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

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Transport Theory

We define the neutral particle transport theory as a framework of study with special attention to neutron transport problem due to its increasing applicability in different areas of science such as Reactor Physics, Nuclear Medicine, Radiological Protection, etc.

Reactor Physics

Nuclear Medicine

Radiological Protection

Two Main Approaches

Probabilistic School

Based on the stochastic nature between neutrons and atomic nuclei interactions

Deterministic School

Based on a mathematical model and different approximations that preserve the main physical processes

Deterministic Methods

Fine-mesh methods	**Finite difference methods**	Diamond Difference (DD)	...	...
	Finite element methods	Step ou Constant Discontinuous (CD)	Linear Discontinuous (LD)	...
Coarse-mesh methods	**Nodal methods**	Constant Nodal (CN)	Linear Nodal (LN)	Linear-Linear Nodal (LLN)
	Spectral nodal methods	Spectral Green's Function (SGF)	Response Matrix (RM)	Analytical Discrete Ordinates (ADO)

Due to the complexity and the increasing of nuclear techniques applied in different areas of science and engineering, it is necessary more accurate numerical methods that use less computational resources and improve the processing time to solve fixed source neutral particle transport problems.

Shielding

Radiological protection

Oil well logging

Nuclear Medicine

Material Science

Geological studies

Formulation

With the development of a new coarse-mesh spectral nodal response matrix method with linear approximation for the leakage terms in the transverse integrated S_N equations, it is expected to generate accurate numerical results and low computational cost in the solution of two-dimensional neutral particle transport problems with fixed source and isotropic scattering.

Neutron Transport Equation as a Balance Equation

Mathematical model that quantifies the average behavior of the population of neutrons migrating within a control volume

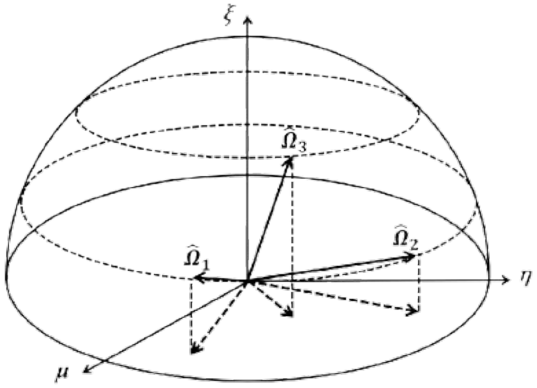
$$\frac{1}{v}\frac{\partial}{\partial t}\Psi(\vec{R},E,\hat{\Omega},t)+\hat{\Omega}\cdot\vec{\nabla}\Psi(\vec{R},E,\hat{\Omega},t)+\sigma_t(\vec{R},E)\Psi(\vec{R},E,\hat{\Omega},t)= \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' f(E',\hat{\Omega}'\rightarrow E,\hat{\Omega})c(E')\sigma_t(\vec{R},E')\Psi(\vec{R},E',\hat{\Omega}',t)+Q(\vec{R},E,\hat{\Omega},t) \qquad (1)$$

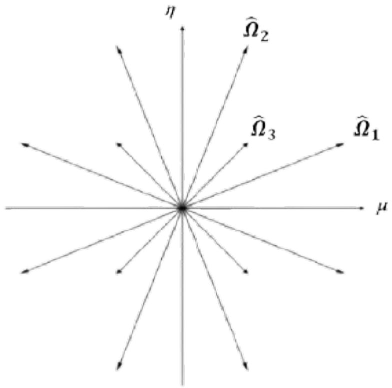
Neutron transport equation for stationary, monoenergetic and non-multiplying media with isotropic scattering

$$\hat{\Omega} \cdot \vec{\nabla}\Psi(\vec{R},\hat{\Omega}) + \sigma_t(\vec{R})\Psi(\vec{R},\hat{\Omega}) = \frac{\sigma_s(\vec{R})}{4\pi}\int_{4\pi} d\hat{\Omega}'\Psi(\vec{R},\hat{\Omega}') + Q(\vec{R},\hat{\Omega}) \qquad (2)$$

Discrete ordinates formulation

The discrete ordinate (S_N) formulation is widely used in numerical modeling of the transport equation and consists of discretizing the angular variable into a finite number of discrete values.

