forbidden subgraphs, Colourings and Applications Chair: Celina de Figueiredo	Cultural Center	
10:00 — 10:50	Coffee Break Poster session 1	Cultural Center Cultural Center	
10:50 — 12:30	Thematic Sessions: BIO 3 / CFM 1 / CPDE 2 / NR 2	Rooms 307 / 308 / 317 / 318	

12:30 — 13:15	Quick Lunch (offered by FGV)	Cultural Center
13:15 — 14:00	Wil Schilders Mathematics: key enabling technology for scientific machine learning Chair: José Alberto Cuminato	Cultural Center

### Thursday, February 2nd

Hour	Event	Location
8:30 — 9:15	Claudia d'Ambrosio Mathematical Optimization for Urban Air Mobility Chair: Alvaro Riascos	Cultural Center
9:15 — 10:00	José Luis Aragón Vera Pattern formation in Turing systems with space varying diffusion Chair: Pablo Martín Rodríguez	Cultural Center
10:00 — 10:30	Coffee Break	Cultural Center
10:30 — 12:10	Christian Vergara Minicourse: Numerical solution of coupled problems in the cardiovascular field <i>Chair: Sônia Gomes</i> Thematic sessions: MFG 3 / SP 2	Cultural Center Rooms 307 / 308
12:10 — 13:40	Lunch	_
13:40 — 15:20	Thematic Sessions: FM 2 / OC 3 / RC 2	Rooms 307 / 308 / 317
15:20 - 15:50	Coffee Break	Cultural Center
15:50 — 17:30	Ana da Silva Minicourse: Graph Coloring — Theory and Application <i>Chair: Celina de Figueiredo</i> Thematic Sessions: BIO 4	Cultural Center Room 307
19:30	Social dinner	Fogo de Chão Botafogo

Friday, February 3rd

Hour	Event	Location
8:30 — 10:10	Thematic Sessions: BIO 5 (starts at 09:20) / CFM 2 (08:55) / IM (08:30)	Rooms 307 / 308 / 317
10:10 - 11:00	Coffee Break	Cultural Center
10:10 - 11:00	Poster session 2	Cultural Center
11:00 — 11:45	Soledad Villar Machine learning that obeys physical law Chair: Juan Carlos de Los Reyes	Cultural Center
11:45 — 13:00	Alvaro Jose Riascos Villegas Mathematical Models of Crime: Prediction, Discrimination, Interpretability and Equilibrium <i>Chair: Pablo Martín Rodríguez</i>	Cultural Center
	Poster awards & Closure	Cultural Center

(\*) All of the rooms are on the 3rd floor of the building just in front of the Cultural Center. You should use the access card.

# **Roundtables**

#### New Challenges in the Modern Industrial Mathematics

Monday, January 30th — 17:40 — 18:40 — Cultural Center *Chair:* José Alberto Cuminato, *USP* (Brazil)

#### **Speakers:**

- Hasnaa Zidani, INSA Rouen Normandie (France);
- ◊ Héctor Ramírez, Universidad de Chile & CMM (Chile);
- ◊ Wil Schilders, *TU Eindhoven & ICIAM* (The Netherlands).

#### Policies focusing on Gender Equality in Applied Math across Latin American Countries

**Tuesday, January 31st — 17:40 — 18:40 — Cultural Center** *Chair:* Maria Eulália Vares, *UFRJ* (Brazil)

#### **Speakers:**

- ◊ Javiera Barrera, Adolso Ibañez University (Chile);
- ♦ Liliane Basso Barichello, UFRGS (Brazil);
- ♦ Marilaine Colnago, UNESP (Brazil).

# **Thematic Sessions**

#### **Biomathematics (BIO)**

**Organizers:** Pedro Gajardo, *Universidad Técnica Federico Santa María-Valparaíso* (Chile) Olga Vasilieva, *Universidad del Valle* (Colombia)

(BIO 1) Monday, January 30th — 10:30 — 12:10 — Room 307

Chair: Olga Vasilieva

- Josenildo Lima (Brazil);
- Jose Luis Orozco Gonzales (Colombia);
- Carmen Alicia Ramírez Bernate (Colombia);
- Edwin Barrios Rivera (Colombia).

#### (BIO 2) Tuesday, January 31st — 15:50 — 17:30 — Room 307

Chair: Olga Vasilieva

- Michael Robert (USA);
- Juan Vicente Bogado Machuca (Paraguay);
- Mario Julian Cañon Ayala (Colombia);
- Heliana Arias Castro (Colombia).
- (BIO 3) Wednesday, February 1st 10:50 12:30 Room 307

Chair: Olga Vasilieva

- Pablo Aguirre (Chile);
- Fernando Córdova-Lepe (Chile);
- Rodrigo Gutierrez (Chile).
- Flávio Codeço Coelho (Brazil).

#### (BIO 4) Thursday, February 2nd — 15:50 — 17:30 — Room 307

Chair: Olga Vasilieva

- Padmanabhan Sechaiyer (USA);
- Viswanathan Arunachalam (Colombia);
- Luiz Max Carvalho (Brazil);
- Victor Riquelme (Chile).

#### (BIO 5) Friday, February 3rd — 09:20 — 10:10 — Room 307

Chair: Olga Vasilieva

• Michel de Lara (France).

# Novel Computational Methods for Coupled and Non-linear Problems Arising in Complex Fluid Mechanics (CFM)

**Organizers:** Sergio González Andrade, *Escuela Politécnica Nacional* (Ecuador) Paúl E. Méndez, *Escuela Politécnica Nacional* (Ecuador)

#### (CFM 1) Wednesday, February 1st - 10:50 - 12:30 - Room 308

- Andrea Ceretani (Argentina);
- Paúl E. Méndez (Ecuador);
- Philippe Devloo (Brazil).

#### (CFM 2) Friday, February 3rd — 08:55 — 10:10 — Room 308

- Sergio González-Andrade (Ecuador);
- Raimund Bürger (Chile);
- Sônia Gomes (Brazil).

#### **Control and Stabilization for Partial Differential Equations (CPDE)**

**Organizers:** Roberto Capistrano Filho, *UFPE* (Brazil) Victor Hugo Gonzalez, *UFPE* (Brazil)

#### (CPDE 1) Monday, January 30th — 10:30 — 12:10 — Room 308

- Juan Límaco (Brazil);
- Fernando Gallego (Colombia);
- Patrício Guzman (Chile);
- Eduardo Cerpa (Chile).

#### (CPDE 2) Wednesday, February 1st — 10:50 — 12:05 — Room 317

- Constanza Sánchez de la Vega (Argentina);
- Victor Hugo Gonzalez Martinez (Brazil).

#### **Financial Mathematics (FM)**

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Organizers: Beatrice Acciaio, Department of Mathematics, ETH Zurich (Switzerland)
Ernesto Mordecki, Centro de Matematica, Universidad de la República (Uruguay)
Yuri Saporito, FGV EMAp (Brazil)
Max O. Souza, UFF (Brazil)
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#### (FM 1) Monday, January 30th — 15:50 — 17:30 — Room 307

- Beatrice Acciaio (Switzerland);
- Max Souza (Brazil);
- Sebastian Jaimungal (Canada);
- Ernesto Mordecki (Uruguay).

#### (FM 2) Thursday, February 2nd — 13:40 — 15:20 — Room 307

- Sergio Pulido (France);
- Yuri Saporito (Brazil);
- Andrés Ricardo Sosa-Rodríguez (Uruguay);
- Julio Backhoff-Veraguas (Austria).

#### Industrial Mathematics in Brazilian research centers (IM)

#### Organizer: LACIAM Organizing Committee

#### (IM) Friday, February 3rd — 08:30 — 10:10 — Room 317

Chair: Cláudio Struchiner (Brazil)

- Geraldo Silva (Brazil);
- Lucas Nissenbaum (Brazil) and Thiago Ramos (Brazil);
- Marcio A. Murad (Brazil);
- Vincent G. Y. Guigues (Brazil).

#### Direct and Inverse Problems in Particle and Radiation Transport (IP)

Organizer: Cássio B. Pazinatto, IFSul, Cordenadoria de Matemática, Pelotas, RS (Brazil)

#### (IP) Monday, January 30th — 15:50 — 17:30 — Room 308

Chair: Liliane Basso Barichello

- Enzo L. Gaggioli (Argentina);
- Mohsen Alaeian (Brazil);
- Ricardo C. Barros (Brazil);
- Cássio B. Pazinatto (Brazil).

#### New developments in Mean Field Games and Hamilton-Jacobi equations (MFG)

**Organizers:** Daniela Tonon, *Università di Padova* (Italy) Adriano Festa, *Politecnico di Torino* (Italy) Francisco José Silva Álvarez, *Université de Limoges* (France)

#### (MFG 1) Monday, January 30th — 10:30 — 12:10 — Room 317

- Francisco J. Silva (France);
- Athena Picarelli (Italy);
- Elisa Calzola (Italy);
- Luis Briceño Arias (Chile).

#### (MFG 2) Tuesday, January 31st — 10:30 — 12:10 — Room 307

- Juliàn Gutiérrez (Saudi Arabia);
- Daniela Tonon (Italy);
- Guilherme Mazanti (France);
- Roberto Guglielmi (Canada).

#### (MFG 3) Thursday, February 2nd — 10:30 — 12:10 — Room 307

- Elisabetta Carlini (Italy);
- Adriano Festa (Italy).

#### Mathematical Linguistics (ML)

#### **Organizers:** Alexandre Rademaker, *FGV EMAp* (Brazil) Leonel Figueiredo de Alencar, *UFC* (Brazil)

#### (ML 1) Monday, January 30th — 13:40 — 15:20 — Room 307

Chair: Alexandre Rademaker

- Katiuscia de Moraes Andrade (Brazil);
- Francis Bond (Czechia);
- Paulo Cavalin (Brazil);
- Pablo Calcina Ccori (Peru).

#### (ML 2) Tuesday, January 31st — 13:40 — 15:20 — Room 307

Chair: Alexandre Rademaker

- Dan Flickinger (USA);
- Alexandre Rademaker (Brazil);
- Guilherme Sales (Brazil);
- João Santos (Brazil).

#### Trends in numerical methods and approximation for PDE-constrained optimization (NPDEOPT)

Organizers: P. Merino (Ecuador) and E. Otarola (Chile)

## (NPDEOPT) Tuesday, January 31st — 15:50 — 17:30 — Room 308

Chair: Pedro Martín Merino Rosero

- Sofía López (Ecuador);
- Christian Meyer (Germany);
- Luis Briceño (Chile);
- Pedro Merino (Ecuador).

## Mathematical methods in Network Reliability (NR)

**Organizers:** Javiera Barrera M., *Faculty of Engineering and Science* (Chile) Eduardo Moreno, *Universidad Adolfo Ibáñez* (Chile) Latin American Congress on Industrial and Applied Mathematics, Rio de Janeiro, Brazil, January 30th - February 3rd, 2023

#### (NR 1) Monday, January 30th — 10:30 — 12:10 — Room 318

Chair: Javiera Barrera

- Pablo Romero (Uruguay);
- Dora Jiménez-Álvarez (Chile);
- Eduardo Moreno (Chile).

#### (NR 2) Wednesday, February 1st — 10:50 — 12:30 — Room 318

Chair: Eduardo Moreno

- Mario Estrada (Colombia);
- Javiera Barrera (Chile);
- Héctor Cancela (Uruguay);
- Gerardo Rubino (France).

#### **Optimal control theory and applications (OC)**

**Organizers:** Geraldo Nunes Silva, *UNESP* (Brazil) Valeriano Antunes de Oliveira, *UNESP* (Brazil)

#### (OC 1) Monday, January 30th — 13:40 — 15:20 — Room 308

Chairs: Geraldo Silva and Valeriano A. de Oliveira

- Héctor Ramírez (Chile);
- Jorge Becerril (Mexico);
- Karla L. Cortez (Mexico).

#### (OC 2) Tuesday, January 31st — 13:40 — 15:20 — Room 308

Chair: Valeriano A. de Oliveira

- Geraldo Silva (Brazil);
- Valeriano Antunes de Oliveira (Brazil);
- Domingo A Tarzia (Argentina).

#### (OC 3) Thursday, February 2nd — 13:40 — 15:20 — Room 308

Chair: Geraldo Silva

- Ulcilea Leal (Brazil);
- Ana Paula Chorobura (Brazil);
- Hasnaa Zidani (France);
- Closing discussion.

#### Mathematical foundations of robot control (RC)

Organizers: Gennaro Notomista, University of Waterloo (Canada) Roberto Guglielmi, University of Waterloo (Canada)

#### (RC 1) Monday, January 30th — 15:50 — 17:30 — Room 317

Chair: Roberto Guglielmi

- Alvaro Javier Prado Romo (Chile);
- Yue Hu (Canada);
- Luis Guerrero-Bonilla (Mexico).

#### (RC 2) Thursday, February 2nd — 13:40 — 15:20 — Room 317

Chair: Gennaro Notomista

- Gennaro Notomista (Canada);
- Valdir Grassi Jr (Brazil);
- Marco H. Terra (Brazil);
- Dylan Shell (USA);
- Closing discussion.

#### Recent contributions in stochastic differential equations (SDE)

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Organizers: Hugo de la Cruz, FGV EMAp (Brazil)
Juan Carlos Jimenez, ICIMAF (Cuba)
Zochil González Arenas, UERJ (Brazil)
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#### (SDE 1) Monday, January 30th — 13:40 — 15:20 — Room 317

Chair: Carlos Mora

- Márcia Cristina Anderson Braz Federson (Brazil);
- Nikolai Vasilievich Chemetov (Brazil);
- Zochil Gonzalez Arenas (Brazil);
- Daniel Barci (Brazil).

#### (SDE 2) Tuesday, January 31st — 13:40 — 15:20 — Room 317

Chair: Márcia Cristina Anderson Braz Federson

- Christian Horacio Olivera (Brazil);
- Hugo de la Cruz (Brazil);
- Carlos Mora (Chile).

#### Special topics in stochastic processes, random structures, and applications (SP)

Organizer: Anatoli Iambartsev, USP (Brazil)

#### (SP 1) Tuesday, January 31st — 10:30 — 12:10 — Room 308

Chair: Pablo Martin Rodriguez (Brazil)

- Aline Duarte (Brazil);
- Anatoly Yambartsev (Brazil);
- Andressa Cerqueira (Brazil);
- Artem Logachev (Russia).

#### (SP 2) Thursday, February 2nd — 10:30 — 12:10 — Room 308

Chair: Anatoli Iambartsev

- Maria Eulalia Vares (Brazil);
- Fabio M. L. S. M. Lopes (Chile);
- Manuel González-Navarrete (Chile);
- Nevena Maric (Serbia).

Latin American Congress on Industrial and Applied Mathematics, Rio de Janeiro, Brazil, January 30th — February 3rd, 2023

# **Detailed Conference Program**

Only the name of the speakers is shown in the program. The name of all co-authors can be found in the corresponding abstract and in the Index of Authors.

Committees

Practical Information

Table of Restaurants

Time Schedule

Roundtables

Thematic Sessions

## **Minicourses**

- 1 Numerical solution of coupled problems in the cardiovascular field *Christian Vergara*
- 3 Graph Coloring Theory and Application *Ana da Silva*

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- 5 Bilevel learning for inverse problems *Juan Carlos De los Reyes*

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- 7 Genetic algorithm for establishing Wolbachia in wild populations of Aedes aegypti mosquitoes Jose Luis Orozco Gonzales, Antone dos Santos Benedito, Helenice de Oliveira, Florentino Silva, Claudia Pio Ferreira and Olga Vasilieva
- 8 A reaction-diffusion model for the control of the Aedes aegypti vector using sterile mosquitoes in the city of Cali Carmen Alicia Ramírez Bernate and Héctor J. Martínez-Romero
- 9 Optimal dengue control in a two-patch model with limited resources *Edwin Barrios Rivera and Olga Vasilieva*

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- 11 Stabilization of a time delayed for a generalized dispersive system *Fernando A. Gallego*
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- 16 On regularized optimal execution problems and their singular limits *Max O. Souza*
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- 79 Graph theory: Forbidden subgraphs, Colourings and Applications *Maya Stein*
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- 91 Limiting behavior of the reliability function for mixed coherent systems with Lévy-frailty Marshall-Olkin dependent failure times Javiera Barrera, Guido Lagos, Pablo Romero, and Juan Valencia
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- 104 On distinct notions of tensor rank and practical implications to the higher-order completion problem João Luiz Santos Gomes and Sandra Augusta Santos
- 105 A shape optimization approach to approximation of measures João Miguel Machado, Antonin Chambolle, and Vincent Duval
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- 109 An Adaptive strategy for avoiding stagnation on restarting GMRES Juan C. Cabral and Christian E. Schaerer
- 110 Food distribution model using the goal programming approach Letícia Ferreira Godoi, Flávia Queiroga Aranha, and Daniela Renata Cantane
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- 153 A RDE-based approach for the numerical simulation of a Stochastic SVIR model *Mario Muños, Hugo De la Cruz, and Carlos Manuel Mora*
- 154 On restricting the infected population peak of a SIR modeled epidemic by a reduced intervention *Martín Ignacio Errázquin and Graciela Adriana González*
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- 156 Final size and error estimates for a two-group SEIRD model Matheus Santos and Alison Melo
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# Numerical solution of coupled problems in the cardiovascular field

#### CHRISTIAN VERGARA

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Keywords: Cardiovascular mathematics, coupled problems, coupling enditions

The cardiovascular system functioning is characterized by the interaction among heterogeneous processes [1]. The mathematical and numerical description of such problems is obtained by considering the coupling among non-linear partial differential equations describing the processes at hand. Heterogeneity of the coupling could be given by:

- (a) the interaction among different physical processes;
- (b) different mathematical models used for the same physical process in different regions;
- (c) the same mathematical model written in domains with different geometric detail.

The numerical solution of such problems is highly challenging and, in particular, it is fundamental to account for the following issues:

- (a) write suitable interface or in general coupling conditions;
- (b) study the numerical solution of the coupled problem by monolithic and partitioned schemes;
- (c) study the stability of partitioned schemes in the cardiovascular regimes;
- (d) verify the applicability of the method to real contexts obtained by medical images;
- (e) discuss the computational effort needed by the numerical schemes.

In this mini-course we provide possible numerical solutions of cardiovascular coupled problems. Examples are: the fluid-structure interaction arising between blood and vessel wall and the electro-mechanical coupling of the cardiac function [1] (for coupling of type a); the Stokes-Darcy coupling arising in the cardiac perfusion modeling [2, 3] (for coupling of type b); the geometric multiscale approach for blood dynamics [4] (for coupling of type c). For each problem we discuss its mathematical formulation together with suitable numerical schemes for its accurate, stable and efficient solution. For some problems also some practical academic examples will be provided by running together some computational codes.

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# Graph Coloring - Theory and Application

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Keywords: Graph coloring, chromatic number, coloring algorithms

Graph coloring problems are without a doubt among the most studied problems in graph theory. This interest can be explained not only by the broad range of real-life situations that can be modeled as graph coloring problems (for instance, it can model frequency assignment, scheduling, clustering, etc), but also by its unapparent relation to other graph parameters (for instance, the Erdős-Stone-Simonovits Theorem relates the chromatic number of a graph G with the maximum edges allowed in any graph H not containing a copy of G). In this course, we will learn some of the classic theoretical results concerning graph coloring, and will then use it to model real-life problems.

Knowledge of basic graph theory concepts is recommended. For the theoretical results, we will be following mainly Douglas West's textbook [1].

#### Bibliography

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# Complex Applications of Industry and Environment for Global Optimization

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Keywords: Global Optimization, Oil and Water Reservoirs, Parameter Identification

We will present two cases of complex problems, that require Global Optimization and analyze the challenges from the optimization point of view:

- (a) Modeling the movement of oil spills in the sea in the case of accidents, and how to model the cleaning process using skimmer ships that follow an optimal trajectory, to minimize the oil that could arrive to the coast.
- (b) Find the solution of an inverse parameter identification problem to characterize the porous media, to be able to predict the production of wells in reservoirs of oil and of water. This inverse problem is highly nonlinear and a big challenge to Optimization.

# Bilevel learning for inverse problems

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Keywords: Inverse problems, bilevel optimization, imaging, data assimilation

In recent years, novel ideas have been applied to several inverse problems in combination with machine learning approaches, to improve the inversion by optimally choosing different parameters of interest. A fruitful approach in this sense is bilevel optimization, where the inverse problems are considered as lower-level constraints, while on the upper-level a loss function based on a training set is used. When confronted with inverse problems with sparsity-based regularizers [3, 5, 4, 2] or nonlinear dynamics [1, 6, 7], however, the bilevel optimization problem structure becomes quite involved, and classical nonlinear or bilevel programming results cannot be directly utilized.

In this talk, I will present the general setting of bilevel inverse problems and discuss the main theoretical challenges, as well as the applicability to relevant practical instances. Particular attention will be paid to imaging problems with sparsity-based regularizers and nonlinear inverse problems arising in variational data assimilation. The main difficulties related to the reformulation as single level problems, the derivation of optimality conditions and the numerical solution will be addressed.

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# Optimization of the Aedes aegypti control using Wolbachia

JOSENILDO LIMA<sup>1</sup>, AMÁLIA VASCONCELOS<sup>2</sup>, AND RODRIGO CARDOSO<sup>3</sup>

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In this study, we developed a partial differential equation model with parameters dependent on temperature and rainfall that analyzes the dynamics of diseases transmitted by the *Aedes aegypti* to humans. We formulated a mono-objective optimization problem to minimize the mosquito population and the time spent in control, applying mosquitoes infected with *Wolbachia* during the summer to decrease the number of infected humans. We used operator decomposition, finite differences, fourth-order Runge-Kutta, and the Real Biased Genetic Algorithm for numerical and computational simulations.

Keywords: Wolbachia, Partial differential equations, Mono-objective optimization

# Genetic algorithm for establishing *Wolbachia* in wild populations of *Aedes aegypti* mosquitoes

Jose Luis Orozco Gonzales<sup>1</sup>, Antone dos Santos Benedito<sup>2</sup>, Helenice de Oliveira Florentino Silva<sup>3</sup>, Claudia Pio Ferreira<sup>4</sup>, and Olga Vasilieva<sup>5</sup>

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Keywords: Wolbachia, Aedes aegypti mosquitoes, genetic algorithm, release strategies

Wolbachia is an endosymbiotic intracellular bacterium that is not naturally present in wild Aedes aegypti mosquitoes but can be transgenically transmitted to them by microinjections. When a female mosquito carries Wolbachia in her cells, she loses the ability to transmit dengue and other arboviral infections when biting people. The bacterium also grants a reproductive advantage to infected mosquitoes over non-infected insects through maternal transmission and cytoplasmic incompatibility phenotype. Depending on the ambient temperatures, these two features may be either perfect or imperfect. The latter defines whether a total population replacement or a stable coexistence of the wild and Wolbachia-infected populations can be achieved. The Wolbachia-based biological control of arboviral human infections consists in releasing Wolbachia-carrying mosquitoes seeking a total or partial replacement of the wild population as a final goal.

This presentation will briefly review a *Wolbachia* invasion model that can be adapted to two major *Wolbachia* strains, *wMel* and *wMelPop*, both of which undergo testing in field releases. Furthermore, we will showcase the implementation of the genetic algorithm to optimize the release strategies for each *Wolbachia* strain by minimizing the total quantity of the released insects together with the overall time and different frequencies of releases.

# A reaction-diffusion model for the control of the *Aedes aegypti* vector using sterile mosquitoes in the city of Cali

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Keywords: Aedes aegypti, sterile mosquitoes, reaction-difusion, control strategies

In recent years, the Public Health agencies in the city of Cali have tried through different mechanisms to reduce the population of the *Aedes aegypti* mosquito, achieving their objective to a certain extent, although these are still insufficient for the eradication of the viruses that this mosquito transmit.

We formulate a model in EDP that considers the effects of geographic dispersion and spatial heterogeneity. In this model, the oviposition, maturation, and natural mortality rates vary according to the temperatures of the city of Cali in the dry and wet periods. Control is introduced by sterile mosquitoes that decrease the population. Numerical simulations are carried out, under different sterile mosquito release strategies, which are analyzed in terms of the distribution and size of the population in space-time in a particular region of the city of Cali. Subsequently, conditions are characterized under which the use of sterile mosquitoes can become an efficient strategy to reduce the population of fertilized females with viable eggs at a low social cost.
## Optimal dengue control in a two-patch model with limited resources

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Keywords: Dengue, Optimal control theory, Isoperimetric constraints

There are many diseases that can be spread by the mobility of people and dengue fever is one of them. This disease is one of the most important public health problems in tropical and subtropical countries. In particular, in and around the city of Cali (Colombia), dengue is endemic. Due to the overpopulation of large cities, many people now decide to reside in smaller municipalities near the big cities and to commute for work, study, or leisure. Therefore, voluntary or forced mobility of people continues to be a key element in the transmission of dengue and other diseases.

In order to study and analyze the impact of mobility of people on dengue transmission, an epidemiological model of type SEI-SEIR(S) was proposed of two patches [1], where the mobility of people occurs by means of the times of permanence of a person in a certain patch [3]. In addition, we include in our model the concept of "effective population" (originally introduced in [2]) which allows to visualize the effect that the intensity of people flow between two patches has on the spread of the disease.

Because the budget allocated to vector control programs is not unlimited, we propose to design the control policies capable of reducing the incidence of dengue fever in a way that suits the total budget assigned for both patches. Using the optimal control approach, the goal of control intervention is to minimize the proportion of infected people residing in both patches while trying to allocate the implementation costs within the frameworks of the common budget constraint.