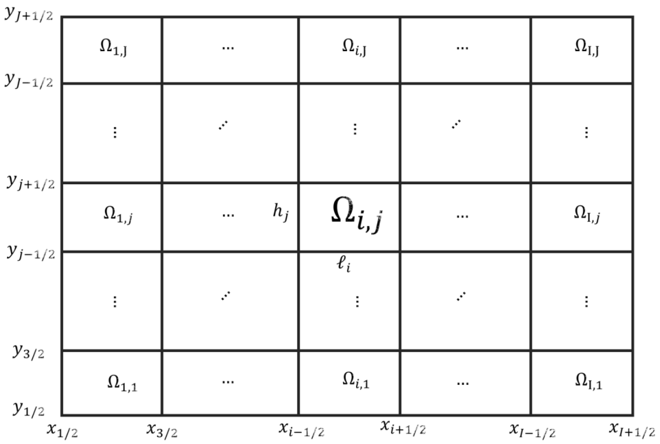




$$\hat{\Omega}_m \cdot \vec{\nabla}\Psi_m(\vec{R}) + \sigma_t(\vec{R})\Psi_m(\vec{R}) = \frac{\sigma_s(\vec{R})}{4}\sum_{n=1}^{M}\Psi_n(\vec{R})\omega_n + Q(\vec{R}) \qquad m = 1:M \qquad (3)$$

Spatial discretization

The rectangular spatial domain is divided into I x J cells and the S_N transport equations are solved inside each one, considering uniform total and scattering macroscopic cross sections, and the fixed sources



$$\mu_m \frac{\partial}{\partial x}\Psi_m(x,y) + \eta_m \frac{\partial}{\partial y}\Psi_m(x,y) + \sigma_{t,i,j}\Psi_m(x,y) = \frac{\sigma_{s,i,j}}{4}\sum_{n=1}^{M}\Psi_n(x,y)\omega_n + Q_{i,j} \qquad m = 1:M \qquad (x,y)\in\Omega_{i,j} \qquad (4)$$

Transverse integrated S_N equations

$$\frac{\mu_m}{\sigma_{t,i,j}}\frac{d}{dx}\widehat{\Psi}_{m,j}(x) + \widehat{\Psi}_{m,j}(x) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widehat{\Psi}_{n,j}(x)\omega_n + \frac{Q_{i,j}}{\sigma_{t,i,j}} - \frac{\eta_m}{\sigma_{t,i,j}h_j}\left[\Psi_m\left(x, y_{j+1/2}\right) - \Psi_m\left(x, y_{j-1/2}\right)\right] \quad (5)$$

$$\frac{\eta_m}{\sigma_{t,i,j}}\frac{d}{dy}\widetilde{\Psi}_{m,i}(y) + \widetilde{\Psi}_{m,i}(y) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widetilde{\Psi}_{n,i}(y)\omega_n + \frac{Q_{i,j}}{\sigma_{t,i,j}} - \frac{\mu_m}{\sigma_{t,i,j}\ell_i}\left[\Psi_m\left(x_{i+1/2}, y\right) - \Psi_m\left(x_{i-1/2}, y\right)\right] \quad (6)$$

$$\frac{\mu_m}{\sigma_{t,i,j}}\frac{d}{dx}\widehat{\varphi}_{m,j}(x) + \widehat{\varphi}_{m,j}(x) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widehat{\varphi}_{n,j}(x)\omega_n + \frac{6\eta_m}{\sigma_{t,i,j}h_j}\widehat{\Psi}_{m,j}(x) - \frac{3\eta_m}{\sigma_{t,i,j}h_j}\left[\Psi_m\left(x, y_{j+1/2}\right) + \Psi_{m,i,j}\left(x, y_{j-1/2}\right)\right] \quad (7)$$

$$\frac{\eta_m}{\sigma_{t,i,j}}\frac{d}{dy}\widetilde{\varphi}_{m,i}(y) + \widetilde{\varphi}_{m,i}(y) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widetilde{\varphi}_{n,i}(y)\omega_n + \frac{6\mu_m}{\sigma_{t,i,j}\ell_i}\widetilde{\Psi}_{m,i}(y) - \frac{3\mu_m}{\sigma_{t,i,j}\ell_i}\left[\Psi_m\left(x_{i+1/2}, y\right) + \Psi_m\left(x_{i-1/2}, y\right)\right] \quad (8)$$