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# Local null controllability of a quasi-linear parabolic equation in dimensions 2 and 3

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Keywords: Controllability, parabolic equations

In this work, we studied the null controllability in dimension 2 and 3 of the following model,

$$\begin{cases} y_t - \nabla \cdot (a(y)\nabla y) = v \mathbf{1}_{\omega}, & (x,t) \in Q = \Omega \times (0,T) \\ y = 0, & (x,t) \in \Sigma = \partial \Omega \times (0,T) \\ y(0) = y_0, & x \in \Omega, \end{cases}$$

where  $a : \mathbb{R} \to \mathbb{R}$  is a  $C^3$  function that possess bounded derivatives and 0 < m < a(r) < M.

## Stabilization of a time delayed for a generalized dispersive system

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Keywords: Stabilization, time-delayed

In this manuscript we study the asymptotic behavior of the solution of the time-delayed higher order dispersive systems posed in the real line. Under suitable assumptions on the time delay coefficients we prove that the system under consideration is exponentially stable in two different ways. First, if the coefficient of the delay term is bounded from below by a positive constant, we use the Lyapunov approach to prove that the energy associated to the solution of the higher order dispersive system decays exponentially. After that, we extend this result to the case in which the coefficient of the undelayed feedback is also indefinite. Both problems are investigated when the exponent p in the nonlinear term ranges over the interval [1, 2j) where 2j + 1 is the order of the dispersive system.

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## Stabilization of partial differential equations with disturbances

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**Keywords:** Heat equation, boundary disturbance, feedback stabilization, Backstepping, Lyapunov techniques

In this talk we shall discuss the stabilization of partial differential equations subjected to disturbances. We shall review some recent results and then we shall address the rapid stabilization of the heat equation with boundary disturbance, where the sign multivalued operator is used to reject the effects of the disturbance.

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## Singular Perturbation Method for a KdV-ODE coupled system

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Keywords: infinite-dimensional systems, time scales, Korteweg-de Vries equation

This talk considers systems coupling an ordinary differential equation (ODE) with a Kortewegde Vries equation through its boundary data. The main focus is put on the role of different time scales on the stability of the coupled system. We study the Singular Perturbation Method [4], which is a well-established tool in finite-dimension. For PDEs there is some recent work considering first-order [6, 7, 8] and second order hyperbolic systems coupled to ODEs [2, 3]. In a joint work with Swann Marx (Nantes) [5] we get stability and Tikhonov-type results for our system involving the Korteweg-de Vries equation. A fundamental tool is the Lyapunov function introduced in [1].

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## Quantifying arbitrage

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Keywords: Arbitrage, Wasserstein distance

In this talk I will present a way to quantify arbitrage, that allows to deal with model uncertainty without imposing the no-arbitrage condition. In markets that admit "small arbitrage', we can still make sense of the problems of pricing and hedging. The pricing measures here will be such that asset price processes are close to being martingales, and the hedging strategies will need to cover some additional cost. We show a quantitative version of the Fundamental Theorem of Asset Pricing and of the Super-replication theorem. We study robustness of the amount of arbitrage and existence of respective pricing measures, showing stability with respect to a new, strong adapted Wasserstein distance.

## On regularized optimal execution problems and their singular limits

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Keywords: Portfolio execution problem, stochastic

We investigate the portfolio execution problem under a framework in which volatility and liquidity are both stochastic. Iliquidity costs arise as temporary price impacts, and are modelled through a power law of the agent turnover rate. We begin by analysing a regularised setting, where the admissible strategies do not ensure full execution. The constraint problem is obtained as a singular limit of the regularised one. As a byproduct of our analysis, we obtain a numerical algorithm with useful convergence properties.

## Risk Budgeting Allocation for Dynamic Risk Measures

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Keywords: Dynamic Risk Measures, Portfolio Allocation, Risk Parity, Reinforcement Learning

We develop an approach for risk budgeting allocation – a risk diversification portfolio strategy – where risk is measured using time-consistent dynamic risk measures. For this, we introduce a notion of dynamic risk contributions that generalise the classical Euler contributions and which allow us to obtain dynamic risk contributions in a recursive manner. Moreover, we show how the risk allocation problem may be recast as a convex optimisation problem and develop an actor-critic approach to solve for risk allocations using deep learning techniques.

## Multiple interval stopping rules in American perpetual options

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Keywords: Perpetual American Options, Optimal stopping, Diffusions

Considering a real-valued diffusion, a real-valued reward function and a positive discount rate, we provide an algorithm to solve the optimal stopping problem consisting in finding the optimal expected discounted reward and the optimal stopping time at which it is attained. Our approach is based on Dynkin's characterization of the value function. The combination of Riesz's representation of excessive functions and the inversion formula gives the density of the representing measure, being only necessary to determine its support. This last task is accomplished through an algorithm. The proposed method always arrives to the solution, thus no verification is needed, giving, in particular, the shape of the stopping region. Generalizations to diffusions with atoms in the speed measure and to non smooth payoffs are analyzed.

Applications to pricing perpetual contracts with multiple disconnected interval stopping regions are discussed.

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## Parallel inverse-problem solver for time-domain optical tomography with perfect parallel scaling

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Keywords: Optical tomography, radiative transfer, inverse problem

This talk presents an efficient *parallel* radiative transfer-based inverse-problem solver for time-domain optical tomography [1]. The radiative transfer equation provides a physically accurate model for the transport of photons in biological tissue, but the high computational cost associated with its solution has hindered its use in time-domain optical-tomography and other areas. In this talk we describe how this problem can be tackled by means of a number of computational and modeling innovations, including 1) The incorporation of a high-order spectral method (Fourier continuation discrete ordinates method (FC–DOM) [2]) 2) A spatial paralleldecomposition strategy with *perfect parallel scaling* for the forward and inverse problems of optical tomography on parallel computer systems; and, 3) A Multiple Staggered Source method (MSS) that solves the inverse transport problem at a computational cost that is *independent of* the number of sources employed, and which significantly accelerates the reconstruction of the optical parameters: a six-fold MSS acceleration factor was demonstrated. Finally, our contribution presents 4) An intuitive derivation of the adjoint-based formulation for evaluation of functional gradients, including the highly-relevant general Fresnel boundary conditions—thus, in particular, generalizing results previously available for vacuum boundary conditions. Solutions of large and realistic 2D inverse problems are presented, which were produced on a 256-core computer system. The combined parallel/MSS acceleration approach reduced the required computing times by several orders of magnitude, from months to a few hours. Further optimization, in progress, which could significantly improve reconstruction accuracy and computing times, will implement the correct resolution of boundary layers [3].

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## PHOTOACOUSTIC TEMPERATURE MEASUREMENTS DURING HYPERTHERMIA THERMAL TREATMENT OF CANCER

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**Keywords:** Kalman filter, state estimation problem, hyperthermia, cancer treatment, photoacoustic temperature measurement, bioheat transfer

Among thermal treatments, Hyperthermia with laser heating can be a noninvasive alternative for the treatment of more superficial tumors in the body. Temperature levels and time of exposure to high temperatures are two facts, on which thermal damage of tissue is dependent; Thus, accurate techniques are required for monitoring the temperature in the target region of interest. In this work, the couple of laser hyperthermia treatment of cancer is to the photoacoustic technique is considered as a direct problem and in continue, temperature measurement of internal tissues is determined by solving a state estimation problem with the Kalman filter. The hyperthermia treatment is defined as the region of interest which is continuously heated by a laser, while another laser is sequentially pulsed over the same heated surface to generate acoustic pressure waves. The observation model is derived from the photoacoustic problem, which is linear with respect to the local internal temperatures of the tissues. The evolution model given by the bioheat transfer problem is also supposed linear and uncertainties are modeled as additive and Gaussian. Therefore, the Kalman filter provides the optimal solution to the state estimation problem considered in this work. Simulated nonintrusive acoustic pressure measurements are used in inverse analyses for two test cases, with different dimensions and locations of a tumor in a two-dimensional region. In order to enhance the local absorption of the laser energy and to reduce thermal damage to normal cells, The simulated tumors are supposed loaded with nanoparticles. The Kalman filter estimated accurate and stable temperature distributions, even in the tumor region that involved large gradients. Moreover, uncertainties in the Kalman filter estimates were smaller than those resulting from the direct simulation of the photoacoustic thermometry problem.

## On a Linear-Linear Response Matrix Spectral Nodal Method for Discrete Ordinates Neutral Particle Transport Computational Modeling

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**Keywords:** Linear-Linear Response Matrix Spectral Nodal Method, Neutral Particle Transport Computational Modeling

In this work, a Linear-Linear Response Matrix Spectral Nodal method for monoenergetic neutral particle transport problems with isotropic scattering and discrete ordinates approximation in rectangular Cartesian geometry is presented. It solves the transverse integrated discrete ordinates transport equations considering linear approximations for the leakage terms in both X and Y coordinate directions by using first-order Legendre polynomials. Also, the scattering terms are treated analytically and the general solution of this highly coupled system of linear ordinary differential equations is used for the Response Matrix reconstruction that can be applied with the Partial or Full Bock Invertion iterative sweep across the spatial discretization grid. With this approach, continuous numerical results between nodes are expected to preserve the linear system's analytical solutions and satisfy the prescribed boundary conditions. Also, the method is expected to be more accurate when compared to the companion spectral nodal methods with constant approximations for the transverse leakage terms.

## On the use of the adjoint operator in estimating neutral particles sources

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Keywords: source estimation problems, analytical discrete ordinates, adjoint operator

The adjoint transport operator has been applied as a mathematical tool to solve several significant problems in nuclear safety, optical tomography, oil well logging, thermal radiation in medical applications, and many others. In such problems, we are often concerned with estimating the spatial distribution and intensity of internal sources of neutral particles. In this work, we use the adjoint to the transport operator to derive a linear model that relates the absorption rate measurements of a series of internal particle detectors with the coefficients of the source expansion on a given basis.

We consider two-dimensional (XY-geometry) monoenergetic transport problems and develop a nodal variant of the adjoint version of the Analytical Discrete Ordinates (ADO) method to write spatially explicit solutions for the averaged x and y adjoint fluxes. This way, we can use explicit expressions to derive closed-form formulas for the absorption rates. Then, we use either the Tikhonov iterative technique or the Metropolis-Hastings algorithm for the Markov chain Monte Carlo method within the Bayesian framework to estimate localized two-dimensional piecewise constant from noise measurements. Considering 1% of white gaussian noise, we were able to localize the sources of neutral particles in every test problem, as well as their magnitude. Moreover, using closed-form expressions provided by the ADO formulation allowed a relevant reduction in computational time.

## A Lagrange-Galerkin scheme for first order mean field games systems

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Keywords: Mean field games, Lagrange-Galerkin schemes, convergence results.

In this work, we consider a standard first order Mean Field Games (MFG) system [4]:

$$\begin{aligned} -\partial_t v + H(x, \nabla v) &= F(x, m(t)) \quad \text{in } [0, T] \times \mathbb{R}^d, \\ v(T, \cdot) &= G(\cdot, m(T)) \quad \text{in } \mathbb{R}^d, \\ \partial_t m - \operatorname{div} \left( \partial_p H(x, \nabla v) \right) &= 0 \quad \text{in } [0, T] \times \mathbb{R}^d, \\ m(0, \cdot) &= m_0(\cdot) \quad \text{in } \mathbb{R}^d. \end{aligned}$$
(MFG)

Discretizations of system (MFG) have been investigated in [1, 2, 3]. Convergence of solutions of the resulting schemes to solutions to (MFG) have been shown in [1, 2], in the one dimensional case by using analytic techniques, and in [3], in general dimensions by using probabilistic techniques.

In this talk, we report on a Lagrange-Galerkin discretization of (MFG) in the spirit of [5] and we provide a convergence result for solutions to the scheme with exact integration and in general dimensions. Finally, we also explain the relation between this scheme and the one in [1].

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## A semi-Lagrangian scheme for Hamilton-Jacobi-Bellman equations with Dirichlet boundary conditions

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**Keywords:** Semi-Lagrangian schemes, Hamilton-Jacobi-Bellman equations, Dirichlet boundary conditions, Viscosity solutions

We study the numerical approximation of parabolic, possibly degenerate, Hamilton-Jacobi-Bellman (HJB) equations in bounded domains. It is well known that convergence of the numerical approximation to the exact solution of the equation (considered here in the viscosity sense) is achieved under the assumptions of monotonicity, consistency and stability of the scheme. While standard finite difference schemes are in general non monotone, the so-called semi-Lagrangian (SL) schemes are monotone by construction. These schemes make use of a wide stencil and, when the equation is set in a bounded domain, this typically causes an overstepping of the boundary. We discuss here a suitable modification of this scheme adapted to the treatment of boundary problems

## A semi-Lagrangian scheme for Hamilton-Jacobi-Bellman equations with oblique boundary conditions

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**Keywords:** Hamilton-Jacobi-Bellman equations, oblique boundary conditions, semi-Lagrangian schemes

We propose a first order explicit semi-Lagrangian method to approximate the solution to the following parabolic Hamilton-Jacobi-Bellman equation on a bounded domain. Let  $\mathcal{O} \subseteq \mathbb{R}^d$ (with d = 1, 2, 3) be an open bounded set, we consider the problem

$$\begin{cases} -\partial_t u(t,x) + \max_{a \in A} H\left(t,x, Du, D^2 u, a\right) = 0 \quad \text{for } (0,T) \times \mathcal{O}, \\ \max_{b \in B} \left\{ \langle \gamma(x,b), Du \rangle - g(t,x,b) \right\} = 0 \quad \text{for } (t,x) \in (0,T) \times \partial \mathcal{O}, \\ u(T,x) = u_T(x) \quad \text{for } x \in \overline{\mathcal{O}}, \end{cases}$$
(1)

where T > 0, A and B are compact sets,  $\langle n(x), \gamma(x,b) \rangle > \nu > 0$  for all  $x \in \partial \mathcal{O}$ , with n outward-pointing normal to  $\mathcal{O}$ , and

$$H(t, x, p, M, a) = -\frac{1}{2} \operatorname{Tr} \left( \sigma(t, x, a) \sigma(t, x, a)^{\top} M \right) - \langle \mu(t, x, a), p \rangle - f(t, x, a),$$

for some  $\mu, \sigma$  and f such that a comparison principle holds.  $\sigma$  is a positive semidefinite matrix, possibly degenerate. Firstly, we discretize the solution of the stochastic SDE for the characteristic curves using the stochastic Euler method, then we reconstruct the numerical solution at the feet of the characteristics using standard interpolation techniques on unstructured spatial grids. The main novelty of our approach is in the treatment of non-linear oblique boundary conditions: each time one of the characteristics falls outside of the spatial domain, it is reflected inside along a direction depending both on the position of the characteristic itself and on the vector field  $\gamma$ . Finally, the numerical solution interpolated in the reflected point is corrected with a term depending on the boundary condition g. We have proved consistency, stability and convergence of this scheme. We underline that these results hold under an inverse parabolic CFL condition, which allows for large time steps. In the end, we conclude our work with some numerical simulations, both in  $\mathbb{R}$  and in  $\mathbb{R}^2$ .

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## Proximal first-order algorithms for solving stationary mean field games with non-local couplings

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**Keywords:** MFG with non-local couplings, proximal algorithms, a priori information, partial inverse

We consider a variational stationary mean field game with non-local couplings given by positive definite symmetric (PDS) kernels. Following the discretization proposed in [1], we propose a finite dimensional convex optimization problem such that the discretized mean field game corresponds to its first order optimality conditions. We further propose several proximal first-order algorithms to solve equivalent formulations of the optimization problem using projections onto suitable vector spaces and a priori information. In the proposed algorithms, the non-local coupling is activated explicitly while the remaining local terms are activated implicitly. We provide numerical comparisons of all the proposed methods by using a particular PDS kernel.

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## Proposal of a chatbot in Portuguese for the legal domain using the Rasa framework

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Keywords: Rasa, virtual assistant, legal domain

Since the COVID-19 pandemic quarantine, the State Court of Ceará (henceforth TJCE, from the abbreviation in Portuguese) has been improving to enable remote access to judiciary, such as WhatsApp Business and Virtual Counters. The Virtual Counters, regulated by Resolutions  $n^{\circ}$  372/21 (CNJ) and  $n^{\circ}$  12/2021 (TJCE), allow direct communication by videoconference with no need to schedule. Despite the extensive list of solutions provided by these service channels, there are limitations due to the assistance being done entirely by the civil servers. Therefore, this project aims to build an attendance chatbot in PT-BR, using Rasa, that will be integrated into WhatsApp Business to automatize the answers to FAQs. In this way, we expect to contribute to the effectiveness of the principle of *jus postulandi*. Unlike other platforms that use decision trees, Rasa is an open source machine learning framework [1]. This architecture provides a huge naturalness and customization to automated text and voice-based conversations. It also allows additional dependencies such as spaCy, MITIE, Python packages and built-in connectors to channels like Telegram, WhatsApp and Facebook. Initially, we intend to take the 17th unit of the TJCE Small Claim Court as a pilot project to develop a Proof of Concept. We will start compiling a legal domain corpus from the WhatsApp Business conversations. Currently, we are dealing with TJCE to get permissions and full access to WhatsApp Business conversations. The next step is to create a *persona* for the chatbot and a conversational flow, complying with UX writing criteria and accessible language.

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## Using Wordnet Senses to Investigate Zipf's meaning-frequency Law

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Keywords: Zipf's law, wordnets, sense-annotated corpora

George K. Zipf [10] observed that more frequent words have more senses. We take advantage of new sense-annotated corpora to test this law using corpora and wordnets of English, Spanish, Portuguese, French, Polish, Japanese, Indonesian and Chinese [1, 2, 3, 4, 5, 6, 7, 8, 9]. We show that the law describes languages accurately for these languages if we take - as Zipf did - mean values of meaning count and averaged ranks. The law only works over aggregates, it does not predict the number of senses for a single lemma. We also provide evidence that slope coefficients of Zipfian log-log linear model may vary from language to language. Finally, we show that the law holds for both single and multi-word expressions.

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## Foundation Models for Language

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Keywords: neural networks, language models, foundation models

In this presentation I will talk about the recently-famous and large neural language models such as BERT, GPT-3, and the like, which have been bringing great impact on NLP applications. More specifically, I will cover the different types of models, their architecture, and how they are developed. With this talk I not only expect to help expanding the portfolio of techniques for those already working with NLP, but also opening up the minds for those designing ML systems for other domains, given the potential of such models as a new paradigm for reuse of ML models.

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### Enhancing a sentiment analysis corpus through paraphrasing

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Keywords: Corpus, Bert, Paraphrasing, Parrot, Pegasus

Nowadays, artificial intelligence has presented many solutions to different problems with very accurate results. Specifically in text classification (TC), many works have been proposed using diverse techniques such as Machine Learning (ML) or Deep Learning (DL) [1].

The DL-based solutions for TC usually works on large datasets and obtains good results. Therefore, the quantity and quality of a dataset determines the success of a DL-based solution for TC.

In this presentation, we show a solution to enhance a dataset by paraphrasing sentences of the original corpus. We tested two automatic paraphrasing techniques: Parrot [2] and Pegasus [3] and we prove the augmented corpus on a classifier based on BERT [4] to measure its performance.

We used the IMDB dataset containing 50k movies reviews categorized in positive and negative . The results showed that without paraphrasing, the Bert model obtained 90% of f-measure; and with paraphrasing we obtained 99.56% and 99.86%.

	Original	Augmented Parrot	Augmented Pegasus
Precision	0.90722	0.99566	0.99860
Recall	0.90691	0.99565	0.99860
F-measure	0.90697	0.99565	0.99860

Table 1: Results of classification methods applying to different corpus

Finally, we would like to encourage the use of paraphrasing techniques to improve the corpus because it provides new sentences that improve any classifier model. Furthermore, the use of paraphrasing increases the richness of any corpus by adding new vocabulary.

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### Nonexistence of most reliable graphs with least corank

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Keywords: Network reliability, uniformly most reliable graphs, corank.

If G is a graph and  $\rho \in [0, 1]$ , the reliability  $R_G(\rho)$  is the probability of G being connected after each of its edges is removed independently with probability  $\rho$ . A simple graph G is a uniformly most reliable graph (UMRG) if  $R_G(\rho) \geq R_H(\rho)$  for all  $\rho \in [0, 1]$  and every simple graph H on the same number of vertices and edges as G. In 1986, Boesch conjectured that, if there is connected graph on n vertices and m edges, there is also a UMRG on the same number of vertices and edges [2]. Some counterexamples to Boesch's conjecture were already given by Kelmans [4], Myrvold et al. [5] and Brown and Cox [3]. It is known that UMRGs do exist whenever the corank m - n + 1 is at most 4 (and the corresponding graphs are fully characterized). Ath and Sobel conjectured that the same holds whenever the corank c is between 5 and 8 as long as  $n \geq 2c - 2$ . In this work, we give an infinite family of counterexamples to Boesch's conjecture with corank 5. These are the first counterexamples that attain the minimum possible corank. As a byproduct, the conjecture by Ath and Sobel [1] is disproved for corank 5.

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## Telecommunication Network Reliability under seismic event considering the dependence on the power supply

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Keywords: Reliability, telecommunication networks, power grid, Monte Carlo simulation

Telecommunication network reliability has become more relevant as these networks are critical to performing our daily activities [1]. On the other hand, earthquakes are one of the least predictable extreme events and, at the same time, have a high impact on the operability of the networks. We propose a seismic risk analysis to estimate the network reliability conditional to the earthquake occurrence. This study uses the Probabilistic Seismic Hazard Analysis method to evaluate the telecommunication network and power grid element state after a seismic event, see [2]. We study the reliability of a telecommunications network dependent on the power grid supply. We evaluate how the operability of a telecommunication network is affected by failures caused by earthquakes, following the approach described in [2]. The seismic event may cause the telecommunications network infrastructure to fail according to the situation model in [3]. Additionally, telecommunication components may be unavailable due to a lack of power supply. We propose a network dependency simple enough to have a reasonable computational cost. It also incorporates the terrain characteristics and the component robustness in network performance analysis. We used the model to quantify the reliability improvement when additional elements are incorporated into the network design. We use connectivity reliability metrics for this analysis; see [3].

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#### Network reliability optimization using convex envelopes

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Keywords: convex envelopes, network reliability optimization, nonlinear optimization

Network design to optimize the reliability of a network is one of the most classic problems in the optimization literature, with applications in many of the aspects of our lives and certainly in many more in the future. Given a simple undirected graph representing a network, edges fail according to a random probability  $p_e$ . The reliability of the network is defined as the probability that a given subset of nodes remains connected. The *network reliability optimization* problem consist on to decide the subset of edges on E to construct (given a predefined budget) in order to maximize the reliability of the resulting network.

In this talk we discuss how to use convex envelopes to approximate this nonlinear nonconvex integer programming problem. More precisely, we use reliability-preserving reductions, classical convex envelopes of bilinear functions, introduce custom cutting planes, and propose a new family of convex envelopes for expressions that appear in the evaluation of network reliability. Furthermore, we exploit the refinements produced by spatial branch-and-bound to locally strengthen our convex relaxations. For series-parallel networks this allows to obtain the optimal solution. For general graphs, this technique allows to reduce considerable the size of the problem, making suitable for other techniques, like sampling approximations.

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## Equivalent formulations of optimal control problems with maximum cost and applications

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Keywords: Optimal control, maximum cost, Mayer problem, state constraints, SIR model.

We revisit the optimal control problem with maximum cost with the objective to provide different equivalent reformulations suitable to numerical methods. We propose two reformulations in terms of extended Mayer problems with state constraints, and another one in terms of a differential inclusion with upper-semi continuous right member without state constraint. For the latter we also propose a scheme that approximates from below the optimal value. These approaches are illustrated and discussed in several examples.

## Characterization of solutions for a class of linear-convex optimal control problems

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**Keywords:** optimal control, linear-convex constraints, necessary conditions, sufficient conditions, mixed constraints

In this talk, we discuss sufficient and necessary optimality conditions for a class of linearconvex optimal control problems with mixed constraints recently developed in [1]. Roughly speaking, by a "linear-convex" problem, we mean that the equality constraints are linear while the inequality constraints are convex jointly in the state-control variables. Since no differentiability is assumed, these conditions are expressed through convex subdifferentials and normal cones.

Both of these optimality conditions are derived using the duality theory developed by Rockafellar in [3] for problems of calculus of variations posed over arcs of bounded variation. According to this theory, the costate is the solution to a suitably defined dual problem and, since it is expected that the costate presents discontinuities at the boundary of the region defined by the constraints, we should also expect a costate of bounded variation.

For the derivation of the sufficient conditions, we do require some technical conditions in order to make the corresponding dual problem more manageable. If, in addition we also impose a Slater-type condition, the sufficient optimality conditions turn out to be also necessary, completely characterizing the solutions of the problem at hand.

Finally, we point out that the conditions we imposed in order to derive the optimality conditions are of a different nature than the usual regularity assumptions on the mixed constraints such as the *Mangasarian-Fromovitz constraint qualification* or the *bounded slope condition* (see for example [2]) and are, in some sense, less restrictive, since all of these regularity conditions imply an absolutely continuous costate while our conditions produce a costate merely of bounded variation. If we also assume the constraint qualification version of the bounded slope condition, it is possible to show that the costate indeed reduces to an absolutely continuous function.

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## A Weierstrass Condition for Affine-Convex Optimal Control Problems with Nonregular Mixed Constraints

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**Keywords:** Optimal control, Necessary conditions, Nonregular mixed constraints, Affine-Convex constraints.

In this talk, we present necessary optimality conditions in the form of a maximum principle for an optimal control problem delimited by non-regular mixed constraints when the data of the problem is affine-convex only in the control variable, meaning that the equality constraints are affine and the inequality constraints, as well as the running cost, are convex with respect to the control variables.

In order to derive first order necessary conditions, most papers dealing with optimal control problems subject to mixed constraints impose some sort of regularity condition on the constraints. This notion of regularity varies depending on the context of the problem and can be formulated as a constraint qualification or as a condition depending on a nominal process; for example, the well-known *Mangasarian-Fromovitz constraint qualification* and the *regularity condition* defined in [3] for smooth mixed constraints or the *bounded slope condition* and the *weak basic constraint qualification* for the nonsmooth case as defined in [2] and [4], respectively.

Recently, in [1], first order optimality conditions were derived over essentially bounded controls imposing only a closedness condition on the image of some functionals associated with the equality constraints, these results are given in terms of a "weak" maximum principle, meaning that they lack the Weierstrass condition (or maximum condition).

Here, we will show that, if the control problem is affine-convex in the sense mentioned above and the equality constraints satisfy a full-rank condition, it is possible to derive the Weierstrass condition in its usual form by using the main result in [1] and following closely the approach in [3] where *sliding modes* are used to derive the maximality condition from the *stationarity conditions* present in the weak version of the maximum principle for regular mixed constraints.

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## Tube-based robust NMPC for motion control of skid-steer mobile robot with terra-mechanical constraints

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**Keywords:** Wheel-terrain interaction, tube-based nonlinear model predictive control, trajectory tracking

The wheel-terrain interaction configures favorable maneuvering conditions on ground vehicles. However, the slip phenomena, as result from such interaction, directly impact on the pure rolling motion of the vehicle's tires and then on the vehicle's chassis, imposing strong dynamics constraints by the ground disturbance propagation. For instance, it may lead to the degeneration of tractive and skid force production capability, and eventually induce destabilization of the vehicle either by slipping during traction, sliding while braking, or skidding while trapping [1]. During the lecture it will be addressed this issue by explaining and discussing numerous interesting kinematic and dynamic properties of uncertain terra-mechanical models, which all can reveal together within a single vehicle model difficult to control. Such a big control difficulty, also observed in practice, may be very inspiring for students, researchers and practitioners looking for an efficient feedback control system that could help the agile trajectory-tracking maneuverability of autonomous ground robots subject to deformable and non-deformable terrain disturbances. In this scenario, it will be covered the robust control design problem by introducing an integral control architecture based on time-varying reachable sets (tubes) and Nonlinear Model Predictive Control (NMPC) schemes [1, 2]. Similarly, it will be explained how the presented motion controllers were made adaptive to terra-mechanical parameters with a Nonlinear Moving Horizon Estimation approach working under a parallel Real-Time Iteration scheme. We will be also discussing in depth about the mathematical conditions that an NMPC should meet to strength robust control properties in terms of performance, feasibility, reachability, and stability. The lecture will be illustrated by selected simulation and experimental results obtained in laboratory and in-field conditions.

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## Model-based optimization for legged locomotion: an overview

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Keywords: legged robots, optimal control, model-based optimization

Legged robots, especially bipedal and quadrupedal ones, are highly complex machines that have been introduced already in the early 1970s. One of the main problems yet to be solved is reliable and stable walking. It is only in the past decade that the capabilities of legged robots have seen a rapid growth thanks to more mature hardware and control frameworks. Especially, optimization-based control methods have delivered reliable locomotion not only on flat grounds, but also in nominal complex situations requiring multiple contacts and challenging terrain. While there is an ongoing shift towards learning based methods, model-based optimization remains the state of the art for this complex task, where simplified models are typically preferred for realtime control and trajectory generation, though thanks to advancements in numerical methods, more complex models are also being considered. There are different approaches in tackling the optimal control problem formulation for walking, depending on the dynamic model of the robot, the contact model, and the desired outcome. This talk will give an overview of current approaches to solving the locomotion problem as a model-based optimal control problem.

## Applications of set-invariance to multi-robot defense and surveillance

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Keywords: control barrier functions, perimeter defense, multi-robot systems

In this talk, a new formulation and solution to the perimeter defense problem will be presented. This novel formulation, based on set-invariance principles, allows for closed-form, reactive, and computationally efficient control strategies that are scalable with respect to the number of robots, making them suitable for real-time implementation. Extensions of this work to robust area defense and surveillance will also be discussed.

## Ecologically-inspired Robots for Long-term Environmental Monitoring

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**Keywords:** Optimization-based control, nonlinear control, multi-robot systems, resilience, heterogeneity

Environmental monitoring tasks typically take place over long time horizons. Therefore, robotic platforms employed to perform such tasks need to be designed and controlled to remain operational in unknown environments under unmodeled and unforeseen conditions. In order to achieve this goal, robotic systems have to necessarily take into account their limited availability of energy, and be resilient to unexpected environmental phenomena and system failures. This talk introduces the concept of *robot ecology*, an optimization-based robot control framework where tasks and specification are encoded as constraints in a convex optimization program used to synthesize the robot controller. The framework generalizes to the execution, prioritization, and allocation of multiple tasks for resilient and energy-aware robot teams. The effectiveness of the proposed approach is illustrated in a scenario where a team of robots is deployed to collectively execute persistent monitoring tasks subject to energy and resilience constraints.

## Operator-valued stochastic differential equations in the context of Kurzweil-like equations

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Keywords: Itô integral, Itô-Henstock integral, Kurzweil-belated integral.

It is well-known that generalized ODEs encompass ordinary and functional differential equations, impulsive and measure differential equations, dynamic equations on time scales, integral equations, and semilinear parabolic PDEs. This time, we will present our forays into stochastic differential equations. We will describe an environment, similar to generalized ODEs, that deals with random variables and stochastic processes. The results we will mention are described carefully in [1].

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## Weak kinetic solution for Stochastic Degasperis-Procesi Equation

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Keywords: long waves, kinetic theory, Jakubowski-Skorokhod theorem

We study the stochastic Degasperis-Procesi equation in the one-dimensional domain  $\mathbb R$ 

$$\begin{cases} du = -(u\partial_x u + \partial_x p) \ dt + \sigma(x, u)d\mathcal{W}_t, \\ \left(1 - \partial_{xx}^2\right) p = \frac{3}{2}u^2 \quad \text{in } \mathbb{R}_T = (0, T) \times \mathbb{R}, \\ u(0) = u_0 \qquad \qquad \text{in } \mathbb{R}, \end{cases}$$
(1)

where u = u(t, x) denotes the velocity of the fluid and  $u_0 = u_0(x)$  is the initial velocity;  $\sigma$  and  $W_t$  are the non-linear diffusion coefficient and the Wiener process.

We establish the global solvability result for the system (1) by the kinetic theory and the Jakubowski-Skorokhod theorem.

N.V. Chemetov acknowledges support from FAPESP, Grant 2021/03758-8.

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## Time-reversal transformation for multiplicative-noise stochastic differential equations

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Keywords: Multiplicative-noise stochastic systems, equilibrium, time reversibility

In this work, we define the time reversal transformation [1, 2] for systems driven by multiplicative-noise stochastic differential equations (SDEs) in order to study equilibrium properties of such systems. To this end, we take into account the dependence of the asymptotic stationary probability distribution on the stochastic calculus prescription. For defining the SDE, we use the generalized Stratonovich or  $\alpha$ -prescription, where  $\alpha$  is a continuous parameter,  $0 \le \alpha \le 1$ , and each of its values corresponds with a different discretization rule (including Itô and Stratonovich prescriptions). We show that, using a careful definition of equilibrium distribution and taking into account the appropriate time reversal transformation, usual equilibrium properties are satisfied for any stochastic prescription.

On the other hand, we consider a simple model of a bistable system under the influence of multiplicative noise [3]. We are interested in the conditional probability of remaining in a minimum of the potential energy. In this setting, we found corrections to the Kramers escape rate produced by the diffusion function which governs the state-dependent diffusion for arbitrary values of the stochastic prescription parameter. Interestingly, we found an expression for the escape rate which exhibits invariance under the time-reversal transformation previously defined.

The Brazilian agencies, Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) are acknowledged for partial financial support.

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## Stochastic dynamics at criticality

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Keywords: Stochastic dynamics, Renormalization Group, Multiplicative noise

Out-of-equilibrium evolution near continuous phase transitions is a fascinating subject. While equilibrium properties are strongly constrained by symmetry and dimensionality, the dynamics is much more involved. The interest in critical dynamics is rapidly growing up in part due to the wide range of multidisciplinary applications in which criticallity has deeply impacted. For instance, the collective behavior of different biological systems has critical properties, displaying space-time correlation functions with non-trivial scaling laws [1]. Other interesting examples come from epidemic spreading models where dynamic percolation is observed near multicritical points [2].

The standard approach to critical dynamics is the "Dynamical Renormalization Group (DRG)" [3]. The simplest assumption is that, very near a critical point, the dynamics of the order parameter is governed by a dissipative process driven by an overdamped *additive noise* Langevin equation. The typical relaxation time near a fixed point is given by  $\tau \sim \xi^z$ , where  $\xi$  is the correlation length and z is the dynamical critical exponent. At a critical point  $\xi \to \infty$ . Therefore, the system does not reach the equilibrium at criticality. Together with usual static exponents, z defines the dynamic universality class of the transition.

A DRG transformation not only generate new couplings in the system Hamiltonian but also modifies the probability distribution of the stochastic process initially assumed. Thus, the probability distribution of the noise evolves with the DRG transformation, *i.e.*, it is scale dependent. By means of a perturbative approach on a simple model of scalar field with  $Z_2$ symmetry, we show that the dynamics flows to a fixed point governed by a *multiplicative noise* stochastic process, even in the case of assuming an additive dynamics as a starting condition.

Using a functional formalism [4], that allows us to deal with any stochastic prescription (such as Itô, Stratonovich, Hänggi-Klimontovich and so on) on the same footing, we show that, at the novel multiplicative fixed point, different stochastic prescriptions belongs to the same universality class.

FAPERJ, CNPq and CAPES are acknowledged for partial financial support.

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#### LACIAM-45

# Modeling of nonlinear/nonconvex aspects in SDDP algorithms: experience in the official models applied to the energy planning of the large-scale Brazilian system.

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**Keywords:** stochastic dual dynamic programming, nonlinear programming, nonconvexities, piecewise linear models.

The power generation planning of the large-scale Brazilian hydrothermal system has been performed for over twenty years [1] with the application of the SDDP algorithm proposed in [2]. Even though in that paper a linear stochastic optimization problem with stage-wise independency has been considered, several improvements have been proposed over time in order to represent interstage dependency of log-normal inflows with a periodic autorregressive model [3], as well as the modeling of nonlinear/nonconvex aspects such as the head-dependent hydro production function [4], evaporation as a function of storage, losses due to spillage, state-dependent hydraulic constraints, among others. This talk aims to describe and put in a more general context some procedures that have been conceived in order to consider, in the SDDP algorithm, convex piecewise-linear models or polynomial functions to approximate such aspects, and how such functions should be addressed when building the Benders cuts that approximate the recourse function for each stage, by taking into account the derivatives/sensitivities of such functions with respect to the state variables of the problem. In addition, we describe the topological analysis that has to be made, both in the shape of these functions and in its effect in the output of the optimization problem, in order to decide whether such approximation can be employed or a linear approximation must be used. Illustrative results are presented for real cases of the official operation planning of the Brazilian system with the NEWAVE model.

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## Diffusion in inverse problems and inverse problems in diffusion

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Keywords: Inverse problem, Regularization, Diffusion, Inpainting

This presentation will be twofold. First we will show how diffusion can be used to successfully solve a certain type of inverse problems and then we will consider an inverse problem in diffusion in which appropriate regularization tools lead to quite satisfactory results.

The first problem originates in the area of inpainting. An image inpainting problem consists of restoring an image from a (possibly noisy) observation, in which data from one or more regions is missing. Several inpainting models to perform this task have been developed, and although some of them perform reasonably well in certain types of images, quite a few issues are yet to be sorted out. For instance, if the original image is expected to be smooth, inpainting can be performed with reasonably good results by modeling the solution as the result of a diffusion process using the heat equation. For non-smooth images, however, such an approach is far from being satisfactory. On the other hand, Total Variation (TV) inpainting models based on high order PDE diffusion equations can be used whenever edge restoration is a priority. The introduction of spatially variant conductivity coefficients on these models, such as in the case of Curvature-Driven Diffusions (CDD) approach, has allowed inpainted images with well defined edges and enhanced object connectivity. The CDD approach, nonetheless, is not suitable wherever the image is smooth, as it tends to produce piecewise constant solutions. Based upon this, we propose using CDD to gather a-priori information used at a second step in a weighted anisotropic mixed Tikhonov plus total-variation model that allows for both edge preservation and object connectivity while precluding the "staircasing" effect that all pure TV-based methods entail. Comparisons between the results of the implemented models will be illustrated by several computed examples, along with performance measures.

The second problem has its origins in the area of design of thermal materials. It consists of determining a non-homogeneous heat conductivity profile in a steady-state heat conduction boundary-value problem with mixed Dirichlet-Neumann boundary conditions over a bounded domain in  $\mathbb{R}^n$ , from the knowledge of the state over the whole domain. We develop a method based on a variational approach leading to an optimality equation which is then projected into a finite dimensional space. Discretization yields a linear although severely ill-posed equation which is then regularized via appropriate ad-hoc penalizers resulting a in a generalized Tikhonov-Phillips functional. No smoothness assumptions are imposed on the conductivity. Numerical examples for the case in which the conductivity can take only two prescribed values (a twomaterials case) show that the approach is able to produce very good reconstructions of the exact solution.

# Improving climate-driven transmission models for mosquito-borne disease emergence

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Keywords: climate change, dengue fever, vector-borne disease, epidemiology

Mosquito-borne diseases historically endemic to areas with tropical climates have been spreading in temperate regions of the world with greater frequency in recent years. Although numerous factors contribute to this spread, changes in temperature, precipitation, and humidity patterns are playing an important role due to climate-driven processes in mosquito life cycles and pathogen transmission cycles. Therefore, it is becoming increasingly important to develop models aimed at understanding influences of climate on mosquito-borne diseases. In this work, we present models incorporating seasonal and diurnal fluctuations in climate to show how different meteorological patterns can influence dynamics of dengue fever, a disease caused by an arbovirus transmitted by the mosquito species Aedes aegypti. We apply these models to the study of dengue emergence in temperate cities of Central Argentina, where dengue outbreaks started occurring for the first time in 2009 and have continued with increasing incidence over the last decade. We evaluate models with different assumptions about the influence of climate on mosquito and dengue dynamics and explore the impacts of potential long-term climate change scenarios on these dynamics. We discuss the implications of this work for surveillance and mitigation strategies with a particular emphasis on improving these strategies in regions experiencing dengue emergence.

# On modeling a Gauss transmission rate and clustering epidemic times series for a Peru Dengue outbreak

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Keywords: Times series classification, LSTM, Dengue, Gaussian transmission rate

Dengue fever is an endemic disease present in tropical and subtropical regions. It has recently appeared in non-tropical areas with dry weather, such as Lima-Peru. Its alarming geographical expansion has raised decision-makers attention even in small outbreaks. In this talk, I will present advances in two directions of research. In the first part, we analyze the Dengue cases in Peru, which rose to 68.000 cases in 2017, spread along 376 districts. Each time series containing weekly reported cases are grouped for detecting the geographical regions where the environmental conditions for mosquitoes combined with local social-economical activities may cause high dengue incidence. We found that feature-based clustering improves short-term forecasting in deep-learning models. However, which features should be used to have meaningful clusters is not always clear. Hence, we perform feature selection experiments to find an optimal set of features.

In the second part, we analyze the outbreak in Lima since the temperature-based reference models failed to fit the data because the temperature and mosquito seasons do not match the outbreaks. This means that other variables are also involved in epidemic outbreaks. Our work introduces a new component to capture these processes, including whether entomological, environmental, or related to population mobility. This new component is a Gaussian function that modulates the human and vector transmission rate. Then a probabilistic model selection experiment evaluated the unknown model parameters. Our results indicate that our model can fit the historical data to extract information about outbreaks by interpreting the new model parameters. This work is part of joint work with colleagues from the Technological University of Peru and Asunción National University.

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# Mathematical and statistical modeling applied for malaria control

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**Keywords:** Malaria, Bayesian modelling, ordinary differential equations, Spatio-temporal modelling

Malaria is one of the main challenges in public health in the Brazilian Amazon basin, where this disease caused 167.097 cases in 2020. The Brazilian malaria control program has dropped malaria incidence toward disease elimination during the XXI century, but a rebound in points in 2017 evidenced the fragility of control efforts. Malaria elimination contains a set of challenges, such as malaria drug resistance, knowing the causes of malaria rebound, and case-notification delay. Drug resistance decreases the effectiveness of antimalarial treatments provoking treatment failure that increases disease transmission. The Brazilian Amazon region has experimented with contrast in human mobility, economic activities, environmental changes, and deforestation that might explain the rebound in cases in 2017. The notification time of malaria cases differs in the Amazon basin where some municipalities can take 30 days or more for notifying a malaria case in the National Surveillance System; this situation can delay the reactions of the malaria control program. In this work, some mathematical tools were adopted for representing malaria drug resistance, estimating the effect of the causes of malaria rebound in 2017, and predicting malaria cases considering reporting delays. This work evidences the usefulness of mathematical tools such as ordinary differential equations, next-generation matrix, the Latin hypercube sampling, and the Spatio-temporal Bayesian models in challenges of biological systems.

# Analysis of tuberculosis dynamics considering vaccinated, treated and latent low-risk populations

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**Keywords:** Tuberculosis, latent low-risk , basic reproductive number, optimal control, vaccination

Tuberculosis, or TB, is caused by *Mycobacterium tuberculosis*, a bacterium that almost always affects the lungs. It is a curable and preventable disease. Worldwide, tuberculosis is the leading cause of death from a single infectious agent (ahead of AIDS). A total of 1.4 million people died from TB in 2019 (including 208,000 people with HIV).

Studies on modeling TB transmission consider different prevention and control strategies, such as vaccination, treatment, quarantine, and isolation ([1], [2]). Some research has considered a combination of these control methods, determining that vaccination and treatment are effective strategies for reducing TB disease transmission [4].

The low-risk latent class, which groups latent individuals who do not progress to infectious TB and recovered individuals (naturally or by treatment), is of great importance in this disease because the rate of disease spread decreases as long as infected individuals remain in this class [3].

In this work we propose a model for the dynamics of tuberculosis, which considers a low-risk latent population, that allows us to evaluate the importance of considering this population in the dynamics of TB, where we consider control mechanisms such as vaccination and treatment, and whether it is necessary to treat and/or control this population.

To this end, we perform a qualitative analysis of the model, analyze which parameters are most relevant in the initial transmission of the disease and calculate the average number of new infections produced by an infectious individual. We pose and solve numerically an optimal control problem, in which we seek to minimize both the number of infected individuals and the economic costs involved in the implementation of the controls in the tuberculosis dynamics proposed. We use numerical simulations to analyze the effects of implementing the obtained controls. Finally, simulations are carried out for Cali, establishing a methodology for the design of control strategies to reduce TB transmission in the city considering a low-risk latent population.

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# A variational approach for price formation models in one dimension

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Keywords: Mean Field Games, Price formation, Potential Function, Lagrange multiplier

This talk considers a class of first-order mean-field games (MFGs) of price formation. We eliminate one of the equations using Poincaré Lemma. The reduced problem for a single function, the potential, offers an alternative approach to obtain the solution of the MFGs system by solving a convex variational problem. We obtain solutions for the variational problem using the direct method in the calculus of variations. Moreover, we establish a correspondence between solutions of the MFGs system and the variational problem. We illustrate our results for the linear-quadratic model.

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# Mean Field Games planning problems with general initial and final measures

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Keywords: PDES, Optimal Control, Optimal Transport

The planning problem in Mean Field Games (MFG) was introduced by P.L. Lions in his lessons, to describe models in which a central planner would like to steer a population to a predetermined final configuration while still allowing individuals to choose their own strategies. In a recent variational approach, see [3, 5], the authors studied the well-posedness of this problem in case of merely summable initial and final measures. This approach uses techniques coming from optimal transport, introduced by Benamou and Brenier in [1], extended to the congestion case in [2], and already used to show the existence and uniqueness of weak solutions for classical MFGs by Cardaliaguet and collaborators. The case of less regular initial and final measures is now studied via techniques introduced by Jimenez in [4], for the analogous problem in optimal transport.

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# A variational mean field game with free final time and control interaction

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Keywords: mean field games, free final time, potential games, optimization

In this talk, we present a mean field game model in which an agent's optimization criterion consists in minimizing a certain cost in free final time with the constraint of reaching a given target set. More precisely, the cost of an agent is made of an individual running cost, a pairwise interaction cost which takes into account both positions and velocities of the agents, and a cost on the time the agent takes to reach a given target set, which is equal to  $+\infty$  if the target set is not reached.

After presenting the framework, its motivation from the modeling of crowd motion, and some previous related results for minimal-time mean field games [1, 2] and other similar mean field game models [3], we present our main result, which provides a potential structure for the game by showing that its equilibria can be characterized as critical points of a functional  $\mathcal{J}$ . This is done by adopting a Lagrangian description of the game, and existence of equilibria is obtained after studying the existence of a minimizer of  $\mathcal{J}$ . The talk is concluded by numerical illustrations.

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# Sensitivity analysis of the value function for semilinear parabolic optimal control problems

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Keywords: value function, PDE-constrained optimization, Riccati operator

We derive sufficient conditions for expressing the first and second order sensitivities of the value function associated with a class of optimal controls problems constrained by parabolic semilinear equations. In particular, we relate the first order sensitivity with the adjoint equation and the second order sensitivity with a suitably defined Riccati equation.

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## Evaluating a semantic algebra on a large grammar of English

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Keywords: Computational linguistics, semantic algebra

One of the ambitious goals of computational linguists is to develop implementations of the grammars of human languages, explicitly modeling for each particular language the lexicon and the inventory of syntactic rules used to compose the well-formed phrases and sentences of that language. The grammar of a language can be taken to define a mapping from form (the observable sequence of words in a sentence) to meaning (the semantic content communicated by the sentence), and thus a grammar implementation should also aim to make explicit the rules of semantic composition into some target logical formalism. Ideally, this method for constructing the meaning of each phrase from its parts would pair each syntactic rule of a language-specific grammar with one or more composition operations drawn from a small library of formally precise and language-independent operations. Such a semantics (MRS: Copestake et al. 2005) which has been used for grammar implementations of a variety of languages, and its basic operations were illustrated using an early version of the English Resource Grammar (ERG: Flickinger 2000, 2011).

In this talk I will present ongoing collaborative work with Stephan Oepen and Emily M. Bender (see Flickinger et al. 2014) to extend and revise this semantic algebra to accommodate most of the wide syntactic and semantic coverage in MRS of the current ERG, and to identify those constructions in the grammar which cannot be readily shown to be compliant with the algebra. We have also implemented a language-independent model of this revised algebra in order to evaluate the compliance of the ERG with the algebra over a representative set of example sentences illustrating the broad range of syntactic phenomena and their corresponding MRS logical forms computed using the grammar. Our goal is to gain a better understanding of the degree to which a small set of composition operations suffices to construct the meanings of the many construction types in a language, and to focus attention on non-compliant constructions defined in the ERG in order to see whether it is the algebra which should be revised, or the grammar's analysis of those constructions.

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# Challenges of modeling Portuguese morphology in a computational grammar of Portuguese in the HPSG formalism

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**Keywords:** deep syntactic parsing, grammar engineering, computational morphology, evaluative suffixes

A comprehensive lexical database is an indispensable component of a linguistic-based computational grammar. This grammar type strives to mathematically model a fluent speaker's knowledge about the structures of their natural language. It has proven to be very useful in natural-language understanding tasks [6, 7]. For languages with a rich inflectional system and productive word-formation processes like Portuguese, one cannot simply limit oneself to the entries of a standard dictionary as a lexical knowledge source. It is mandatory to model the combinatorics of stems, inflectional, and derivational affixes, as well as the orthographic and morphophonological that apply to the output of these combinations [3]. In this talk, we report on our experience in developing PorGram [1], an open-source, free software computational grammar of Portuguese in the HPSG formalism, encoded in the Type Description Language (TDL) [5]. The construction of PorGram so far has combined the Grammar Matrix [4], which automatically generates TDL code from choices in a customization questionnaire, and hand-coding of TDL specifications. PorGram's ultimate goal is to parse unrestricted text. Therefore, it needs to incorporate a vast amount of lexical knowledge. We discuss the solutions implemented to handle inflectional and derivational morphology and the envisaged strategies to tackle problems that remain unsolved. These strategies draw on existing resources, such as MorphoBr [2], a large full-form lexicon, and the UD\_Portuguese-Bosque treebank [8]. The focus of the presentation will be the implementation of evaluative suffixation. A hallmark of Portuguese morphology, it comprises diminutive, augmentative, and absolute superlative suffixes, which are extremely productive, potentially applicable to any noun and/or adjective [9, 10]. Since they involve intricate interactions between inflectional and derivational processes, their implementation is an ideal test case for assessing the strengths and weaknesses of a framework for computational morphology.