$$\widehat{\Psi}_{m,j}(x) = \frac{1}{h_j}\int_{y_{j-1/2}}^{y_{j+1/2}}\Psi_m(x,y)dy$$

$$\widetilde{\Psi}_{m,i}(y) = \frac{1}{\ell_i}\int_{x_{i-1/2}}^{x_{i+1/2}}\Psi_m(x,y)dx$$

$$\widehat{\varphi}_{m,j}(x) = \frac{6}{h_j^2}\int_{y_{j-1/2}}^{y_{j+1/2}}\left(y - y_j\right)\Psi_m(x,y)dy$$

$$\widetilde{\varphi}_{m,i}(y) = \frac{6}{\ell_i^2}\int_{x_{i-1/2}}^{x_{i+1/2}}(x - x_i)\Psi_m(x,y)dx$$

$$\Psi_m(x, y_{j\pm1/2}) \cong \widetilde{\Psi}_{m,i,j\pm1/2,} + \frac{2(x-x_i)}{\ell_i}\widetilde{\varphi}_{m,i,j\pm1/2} \quad (9)$$

$$\Psi_m(x_{i\pm1/2}, y) \cong \widehat{\Psi}_{m,i\pm1/2,j} + \frac{2(y-y_j)}{h_j}\widehat{\varphi}_{m,i\pm1/2,j} \quad (10)$$

Linear approximation for the leakage terms

Transverse integrated S_N equations with linear approximations for the leakage terms

$$\frac{\mu_m}{\sigma_{t,i,j}}\frac{d}{dx}\widehat{\Psi}_{m,j}(x) + \widehat{\Psi}_{m,j}(x) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widehat{\Psi}_{n,j}(x)\omega_n + \frac{Q_{i,j}}{\sigma_{t,i,j}} - \frac{\eta_m}{\sigma_{t,i,j}h_j}\left(\widetilde{\Psi}_{m,i,j+1/2} - \widetilde{\Psi}_{m,i,j-1/2}\right) - \frac{2(x-x_i)}{\ell_i}\frac{\eta_m}{\sigma_{t,i,j}h_j}\left(\widetilde{\varphi}_{m,i,j+1/2} - \widetilde{\varphi}_{m,i,j-1/2}\right) \quad (11)$$

$$\frac{\eta_m}{\sigma_{t,i,j}}\frac{d}{dy}\widetilde{\Psi}_{m,i}(y) + \widetilde{\Psi}_{m,i}(y) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widetilde{\Psi}_{n,i}(y)\omega_n + \frac{Q_{i,j}}{\sigma_{t,i,j}} - \frac{\mu_m}{\sigma_{t,i,j}\ell_i}\left(\widehat{\Psi}_{m,i+1/2,j} - \widehat{\Psi}_{m,i-1/2,j}\right) - \frac{2(y-y_j)}{h_j}\frac{\mu_m}{\sigma_{t,i,j}\ell_i}\left(\widehat{\varphi}_{m,i+1/2,j} - \widehat{\varphi}_{m,i-1/2,j}\right) \quad (12)$$

$$\frac{\mu_m}{\sigma_{t,i,j}}\frac{d}{dx}\widehat{\varphi}_{m,j}(x) + \widehat{\varphi}_{m,j}(x) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widehat{\varphi}_{n,j}(x)\omega_n + \frac{6\eta_m}{\sigma_{t,i,j}h_j}\widehat{\Psi}_{m,j}(x) - \frac{3\,\eta_m}{\sigma_{t,i,j}h_j}\left(\widetilde{\Psi}_{m,i,j+1/2} + \widetilde{\Psi}_{m,i,j-1/2}\right) - \frac{2(x-x_i)}{\ell_i}\frac{3\,\eta_m}{\sigma_{t,i,j}h_j}\left(\widetilde{\varphi}_{m,i,j+1/2} + \widetilde{\varphi}_{m,i,j-1/2}\right) \quad (13)$$