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## Using a Knowledge-based Approach for Data Augmentation

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**Keywords:** Text Data Augmentation, Boosting Performance, Computational Grammars, Methods

Despite the stunning achievements of data-driven models on many areas of Natural Language Processing (NLP), there is still a problem when it is necessary to use machine learning techniques with a small data set, this combination normally generates inaccurate models because of the high overfitting. The state-of-the-art solution to this problem has an automated treatment based on random data augmentation systems, such as Easy Data Augmentation (EDA)[1] that uses 4 operations: Synonym Replacement, Random Insertion, Random Swap, and Random Deletion. These methods can in fact improve the performance of the models by expanding the dataset with synthetic sentences, but they can also introduce new problems as cited in [2], falling shorts in producing semantically equivalent texts and sentences acceptable to native speakers. Another way to augment datasets is by using the back-translation technique, that proceeds by translating a sentence from a language x to a language y, and then, translating the sentence back to the language x, possibly resulting in new sentences. This method can generate new sentences but given the inherently nuanced and subjective nature of language, it will often produce very literal and unnatural expressions if it is based on a probabilistic model only. Aiming at a solution to the problem of overfitting in small datasets, using synthetic text data generated from automatic transformations, but preserving the semantic equivalence to the original sentences and their acceptance by natives, we investigated if using methods similar to that used in EDA and back-translation, but guided by knowledge, can help to produce more accurate models or even models that can better categorize, recognize or generate new acceptable sentences. For this investigation, we used computational grammars in the Grammatical Framework (GF) formalism [3] as an alternative to traditional methods of textual data augmentation (TDA). We modeled English and Portuguese linguistic phenomena to generate a controlled corpus of sentences from a dataset of 50 sentences. This modeling included linguistic treatment and manipulations, such as identification of synonymy relationships between words, insertion and deletion of adjuncts, displacement of phrases in the sentence, etc., all based on the knowledge linguists possess of these languages. As a result, we have shown that with the use of computational grammars, the dataset grows quickly without losing data quality.

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## Feature extraction and LSA in automatic essay evaluation

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## 1 Abstract

The technological advances in the field of education have enabled a variety of online activities, among which are the answers to discursive questions [2]. Such questions serve the purpose of verifying and gauging students' learning, in particular the abilities to write and structure the argumentative discourse [4, 3, 7]. Within this context, the development of approaches to foster automate correction gains relevance, as it presents advantages such as:

i) it reduces the correction time, proving more stable in the correction procedure, reducing the possibility of errors;

ii) it provides immediate feedback which can support students in solving questions;

iii) it allows multiple submissions at a time and place determined by the user;

iv) it has low cost [6].

The main focus of the experiments here presented is the development of a set of algorithms for the automatic evaluation of written answers to discursive questions based on Natural Language Processing and Artificial Intelligence techniques. The main techniques used:

- 1. The initial work was to apply a latent semantic analysis (LSA) model for the automatic evaluation of short answers (25 to 70 words) to open-ended questions of the entrance examinations from the Federal University of Pará (Ufpa) [1];
- 2. Next, we conducted experiments using a method based on n-gram similarity and a categorization process [5];
- 3. Next, we conducted experiments using a method based on machine learning techniques to a corpus constituted of a sample covering 1000 essays from a public exam for admission to the career of Administrative Technician in Education.

A system is considered to perform well when the system versus human agreement index approaches or is higher than the human versus human agreement index. Considering a study corpus constituted of 1,000 (thousand) essays obtained from a selection process and previously evaluated by two human specialists, the quadratic kappa index (QK) among human evaluators was 0.68. For this same corpus, in our experiments, we obtained a system versus human index QK of 0.8412. In light of the results, we can consider that this technology is achieving a good performance, thus, the method can be used in combination with human evaluation in real tests with written answers to discursive questions.

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# A SECOND-ORDER DESCENT METHOD WITH ACTIVE-SET PREDICTION FOR GROUP SPARSE OPTIMIZATION

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Keywords: Nonsmooth Sparse Optimization, Penalization Method, Second Order Method

In this paper, we propose a second-order algorithm for the solution of finite and infinite dimensional group sparse optimization problems. Group sparse optimization has gained a lot of attention in the last years due to several important classification problems requiring group sparse solutions. The most prominent application example is the group LASSO problem, which consists in minimizing a least-squares fitting term together with the group sparsity  $l_1/l_2$  norm.

The method is built upon the steepest descent directions of the nonsmooth problem, which are further modified by using second-order information. A prediction step is also proposed for faster identification of the strong active set. A general convergence result is proved, and the active set behavior is analyzed. The work ends with comparative computational experiments to test the performance of the devised algorithm.

## Quadratic regularization of bilevel optimal transport problems

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Keywords: Optimal transport, Kantorovich problem, bilevel optimization

We consider a bilevel optimization problem, where the lower level problem is given by the Kantorovich problem of optimal transportation. The upper level optimization variables are the optimal transport plan and one of the marginals. A possible application of the problem under consideration is the identification of a marginal based on measurements of the transportation process. Due to the curse of dimensionality associated with the Kantorovich problem, regularization techniques are frequently employed for its numerical solution. A prominent example is the entropic regularization leading to the well-known Sinkhorn algorithm. Here, we pursue a different approach and apply a quadratic regularization leading to transport plans in  $L^2(\Omega_1 \times \Omega_2)$ , where  $\Omega_1$  and  $\Omega_2$  are the domains of the marginals. The dual problem is a problem in  $L^2(\Omega_1) \times L^2(\Omega_2)$ , which yields the desired reduction of the dimension. We investigate the convergence behavior of the regularized bilevel problems (where the Kantorovich problem as lower level problem is replaced by its quadratic regularization) for regularization parameter tending to zero. It turns out that, under additional assumptions, weak-\* accumulation points of sequences of optimal solutions of the regularized bilevel problems are solutions of the original bilevel Kantorovich problem.

# Numerical methods for solving variational mean field games with proximity operators

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**Keywords:** MFG with local and non-local couplings, stationary MFG, proximal splitting algorithms

We first consider a variational stationary mean field game with local couplings, whose solution can be approximated by the finite-difference scheme proposed in [1]. We propose a finite dimensional convex optimization problem such that the discretized mean field game corresponds to its first order optimality conditions. We further apply and propose several proximal first-order algorithms to solve equivalent formulations of the optimization problem using projections onto suitable vector spaces and a priori information. We compare their numerical performance in some academic examples and we briefly discuss approaches for time-dependent MFG and MFG with non-local couplings.

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# State–constrained elliptic optimal control problems with $L^q$ –quasinorm penalization

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**Keywords:** Elliptic optimal control problem, point type state constraints, non-convexity, difference of convex functions, Huber regularization, Lavrentiev regularization, Newton's semismooth method.

Let  $\Omega \subset \mathbb{R}^n$ , with n = 2 or n = 3, be a Lipschitz bounded domain with boundary  $\Gamma$ . For p > 1, we define

$$\Upsilon_p: L^2(\Omega) \to \mathbb{R}$$
$$u \mapsto \int_{\Omega} |u|^{1/p}.$$

Let  $\alpha, \beta > 0$ . We consider the following elliptic optimal control problem:

$$\begin{cases} \min_{\substack{(y,u)\in H^1(\Omega)\times L^2(\Omega)}} J(y,u) &:= \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2\Omega}^2 + \beta \Upsilon_p(u) \\ \text{subject to:} \\ -\Delta y(x) + y(x) = u(x), \quad x \in \Omega, \\ \partial_{\vec{n}} y(x) = 0, \qquad \qquad x \in \Gamma, \\ y_a \leq y(x) \leq y_b, \qquad \qquad x \in K \subset \Omega, \end{cases}$$

with  $y_a, y_b \in \mathbb{R}$ . Notice that the term  $\Upsilon_p$  in the cost function produces a lost of convexity on it, and thereby the usual tools from convex analysis cannot be applied directly for formulating an optimally system for the problem. Therefore, it is necessary to introduce some non-smooth analysis techniques, such as those provided by the difference of convex functions (DC) theory, together with the introduction of a Huber-type regularization (see [2]) of the term  $\Upsilon_p$ . The optimal control problem also has point-wise sate constrains. It is known that this situation leads to optimally systems whose associated Lagrange multipliers have poor regularity, making its numerical treatment difficult (see [1]). To avoid the appearance of multipliers with such characteristics, we introduce a Lavrentiev-type regularization. Thanks to the two previously mentioned regularizations, it is possible to formulate a family of optimal control problems (depending on the associated regularization parameters) for which we respectively obtain an optimal systems using the Difference of Convex Functions (DC) theory, and whose multipliers of Lagrange are more regular.

After that, we solve the regularized problem numerically by applying Newton's semi-smooth algorithm (see [4, 3]). We analyze the qualitative form of the solution of the regularized problem, and we study numerically what happens with the regularized solutions as the regularization parameters vary. Finally, we study the convergence rate of the proposed algorithm, and we give our conclusions about the work.

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## Minimax control problems and necessary optimality conditions

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Keywords: Minimax optimal control problems, mixed constrained, maximum principle

We furnish a weak maximal principle for minimax optimal control problems in the presence of mixed state-control equality and inequality constraints. We allow for parameter uncertainties in the cost function, in the dynamical control system and in the equality and inequality constraints. The necessary optimality conditions is obtained by assuming a new constraint qualification of Mangassarian-Fromovitz type. Optimality conditions under a full rank conditions type are provided as corollary of the Mangassarian-Fromovitz conditions case. We present some examples to illustrate the results.

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## An Asymptotic Weak Maximum Principle

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Keywords: Optimal control, optimality conditions, maximum principle, mixed constraints

We are concerned with optimal control problems with mixed constraints posed as follows.

 $\begin{array}{l} \text{Minimize } l(x(0), x(1)) \\ \text{over } x \in W^{1,1}([S,T]; \mathbb{R}^n) \text{ and measurable functions } u:[0,1] \to \mathbb{R}^m \text{ satisfying} \\ \dot{x}(t) = f(t, x(t), u(t)) \text{ a.e. in } [0,1], \\ b(t, x(t), u(t)) = 0 \text{ a.e. in } [0,1], \\ g(t, x(t), u(t)) \leq 0 \text{ a.e. in } [0,1], \\ u(t) \in U(t) \text{ a.e. in } [0,1], \\ (x(0), x(1)) \in C, \end{array} \tag{OCP}$ 

where  $l : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ ,  $(f, b, g) : [0, 1] \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n \times \mathbb{R}^{m_b} \times \mathbb{R}^{m_g}$  are given functions,  $U(t) \subset \mathbb{R}^m$  for all  $t \in [0, 1]$  and  $C \subset \mathbb{R}^n \times \mathbb{R}^n$ .

As it is pointed out in [3], it is well known that the maximum principle is not in general valid for (OCP). It is necessary to impose some regularity conditions on the mixed constraints or to assume interiority-type hypotheses. In this work, inspired by some previous works from the literature ([1] and [2], e.g.), we consider processes which satisfy asymptotically (or approximately) the conditions in the weak maximum principle. Such processes are termed asymptotic weak maximum principle (AWMP) processes. We, then, prove that every weak local optimal process of (OCP) is, necessarily, an AWMP one. In other words, the conditions satisfied by the AWMP processes can be viewed as necessary optimality conditions. No regularity condition (or constraint qualification) or interiority hypothesis is imposed on the mixed constraints. In addition, we propose an augmented Lagrangian-type method which generates sequences whose limits, when they exist, are AWMP processes. The results are applied to some simple academic instances of (OCP). (Work supported by grant 2013/07375-0, São Paulo Research Foundation (FAPESP).)

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# Optimal Control Problems for Elliptic Hemivariational Inequalities

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Keywords: Optimal controls, Elliptic hemivariational inequality, Asymptotic behavior.

We consider a bounded domain  $\Omega$  in  $\mathbb{R}^d$  whose regular boundary  $\Gamma$  consist of the union of three disjoint portions  $\Gamma_i$ , i = 1, 2, 3 with  $meas(\Gamma_i) > 0$ . We formulate the following nonlinear elliptic problem with mixed boundary conditions [3]:

$$-\Delta u = g \text{ in } \Omega, \quad u\big|_{\Gamma_1} = 0, \quad -\frac{\partial u}{\partial n}\big|_{\Gamma_2} = q, \quad -\frac{\partial u}{\partial n}\big|_{\Gamma_3} \in \alpha \,\partial j(u), \tag{1}$$

where  $\alpha$  is a positive constant,  $g \in L^2(\Omega)$ ,  $q \in L^2(\Gamma_2)$  and the function  $j: \Gamma_3 \times \mathbb{R} \to \mathbb{R}$ , called a superpotential (nonconvex potential), is such that  $j(x, \cdot)$  is locally Lipschitz for a.e.  $x \in \Gamma_3$  and not necessary differentiable. Such multivalued condition on  $\Gamma_3$  is denoted for a nonmonotone relation expressed by the generalized gradient of Clarke [2]. The weak formulation of (1) is given by the elliptic hemivariational inequality [3, 5]:

find 
$$u \in V_0$$
 such that  $a(u,v) + \alpha \int_{\Gamma_3} j^0(u;v) \, d\Gamma \ge L(v), \quad \forall v \in V_0,$  (2)

where  $j^0$  represent the generalized (Clarke) directional derivative,  $a(u, v) = \int_{\Omega} \nabla u \, \nabla v \, dx$ ,  $L(v) = \int_{\Omega} gv \, dx - \int_{\Gamma_2} qv \, d\gamma$  and  $V_0 = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_1\}$ .

We formulate for each  $\alpha > 0$ , different optimal control problems  $(C_{\alpha})$ , on the internal energy g and the heat flux q, for quadratic cost functional and we prove existence results for the optimal solutions (see [1, 4]). We also consider a problem as (1), with a Dirichlet condition on  $\Gamma_3$  and we formulate similar optimal control problems (C), on control variables g and q. We obtain, convergence results for optimal controls and system states  $(C_{\alpha})$  to the corresponding optimal control and system state (C), when the parameter  $\alpha$  goes to infinity.

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# Quantitative particle approximation of nonlinear Fokker-Planck equations with singular kernel

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Keywords: Interactive particle systems, convergence, well-posedness

In this work, we study the convergence of the empirical measure of interacting particle systems with singular interaction kernels. First, we prove quantitative convergence of the time marginals of the empirical measure of particle positions towards the solution of the limiting nonlinear Fokker-Planck equation. Second, we prove the well-posedness for the McKean-Vlasov SDE involving such singular kernels and the convergence of the empirical measure towards it (propagation of chaos).

Our results only require very weak regularity on the interaction kernel, which permits to treat models for which the mean field particle system is not known to be well-defined. For instance, this includes attractive kernels such as Riesz and Keller-Segel kernels in arbitrary dimension. For some of these important examples, this is the first time that a quantitative approximation of the PDE is obtained by means of a stochastic particle system. In particular, this convergence still holds (locally in time) for PDEs exhibiting a blow-up in finite time. The proofs are based on a semigroup approach combined with a fine analysis of the regularity of infinite-dimensional stochastic convolution integrals.

This work is in collaboration with A. Richard and M. Tomasevic.

# Steady-state density preserving method for second-order SDEs

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**Keywords:** Nonlinear damped stochastic systems, stationary distribution, numerical approximation, computer simulation

We devise a method for the long-time integration of a class of damped second-order stochastic mechanical systems. The introduced numerical scheme has the advantage of being completely explicit for general nonlinear systems while, in contrast with other commonly used integrators, it has the ability to compute the evolution of the system with high stability and precision in very large time intervals. Notably, the method has the important property of preserving, for all values of the stepsize, the steady-state probability density function of any linear system with a stationary distribution. Numerical experiments are presented to illustrate the practical performance of the introduced method.

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# Numerical solution of stochastic differential equations appearing in open quantum systems

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**Keywords:** Stochastic differential equation, Euler-Exponential scheme, weak convergence, locally Lipschitz SDE, numerical solution

The talk addresses the numerical simulation of quantum systems by using stochastic differential equations (SDEs). First, we focus on the numerical solution of the non-linear stochastic Schrödinger equation, which is also called non-linear Belavkin equation. We present an Exponential-Euler scheme for this locally Lipschitz SDE that describe open quantum systems. We provide recent results on the weak convergence of this numerical method, which includes the study of the leading order term of the weak error expansion with respect to the step-size. Thus, we develop the Talay-Tubaru extrapolation procedure in quantum simulations. Second, we introduce a quantum-trajectory method for solving stochastic quantum master equations with mixed initial states. We obtain the solution of the stochastic master equation by means of a system of coupled SDEs of Schrödinger type, inspired by classical particle systems. Then, we construct exponential schemes for the resulting SDEs.

The talk is based on joint works with R. Biscay, J. Fernández. M. Muñoz.

# Models selection procedures for random objects driven by context tree models

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Keywords: model selection, contex tree

In several research problems we deal with stochastic sequences of inputs from which a volunteer generates a corresponding sequence of responses, and it is of interest to model the relation between them. A new class of stochastic processes, namely sequences of random objects driven by context tree models, has been introduced to model this relation. In the talk I will formalize this class of stochastic processes and present model selection procedures to make inference on it.

# Large deviations for birth-death processes with polynomial rates

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Keywords: large deviation principle, birth and death process

Birth-death processes form a natural class where ideas and results on large deviations can be tested. In the talk I overview our results about large deviations for birth-death processes where the jump rate has an asymptotically polynomial dependence on the process position. Almost all considered cases have not the large deviation principle, but there is a special case, where the principle is established: the rate of a downward jump (death) is growing asymptotically linearly with the population size, while the rate of an upward jump (birth) is growing sub-linearly. We also consider various forms of scaling the original process and normalizing the logarithm of the large deviation probabilities. The results [1] show interesting features of dependence of the large deviation functional on the parameters of the underlying process.

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# Recovering communities in networks

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Keywords: Stochastic Block Model, EM algorithm, Random Networks

Network models have received increasing attention from the statistical community, in particular in the context of analyzing and describing the interactions of complex random systems. In this context, community structures can be observed in many networks where the nodes are clustered in groups with the same connection patterns. In this talk, we address the community detection problem for weighted networks in the case where, conditionally on the node labels, the edge weights are drawn independently from a Gaussian random variable with mean and variance depending on the community labels of the edge endpoints. We will present a fast and tractable EM algorithm to recover the community labels that achieves the optimal error rate.

# The law of the iterated logarithm for solutions of stochastic differential equations with random coefficients

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Keywords: law of the iterated logarithm, stochastic differential equations

The functional law of the iterated logarithm is obtained for solutions of stochastic differential equations with random coefficients and Poisson noise.

# Machine learning algorithms for making inferences on networks and answering questions in biology, medicine and pharmacology

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**Keywords:** Complex networks, machine learning, protein function, disease genes, drug side effects

A cell can be viewed as a set of complex networks of interacting biomolecules, and genetic disease as the result of abnormal interactions within these networks. In this talk, I will present novel machine learning algorithms for solving problems in systems biology, medicine and pharmacology that can be phrased in terms of inference in such large-scale networks.

I will begin by describing a semi-supervised learning method that can accurately predict protein function for newly sequenced organisms and is currently the state-of-the-art method for predicting function in bacteria. I will then describe a method to quantify a distance between disease modules on the human interactome that uses only disease phenotype information. I will show how this measure can be exploited by a learning algorithm for inferring disease genes for heritable disease. Importantly, our approach allows the prediction of disease genes for diseases for which no disease gene is already known. Finally, I will present a method for the prediction of drug side effects. This algorithm, which is based on matrix factorization, is the first that can predict the frequency of drug side effects in the population.

# Graph theory: Forbidden subgraphs, Colourings and Applications

### MAYA STEIN

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### Keywords: graph, subgraph

A fundamental structure in discrete mathematics are graphs, which are used to model pairwise relations between abstract objects. A graph consists of points (called vertices), some of which are connected by lines (called edges). The simplicity and generality of this concept made graphs widely applicable and popular. Many interesting applications can be modeled by graph colourings, where one seeks to colour the vertices with few colours in a way that no two endvertices of an edge receive the same colour.

In this talk, we will survey some of the basic structural properties of graphs, with a special focus on forbidden subgraphs. We will examine two algorithmic applications in greater detail: first, algorithms for graph colouring and second, algorithms for training data for machine learning.

# Mathematics: key enabling technology for scientific machine learning

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Keywords: scientific computing, machine learning, neural networks, artificial intelligence

Artificial Intelligence (AI) will strongly determine our future prosperity and well-being. Due to its generic nature, AI will have an impact on all sciences and business sectors, our private lives and society as a whole. AI is pre-eminently a multidisciplinary technology that connects scientists from a wide variety of research areas, from behavioural science and ethics to mathematics and computer science.

Without downplaying the importance of that variety, it is apparent that mathematics can and should play an active role. All the more so as, alongside the successes of AI, also critical voices are increasingly heard. As Robert Dijkgraaf (former director of the Princeton Institute of Advanced Studies) observed in NRC in May 2019: "Artificial intelligence is in its adolescent phase, characterised by trial and error, self-aggrandisement, credulity and lack of systematic understanding." Mathematics can contribute to the much-needed systematic understanding of AI, for example, greatly improving reliability and robustness of AI algorithms, understanding the operation and sensitivity of networks, reducing the need for abundant data sets, or incorporating physical properties into neural networks needed for superfast and accurate simulations in the context of digital twinning.

Mathematicians absolutely recognise the potential of artificial intelligence, machine learning and (deep) neural networks for future developments in science, technology and industry. At the same time, a sound mathematical treatment is essential for all aspects of artificial intelligence, including imaging, speech recognition, analysis of texts or autonomous driving, implying it is essential to involve mathematicians in all these areas. In this presentation, we highlight the role of mathematics as a key enabling technology within the emerging field of scientific machine learning. Or, as I always say: "Real intelligence is needed to make artificial intelligence work."
### Conservation and dynamical interaction of plant communities

<u>Pablo Aguirre</u><sup>1</sup>, Elisa Domínguez-Hüttinger<sup>2</sup>, Jaime Acosta-Arreola<sup>3</sup>, Jorge A. Meave<sup>4</sup>, and Nicolás González Muñoz<sup>5</sup>

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**Keywords:** Ecological reserve management, exotic species control, dynamical systems, invariant manifolds

We propose a mathematical model that integrates several different sources of field data of the San Angel Pedregal Ecological Reserve, Mexico City. The model considers two species of native trees, *Pittocaulon praecox* and *Buddleja cordata* and the exotic tree of Australian origin Euclyptus camaldulensis. Our aim is to establish conservation strategies of native trees facing invasion of the exotic species. Mathematically each of the asymptotically stable states of the model is associated with a given basin of attraction [3, 4]. Crossing from one basin of attraction into another is possible whenever the initial state is pushed beyond the relevant basin boundary. Generically, these separatrices correspond to stable manifolds of saddle objects in phase space. We set up a scheme in which the first step is to identify and describe the relevant stable manifold as a global object in phase space and understand its role as a separatrix of different basins of attraction [1, 2]. Once this "critical" boundary has been isolated, variation of a control variable —modelling an external intervention—should drive the system through the stable manifold and into the basin of attraction of the desired equilibrium state. Thus, our investigation allows us to understand the nonlinear negative effects of exotic species and to propose possible strategies for their control, to predict the effects of perturbations (biotic and abiotic) on the basins of attraction of ecosystems and ultimately to help design reserve management strategies aimed at decision makers by assessing what is the most likely long term ecologic interaction between the tree species.

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# An animal population going after a mobile resource. A complete-migration mathematical model.

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Keywords: complete migration, mobile resource, population abundance

We consider an animal population that develops in a planar habitat  $\Gamma \subset \mathbf{R}^2$ , in which its position at each instant can be represented by a point on  $\Gamma$  and whose abundance is accounted for by a non-negative time function N(t). Assuming the case where its primary basal resource has a density distribution that decreases radially but whose point of the maximum value is mobile, defining an annual cycle  $\gamma : \mathbf{R} \to \Gamma$ ,  $\gamma(t+1) = \gamma(t)$ ,  $\forall t \in \mathbf{R}$ , we model the trajectory that this animal population must follow and the one that must converge if it is mobilized (completely) after this resource, weighing the times of foraging and reproduction. So, if a function  $t \to \alpha(t) = \gamma(a(t)) \in \Gamma$ , represents the position of the population, then

$$\begin{cases} N' = r[||\alpha'||] \left(1 - \frac{N}{K[\mathcal{D}(\alpha,\gamma)]}\right) N\\ a' = \lambda(N)(K[0] - K[D(\alpha,\gamma)]), \end{cases}$$

where the carrying capacity K[] is negatively correlated with the distance  $\mathcal{D}(\alpha, \gamma)$  between the population and the center point of the resource. Furthermore, the intrinsic growth rate r[] is negatively correlated with the displacement rate  $||\alpha'||$ . On the other hand, the variation (always positive) of the administration of time a(t) in its path by the population decreases with population size through an auxiliary function of N and, on the other hand, increases more being further from the central point of the resource, that is, with a lower carrying capacity.

The work obtained analytical and numerical conclusions about the population dynamics of the abundance-location pair.

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# Spatio-temporal dynamics of anuran male choirs as an energetically limited swarmalator system

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Keywords: Swarmalators, mobile coupled oscillator, adaptive calling rate

Anuran males vocalize together forming choral congregations with the aim of attracting females. A choir can be understood as a dynamic acoustic network, which varies both in time and space, with communication rules determined by competition and/or cooperation, which are conceptual frameworks that explain the synchrony and alternation of co-occurring calls. From a mathematical approach, the choirs have been modeled as a static coupled oscillators system whose formulation is inspired by the traditional phase delay model, where the intrinsic rates of singing are represented as natural frequencies of constant value. Recently, a new modeling paradigm called Swarmalators (a contraction between swarm and oscillators) makes it possible to study the collective behavior of multi-agents, such as occurs in anuran choirs, where they self-organize spatially and temporarily. In this work, we analyze which spatial-temporal structures arise from the interaction between anuran males with adaptive calling rates and energetically limited position changes, describing the dynamics of self-organization by a system of mobile coupled oscillators.

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# Modeling Feline Sporotrichosis

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**Keywords:** epizooty, next generation matrix,  $R_0$ , infectious disease, disease control

Sporotrichosis is a subcutaneous mycosis with a global distribution, also known as "rose gardener's disease". Brazil is experiencing a rapid spread of the zoonotic transmission of Sporothrix brasiliensis, the main etiological agent of this disease in this country, affecting domestic felines. Cost-effective interventions need to be developed to control this emergent public health problem. To allow for the comparison of alternative control strategies, we propose in this paper, a mathematical model representing the transmission of S. brasiliensis among cats, stratified by age and sex. The model presented is the first attempt in the literature to describe the transmission of sporotrichosis. We derived the expected endemic equilibria based on what is known about the disease and the biology and behavior of cats. Through the next generation matrix, we derived the  $R_0$  for this disease. Other analytical properties of the model and numerical simulations showed possible strategies for reducing the endemic levels of the disease in the cat population, with a positive impact on human health. The scenarios included mass treatment of infected cats and mass implementation of contact reduction practices, such as neutering. The results indicate that mass treatment can reduce substantially the disease prevalence, and this effect is potentialized when combined with neutering or other contact-reduction interventions. On the other hand, contact-reduction methods alone are not sufficient to reduce prevalence.

### Shape optimization for flows under mixed boundary conditions

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**Keywords:** Navier-Stokes/energy equations, mixed boundary conditions, do-nothing conditions, shape optimization

We are interested in shape optimization problems of the form

Find  $\Omega^* \in \mathcal{O}$  such that  $\mathcal{J}(u_{\Omega^*}, \boldsymbol{v}_{\Omega^*}, \Omega^*) = \inf_{\Omega \in \mathcal{O}} \mathcal{J}(u_{\Omega}, \boldsymbol{v}_{\Omega}, \Omega),$ 

where  $\mathcal{O}$  is a set of admissible domain perturbations,  $\mathcal{J}$  is a given cost functional, and  $u_{\Omega}$ ,  $v_{\Omega}$  represent the temperature distribution and the velocity field, respectively, of an incompressible fluid in a domain  $\Omega$ . The special feature here is the presence of a domain boundary portion where the fluid can leave or re-enter freely, sometimes called *open* boundary part.

We assume that v is governed by the Stokes or Navier-Stokes equations, while u is governed by an energy equation. The presence of the open boundary part naturally introduce mixed boundary conditions for u and v. In particular, we consider do-nothing type conditions for the fluid flow and the heat transfer at the open boundary. The presence of mixed boundary conditions requires to carefully define the set admissible domain perturbations to have the existence of weak solutions, with the regularity possibly required by the evaluation of the cost functional. Further, the existence of the shape derivative may be affected by the choice of the boundary conditions on the open boundary part.

In this talk we first discuss the existence, uniqueness, and regularity of weak solutions for a Boussinesq system (coupled Navier-Stokes and energy equations according to the Boussinesq approximation) with mixed boundary conditions, considering either a do-nothing or a directional do-nothing condition for the fluid flow, and a new boundary condition for the heat transfer that couples nonlinearly the fluid velocity and temperature. This part of the talk correspond to a joint work with Carlos N. Rautenberg and Rafael Arndt (George Mason University, USA); see [1,2]. Then, we present some initial results on PDE-constrained shape optimization problems that involve mixed boundary conditions: The optimal conduit shape for a Stokes flow; and the optimal shape design for a one-way coupled Navier-Stokes/energy equations (no bouyancy effects). This second part of the talk correspond to a joint work with Carlos N. Ratenberg and Weiwei Hu (University of Georgia, USA); see [3].

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# A Dual-Mixed Approximation for a Huber Regularization of Generalized p-Stokes Viscoplastic Flow Problems.

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**Keywords:** Viscoplastic fluids, Dual-mixed methods, Twofold saddle point, Semismooth Newton methods.

In this work, we propose a dual-mixed formulation for stationary viscoplastic flows with yield, such as the Bingham or the Herschel-Bulkley flow. The approach is based on a Huber regularization of the viscosity term and a two-fold saddle point nonlinear operator equation for the resulting weak formulation. We provide the uniqueness of solutions for the continuous formulation and propose a discrete scheme based on Arnold-Falk-Winther finite elements. The discretization scheme yields a system of slantly differentiable nonlinear equations, for which a semismooth Newton algorithm is proposed and implemented. Local superlinear convergence of the method is also proved. Finally, we show several numerical experiments in two and three dimensions to illustrate the behavior and efficiency of the method [1].

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### Multiscale simulation of discrete fracture networks

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Keywords: Discrete fracture, mixed finite elements, multiscale

We present a technique for the numerical simulation of coupling discrete fracture flow with the surrounding matrix flow in a multiscale setting. The research effort is the combination of three projects: 1) a mesh generation project; 2) a mixed finite element approximation where matrix flow is coupled to fracture flow and fracture intersection lines (DFM) and 3) a MHM(Hdiv) - multiscale mixed hybrid formulation applied to the discrete fracture matrix flow.

The mesh generation considers the intersection of a plane polygon with an existing mesh ([3]). The main challenge in this research is to handle intersecting faces with small angles and/or distances. A *snapping* algorithm is proposed such as to avoid very small and/or distorted elements. Consequently, the resulting fracture representation may seize to be plane. Also, fracture that are very close may overlap after their insertion.

The mixed element approximation couples three dimensional matrix porous media flow with two dimensional flow over a manifold (i.e. fracture) ([1]). The fracture acts as a pressure boundary condition for the matrix flow. The conservation of mass over the manifold considers the sum of the boundary flow of the three dimensional domain and the flow over the manifold. The resulting system is a symmetric saddle point problem.

The resulting numerical problem is reduced by restraining the fluxes between the macro domains to macro fluxes with reduced number of degrees of freedom ([2]). These restraints allow to substructure the problem where internal degrees of freedom are condensed on the coarse-scale degrees of freedom. The resulting system of equations is much smaller than the full system.

Finally, the simulation technique is applied to different DFM benchmark problems. The effect of coarsening the mesh is numerically explored. When the multiscale meshes lead to poor quality results, we show how these results can be improved.

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### Optimal control of nematic liquid crystals

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**Keywords:** optimal control, nematic liquid crystals, coupled Schrödinger-elliptic system

Solitary waves are nonlinear and self-reinforcing waves that appear in diverse areas of the physics. In particular, in a physical medium of nematic liquid crystals (NLC), it is possible to observe that they are able to support spatial optical solitary waves, so-called Nematicons. These waves arise from a polarized electromagnetic beam (a laser) propagating in a thin slab of NLC previously preconditioned by a bias low frequency electric field. This electric field is externally applied in order to pre-tilt the NLC molecules. The experimental set-up for this phenomena was studied extensively by Assanto and collaborators [3]. The complete model was obtained by minimizing the free elastic energy deriving a nonlinear coupled system of an NLS and an elliptic Poisson-type equations for which it is proved well posedness and existence of soliton solutions [1]. In this talk we will consider a simplification of the complete model given by

$$0 = i\partial_z u + \frac{1}{2}\nabla^2 u + 2u\theta, \tag{1a}$$

$$0 = \nu \nabla^2 \theta - q\theta + |u|^2, \tag{1b}$$

where the variable u represents the complex amplitude of the polarized laser beam, and the real variable  $\theta$  is related to the director field angle describing the macroscopic orientation of the molecules of the NLC.

In [2] the authors show the well-posedness and existence of soliton solutions (nematicons) for this system. Using these nematicon solutions it is possible to design and test optical switching and routing circuits in reconfigurable settings. Thus, it is interesting to wonder about the possibility to manipulate, mathematically and physically, diverse parameters of the model in order to achieve desired states. In this way, we study an optimal control problem for the coupled system (1) considering the control q = q(z) depending on the optical axis coordinate.

The goal consists in finding an optimal control for which the solution u of equation (1) with a given initial state reaches a terminal state at  $z = \zeta$  near a desired target with minimum global rate of change of q. We will show well-posedness, existence and first order necessary conditions for an optimal solution. The result can be interpreted as the attainment of the optimal bias electric field necessary to take the intensity of the laser beam to a desired final state.

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# STABILIZATION RESULTS FOR DELAYED FIFTH-ORDER KDV-TYPE EQUATION IN A BOUNDED DOMAIN

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Keywords: KdV-type system, Delayed system, Damping mechanism, Stabilization

In this talk we shall discuss stabilization results for the Kawahara equation, a fifth order Korteweg-de Vries type equation, with time-delayed internal feedback. Under suitable assumptions on the time delay coefficients we prove that solutions of this system are exponentially stable. First, considering a damping and delayed system, with some restriction of the spatial length of the domain, we prove that the Kawahara system is exponentially stable for  $T > T_{\min}$ . After that, introducing a more general delayed system, and by introducing suitable energies, we show using Lyapunov approach, that the energy of the Kawahara equation goes to zero exponentially, considering the initial data small and a restriction in the spatial length of the domain. To remove these hypotheses, we use the compactness-uniqueness argument which reduces our problem to prove an observability inequality, showing a semi-global stabilization result.

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# Network Reliability Analysis Subject to Dependent Failures due to the occurrence of Ice Storms

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**Keywords:** Network reliability, Monte Carlo, Variance reduction, Geographically correlated failures

Although it began more than 60 years ago, network reliability is an area of study that still has much room for further development. Evidence of component failure dependences and the critical role played by these networks after natural disasters make them an area that needs further analysis. Ice storms are natural disasters affecting power grids that have become more recurrent. They correspond to a climatic phenomenon where freezing precipitation and wind speed can severely damage the networks due to the accumulation of ice and the impact of wind. We consider a Power grid where transmission lines fail due to a combination effect of wind and freezing precipitation (see [1]). We calibrate a Marshall-Olkin multivariate vector ([2]) that models the transmission lines' lifetimes. After the multivariate model parameters are determined, an accurate reliability estimation is obtained using variance reduction methods ([3]). We applied the technique to study the reliability of the Chilean Power Grid in the regions of Nuble and Bio Bio against the occurrence of ice storms.

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# Limiting behavior of the reliability function for mixed coherent systems with Lévy-frailty Marshall-Olkin dependent failure times

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**Keywords:** Asymptotic approximation, Reliability, Marshall-Olkin distribution, Dependent random variables

The study of network reliability is a topic where practical and theoretical questions have challenged the researchers for the las 60 years. Recently, we seek to set higher standards for network services because, as a society, more activities rely on them. With these new standards, correlations between components' lifetimes cannot be neglected anymore, and incorporating dependency has become a central challenge in Reliability. In this work, we study the asymptotic behavior of the system's reliability when we assume the system's components have a Lévy-frailty Marshall-Olkin (dependent) lifetimes. This model is of interest because, first, it is a flexible family that allows considering mild or strong failure dependence. Second, it is exchangeable, which allows the use of the Samaniego system signature result and also have a better interpretation of the results. Third, it is a subfamily of the Marshall-Olkin models [1], so any findings can be used as benchmarks for more general results (see [3]). Our results show that, as the number of components grows, the probability that the system is still functional converges to the probability of the first-passage time of a Lévy subordinator process. More specifically, we consider a sequence of mixed coherent systems ([4]) whose components are homogeneous and non-repairable, with failure-times governed by a Lévy-frailty Marshall-Olkin distribution — a distribution that allows simultaneous component failures. We show that under measurability conditions the reliability function converges to the probability of a first-passage time of a Lévy subordinator process. The proof combines the asymptotic behavior of the Samaniego's signature ([4]) with the asymptotic behavior of the k out of n component to fail as studied in [5].

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# Explicit formulas for the variance of the Creation Spectrum and the F- Monte Carlo network reliability estimation methods

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Keywords: network reliability, Monte Carlo, variance reduction

In this work we revisit a classical static homogeneous network reliability model, where the system under study is represented by a graph G = (V, E), where a set of nodes V is connected by a set of links E, with |V| = n and |E| = m. Nodes are perfect, but links fail, independently from each other, with identical distributions (failure probability q = 1 - p).

A configuration or state of the network is the vector containing the up/down state of each link. The network state space  $\Omega$  contains all the possible states, and it is the union of two disjoint subspaces, one of which includes all states associated to a network up condition, and the other one includes all states associated to a network down condition. Usually, network up means that a subset  $K \subseteq V$  of nodes is connected by means of the operational links, and network down means that the subset K is disconnected. The network reliability is expressed by the polynomial  $R = \sum_{j=1}^{m} \alpha_j {m \choose j} p^j q^{m-j}$ , where  $\alpha_j$  is the fraction of network up states with exactly j operational links. Its computation is an NP-hard problem, so that it is usual to estimate its value for a given p by means of Monte Carlo methods.

In this work, we discuss the standard Monte Carlo method and two variance reduction methods from literature, the Creation Spectrum [3] and the F–Monte Carlo [1] [2] methods, and we present novel analytical expressions for the variance of the reliability simulation estimators, contributing to the study of these methods and their performance.

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# Network Performability, Rare Events and Standard Monte Carlo

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**Keywords:** network reliability, network performability, resilience, rare events, standard Monte Carlo, sensitivity analysis

In this talk, we underline the interest in moving from the typical reliability binary world where components and systems are either up or down, to a multi-variate one, where the up state is decomposed into several performance levels. This is also called a *performability* view of the system. After discussing a very representative metric in this class, called *resilience* in the area, defined as the expected number of pairs of nodes that can communicate, we briefly describe a Monte Carlo approach where instead of trying to reduce the variance of the estimators, we focus on reducing their time complexities. This view allows a first straightforward way of exploring resilience and related metrics. It also allows performing a sensitivity analysis of them with respect to the individual reliabilities of the components, without a significant overhead of the procedure that estimates the resilience metric alone. We limit the development to a static context. Numerical examples illustrate these procedures.

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## Inflation forecast with Artificial Intelligence

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Keywords: Core inflation, Forecasting, Artificial Intelligence

Inflation is the continuous and generalized increase in prices in an economy. A small inflation rate is natural and associated with a healthy growth of an economy, however, uncertainties related to the volatility and predictability of inflation bring issues to maintain purchasing power and, at the macroeconomic level, in monetary policy design. Recently, because of the pandemic event of Covid-19, central banks once again are concerned about the increase of inflation worldwide. To observe the tendency of the inflation, several central banks use core inflation to decompose the inflation in persistent and transient components [1, 2]. In Brazil, inflation targets are defined using the Extended National Consumer Price Index (IPCA), which is sensitive to seasonal behaviour and demand shocks. Such effects add adversities to the analysis of the inflation, which in turn, impose extra difficulties to the design of monetary policies. In this sense, the use of core inflation as a target would allow the design less rigid monetary policies. Thus, in this work, we propose a wavelet approach to calculate the core inflation using Daubechies families, which allow exclusion of transient components of the inflation without the need of additional hypothesis. To compute wavelet core inflations, we use the IPCA time series, between July 2006 and December 2021. We consider, additionally, macroeconomics indexes to increase idiosyncrasy of the economic context, such as life cost index, minimum wage and market expectation. For the forecast, artificial intelligence techniques are adopted, such as neural networks. We point out that the use of neural networks make it possible to analyse highly complex problems that cannot always be described by analytical models [3]. We analyse confidence intervals to estimate bounds for inflation forecast probable values. Among the main conclusions, our inflation forecast generated smoothed signals, allowing to identify the trend of inflation up to twelve months.

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# Optimization-based control for nonlinear dynamical systems with narrow feasible region and recycles

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**Keywords:** Recycles, Feasible operation, Plant-wide control, Distance Field Map, Dynamic behavior

Recycle of mass and energy is a feature present in almost all processes and industries [5]. It is an inevitable characteristic found in actual industries due to the differences between the designed processes and the actual implementation. When a process is set in, it is possible to identify inefficiencies in the planned performance, and the use of recycle tries to reduce this difference [2]. Although recycling helps to improve the plant's overall performance compared with the serial arrangement, its effect on plant dynamic behavior is seldom considered, and those changes start to affect features of the process like controllability and stability. Similarly, recycling affects the feasible region of individual equipment and its effect is not verified either. Furthermore, it is crucial to take into account the difficulty to keep the feasibility of processes. Usually, the process is thought of as possible over a wide range of operative conditions. But in fact, actual processes only exist over a narrow set of conditions [4] that are not only defined by security but by physical phenomena viability [3]. Nonlinear dynamical systems are designed to operate over a unique nominal state without foreseeing that disturbances could carry the process to other operative points or out of the feasible region.

Several works have demonstrated that advanced control strategies allow the improvement of the dynamic behavior of complex plants. Different techniques, like Model-Based Predictive Control (MPC) and Plantwide Control (PWC), show that their implementation reduces the recycling effects [1]. However, there is no explicit methodology to design those controllers to face the impacts of recycling over dynamic behavior and/or feasibility. Even, there is no tuning procedure to design the controllers that allow the optimization of the dynamic performance of plants, including the control system.

In this sense, this work presents a methodology to characterize the effects of recycles over dynamic behavior of plants and how they affect the feasible operative region. Based on the previous analysis, a methodology of control is proposed to design an optimization-based control strategy, facing explicitly the dynamical phenomena of recycling on processes.

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# Computational Modeling of Pharmacokinetic Profiles Measured by Alternate Current Biosusceptometry

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Keywords: Ordinary Differential Equations, Parameter Estimation, Identifiability.

This work is on the development and implementation of an ordinary differential equation (ODE) model for drug biodistribution aimed at the pharmacokinetics of magnetic nanoparticles. The data that we have used comes from in vivo experiments in which one injected nanoparticles into the bloodstream and measured them both in the heart and liver by using alternate current biosusceptometry [1, 2]. The proposed linear ODE model comprises three compartments, one for the heart and the other two for the liver, from which the nanoparticles partially return to the bloodstream. Reported results include suitable calibrations of curves and parameters performed in *Mathematica* software using NLMEModeling and IdentifiabilityAnalysis packages [3, 4]. Besides other metrics and the optimal value for each parameter of the model, we also provide their respective standard errors achieved by a successful covariance step.

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## Edge-colorings avoiding patterns in a $K_4$

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Keywords: Extremal Graph Theory, Erdős-Rothschild Problem, Edge Coloring

This paper consists of a multicolored variation of the problem proposed by Erdős and Rothschild. The problem consists of characterizing graphs that admit the largest number of r-edgecolorings avoiding a fixed pattern of a graph F, where r and the pattern of F are given. A *pattern* P of F is a partition of its edge set. An r-coloring of a graph G is said to be (F, P)-free if G does not contain a copy of F in which the partition of the edge set induced by the coloring is isomorphic to P. Let  $\mathcal{P}$  be a pattern family, i.e., a set of pairs (F, P). We say that an r-colored graph  $\widehat{G}$  is  $\mathcal{P}$ -free if  $\widehat{G}$  is (F, P)-free for all pairs  $(F, P) \in \mathcal{P}$ . Let  $\mathcal{C}_{r,\mathcal{P}}(G)$  be the set of all  $\mathcal{P}$ -free rcolorings of a graph G. We write  $c_{r,\mathcal{P}}(G) = |\mathcal{C}_{r,\mathcal{P}}(G)|$  and  $c_{r,\mathcal{P}}(n) = \max \{c_{r,\mathcal{P}}(G) \colon |V(G)| = n\}$ . We say that an n-vertex graph G is  $(r, \mathcal{P})$ -extremal if  $c_{r,\mathcal{P}}(n) = c_{r,\mathcal{P}}(G)$ .

In the current paper, we focus on the complete graph  $F = K_4$  and we consider pattern families that do not contain the rainbow pattern, particularly the family  $\mathcal{P}^*$  of all patterns of  $K_4$  except  $K_4^R$ , which we call the non-rainbow patterns of  $K_4$ . This means that colorings in  $\mathcal{C}_{r,\mathcal{P}^*}(G)$  are such that all copies of  $K_4$  are rainbow.

It is known that for families  $\mathcal{P}^*$  with the properties of the previous paragraph, there exists  $r_1$  such that the Turán graph  $T_3(n)$  cannot be  $(r, \mathcal{P}^*)$ -extremal for any  $r \geq r_1$ . Here, we are interested in the largest possible value  $r_0$  such that  $T_3(n)$  is  $(r, \mathcal{P}^*)$ -extremal for all r with  $2 \leq r \leq r_0$ . The best known lower bound on  $r_0$  is 91, see [2]. We have already proven that this bound has been improved to 155, and we believe that it is possible to increase this value to a obtain a better bound.

To be more precise, we show that for  $2 \le r \le 155$ , there exists  $n_0$  such that, for every  $n \ge n_0$ and every *n*-vertex graph G, we have  $c_{r,\mathcal{P}^*}(K_4) \le r^{\exp(n,K_4)}$ . Moreover, equality holds in this equation if and only if G is isomorphic to the tripartite Turán graph  $T_3(n)$ .

The proof of our results combines the general strategy in [1] and [3] with linear programming. In some previous applications of this method, the general bounds provided by linear programming were not strong enough to extend the conclusion of this results to the entire range of r. Our main contribution in this works is to extend the technique of [3], which uses an inductive component in the proof, and allows us to better exploit local restrictions and to extend the result to better values of r. In [3], the bounds were extended to the best possible value.

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# Closed expression for the final size vector for a stochastic SIR model

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Keywords: Stochastic Epidemiological Modeling, SIR CTMC Model, Epidemic Final Size

Epidemiological modeling helps in analyzing the spread of diseases and identifying measures that can be adopted to contain them. The use of stochastic models allows us to study properties that are not accessible through deterministic models. In epidemiology, a very important property to be established, both for inference about an epidemic and for decision-making applied to public health, refers to the final size of the epidemic. The final size is the total number of individuals who contracted the disease over the duration of the epidemic. Final size estimation is a current research topic of wide interest, tackled through several approaches [1, 3, 2]. A common approach for obtaining the probability distribution for the final size of an epidemic is given by calculating powers of matrices that can be excessively large depending on the size of the population [4, 5]. Therefore, the modeling becomes unfeasible because of the computational cost. As an alternative way, in this work, we deduce an expression to find the closed form of the final size vector of the epidemic in the case of a stochastic SIR model defined by Continuous Time Markov Chain. The obtained expression allows accessing this distribution for the final size of the epidemic without needing the computation of high-order powers of large matrices.

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# A high-order scheme with multidimensional limiting process coupled to a nonlinear finite volume method for simulation of miscible displacement in porous media

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Keywords: Miscible displacement, Oil reservoir simulation, Full finite volume method

The phenomenon of miscible displacement of one incompressible fluid by another in a porous medium occurs in petroleum reservoirs, in saltwater intrusion on ocean coasts, and in the dispersion of polluted fluids in groundwater. The governing equations for the displacement process consist of a nonlinear differential equation, one of which has an elliptical form for pressure and a parabolic form for concentration. Traditionally, the governing equation is solved numerically by finite difference or finite element methods, i.e., the pressure and fluid velocity have traditionally been approximated by a mixed finite element method or discontinuous Galerkin methods, and the concentration by a finite difference method based on the use of a modified method of the characteristic procedure or the classical first order method or even by higher order Gudonov methods ([1], [2]). The objective of this work is to present a robust discretization based full finite volume method for such convection-dominated two-phase flow problems. This numerical formulation must be able to deal with unstructured meshes and with highly anisotropic and heterogeneous porous media. Both the pressure equation and the Darcy flux are approximated using the nonlinear two-point flux approximation (NL-TPFA), which produces monotonic solutions. These advantages are very important for oil reservoir simulation [3]. The nonlinear system is solved using Picard iteration and Anderson acceleration method. The concentrations are approximated by the high-order MUSCL-type scheme, together with the multidimensional limiting process (MLP) used to control the spurious oscillations. This limitation strategy was originally proposed by [4] for solving aerodynamic problems. To show the potential of the proposed scheme, we solve some benchmark we compare our scheme with other numerical formulations found in literature.

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# The application of a time exponential integrator to the wave equations, oriented to seismic imaging.

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Keywords: exponential integrator, Faber polynomials, wave equations

Exponential time integrators have been applied successfully in several physics-related differential equations [1, 2, 3]. However, their application in hyperbolic systems with absorbing boundaries, like the ones arising in seismic imaging, still lacks theoretical and experimental investigations.

The present work is an in-depth study of the Faber polynomials for exponential integration, consisting of a generalization of a popular exponential method that uses Chebyshev polynomials. This allows solving non-symmetric operators that emerge from classic seismic wave propagation problems with absorbing boundaries.

Theoretical, as well as numerical, results are presented for Faber approximations. We also the practical importance of determining an optimal ellipse encompassing the full spectrum of the discrete operator, in order to ensure and enhance convergence of the Faber exponential series. Furthermore, based on estimates of the spectrum of the discrete operator of the wave equations with a widely used absorbing boundary method, we numerically investigate stability, dispersion, convergence and computational efficiency of the Faber exponential scheme.

Overall, we conclude that the method is suitable for seismic wave problems and can provide accurate results with large time step sizes, and the computational cost diminishes with the increase of the approximation degree.

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# Evaluation of Football Forecasting Models: 2021 Brazilian Championship Case Study

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Keywords: football data analysis, forecasting models, accuracy evaluation, data visualization

Football forecasting models are computer programs/algorithms that use data such as previous results, match statistics, player performances and club economics to predict the probabilities for the results of future matches. In the present work, we analyse the performance of football results forecasts. We have collected data from eight different forecasting models during the 2021 Brazilian football season. First, we guide the analysis through visual representations of the data using a 2-simplex triangle to investigate visual patterns from the forecasting models. It highlights the most prominent features and enhances the interpretation of differences and similarities between models. Then, we evaluate forecasts' accuracy using the Ranked Probability Score (RPS) and analyse its evolution as championship matches were played; models comparison accounts for minor scale differences that may become consistent in time. Our primary goal is to encourage football forecasts' performance discussion. We hope to accomplish it by presenting appropriate criteria and easy-to-understand visual representations that can point the relevant factors of the subject.