$$\frac{\eta_m}{\sigma_{t,i,j}}\frac{d}{dy}\widetilde{\varphi}_{m,i}(y) + \widetilde{\varphi}_{m,i}(y) = \frac{c_{0,i,j}}{4}\sum_{n=1}^{M}\widetilde{\varphi}_{n,i}(y)\omega_n + \frac{6\mu_m}{\sigma_{t,i,j}\ell_i}\widetilde{\Psi}_{m,i}(y) - \frac{3\,\mu_m}{\sigma_{t,i,j}\ell_i}\left(\widehat{\Psi}_{m,i+1/2,j} + \widehat{\Psi}_{m,i-1/2,j}\right) - \frac{2(y-y_j)}{h_j}\frac{3\,\mu_m}{\sigma_{t,i,j}\ell_i}\left(\widehat{\varphi}_{m,i+1/2,j} + \widehat{\varphi}_{m,i-1/2,j}\right) \quad (14)$$

Analytical solution of the transverse integrated S_N equations with linear approximations for the leakage terms (matrix representation)

$$\widehat{\Psi}^{out} = \overline{\mathrm{MX1}}\widehat{\Psi}^{in} + \overline{\mathrm{MX2}}\left(\widetilde{\Psi}^{out} - \widetilde{\Psi}^{in}\right) + \overline{\mathrm{MX3}}(\widetilde{\varphi}^{out} - \widetilde{\varphi}^{in}) + \overline{\mathrm{SX}} \quad (15)$$

$$\widetilde{\Psi}^{out} = \overline{\mathrm{MY1}}\left(\widehat{\Psi}^{out} - \widehat{\Psi}^{in}\right) + \overline{\mathrm{MY2}}\widetilde{\Psi}^{in} + \overline{\mathrm{MY3}}(\widehat{\varphi}^{out} - \widehat{\varphi}^{in}) + \overline{\mathrm{SY}} \quad (16)$$

$$\widehat{\varphi}^{out} = \overline{\mathrm{MXX1}}\widehat{\Psi}^{in} + \overline{\mathrm{MXX2}}\left(\widetilde{\Psi}^{out} - \widetilde{\Psi}^{in}\right) + \overline{\mathrm{MXX3}}\left(\widetilde{\Psi}^{out} + \widetilde{\Psi}^{in}\right) + \overline{\mathrm{MXX4}}\widehat{\varphi}^{in} + \overline{\mathrm{MXX5}}(\widetilde{\varphi}^{out} - \widetilde{\varphi}^{in}) + \overline{\mathrm{MXX6}}(\widetilde{\varphi}^{out} + \widetilde{\varphi}^{in}) + \overline{\mathrm{SXX}} \quad (17)$$

$$\widetilde{\varphi}^{out} = \overline{\mathrm{MYY1}}\left(\widehat{\Psi}^{out} - \widehat{\Psi}^{in}\right) + \overline{\mathrm{MYY2}}\left(\widehat{\Psi}^{out} + \widehat{\Psi}^{in}\right) + \overline{\mathrm{MYY3}}\widetilde{\Psi}^{in} + \overline{\mathrm{MYY4}}(\widehat{\varphi}^{out} - \widehat{\varphi}^{in}) + \overline{\mathrm{MYY5}}(\widehat{\varphi}^{out} + \widehat{\varphi}^{in}) + \overline{\mathrm{MYY6}}\widetilde{\varphi}^{in} + \overline{\mathrm{SYY}} \quad (18)$$

Response Matrix representation

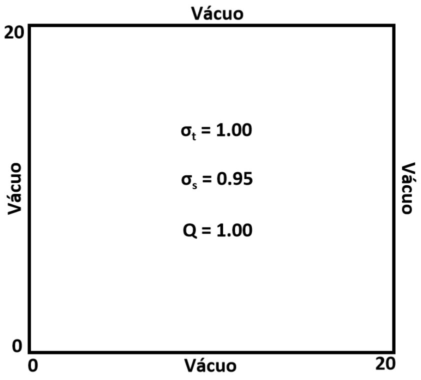
Solving for the vectors in the outgoing directions of motion, we obtain the characteristic equation of the offered method

$$F^{out} = \overline{\mathrm{RM}}F^{in} + \overline{\mathrm{P}} \quad (19)$$

S_N Transport sweeps

The RM-LLN method implements the FBI (Full Block Inversion) iterative scheme where the average emergent angular fluxes are computed from estimates of the incident node-edge average angular fluxes on each spatial discretization node