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#### LACIAM-102

# Melanoma dynamics involving macrophages and CAR T-cell immunotherapy

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Keywords: tumour-associated macrophages, mathematical modelling, T lymphocytes

Melanoma skin cancer is considered one of the most aggressive types of cancer due to its high capacity to cause metastases, reducing the chances of patient survival if discovered late. In addition, melanoma has very immunogenic characteristics that make its treatment difficult, increasing the need to develop more effective techniques of therapy. In terms of oncology, mathematical modeling enables the analysis and distinction of the various mechanisms involved in tumor progression, allowing many scenarios, which would be impractical experimentally or very expensive. The present work gathers as main objectives to develop a mathematical model to describe the dynamics of melanoma in the presence of macrophages and an immunotherapy treatment with CAR-T cells and to simulate computationally scenarios of failure and success of the treatment. The results showed that without the presence of macrophages, when the tumour is immunosuppressive, the immunotherapy treatment is less effective in controlling the tumour cell population, agreeing with literature data on immunosuppression caused by melanoma, especially when immunotherapy treatments are used. Furthermore, under immunosuppressive conditions and in the presence of macrophages, failure of immunotherapy treatment occurs.

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# On distinct notions of tensor rank and practical implications to the higher-order completion problem

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Keywords: tensor rank, tensor decomposition, tensor train, higher-order completion problem

Matrix linear algebra provides powerful tools for organizing and handling data. Mathematical refinements and algorithmic developments resting, for example, upon the Singular Value Decomposition (SVD), have benefited many areas, such as image processing, physics, biomedicine, signal analysis, and neural networks, among others. As data structures become increasingly larger and more complex, more degrees of freedom are required to handle and interpret the data, so the study of multidimensional objects – the so-called tensors – became necessary.

In this work, we consider a tensor of order N, i.e., an array of N dimensions that is an element of a tensor product of N vector spaces. As for matrices, which can be seen as tensors of order 2, it is desired to study adequate decompositions of tensors to extract significant information from the data. Compared to matrices, the addition of just one order is already enough to demand new concepts for accommodating the introduced extension [1].

There exist classical decompositions such as the *Parallel Factor Decomposition* (PARAFAC) or the *High-Order SVD* (HOSVD). For each of these, a proper notion of rank is used and both have diverse applications and results in several areas. However, they suffer from drawbacks that can hinder the analysis of large tensors.[1].

The focus of our study is on the Tensor Train (TT) decomposition, together with the TT-rank [2], which does not suffer from the drawbacks of the aforementioned decompositions, as its number of estimated parameters grows linearly with dimension. This fact qualifies TT decomposition as a powerful tool for dealing with high-order problems. Furthermore, we apply the related notions of rank to address the so-called tensor completion problem [3], which can be solved by optimization techniques applied to an appropriate model. In this case, the choice of the rank definition and adequate parameters are fundamental to the quality of the solution that approximates the original tensor. Results of the literature on TT decomposition show its flexibility to address higher-order problems. For the case of the tensor completion problem, the methods that are based on the TT-rank usually capture better the global correlation between the tensor entries, being able to produce an approximation with superior quality.

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### A shape optimization approach to approximation of measures

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Keywords: 1D shape optimization, optimal transport, geometric measure theory

In this work we study the following 1 dimensional shape optimization problem: given a compact set  $\Omega \subset \mathbb{R}^2$ , a probability measure  $\rho_0 \in \mathcal{P}(\Omega)$  (which can be viewed for instance as an image) we seek to minimize the following

$$\inf_{\Sigma \in \mathcal{A}} W_2^2(\rho_0, \nu_{\Sigma}) + \Lambda \mathcal{H}^1(\Sigma),$$
(SO)

where the measure  $\nu_{\Sigma}$  is defined as

$$\nu_{\Sigma} := \frac{1}{\mathcal{H}^{1}(\Sigma)} \mathcal{H}^{1} \sqcup \Sigma, \text{ for } \Sigma \in \mathcal{A} := \left\{ \Sigma \subset \mathbb{R}^{2} : \begin{array}{c} 0 < \mathcal{H}^{1}(\Sigma) < +\infty \\ \text{compact, connected.} \end{array} \right\}.$$
(1)

Here  $\mathcal{H}^1$  denotes the 1-dimensional Hausdorff measure in  $\mathbb{R}^2$ , [1], and  $W_2$  denotes the Wasserstein distance on the space of probability measures, defined through the value function of the optimal transport problem [2].

To show existence of solution to (SO) one cannot easily resort to the direct method in the calculus of variations as the family of measures  $\nu_{\Sigma}$  defined in (1) is not compact. Therefore, we propose a relaxed formulation, whose competitors are taken in the space of Radon measures  $\mathcal{M}(\Omega)$ , and show through a blow-up argument that the solutions to this relaxed problem are of the form  $\nu_{\Sigma}$ , being therefore solutions to the original problem.

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### An Approach to Obtain the Prandtl's Equations

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Keywords: Prandtl's equations, boundary layer, Blasius equations

The inclusion of more dimensions in solving problems in both physics and mathematics has a long collection of successes and failures. There are plenty of examples, the general theory of relativity being perhaps the most famous. To a certain extent this short note engages the same idea: extend the problem in one dimension and then project it back with the intention of recovering the equations of the real incompressible flow in the presence of a surface. This innovation may be justified, or help us see the old problem from a new angle, due to the fact that, until today, there has been no formal operation that attends to the problem through the synthesis of the equations of the boundary layer along a thin, flat-plate with zero pressure gradient. Thus, the question that drives this short note is as follows: given a modified Navier-Stokes operator in three dimensions, does its projection to a subspace of two dimensions capture a Prandtl's[1] equations? The lead idea that guides the work consists of jumping into threedimensional space in order to build an operator, that being a modification of the Navier-Stokes operator, that simultaneously possesses a projection in two dimensions where it coincides with the Prandtl's equations. The proposed form of the operator is as follows:

$$N(\bar{u},\nu) + P(\bar{u},\nu) - \wp(\bar{u}) = 0, \tag{1}$$

$$div(\bar{u}) = 0, (2)$$

where  $\nu$ , is the dynamic viscosity,  $\bar{u} = (u_1, u_2, u_3)^t$  is the velocity field,  $N(\bar{u}, \nu)$  the Navier-Stokes operator [2] in 3-dimensional Euclidean space with  $(dp)^{\sharp} = 0$  and  $\partial_t \bar{u} = 0$ ,

$$N(\bar{u},\nu) = (\bar{u}\cdot\nabla)\bar{u} - \nu\nabla^2\bar{u},\tag{3}$$

We are looking for a specific function that connects the subspace with the three-dimensional global space, which we define as

$$\alpha(\|\bar{u}\|) = (1 - \|\bar{u}\| + \|\bar{u}^{\perp}\|), \tag{4}$$

 $\| * \|$  is the usual Euclidean norm and  $\bar{u}^{\perp} = (u, v, 0)^t$ . Given the following operators:

$$P(\bar{u},\nu) = \nu\alpha(\|\bar{u}\|)(\partial_{x^2}^2\bar{u} + \partial_{y^2}^2(\bar{u}^t(\bar{e}_2 \otimes \bar{e}_2)\bar{u})^{\frac{1}{2}}\bar{e}_2),$$
(5)

$$\wp(\bar{u}) = \alpha(\|\bar{u}\|) (\partial_y(\frac{\bar{u}^t(\bar{e}_2 \otimes \bar{e}_2)\bar{u}}{2}) \bar{e}_2 + (\bar{u}^t(\bar{e}_1 \otimes \bar{e}_1)\bar{u})^{\frac{1}{2}} \bar{e}_1 \times \{\nabla \times (\bar{u}^t(\bar{e}_2 \otimes \bar{e}_2)\bar{u})^{\frac{1}{2}} \bar{e}_2\})$$
(6)

them if we take:

$$\bar{u} = \bar{u}^{\perp} = (\partial_y \Phi(x, y), -\partial_x \Phi(x, y), 0)^t,$$
(7)

we can project naturally in a way that suits us:

$$N^{\perp}(\bar{u}^{\perp},\nu) + P^{\perp}(\bar{u}^{\perp},\nu) - \wp^{\perp}(\bar{u}^{\perp}) = 0,$$
(8)

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Latin American Congress on Industrial and Applied Mathematics, Rio de Janeiro, Brazil, January 30th — February 3rd, 2023  $\nabla \cdot \bar{u}^{\perp} = 0,$ (9)

Equation (8) and Eq.(9) are the Prandtl's equations. It is necessary to notice that if we take:

$$\Phi(x,y) = \sqrt{\nu U x} f(\eta), \tag{10}$$

where

$$\eta = y \sqrt{\frac{U}{\nu x}},\tag{11}$$

then equation (8) becomes the Blasius [3] boundary layer equation:

$$(2f''' + f''f, 0, 0)^t = \bar{0}.$$
(12)

The Prandtl's equations are the result of the subtle combination of experimental methods with an asymptotic analysis of the Navier-Stokes equations. The success achieved by the boundary layer theory in the last century is indisputable. On the other hand, the path developed in this work reflects that there is a connection between these equations and an equation that operates in a higher dimension, and they appear, naturally, from a projection. Notably, at no time have we used the traditional procedure that led to these equations, nor the physical or mathematical reasoning [4] of the boundary layer theory. Is it possible to speculate that perhaps, in the near future, real flows can be rationalized from the theory of fiber spaces[5]? Is the boundary layer, as an important part of a real fluid, a kind of fiber, in the mathematical sense of the concept? In addition, a natural question that arises concerns Prandtl's equations for three dimensions. Although there is the hope that a similar connection exists for higher dimensions, at this time, we have no idea what it would be like.

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# A NON-LINEAR FINITE VOLUME SCHEME PRESERVING EXTREMUM PRINCIPLE FOR SIMULATION OF AQUIFERS

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Keywords: Pollutant, Contaminant transport, Groundwater, NLFV-DMP, MUSCL-type

Aquifers modeling is used to analyze sustainable use of water resources, migration of contaminants, and vulnerability of aquifers to contribute to decision making in resource management. The contaminant migration in aquifers with highly heterogeneous and anisotropic properties represents an important multidisciplinary challenge ranging several fields of study. The governing equations of this flow are mainly the Advection-Dispersion-Reaction Equation (ADRE) and the pressure equation, which are based on the Darcy flux. They are solved using a method called IMPEC (Implicit Pressure and Explicit Concentration). Currently, as observed in [1], most numerical models approach the pressure field considering only the potential deviations in their discretized form, ignoring the effects of gravity. In this work, the pressure equation is discretized using the non-linear finite volume method with multipoint flux-approximation that preserves the discrete maximum principle (NLFV-DMP) considering the gravitational term. The advective term is solved using a higher-order method type MUSCL. The method used, described in [1,2,3], can be used with any polygonal meshes having the following main characteristics: it is locally conservative; it allows full heterogeneous diffusion tensors; it has second-order precision for smooth solutions and first-order precision for flow; it preserves linearity for the vast majority of cases; and it presents consistent discretization that treats the gravitational term as part of the discrete flow operator even for nonhomogeneous gravity. Thus, the formulation presented is validated from examples in the literature and the tests show that robust solutions and consistent discretization of the equations are provided to simulate flow processes of porous media in the presence of gravity, especially in systems with complex physical and geological properties.

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# An Adaptive strategy for avoiding stagnation on restarting GMRES

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#### Keywords: linear systems, GMRES, stagnation

The Restarted Generalized Minimal Residual, denoted as GMRES(m), is normally used for the solution of large, sparse, and nonsymmetric linear systems, which is often the most time-consuming part of numerical simulation in science and engineering. In practice, it has the drawback of eventually presenting at certain re-starting cycles a stagnation or a slowdown rate of convergence. In this work, we are going to discuss strategies for avoiding stagnation and how a combination of them can exploit better their individual properties. The combination is implemented as a switching controller that changes the structure of the GMRES(m) when the stagnation is detected. The switching controller chooses conveniently from several techniques, how to augment the Krylov subspace for enriching it. Moreover, the controller varies the restarting parameter to modify the dimension of the Krylov subspace is needed. This strategy makes the adaptive switching controller competitive from the point of view of avoiding the stagnation and acceleration of the convergence respect to the number of iterations and the computational time. We are going to present computational experiments show the advantages and the main issues raised from the perspective of the adaptive switching controller. For instance, when to perform the switching, what information is more important at each stage and when to modify the restart parameter.

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### Food distribution model using the goal programming approach

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Keywords: food distribution, optimization, goal programming

Food insecurity represents the situation where people do not have physical or economic access to sufficient food to cover their dietary needs. This situation is seen worldwide and with the negative impact of the Covid-19 pandemic on the world economy, millions of people have experienced hunger or difficulty in accessing food. In 2020 there was an increase in moderate and severe food insecurity and the situation have been persisting [1]. To reduce this problem, Food Banks are responsible for distributing food that normally no longer has commercial value but still has nutritional properties [2]. Therefore, the distribution process is able to reduce waste redirecting surplus food for people who are in a food insecurity situation. The process must be carried out under conditions of equity, effectiveness and efficiency in order to reach the greatest number of those in need [3]. The challenge is that often the total amount of food may not be sufficient to cover all the existing demands of the population. This work aims to propose an optimization model applied to the problem of food distribution using the goal programming approach, which consists in a widely used method for solving multi-objective problems [4]. Instances have been created to analyze the behavior of the model and its solutions.

### Acknowledgements

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# A variable-stepsize scheme for stochastic differential equations with additive noise

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Keywords: Stochastic Differential Equations, Local Linearization, Runge-Kutta

We present a new stable adaptive algorithm to solve Stochastic Differential Equations (SDEs) with additive noise, this algorithm features two new LL schemes using the Runge-Kutta alike approach embedded in an unconventional way, an adaptive strategy to choose the stepsizes and a way to reconstruct the generated brownian path. This results in an A-stable method that allows to solve SDEs with less timesteps than other adaptive schemes in the literature for the same level of error, resulting in less computational effort.

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### Mathematical Optimization for Urban Air Mobility

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**Keywords:** air traffic management, mixed integer linear programming, tactical deconfliction, reoptimization

We focus on how mathematical optimization (MO) could help build the bricks to develop Urban Air Mobility (UAM). In particular, we focus on passengers' transportation via eVTOLs, i.e., electric flying vehicles that will allow exploiting the sky to help smooth ground traffic in densely populated areas. Clearly, one of the biggest challenges in UAM is to ensure safety. From an operational viewpoint, the flights planning can be highly affected by different kinds of disruptions, which have to be solved at the tactical deconfliction level. Inspired by the classical aircraft deconfliction (see, for example, [1, 2, 3]), we propose a MO formulation based on a mathematical definition of vehicles separation, specialized in the UAM context. The deconfliction is based on speed changes or delayed takeoff, when possible. To the best of our knowledge, our MO model is the first that considers the whole set of conflicts at the same time. In the computational study, we, thus, compare our approach against a variant considering only pairwise conflicts, on three sets of realistic scenarios. More details can be found in Pelegrin et. al [4].

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# Pattern formation in Turing systems with space varying diffusion

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**Keywords:** Turing patterns, Nonlinear analysis, Sturm-Liouville problem, Inhomogeneous diffusion

For many years, Turing systems [1] have been proposed to account for spatial and spatiotemporal pattern formation in various contexts, such as developmental biology and ecology [2]. Experimental evidence that in some biological systems, spatial inhomogeneities are important for regulating patterns has led to several generalizations of the original reaction-diffusion mechanism. Here, we consider a two-morphogen reaction-diffusion system with a diffusion coefficient that depends explicitly on the space variables, for the case when the operator of the spectral Sturm-Liouville problem associated with the general reaction-diffusion system has Legendre polynomials as eigenfunctions. Although it is a special case, we show that it produces new types of patterns with variable wavelengths, and it allows us to propose a generalization of the standard weakly nonlinear analysis using these eigenfunctions instead of the eigenfunctions of the Laplace operator. The parameter regions for producing stripes or spots can be identified from the developed general nonlinear analysis, which is verified numerically using the BVAM reaction-diffusion system [3]. The types of patterns generated by this particular problem enrich the field of pattern formation, and the proposed generalization of the weakly nonlinear analysis may be of interest in other fields and can motivate further generalization by using orthogonal eigenfunctions of other Sturm-Liouville problems.

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# Modeling, Analysis and Simulation of Disease Dynamics through Physics Informed Neural Networks

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**Keywords:** Compartmental Models, Machine Learning, Physics Informed Neural Networks

Understanding the early transmission dynamics of infectious diseases such as COVID-19 has made us to re-envision how we mathematically model, analyze and simulate the spread of infectious diseases and evaluate the effectiveness of non-pharmaceutical control measures as important mechanisms for assessing the potential for sustained transmission. Along with development of mathematical modeling, there have also been a variety of approaches that have been introduced to estimate the parameters such as the transmission, infection, quarantine and recovery rate using real data sets [1]. These include parametric and non-parametric approaches, agent based models, optimal control, Bayesian frameworks, particle swarm optimization, inverse methods and many others. Along with these, there have also been several works recently showing how differential equations can be learned from data. An example of this is using physics informed neural network models (PINNs) [2, 3] that has been applied successfully to linear and non-linear Ordinary and Partial differential equations. Recently, the approach has been applied to understand system-biology and spread of infectious diseases [3, 4].

In this work, we present modeling, analysis and simulation through Disease Informed Neural Networks [4] and its application to real data modeled using non-linear partial differential equations (PDEs). We discuss how these approaches are capable of predicting the behavior of a disease described by modified compartmental models that include parameters and variables associated with the governing PDEs describing the dynamics of the disease. Through benchmark problems, we will show that our model validates real-data and demonstrate how such PINNs based methods can predict optimal parameters for a given dataset. We will also show this proposed approach that takes advantage of parallel computing and the power of GPU computation makes it a robust and reliable candidate for predicting infectious diseases.

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# A stochastic epidemic model with random transmission rate and false negative tests: Explaining the dynamics of COVID-19.

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Keywords: Stochastic perturbations, Infectious diseases, Compartment model, COVID-19

The epidemic disease model is often used to predict an epidemic's characteristics and help plan an effective control strategy. We develop a stochastic model that considers random perturbations in transmission rates with a diagnostic test to describe the dynamics of the spread of COVID-19 in the Pacific Narinense region in Colombia. The stochastic epidemic model is stratified in the Susceptible-Exposed-Infectious-Recovered, SEIR type compartment model with a false negative rate of diagnostic tests for detecting an active SARS-CoV-2 infection. We discuss the effect of vaccination as a control measure and compare the basic reproduction number for the proposed model for two different times, before and after vaccination. The outbreak in the economically backward coastal region of Pacific Nariñense is considered for the study and compared with Bogotá city. We estimate model parameters using reported COVID-19 epidemic data from the National Institute of Health(INS), Colombia. The computer experiments for the proposed model with random perturbations were performed, and the model is validated through numerical simulations for actual data.

### On the prior modelling for the basic reproductive ratio

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Keywords: Epidemic models, basic reproductive number, prior modelling, Bayesian inference.

The basic reproductive number is a central quantity in theoretical epidemiology, defining the threshold between disease-free equilibria and epidemics. It can usually be written as a ratio between the rates of creation and the removal of infected individuals of infected individuals. Bayesian inference for epidemic models usually proceeds by assigning Gamma or log-normal priors to these rates, obtaining posterior distributions and often computing their ratio to recover a posterior distribution for  $\mathcal{R}_0$ . In this talk we show that these modelling choices lead to induced distributions on the quantity of interest that have poor statistical properties. We propose new classes of priors and also extend the usual approach by correcting the distribution of  $\mathcal{R}_0$  to explicitly consider the population size. Our findings show that care is needed when constructing priors for inference of epidemic models to ensure valid conclusions about the quantities of interest.
# Inmate population models with non-homogeneous sentence lengths and their effects in an epidemiological model

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**Keywords:** Prison population dynamics, sentencing length structure, McKendrick equation, SIS epidemiological model, health in prisons

In this work, we develop an inmate population model with a sentencing length structure. The sentence length structure of new inmates represents the problem data and can usually be estimated from the histograms corresponding to the sentences imposed on a given population. We obtain a transport equation, typically known as the McKendrick equation, the homogenous version of which is included in population models with age structures. Using this equation, we compute the inmate population and entry/exit rates in equilibrium, which are the values to consider in the design of a penitentiary system. With data from the Chilean penitentiary system, we illustrate how to perform these computations. In classifying the inmate population into two groups of sentence lengths (short and long), we incorporate the SIS (susceptible-infected-susceptible) epidemiological model, which considers the entry of infective individuals. We show that a failure to consider the structure of the sentence lengths—as is common in epidemiological models developed for inmate populations—for prevalences of new inmates below a certain threshold induces an underestimation of the prevalence in the prison population at steady state. The threshold depends on the basic reproduction number associated with the non-structured SIS model with no entry of new inmates.

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## The rough Hawkes Heston model

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Keywords: Rough volatility, Hawkes processes, joint calibration of S&P 500 and VIX smiles

We introduce an extension of the Heston stochastic volatility model that incorporates rough volatility and jump clustering phenomena. In our model, the spot variance is a rough Hawkes-type process proportional to the intensity process of the jump component appearing in the dynamics of the spot variance itself and the log returns. The model belongs to the class of affine Volterra models. In particular, the Fourier-Laplace transform of the log returns and the square of the volatility index can be computed explicitly in terms of solutions of deterministic Riccati-Volterra equations, which can be efficiently approximated using a multi-factor approximation technique. Prices of options on the underlying and its volatility index can then be obtained using Fourier-inversion techniques. We show that a parsimonious setup, characterized by a power kernel and an exponential law for the jumps, is able to simultaneously capture the behavior of the implied volatility smile for both S&P 500 and VIX options. Our findings demonstrate the relevance, under an affine framework, of rough volatility and self-exciting jumps in order to jointly calibrate S&P 500 and VIX smiles.

## **Optimal Trading with Signals and Stochastic Price Impact**

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Keywords: Algorithmic trading, singular perturbation, multiscale modeling, non-linear PDE

Trading frictions are stochastic. They are, moreover, in many instances fast-mean reverting. In this talk, we present how to optimally trade in a market with stochastic price impact and study approximations to the resulting optimal control problem using singular perturbation methods. We prove, by constructing sub- and super-solutions, that the approximations are accurate to the specified order. Finally, we show some numerical experiments to illustrate the effect that stochastic trading frictions have on optimal trading.

## Zero Black-Derman-Toy interest rate model

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**Keywords:** Black-Derman-Toy model, Zero Interest Rate Policy, Bond Option Pricing, Financial Crisis, Term Structure.

We propose a modification of the classical Black-Derman-Toy (BDT) interest rate tree model, which includes the possibility of a jump with a small probability at each step to a practically zero interest rate. The corresponding BDT algorithms are consequently modified to calibrate the tree containing zero interest rate scenarios. This modification is motivated by the 2008–2009 crisis in the United States and it quantifies the risk of future crises in bond prices and derivatives. The proposed model is useful to price derivatives. A comparison of option prices and implied volatilities on US Treasury bonds computed with both the proposed and the classical tree model is provided in different scenarios along the different periods comprising the years 2002–2017.

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## Quantitative Fundamental Theorem of Asset Pricing

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Keywords: FTAP, martingales, Wasserstein distance

We provide a quantitative analysis to the concept of arbitrage, that allows to deal with model uncertainty without imposing the no-arbitrage condition. In markets that admit "small arbitrage", we can still make sense of the problems of pricing and hedging. The pricing measures here will be such that asset price processes are close to being martingales, and the hedging strategies will need to cover some additional cost. We discuss a quantitative version of the Fundamental Theorem of Asset Pricing and of the Super-Replication Theorem. Finally, we study robustness of the amount of arbitrage and existence of respective pricing measures, showing stability of these concepts with respect to a strong adapted Wasserstein distance.

# A numerical scheme for evolutive Hamilton Jacobi equations on Networks

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Keywords: Hamilton-Jacobi equations, Networks, Numerical Analysis

We present a numerical scheme for evolutive Hamilton-Jacobi equations on networks. The method is based on a recent definition of viscosity solution given in [1] and consists of two steps. First, the individual equations, defined on each branch of the network, are approximated by a Semi-Lagrangian scheme. Then, the multiple values obtained at the vertices, one for each branch incident on a given vertex, are processed to select a single value that verifies the definition of viscosity solution. The main advantage over the pure semi-Lagrangian scheme developed in [2] is in terms of computational cost. We present a convergence analysis and some numerical tests.

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# Navigation system based routing strategies in traffic flows on networks

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### Keywords: Traffic flows, Controlled systems, Macroscopic models

Navigation choices play an important role in modeling and forecasting traffic flows on road networks. We introduce a macroscopic differential model coupling a conservation law with a Hamilton-Jacobi equation to respectively model the nonlinear transportation process and the strategic choices of users. Furthermore, the model is adapted to the multi-population case, where every population differs in the level of traffic information about the system.

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## Interval optimal control for problems with uncertainties

<u>Ulcilea Leal</u><sup>1</sup>, Weldon Lodwick<sup>2</sup>, Geraldo Silva<sup>3</sup>, and Gino Maqui-Haumán<sup>4</sup>

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Keywords: Interval-valued functions, Interval optimal control

This thematic session we will address optimal control problems with an interval-valued objective function. We consider the lower and upper order relation on the interval space and with this order relation we obtain optimality conditions. Using two different derivative concepts we propose necessary and sufficient conditions for the interval optimal control problems. For better understanding some numerical examples are presented.