Homogeneous Model Problem

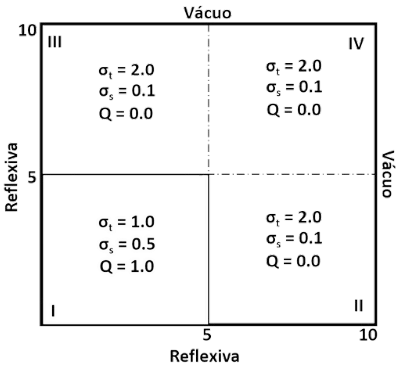


Ref. Sol (500x500, RM-CN)

Numerical results for DD, LD, CN, RM-CN and RM-LLN methods, and LQ_6 quadrature

Mesh	Method	Iterations	CPU(s)	Φ (n cm^{-2} s^{-1})	leak (n cm^{-1} s^{-1})
2 x 2	DD	124	1.6204E-03	1.4210E+01	5.7871E+01
				(8.81%)	(16.62%)
	LD	133	1.4538E-03	1.2266E+01	7.7319E+01
				(6.08%)	(11.41%)
	CN	90	1.3310E-03	9.7243E+00	1.0274E+02
				(25.54%)	(48.03%)
	RM-CN	5	2.0481E-03	1.3276E+01	6.7236E+01
				(1.66%)	(3.12%)
	RM-LLN	5	5.7634E-03	1.3098E+01	6.9018E+01
				(0.29%)	(0.56%)

Heterogeneous Model Problem



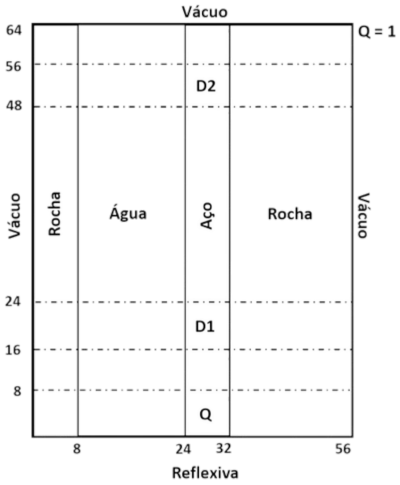
Ref. Sol (500x500, RM-CN)

Numerical results for DD, LD, CN, RM-CN and RM-LLN methods, and LQ_6 quadrature

Mesh	Method	Iterations	CPU(s)	Φ[I](n cm^{-2} s^{-1})	Φ[II](n cm^{-2} s^{-1})	Φ[IV](n cm^{-2} s^{-1})
4 x 4	DD	20	9.5570E-04	1.6875E+00	2.5716E-02	1.1818E-03
				(0.44%)	(37.49%)	(37.49%)
	LD	19	1.1397E-03	1.6728E+00	4.1673E-02	2.0816E-03
				(0.44%)	(1.3%)	(10.11%)
	CN	21	1.3606E-03	1.6540E+00	4.4431E-02	2.1853E-03
				(1.56%)	(8%)	(15.6%)
	RM-CN	9	1.0964E-02	1.6815E+00	4.0901E-02	2.0089E-03
				(0.08%)	(0.58%)	(6.26%)
	RM-LLN	9	3.7412E-02	1.6803E+00	4.1115E-02	1.9063E-03
				(0.01%)	(0.06%)	(0.83%)