# Undiscounted infinite horizon multi-objective optimal control problems

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**Keywords:** Multi-objective programming, Hamilton-Jacobi-Bellman approach, Infinite horizon optimal control problem,  $\varepsilon$ -Pareto solutions

In this talk, we present a characterization of the Pareto fronts for undiscounted infinite horizon multi-objective optimal control problems with state constraints and non-linear dynamics. This work extends the results obtained in [2] for finite horizon problems and in [1] for discounted infinite horizon problems. First, we define an auxiliary optimal control problem without state constraints and show that the weak Pareto front is contained in the boundary of the zero level set of the corresponding value function. Then we establish a characterization of the Pareto front. We also investigate the uniqueness of solutions of the Hamilton-Jacobi-Bellman equation arising in this setting. Finally, we consider undiscounted infinite horizon problems in the absence of the convexity assumption. In that case the existence of Pareto solutions is not guaranteed, so we consider a relaxed problem and relate the Pareto front of this problem with the  $\varepsilon$ - Pareto front of the original problem.

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## Optimal control problems in some metric spaces

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Keywords: Optimal control problems, chance-constraints, Pontryagin's principle

In this talk, we present a class of control problems with uncertainties. Let T be a given finite horizon, and let  $(\Omega, \mathcal{F}, \mathbb{P})$  be a complete probability space. Consider an ensemble of controlled state equations parametrized by the random variable  $\omega \in \Omega$ 

$$\begin{cases} \dot{\mathbf{x}}_{\omega}(t) = A\mathbf{x}_{\omega}(t) + B(\omega)\mathbf{u}(t) + f(t,\omega) & \text{for a.e. } t \in [0,T], \\ \mathbf{x}_{\omega}(0) = x_0, & \\ \mathbf{u}(t) \in U, & \text{for a.e. } t \in [0,T], \end{cases}$$
(1)

where U is a closed metric space,  $x_0$  is an initial data, A and  $B(\omega)$  are linear operators in appropriate spaces (of finite or infinite dimension), and f is a smooth source term. An admissible control input  $u : [0,T] \to H$  is a measurable function assumed to be  $\omega$ -independent, which means that the *parametrized family of states* are driven by the same control. The optimal control problem is as follows

Maximize 
$$\{\mathbb{P}(\Psi(\mathbf{x}_{\omega}(T)) \leq 0) \mid (\mathbf{x}_{\omega}, \mathbf{u}) \text{ satisfies } (1)\}$$

where  $\Psi : H \to \mathbb{R}$  is a given function. The cost function evaluates the probability that the ensemble of controlled states verify a constraint at the final time.

In this talk, we will discuss the optimality conditions of the probust control problem and show that these conditions can be expressed as a Pontryagin principle.

This is a joint work with W. van Ackooij (EDF Lab, France) and R. Henrion (Wias, Berlin)

# Learning-based visual perception and control applied to autonomous vehicles and manipulators

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Keywords: learning-based control, autonomous vehicles, manipulators

Autonomous vehicles is a robotic application with potential to reduce fatalities, accidents and traffic collisions. In the last decade, an evident progress towards the development of autonomous vehicles has been observed. However, long term autonomy in dynamic urban environments is still a challenge due to the variety of situations that can be found within an urban environment, in addition to the uncertainties associated with perception and other participants in traffic. Personal service robot manipulator is another application with potential to improve the life quality of people who need assistance in performing everyday manipulation tasks. Motivated by these two main applications, this talk presents an overview of recent contributions achieved by the researcher's group at University of São Paulo in the following topics: deep learning for monocular depth estimation and grasp detection; visual servoing control of manipulators; multi-task learning; and learning-based control of autonomous ground vehicles.

# Markov Jump Linear System Robust Regulator Applied to Autonomous Truck: Complementary Results

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**Keywords:** Robust Regulator; Markovian Jump Linear Systems, Politopic Uncertainties, Autonomous Truck

We have proposed in the literature robust and computationally efficient methods to algebraically compute state feedback gains for discrete Markovian jump linear systems subject to polytopic uncertainties. We have defined an optimization problem based on regularized leastsquares with bounded uncertain data and penalty functions, for which we introduce a cost function to accommodate and weight the vertices altogether. We have obtained, thenceforth, a recursive and robust solution whose symmetric matrix structure allows for convergence and stability analyses via algebraic Riccatti equations. The penalty parameter is straightforwardly tuned and remains fixed throughout operation. Convergence and stability are guaranteed for any positive value of the penalty parameter, which is convenient for practical implementation. We recast the classic regularized least-squares problem from a polytopic perspective to present a recursive framework for regulation of polytopic systems. We demonstrate the potential of application in real-world systems by means of simulations with an autonomous heavy-duty vehicle model based on experimentally acquired data. A Markov jump linear system represents the drivetrain model of an autonomous heavy duty Scania truck, whose matrices were identified based on data collected by driving the truck around the University of Sao Paulo. The model consists of 7 Markov modes related to the transmission rates from 4th to 10th gears. Each mode has three polytopic vertices to compose the uncertainties. All vertices were identified based on experimental data in order to represent different road slopes (uphill, downhill and flat). The errors to be minimized in the regulation process are related with the driveshaft torsion, engine speed and wheel speed. The transition probabilities were identified through readings of the CAN bus. We will show in this paper complementary results of the paper presented in [?] and [?]. We will show a comparative study with other robust controller based on H-infinity approach. The linear matrix inequality conditions of the robust H-infinity controller designed were satisfied. However, it provided unfeasible torques and the truck could not track the references. On the other hand, the robust recursive regulator successfully tracked the references with small errors.

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## Discrete filters, policy machines, and their reduction problem

#### Dylan Shell

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### Keywords: Filter compression

This talk will examine discrete finite-state transition systems employed as incremental stream transducers, objects that have direct application to robotics: for example, as might be used to model combinatorial estimators (or filters) and also as concise encodings of feedback plans/policies. The problem of their reduction arises from specific ways in which design automation may help to achieve minimalism, to help build better, simpler robots. Assuming no prior familiarity with these objects, the talk will describe what they are and how they are applicable to robotics problems. It will then examine their specific differences from classical automata, including the contrast in their minimization problems, and cases where causality plays a role to constrain non-determinism. Finally, we will describe the parameterized complexity of an exact minimization algorithm.

## Critical scaling for an anisotropic percolation system on $\mathbb{Z}^2$

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Keywords: bond percolation, phase transition, scaling

My basic goal in this talk is to give an example of interplay between SPDEs and percolation methods. We consider a highly anisotropic finite-range bond percolation on  $\mathbb{Z}^2$ : on horizontal lines we have edges connecting two vertices within distance N and vertical edges are only between nearest neighbor vertices. On this graph we consider the following independent percolation model: horizontal edges are open with probability 1/(2N), while vertical edges are open with probability  $\epsilon$  to be suitably tuned as N grows to infinity. The main result tells that if  $\epsilon = \kappa N^{-\frac{2}{5}}$ , then we see a phase transition in  $\kappa$ : there exist positive and finite constants  $C_1, C_2$  so that there is no percolation if  $\kappa < C_1$  while percolation occurs for  $\kappa > C_2$ . The question is motivated by a result on the analogously layered ferromagnetic Ising model at mean field critical temperature. This is based on a joint work with Thomas Mountford and Hao Xue [1].

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# Law of large numbers for the spread of an infectious disease with casual and non-casual transmissions in a configuration model network

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Keywords: SIR epidemic model, configuration model, limit theorem

We consider a stochastic SIR epidemic model in which individuals make non-casual contacts with their neighbors within the social network of the population and casual contacts with people chosen uniformly at random from the population. We will present a low dimensional ODE system describing the limiting behavior of certain quantities of interest to describe the evolution of this model and comment on results on the convergence of the stochastic model to the solution of this deterministic system. Aiming at applications of this model, we also present extensions in which the population is partitioned into subpopulations and with more general epidemic models.

## Reinforced random walks under memory lapses

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Keywords: reinforced dynamics, central limit theorem, law of iterated logarithm, martingale

We introduce a one-dimensional random walk, which at each step performs a reinforced dynamics with probability  $\theta$  and with probability  $1 - \theta$ , the random walk performs a step independent of the past. We analyze its asymptotic behavior, showing a law of large numbers and characterizing the diffusive and super-diffusive regions. We prove central limit theorems and law of iterated logarithm based on the martingale approach.

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# A branching random walk with barriers as a model of seed dispersal on islands

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Keywords: bond percolation, phase transition, scaling

We consider a branching random walk on  $\mathbb{R}$  that cannot evolve past two symmetric barriers as a one dimensional model of seed dispersal on (shrinking) islands. We study survival of the species in relation to the habitat size and seeds production rate. Using multi-type branching processes in conjunction with coupling techniques we are able to find the critical rate for a typical barrier length.

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## Machine learning that obeys physical law

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Keywords: equivariant machine learning

In this talk we will give an overview of the enormous progress in the last few years, by several research groups, in designing machine learning methods that respect the fundamental symmetries and coordinate freedoms of physical law. Some of these frameworks make use of irreducible representations, some make use of high-order tensor objects, and some apply symmetry-enforcing constraints. Different physical laws obey different combinations of fundamental symmetries, but a large fraction (possibly all) of classical physics is equivariant to translation, rotation, reflection (parity), boost (relativity), units scalings, and permutations. In [?] we show that it is simple to parameterize universally approximating polynomial functions that are equivariant under these symmetries, or under the Euclidean, Lorentz, and Poincaré groups, at any dimensionality d. The key observation is that nonlinear O(d)-equivariant (and related-group-equivariant) functions can be universally expressed in terms of a lightweight collection of (dimensionless [?]) scalars – scalar products and scalar contractions of the scalar, vector, and tensor inputs. We complement our theory with numerical examples that show that the scalar-based method is simple, efficient, and scalable [?], and mention ongoing work on cosmology simulations.

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# Mathematical Models of Crime: Prediction, Discrimination, Interpretability, Under-reporting and Equilibrium

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**Keywords:** Crime modelling, under-reporting, spatio-temporal events, criminals strategic reaction.

I will summarize part of a three year research project on the mathematical modeling of crime in Bogotá, Colombia. This research project was financed by the Colombian Government and conducted by the National University of Colombia, the Secretary of Security of Bogotá and the private firm Quantil.<sup>1</sup> I will briefly describe the main results and techniques regarding crime prediction, interpretability and discrimination or algorithmic bias. Then, I will dive deeper into two of the most challenging problems we faced: the under-reporting of events and the strategic reaction of criminals.

Under-reporting of socially sensitive events can undermine the credibility of official figures and can be used strategically by official agents or the general public. Models that simultaneously estimate incidence and under-reporting rates of events can be used to improve the allocation of public resources. To solve this problem we modify well-known combinatorial multi-armed bandit algorithms that we validate using simulations and show the effectiveness of the Combinatorial Upper Confidence Bound (CUCB) algorithm in identifying the fundamental parameters of our model: the true rates of incidence and under-reporting of events. Finally, we use real crime data from a large city, Bogotá - Colombia, showing that the model is able to estimate the true crime and under-reporting rates.

A key missing point of this research agenda and most of the specialized literature is the incorporation of criminals strategic response to police presence. This endogenous response is a huge challenge to current models and puts into question many of the previous studies. Identifying criminal response is a first step towards an equilibrium theory of criminal activity. To approximate this problem, we use a unique experimental data set tailored to identify the causal impact of police patrolling on crime. Using this data set we exploit an identification strategy based on a random utility model of crime location choice. The model allows us to identify agents' utilities from observable data. We were able to estimate own-and cross-elasticities of crime to patrolling time allowing us to evaluate alternative patrolling strategies (i.e., interventions or policy scenarios). To the extent of our knowledge, both the identification of elasticities and the counterfactual analysis are novel features in this literature. Our estimates show that the elasticity of crime to police presence (i.e., time) is, on average across spatial locations, -0.26 for violent crime, -0.38for property crime and -0.38 for total crime, all statistically significant with 95% confidence. Estimates of cross-elasticities are close to zero and suggest that, if anything, crime displacement is negligible. Counterfactual analysis of different police deployment strategies show, for the best allocating algorithm, an average reduction in property crimes of 10, 3% and a reduction in total crimes of 7.9% at no additional cost.

<sup>&</sup>lt;sup>1</sup>Diseño y validación de modelos de analítica predictiva de fenómenos de seguridad y convivencia para la toma de decisiones en Bogotá financed by Colciencias with resources from the Sistema General de Regalías, BPIN 2016000100036.

# Resilience, Sustainability and Decision Under Uncertainty

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Keywords: resilience, sustainability, viability, stochastic optimization, risk

In this talk, I will

- scan through the vocabulary of sustainability in the IPCC (climate) and IPBES (biodiversity) international bodies reports: goals, indicators, vulnerability, adaptive capacity, stress, risk, scenarios, models, etc.,
- address theoretical aspects: how can we formalize sustainability and resilience with tools from control theory (including viability) and decision under uncertainty?
- present methods: how can we tackle the resolution of problems, once mathematically formalized?
- outline examples: biodiversity (fisheries, epidemiology), energy and climate,
- raise open questions and challenges.

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# A Huber computational approach to the non-isothermal viscoplastic flow

#### SERGIO GONZÁLEZ-ANDRADE

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**Keywords:** Viscoplastic fluids, Bingham and Herschel-Bulkley models, Huber regularization, Semismooth Newton methods.

This talk is devoted to the numerical solution of the non-isothermal instationary viscoplastic flow with temperature dependent parameters, by semismooth Newton methods. We discuss the main theoretical aspects regarding this problem. Mainly, we focus on existence of solutions and a multiplier formulation which leads us to a coupled system of PDEs involving a Navier-Stokes type equation and a parabolic energy PDE. Further, we propose a Huber regularization for this coupled system of partial differential equations, and we briefly discuss the well posedness of these regularized problems. A detailed finite element discretization is proposed for the space variable, involving weighted stiffness and mass matrices. After discretization in space, a second order BDF method is used as a time advancing technique, leading, in each time iteration, to a nonsmooth system of equations, which is suitable to be solved by a semismooth Newton algorithm. Finally, we show two detailed computational experiments that exhibit the main properties of the numerical approach.

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15 Singular Perturbation Method for a KdV-ODE coupled system Eduardo Cerpa Pontificia Universidad Católica de Chile, Chile, eduardo.cerpa@uc.cl Keywords: infinite-dimensional systems, time scales, Korteweg-de Vries equation This talk considers systems coupling an ordinary differential equation (ODE) with a Korteweg- de Vries equation through its boundary data. The main focus is put on the role of different time scales on the stability of the coupled system. We study the Singular Perturbation Method [4], which is a well-established tool in finite-dimension. For PDEs there is some recent work con-sidering first-order [6, 7, 8] and second order hyperbolic systems coupled to ODEs [2, 3]. In a joint work with Swann Marx (Nantes) [5] we get stability and Tikhonov-type results for our system involving the Korteweg-de Vries equation. A fundamental tool is the Lyapunov function introduced in [1]. Bibliography [1] I. Balogoun, S. Marx, D. Astolfi, ISS Lyapunov strictification via observer design and integral action control for a Korteweg-de Vries equation. Preprint, 2022. [2] E. Cerpa and C. Prieur, Effect of time scales on stability of coupled systems involving the wave equation. IEEE Conference on Decision and Control, Melbourne, 2017. [3] E. Cerpa, C. Prieur, Singular perturbation analysis of a coupled system involving the wave equation. IEEE Trans. Automat. Control, Vol. 65, No. 11, pp. 4846–4853, 2020. [4] P. Kokotović, H. K. Khalil, and J. O'Reilly, Singular pertrubation methods in control: analysis and design, Academic Press, 1986. [5] S. Marx, E. Cerpa, Singular perturbation method for a KdV-ODE system. Preprint, 2022. [6] Y. Tang and G. Mazanti, Stability analysis of coupled linear ODE-hyperbolic PDE sys- tems with two time scales. Automatica J. IFAC, 85:386–396, 2017. [7] Y. Tang, C. Prieur, and A. Girard, Tikhonov theorem for linear hyperbolic systems. Automatica J. IFAC, 57:1–10, 2015. [8] Y. Tang, C. Prieur, and A. Girard, Singular perturbation approximation of linear hyperbolic systems of balance laws. IEEE Trans. Automat. Control, 61(10):3031–3037, 2016. Latin American Congress on Industrial and Applied Mathematics, Rio de Janeiro, Brazil, January 30th — February 3rd, 2023 LACIAM-14

# A degenerating convection-diffusion system modelling froth flotation with drainage

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Keywords: keyword1, keyword2, keyword3

Froth flotation is a common unit operation used in mineral processing [5, 6]. It serves to separate valuable mineral particles from worthless gangue particles in finely ground ores. The valuable mineral particles are hydrophobic and attach to bubbles of air injected into the pulp. This creates bubble-particle aggregates that rise to the top of the flotation column where they accumulate to a froth or foam layer that is removed through a launder for further processing. At the same time, the hydrophilic gangue particles settle and are removed continuously. The drainage of liquid due to capillarity is essential for the formation of a stable froth layer. This effect is included into a previously formulated hyperbolic system of partial differential equations that models the volume fractions of floating aggregates and settling hydrophilic solids [1, 2]. The construction of desired steady-state solutions with a froth layer is detailed and feasibility conditions on the feed volume fractions and the volumetric flows of feed, underflow and wash water are visualized in so-called operating charts [3]. A monotone numerical scheme is derived and employed to simulate the dynamic behaviour of a flotation column. It is also proven that, under a suitable Courant-Friedrichs-Lewy (CFL) condition, the approximate volume fractions are bounded between zero and one when the initial data are. The presentation summarizes research detailed in [4].

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# A semi-hybrid mixed finite element method for coupled Stokes-Darcy flows with H(div)-conforming velocity fields

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Keywords: Stokes-Darcy's flows. Hybridization. Divergence-free simulation.

We consider a semi-hybrid mixed finite element formulation for the simulation of coupled Stokes-Darcy fluids. Using  $\mathbf{H}(div)$ -conforming approximate velocity fields in the whole domain, the continuity of normal components over element interfaces is taken for granted, and pressure is searched in discontinuous spaces preserving the divergence compatibility property. Tangential continuity of the Stokes velocity is weakly imposed by a traction Lagrange multiplier. The term modeled by Beaver-Joseph-Saffman is elegantly approximated adding an  $L^2$  product term in the tangent velocity space. The method is strongly mass-conservative, leading to exact divergencefree simulations of incompressible flows. The multiplier space requires specific choices according to the velocity approximations implemented in each element geometry. In certain cases, classic divergence-compatible pairs adopted for Darcy's flows may require divergence-free bubble enrichment to enforce tangential continuity of the Stokes velocity in some extent, avoiding any extra stabilization technique. Considerable improvement in computational performance is achieved by the application of static condensation: the global system is solved only for a piecewise constant pressure variable, velocity normal trace and tangential traction over element interfaces. The remaining solution components are recovered by solving independent local Neumann problems in each element. Numerical results shall be presented for verification of the main convergence properties of the method for a problem having known exact solution. The application to a carbonate karst reservoir composed of multiple vugs with different shapes and sizes shall also be illustrated.

# Routes of Innovation and Technological Transfer in Mathematical Sciences: The CeMEAI case

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Keywords: Mathematical Sciences, Product Development, Innovation, Technology Transfer

The Center for Mathematical Sciences Applied to Industry (CeMEAI), headquartered at USP's Institute of Mathematical and Computing Sciences (ICMC), in São Carlos, is structured to promote the use of mathematical sciences as an industrial resource, with the aim of reduce costs, increase production and offer innovative products. In principle, in order to increase competitiveness and strengthen the national industry. In this conference, we present the main routes that CeMEAI has taken to be able to produce innovative products and promote technology transfer to the productive sector and to the community. Focus is placed on our holistic vision of work and on the development of different actions and activities offered concurrently that culminated in the success of the Center in transferring knowledge of the technological developments obtained to our industrial partners.

## Industrial Collaborations and Entity Resolution

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Keywords: Centro Pi, recommendation systems, entity resolution

Centro de projetos e inovação (Centro Pi) is a new research center from Instituto de Matemática Pura e Aplicada (IMPA) whose goal is to conduct industrial collaborations in applied mathematics. Over the first semester of 2022, Centro Pi developed a project with Globo on keyword extraction and recommendation systems. Through our work in this project, we had the opportunity of working on entity resolution, and specifically conducted research in blocking, which consists of reducing the pool of possible matches as a pre-processing stage of the data.

# Computational Models of Geofluid Flow in the Subsurface Environment: A Fascinating Challenge to Academics and Industry

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**Keywords:** Porous media science, Computational Geo-sciences, Co2 storage, Energy withdrawal, Mixed dimensional PDEs

We present some recent advances achieved by the COMOPORE team at LNCC in the computational modeling of porous materials with particular emphasis on applications stemming from hydrocarbon withdrawal in pre-salt formations combined with carbon dioxide geological sequestration to mitigate global warming effects. We construct multiscale mixed-dimensional partial differential equations to describe coupled flow and geomechanics capable of dealing with geological heterogeneity of high-aspect ratios, arising from the presence of discrete fracture networks and cave-conduits slender structures which stem from the dissolution of the carbonate rock. Numerical simulations illustrate the necessity of upscaling flow patterns in different scenarios and compute equivalent petrophysical properties to be inserted in commercial flow simulators. New directions for extending the models to renewable energy stored at the subsurface are also discussed.

# Constant Depth Decision Rules for multistage optimization under uncertainty

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**Keywords:** Stochastic Programming, Robust Optimization, Decision rules, Stochastic Dual Dynamic Programming

In this paper, we introduce a new class of decision rules, referred to as Constant Depth Decision Rules (CDDRs), for multistage optimization under linear constraints with uncertaintyaffected right-hand sides. We consider two uncertainty classes: discrete uncertainties which can take at each stage at most a fixed number d of different values, and polytopic uncertainties which, at each stage, are elements of a convex hull of at most d points. Given the depth mu of the decision rule, the decision at stage t is expressed as the sum of t functions of mu consecutive values of the underlying uncertain parameters. These functions are arbitrary in the case of discrete uncertainties and are poly-affine in the case of polytopic uncertainties. For these uncertainty classes, we show that when the uncertain right-hand sides of the constraints of the multistage problem are of the same additive structure as the decision rules, these constraints can be reformulated as a system of linear inequality constraints where the numbers of variables and constraints is  $O(1)(n+m)d^m uN^2$  with n the maximal dimension of control variables, m the maximal number of inequality constraints at each stage, and N the number of stages. As an illustration, we discuss an application of the proposed approach to a Multistage Stochastic Program arising in the problem of hydro-thermal production planning with interstage dependent inflows. For problems with a small number of stages, we present the results of a numerical study in which optimal CDDRs show similar performance, in terms of optimization objective, to that of Stochastic Dual Dynamic Programming (SDDP) policies, often at much smaller computational cost.

## Data augmentation techniques and clustering to improve Deep Learning forecasts of Dengue cases

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**Keywords:** lstm, epidemiology, bayesian, cluster

Dengue fever represents a public health problem and accurate forecasts can help governments take the best preventive actions. As the volume of data provided continuously increases, machine learning and deep learning (DL) models have become an attractive approach. However, it is difficult to perform accurate predictions in areas with fewer cases or with a lack of available data. In this work, we compare traditional approaches such as LASSO Regression (LR), Random Forest (RF), Support Vector Regression (SVR) vs DL models based on long short-term memory (LSTM), considering weekly dengue incidence and climate, in 217 cities in Paraguay. Several city models may present heterogeneous behaviors and poor accuracy. To mitigate this problem, we propose to enrich the data already available through clustering and data augmentation techniques. To establish a benchmark model, we compare the performance of several traditional (LR, RF and SVR) and deep leaning machine learning models (LSTM). Then, a grouping is implemented based on the similarity of the incidence time series, using clustering techniques. We also explore Data Augmentation (DA) that is a standard technique to improve the performance of deep learning models in several applications. In this paper, we use some image processing inspired DA techniques *e.q.* multiply by a scalar, add noise and shift. We also use an epidemiological compartmental model (SIR) to impose the temporal causality of the generated data to perform the data augmentation, and then we use Bayesian inference to obtain a parameter distribution, we call this technique BIDA.

The LSTM model was selected as benchmark model according to the Root Mean Square Error metric. Although both models showed improvements in the performance of the models (See fig. 1) the *Cluster* model was not always the best in all cases, unlike the *Bayesian* model. But the improvement of the *Cluster* model is always greater.



Figure 1: Comparison of the *Bayesian*, *Cluster* and *Imagebased* models.

Both models presents the best performance, especially in cities with an incidence higher or lower than the average, which is where the other models fail. With data clustering and BIDA, we were able to improve the performance of the models. We believe that this approach is applicable to wide geographic regions and to other mosquito-borne diseases. In future works, we will aim at optimizing the clustering of the time series by designing more experiments, and also combining data augmentation techniques with clustering.

# Metaheuristic Optimization Applied to Astrophysical Blazar Modeling.

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Keywords: Astroparticle physics, Blazars, Metaheuristics, Optimization

Recent astroparticle experiments indicate blazars as very likely multimessenger (MM) emitters, more specifically, sources of simultaneous electromagnetic and neutrino signals [1]. The modeling of blazar observations (leptonic and/or hadronic models), typically requires to specify around 10 free parameters (accordingly) [2]. With such number of free parameters, an exhaustive deterministic exploration of the model parametric space can be computationally prohibitive, when searching for model curves fitting a given spectral energy distribution (SED) data set. Motivated by the ability of population-based metaheuristic algorithms in addressing highdimensional optimisation problems [3, 6], here we study their performance for fitting SED blazar models. We consider different types of swarm optimization and genetic algorithms [4, 5], namely, particle swarm optimization (PSO), mean particle swarm optimization (MPSO), chicken swarm optimization (CHSO), grey wolf optimization (GWO), differential evolution (DE), and asexual genetic algorithm (AGA), among others. For building the optimization objective function we employ a  $\chi^2$  criterion and consider the cases of leptonic and hadronic radiative models. The best performance for our problem was obtained with the PSO and DE algorithms. We also leave as open source the Python optimization code developed for this study, which allows the user to customize the radiative blazar MM model.