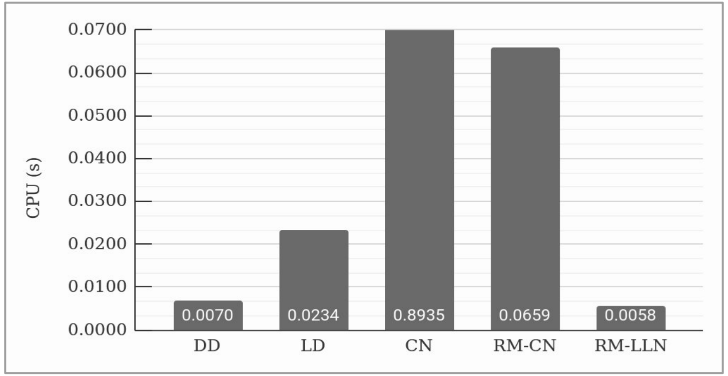
Oil Well Logging Problem

Numerical results for DD, LD, CN, RM-CN and RM-LLN methods, and LQ_4 quadrature



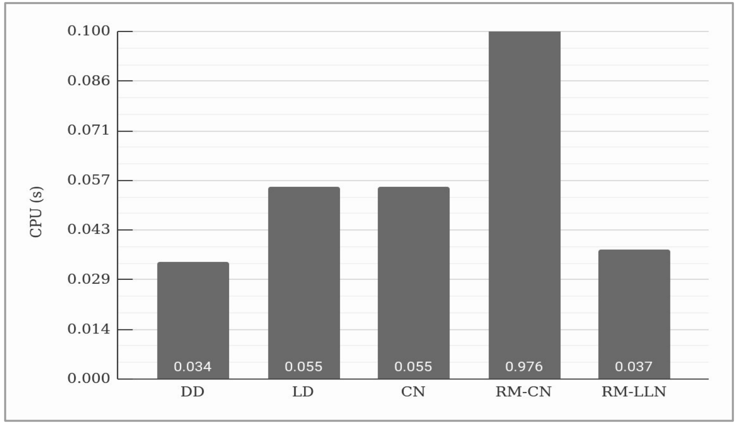
Ref. Sol (224x256, RM-CN)

Mesh	Method	Iterations	CPU(s)	Φ[D1](n cm^{-2} s^{-1})	Φ[D2](n cm^{-2} s^{-1})
7 x 8	DD	307	1.2470E-02	8.7650E-01	-3.9502E-03
				(48.73%)	(131.82%)
	LD	319	1.8583E-02	9.9182E-01	6.7988E-03
				(41.98%)	(45.23%)
	CN	212	1.8153E-02	1.7291E+00	4.6393E-02
				(1.14%)	(273.72%)
	RM-CN	30	3.4365E-02	1.3355E+00	9.3063E-03
				(21.88%)	(25.03%)
	RM-LLN	29	1.1598E-01	1.7139E+00	1.2459E-02
				(0.25%)	(0.37%)

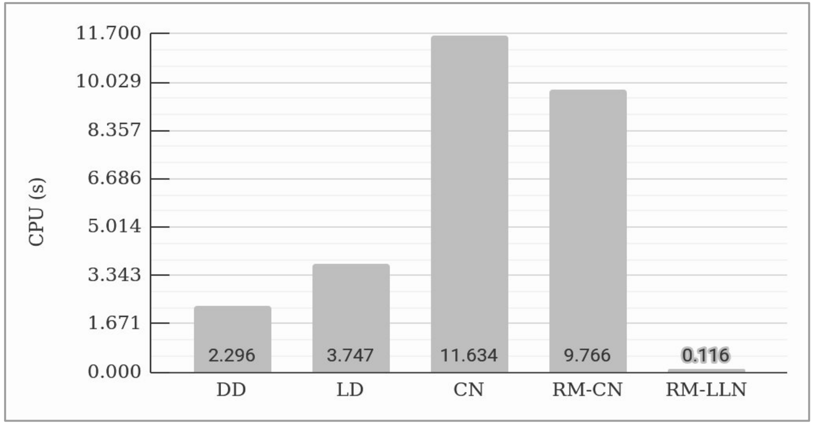


Homogeneous Model Problem

Processing time measured in CPU(s) for numerical results with relative deviation less than 1% with respect to the reference solution.



Heterogeneous Model Problem



Oil Well Logging Problem

Remarks

The mathematical formulation of the RM-LLN method based on a linear response matrix scheme is presented. The method analytically solves the system formed by the S_N equations cross-integrated using linear approximations for the transverse leakages.

The method implements the FBI iterative scheme where the analytical solutions of the system are preserved. Numerical solutions are continuous at the node interfaces and satisfy the boundary conditions.

The RM-LLN method shows to have a high performance as far as accuracy and computational cost are concerned.

Future work

Numerical instability

Numerical solutions show an oscillatory pattern of the angular flux between nodes and, in some cases, negative numerical values are reported.

Ill-conditioned

The matrices involved in the response matrix scheme show poor conditioning resulting from the presence of elements with expressive differences of orders of magnitude.

References

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