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#### LACIAM-146

# Mathematical modelling of COVID-19 and analysis of Rio de Janeiro city outbreak in 2020

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**Keywords:** COVID-19 Epidemiological Modeling, Parameter Estimation, Differential Equations, B-Splines, Uncertainty Quantification

The virus SARS-CoV-2 is the causer agent of COVID-19 disease, which was first noticed in late December 2019 and rapidly spread over the world. Most COVID-19 infections are asymptomatic or present mild symptoms but may progress to viral pneumonia and multi-organ failure, leading to hospitalization and death. Around the world, governors declared a public health emergency, including the state of Rio de Janeiro, in March 2020. That month, a decree ordered the closure of schools, restaurants and theatres, restricted beach access, shopping centres and non-essential commerce, and suggested a decrease in gatherings. Despite these measures, the outbreak of the virus in the region happened.

This work aims to provide a quantitative estimate of crucial parameters related to the COVID-19 outbreak in Rio de Janeiro city from March to July 2020. In particular, to estimate the rate of unreported cases. It is a crucial step to assess the extent and impact of the disease on the population since most of the infections are likely to remain undetected by the health department. The analysis is based on fitting the SEIAQR (Susceptible — Exposed — Infectious — Asymptomatic — Quarantined — Recovered) compartmental model introduced by [1] to data retrieved from the public health agency [3]. This epidemiological model considers isolation, quarantine of confirmed cases, and testing of asymptomatic individuals as non-pharmaceutical strategies to contain the spread of the virus among the population. Since asymptomatic testing was low in Rio de Janeiro, the asymptomatic proportion estimate is a proxy for the under-reporting. From the analytical expression for the basic reproduction number  $\mathcal{R}_0$  and time-dependent reproduction number  $\mathcal{R}_t$  derived by [1], we also are able to derive important conclusions of the evolution of the pandemic.

The evaluation of the model's parameters uses the error-weighted least squares method, which was supported by the normal assumption of the errors, and B-splines for the time-varying parameters: mortality, which depends on the health system, and rate of contact, which depends on the contact rate. The structural and practical identifiability is analyzed to support the feasibility and robustness of the estimation. We use the Bootstrap method to quantify the uncertainty of the estimates. For the outbreak of March-July 2020 in Rio de Janeiro, we estimate about 90% of unreported cases, with a 95% confidence interval (85%, 93%).

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# A one-phase space–fractional Stefan problem with no liquid initial domain

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**Keywords:** Space fractional diffusion equation, Stefan problem, Moving boundary problem, Caputo derivative

We consider a phase-change problem for a one dimensional material with a non-local flux, expressed in terms of the Caputo derivative, which derives in a space-fractional Stefan problem. We prove existence and uniqueness of a regular solution to a phase-change problem with a fractional Neumann boundary condition at the fixed face x = 0, where the domain, at the initial time, consists of liquid (0 < x < b) and solid (b > x). Then we use this result to prove the existence of a limit solution to an analogous problem with non-liquid initial domain (b = 0).

The approach for the liquid and solid case is based on the transformation of domain into a cylindrical one, the use of fractional extremum principles, and the semigroup theory. For the non-liquid case, when it is not possible to transform the domain into a cylinder, we approximate the problem by a sequence of problems with liquid and solid domain, we will find *b*-independent energy estimates for the solutions to appoximated problems, and then consider the limit when b tends to zero.

In addition to the extremum principle and energy estimates, we deduce some interesting properties for space-fractional Stefan problem with fractional Neumann boundary condition, such as an integral condition equivalent to the fractional Stefan condition, and a monotonicity result.

# Determination of the Finite Differences Method (FDM) coefficients

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Keywords: FDM coefficients, Ordinary Differential Equations, Finite Difference Method

In this article, a way to determine the coefficients of the Finite Difference Method will be presented. In addition, a problem of bending a prismatic bar under transverse loading will be solved, which is a fourth order Ordinary Differential Equation (ODE). The study consists of approximating the derivatives from the first terms of the Taylor Series by inserting a set of points centered on the i-th point, where the number of points depends on the order of the derivative to be approximated. For this, a way was developed to determine the FDM coefficients to approximate the nth order derivative. These coefficients are important in the construction of the Finite Difference Equation, which uses the coefficients for derivative approximations and allows solving an ODE. With the generalization of the form of determination of such guidelines presented in this article, there is, consequently, the possibility of applying the FDM to solve an ODE of any order. As a result, the study of an application in the resolution of a fourth resolution ODE related to the problem of bending under transverse loading.

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# Relating SARS-CoV-2 variants using cellular automata imaging

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Keywords: SARS-CoV-2, Cellular Automata, Protein

The disruption caused during the last two years by the COVID-19 pandemic is hard to be underestimated, from more than six million deaths and 600 million cases according to official sources, [1], to economic disruption in most countries [2].

The SARS-CoV-2 is a single-stranded RNA virus, with a genome size of 30 Kb, and four structural proteins: Nucleocapsid (N), Matrix (M), Envelope (E) and the Spike (S) [3, 4]. The latter is responsible for recognizing and allowing the virus to enter the cell, possibly the main reason why this protein has been widely studied. Mutations in the SARS-CoV-2 viruses result in new variants with mutations in the spike protein increasing replication within cells, and an increased transmissibility [5].

Cellular Automata have been widely used to model complex systems with simple, easyto-understand rules [6], and in recent years many papers were devoted study protein related problems using this approach. Sleit and Madain [7] proposed a protein folding model based on cellular automata, with straightforward evolutionary rules based on the hydrophobicity of amino acids. Other works dedicated to the same problem include [8, 9, 10]. Cellular Automata Image (CAI) analysis [11] is a powerful tool to classify protein structure [12, 13, 14] and virus taxonomy [15]. These images can contain important information on the modeled system, for example, CAI allows to differentiate similar systems with respect to those significantly different. The identification of functions, structures, location, and common ancestry of a protein sequence can be performed by a comparison with other know proteins in databases, using alignment, similarity, and homology techniques [16].

In the present paper we propose a protein comparison approach using a cellular automaton image and the information theoretic Hamming metric for the distance between such images, as a measure of similarity and difference, applied to the spike protein. The distance is measured with respect to the S protein in the initial virus strain as first detected in Wuhan, and for the following Variants Of Concern (VOCs) with mutations of the Spike protein: Alpha (first identified in the United Kingdom), Beta (South Africa), Gamma (Brazil), Delta (India), and the more recent Omicron (South Africa), B.1.1.28, and P2 (Brazil). Our goal is to explicitly obtain the evolutionary relationships between these SARS-CoV-2 variants. This work was published in the paper [17]

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# A RDE-based approach for the numerical simulation of a Stochastic SVIR model

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**Keywords:** stochastic systems, ergodic solution, stationary distribution, numerical approximation, stochastic SVIR model

We propose a novel approach for the precise numerical integration of a stochastic SVIR model, which is a stochastic ordinary differential equation (SODE) with non-globally Lipschitz continuous coefficients and multiplicative noise. This SODE is based on a compartmental epidemic model and describes a continuous vaccination strategy with environmental noise effects [1]. By means of a suitable continuous transformation, we link the stochastic SVIR model to an auxiliary random ordinary differential equation (RODE) system that depends on a suitable Ornstein-Uhlenbeck process. In this way, the stochastic SVIR model can be numerically approximated by computing a numerical approximation to this auxiliary RODE system. Based on the conjugacy between the SODE defining the model and the corresponding RDE, an exponential scheme is proposed. Numerical simulations are presented to illustrate the practical performance of the introduced method. Remarkably, the proposed method outperforms other integrators in the literature and is able to approximate, with high stability, meaningful probabilistic features of the continuous system, including its stationary distribution and ergodicity.

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# On restricting the infected population peak of a SIR modeled epidemic by a reduced intervention

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Keywords: epidemiology, SIR model, non-pharmaceutical-intervention

The well known SIR model [1] is one of the simplest but efficient epidemiological models. It is determined by a set of differential equations which represent the dynamics of the susceptible, infected and recovered population groups. These dynamics depend on the parameters  $\beta$  (infection rate) and  $\gamma$  (mean recovery rate). The disease outbreak closely hinges on  $\mathcal{R}_0 = \frac{\beta}{\gamma}$ , known as the reproduction number.

If  $\mathcal{R}_0$  is too large, a great proportion of the susceptible population becomes infected yielding to an undesirable peak of the infected population. This peak may be reduced by implementing a set of actions, referred to as "non-pharmaceutical intervention" (NPI) [2]. The SIR-with-NPI can be modeled by introducing q(t), the fraction of contact prevented through intervention which varies between 0 and 1. Increasing the value of q is equivalent to decreasing  $\beta$  and hence, reducing the peak of the crisis.

This effect is colloquially known as "flattening the curve" which persists as long as the intervention is held on. A premature relax or removal of the intervention, that is, to make q take values near or equal to zero early, may yield to a second outbreak. On the other hand, holding restrictions for a long term results unviable. This work aims to identify strategies q for controlling the peak of the infected population curve by means of a reduced intervention.

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# Hyper-heuristics for the Time-dependent ATSP with Time Windows and Precedence Constraints applied to Air Travel

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**Keywords:** Asymmetric Traveling Salesman Problem, Time Windows, Precedence Constraints, Hyper-heuristic, Reinforcement Learning, Applied Mathematics for Industry and Engineering.

The traveling salesman problem is well known and studied. Given its complexity, we do not have polynomial deterministic algorithms to solve it and we often resort to heuristic methods to obtain solutions close to optimality. In addition, there are several variations associated with TSP that represent applications found in everyday life. We based our studies on the work presented by Saradatta and Pongchairerks [1] on Time-Dependent Asymmetric Traveling Salesman problem with Time Window and Precedence Constraints (TD-ATSP-TWPC). They presented two local searches with the SWAP and INSERT heuristics in the context of air travel. We reproduce the experiments in [1] and embed their heuristic methods into a hyper-heuristic framework, similarly to what was done by Pylyavskyy, Kheiri, and Ahmed to another ATSP variant [2], in order to extract the best performance of each heuristic when applied to different instances.

The cost of a flight between two locations differs depending on the day and direction of travel. Thus, the problem of planning a tour between several locations with air travel is best represented by the TD-ATSP. In addition, we may have precedence and time window constraints associated with the order of visits, in this case one point must be immediately followed by another or must be in a specific position on the tour. In the SWAP heuristic, two points are randomly selected to exchange positions between them, and in the INSERT, a position and a point are drawn, so we remove the point from the current position and insert it into the new. In both cases, there are checks and reordering to ensure that the specific characteristics of the problem are not violated, so that the search for good feasible solutions is guaranteed. At each iteration in the hyper-heuristic, we can select which heuristic to use and stop the search when we reach  $O(n^2)$ iterations without improvement.

We have implemented and compared different heuristic selection methods, such as Simple Random, Random Descent, Random Permutation, and Reinforcement Learning. Using the C++ language, we were able to achieve good solutions in less than 10 ms, and find solutions with costs lower than the ones obtained in [1] in at least one of the hyper-heuristic variants when compared to their local searches. Moreover, regarding simple instances, we obtained a decrease in the standard deviation in their average cost. Lastly, we are currently looking for a pattern of improvement in the standard deviation in more complex instances.

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## Final size and error estimates for a two-group SEIRD model

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Keywords: Epidemic mathematical model, latency period, final size

We consider a SEIRD epidemic model for a population composed by two groups of individuals with asymmetric interaction. Given an approximated solution for the two-group model, we estimate the error of this approximation related to the second group based on the error for the first one. We also study the final size of the epidemic for each group. We illustrate our results with the spread of coronavirus disease 2019 (COVID-19) pandemic in the New York County (USA) for the initial stage of the contamination, and in the cities of Petrolina and Juazeiro (Brazil).

# Modeling and control of malaria dynamics in fish farming regions

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**Keywords:** malaria modelling, monotone dynamical system, cooperative system, impulsive ordinary differential equations

In this work we propose a model that represents the relation between fish ponds, the mosquito population and the transmission of malaria. It has been observed that in the Amazonic region of Acre, in the North of Brazil, fish farming is correlated to the transmission of malaria when carried out in artificial ponds that become breeding sites. Evidence has been found indicating that cleaning the vegetation from the edges of the crop tanks helps to control the size of the mosquito population.

We use our model to determine the effective contribution of the fish tanks to the epidemic. The model consists of a nonlinear system of ordinary differential equations with jumps at the cleaning time, which act as *impulsive controls*. We study the asymptotic behaviour of the system in function of the intensity and periodicity of the cleaning, and the value of the parameters. In particular, we state sufficient conditions under which the mosquito population is exterminated or prevails, and under which the malaria is eradicated or becomes endemic. We prove our conditions by applying results for cooperative systems with concave nonlinearities.

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## QRDOM's ray effect mitigation to particle transport problems with anisotropic scattering

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Keywords: quasi-Monte Carlo integration, discrete ordinates method, ray effect mitigation

The modeling of the transport of particles like photons and neutrons has many important applications in manufactures that involve high temperature processes, energy generation, medical imaging, and others. It usually requires the solution of the linear Boltzmann equation, which turns to be an integro first order differential equation [2, 3]. The Quasi-Random Discrete Ordinates Method (QRDOM, [1]) has been proposed as an alternative to the classical Discrete Ordinates Method (DOM) to mitigate the ray effects, a nonphysical phenomenon that arises as a consequence of the angular discretization. The main idea is to use a quasi-Monte Carlo integration instead of a fixed quadrature to approximate the equation's integral term. Initially developed for transport problems with isotropic scattering, the method is here extended to novel applications with anisotropic scattering. Its advantages and limitations are discussed for selected benchmark problems in rectangular domains. Once applied to such transport problem, the QRDOM requires the solution of a sequence of first order linear differential equations, which can be solved with classical numerical methods for PDE's. Here, the Finite Element Method (FEM) with the Streamline Upwind Petrov-Galerkin stabilization and the GMRES as the linear solver are applied to compute solutions for selected test cases. The evaluation of the QRDOM as an alternative to generate approximated solutions with mitigated ray effects for problems with anisotropic scattering is a fundamental step in investigating its potential to address more realistic particle transport problems.

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## Modeling the Impact of COVID-19 Lockdown in Regional Cities

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Keywords: COVID-19, SIR model, Lockdown

COVID-19 is a Severe Acute Respiratory Syndrome (SARS): a new respiratory disease caused by SARS-CoV-2 virus that emerged in China in December 2019, which has resulted in more than 6 million deaths globally according to the World Health Organization (WHO). In this work, we formulate a new mathematical model that determines the dynamics of COVID-19 transmission in a conglomerate of contiguous cities from São Paulo State – Brazil, more specifically in the region of Presidente Prudente's city. Our goal is to assess the impact that a potential lockdown in a principal city could have on its adjacent towns.

The so-called SCIRD model, formulated from the well-established epidemiological model SIR (Susceptible–Infected –Recovered) [1], splits the population into five compartments: Susceptible (S), Confined (C), Infected (I), Recovered (R) and Dead (D). Such a compartmental-type model is formulated in terms of the following coupled Ordinary Differential Equations:

$$\begin{cases} \frac{dS_{Ci}}{dt} = -\alpha_i S_{Ci} I_{Ci} - \theta_i S_{Ci} + \delta R_{Ci} + \eta C_{Ci} - \sum_{i,j=1}^6 f_{ij} S_{Ci} \alpha_i I_{Cj} \\ \frac{dC_{Ci}}{dt} = \theta_i S_{Ci} - \alpha_c C_{Ci} I_{Ci} - \eta C_{Ci} \\ \frac{dI_{Ci}}{dt} = \alpha S_{Ci} I_{Ci} + \alpha_c C_{Ci} I_{Ci} - \beta I_{Ci} - \gamma I_{Ci} + \sum_{i,j=1}^6 f_{ij} S_{Ci} \alpha_i I_{Cj} , \qquad (1) \\ \frac{dR_{Ci}}{dt} = \beta I_{Ci} - \delta R_{Ci} \\ \frac{dD_{Ci}}{dt} = \gamma I_{Ci} \end{cases}$$

where  $f_{ij}(i \neq j)$  represents the flow of people between small cities and the principal center [2],  $\alpha$ and  $\alpha_c$  account for the infection rates of the susceptible and confined populations, respectively,  $\theta_1$  and  $\theta_2$  are the confinement rates for cities 1 and 2, respectively;  $\delta$  is the immunity loss rate;  $\eta$  defines the insulation loss rate;  $\beta$  establishes the proportion of the population that left the infected and went to the recovered; and  $\gamma$  determines the death rate due to the disease.

By solving the set of equations (1) while simulating a lockdown in the municipality of Presidente Prudente, it is possible to get the epidemiological curves for each adjacent town so that the impact of full confinement in the principal city can be properly measured and analyzed.

## Acknowledgments

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# A Fokker-Planck-Based Acceleration Technique for Multi-Physics Problems in Highly Forward-Peaked Scattering Settings

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Keywords: Fokker-Planck, Multi-Physics, Forward-Peaked, Highly Scattering, Transport Equation

Problems with high energy charged particles are usually characterized by extremely small mean free paths with almost singular differential scattering cross sections in the forward direction. Such problems are encountered in several applications related to plasma physics, X-ray machines, astrophysics etc. Transport problems involving such particles are highly optically thick and have low energy lost in the collisions. The usual discrete ordinates method is accurate in modeling those kinds of problems, but standard iterative methods converge very slowly for such physical characteristics. Acceleration techniques such as diffusion synthetic acceleration (DSA) [1] and nonlinear diffusion acceleration (NDA) [2] improve the convergence but still quite ineffective in accelerating problems with highly forward-peaked scattering. In the present work we develop a acceleration technique for multi-physics problems with highly forward-peaked scattering, following what was done in [3, 4]. The technique is Fokker-Planck-based, which is an asymptotic limit of the transport equation in highly forward-peaked scattering settings. We run simulations using the Fokker-Planck-based method and compare the runtimes and convergence rates with non-accelerated methods.

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## On the lumpability of tree-valued Markov chains

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Keywords: Markov chains; lumpability; quasi-lumpability; phylogenetics; random walk.

Phylogenetic trees are an important tool for biologists to understand how biological entities evolve through time, informed by data from molecular sequences of DNA or RNA. Tree space is complicated and high-dimensional, which makes extremely it hard to traverse. Moreover, it admits many representations, each with its strengths and weaknesses. These characteristics complicate the use of Markov Chain Monte Carlo (MCMC) methods for computing expectations with respect to probability measures defined on phylogenetic space.

One possible strategy for performing and studying MCMC in phylogenetic space is to find lower-dimensional projections that preserve the Markov property, either exactly or approximately. In this talk we will discuss how to perform such a dimension reduction in the space of rooted trees using lumpability or quasi-lumpability with respect to subtrees, also known as clades. We study Metropolis-Hastings and lazy random walks on the rooted subtree prune-andregraft (rSPR) graph and give bounds on the lumping error and total variation with respect to clades.

# Theoretical and numerical analysis of the behavior of a particle at an asymmetric bistable potential

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Keywords: Langevin equation, Stochastic resonance, Bistable potential, Numerical methods

Until the end of the 19th century, noise was seen as something unpleasant, in which there was a need to avoid or even discard it. Recently it has been realized that noise can bring benefits to a system in terms of order. In stochastic resonance [3], noise generates an organized and structured behavior of the system. Regardless of whether it is desirable or not, it appears in different ways in the representation of some physical systems.

The model studied in the present work concerns a classical particle in an asymmetric bistable potential. Its dynamics is governed by the super-damped Langevin equation, based on Newton's second law, under the effect of a multiplicative white noise [4]. The iterative methods of Euler-Maruyama, Itô-Taylor and stochastic Runge-Kutta [2, 5] were theoretically revised and implemented computationally in Matlab. These methods were used in numerical simulations to find the solution of the stochastic differential equation. The Kramer rate [1], which estimates the time for a particle to escape from a potential minimum, is a very important physical measurement. The theoretically calculated Kramer rate was compared with the Kramer rate obtained from numerical simulations with additive and multiplicative noise. One of the objectives of the work is the study of stochastic resonance.

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# Distributionally robust chance-constrained minimum cost multi-commodity flow problem in time-varying networks

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**Keywords:** Uncertainty modelling; Dynamic multi-commodity flow; Robust optimization; Chance-constrained optimization; Distributionally robust.

The multi-commodity network flow (MCNF) problem is one of the most attractive problems in the network literature due to its wide application in various fields, such as the communication systems, urban traffic systems, rail-way systems and the logistic systems. MCNF problems are raised in a network when we need to transfer more than one commodity from the specific sources to the specific sinks in the situation that each arc has a certain capacity. See Karsten et al. [3], Kabadurmus and Smith [2] for more details. The MCNF problem in the presence of the uncertain parameters has attracted attentions of several scholars. In summary, three different types of approaches can be adopted to model imprecise data in MCNF problems including fuzzy approaches, stochastic optimization (SO) methods and robust optimization-based techniques. See Kureichik and Evgeniya [5], Mejri et al. [7] and Calafiore and El Ghaoui [1] for more details. On the other hand, in many real-world applications, such as road or air traffic control, production systems and communication networks, the flow can change over time. See Lu et al. [6], Rahmaniani et al. [8] and Khodayifar et al. [4] for more details.

Given that the decision analysis based on the uncertain data is inevitable in many realworld applications, therefore, this study focuses on the discrete dynamic multi-commodity flow (DDMF) in the presence of the uncertain parameters, such as the cost uncertainty, the demand uncertainty and the arc capacity uncertainty. For this purpose, we develop the dynamic path formulation of the DDMF model proposed by Khodayifar [4] into the case of parameter uncertainty. To study the parameter uncertainty in the DDMF, three different viewpoints are considered. In the first viewpoint, we study the robust counterpart (RC) of the DDMF by considering two different uncertainty sets, the interval and the ellipsoidal. The second viewpoint discusses the chance-constrained DDMF problem and analyses the probability constraints for the probability distributions and construct the deterministic convex counterparts of the chance constraints for any distribution. For the first time, we consider the viewpoint which deals with the chance constraints in the DDMF problem under the distribution uncertainty and obtain the deterministic restrictions such that the probability constraints are guaranteed. All proposed models (except for the robust counterpart model in the case of ellipsoidal uncertainty) in this paper are LP problems which can be solved with the existing algorithms in the LP context.

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# Periodic infinite horizon optimization problems with multiple solutions of mismatching period

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Keywords: Infinite horizon, multistage problems, convex optimization

Several multistage stochastic optimization problems can be framed as periodic, infinite horizon problems. This avoids dealing with thorny questions such as boundary conditions—as in the long term operation of the Brazilian interconnected power system—, and opens new questions as to the (time) limits of such solutions. We investigate several properties of the solutions to such periodic optimization problems, in the convex multistage setting, especially regarding their uniqueness and periodicity. We illustrate with simple examples that such solutions exhibit more complex behavior than the problem they arise from.

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# Planning the production and energy supply minimizing the costs of a factory.

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Keywords: Stochastic Optimization, Renewables Energies, Production Planning

Industrial processes can be highly energy consuming. Industrial actors are increasingly trying to integrate renewable energies to their energy supply for economic and environmental reasons. Recent reviews on related research can be found in [2] and [3].

In this work, we present a mixed-integer multistage stochastic problem optimizing both the production planning and the energy supply management of an industrial complexity. The goal is to minimize the expected energy supply costs of the factory. The mathematical problem is difficult to address first due to the stochasticity of renewable energy, coupled with a large number of time-step and the presence of (a few) binary variables.

We consider two classic methods to resolve our problem: dynamic programming and model predictive control. Those methods are computationally time-consuming, leading us to explore two heuristics based on stochastic dual dynamic programming (SDDP, [4, 5]), an algorithm solving the continuous relaxation of the problem fast. The heuristic uses the cost-to-go approximation of the continuous relaxation (obtained through SDDP) and computes a policy (satisfying integer constraints) with dynamic programming. The second heuristic adapt this idea by computing a policy over two time-step instead of one.

Exactly solving the mixed integer multistage stochastic linear program would be to use an extension of SDDP known as SDDiP ([1]). Unfortunately this algorithm approximate all continuous variables with binary ones, which in our problem with few binary variables doesn't seem reasonable. Instead we develop an alternative approach based on branch & cut methodology.

We run the proposed method on two different study cases modeling a real-case factory. In one of them we consider only time-of-use electricity prices, in the other it is also possible to buy electricity a day-ahead (at preferential rates). We compare and analyze the MPC results to the heuristics exploiting SDDP's cuts on both study case.

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# Periodic variants of stochastic dual dynamic programming in energy operation planning

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**Keywords:** Multistage stochastic optimization, energy planning problem, stochastic dual dynamic programming

The energy planning problem can be modeled as a multistage stochastic program, where at each stage (at each month of the year) an agent needs to choose a generation quantity from thermal and hydro such that minimize a performance index (operation costs) subject to the energy balance equation and the reservoir dynamics. A characteristic of the uncertainties in the problem of interest is their periodic behavior (typically the inflows to the reservoirs follow the annual rainfall regime). The stochastic dual dynamic programming (SDDP) [1, 2, 3] is a method for solving the energy planning problem, where the "curse of dimensionality" of dynamic programming is avoided. In order to reduce the computational effort for solving the energy planning problem, in this work we study and analize multistage stochastic optimization methods that explore periodic structures. To achieve this, we analize the proposals [4, 5] and consequently model and simulate the energy planning problem as a linear policy graph [6, 7].

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