Martina Smitková; Marek Brandner

Numerical modeling of neutron transport - finite volume method, residual distribution schemes

In: Jan Chleboun and Petr Přikryl and Karel Segeth and Jakub Šístek (eds.): Programs and Algorithms of Numerical Mathematics, Proceedings of Seminar. Dolní Maxov, June 6-11, 2010. Institute of Mathematics AS CR, Prague, 2010. pp. 171–176.

Persistent URL: http://dml.cz/dmlcz/702756

NUMERICAL MODELING OF NEUTRON TRANSPORT – FINITE VOLUME METHOD, RESIDUAL DISTRIBUTION SCHEMES

Martina Smitková, Marek Brandner

1 Introduction

Thanks to nuclear renaissance, numerical modeling of reactor physics has become an important field of study. This contribution deals with methods for numerical solving of the neutron transport equation. For its angular discretization we use the P_N approximation, then we discuss two approaches to the spatial discretization – the Finite Volume Method and the Residual Distribution Schemes. Finally we present numerical results.

2 The neutron transport equation

Time-dependent transport of all neutral particles can be described by the one energy group Boltzmann transport equation [1]

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(\mathbf{x}, \boldsymbol{\Omega}, t) + \boldsymbol{\Omega} \cdot \nabla\psi(\mathbf{x}, \boldsymbol{\Omega}, t) + \Sigma_t\psi(\mathbf{x}, \boldsymbol{\Omega}, t) =$$
$$= \frac{\Sigma_s}{4\pi}\int_{4\pi}\psi(\mathbf{x}, \boldsymbol{\Omega}', t)\mathrm{d}\boldsymbol{\Omega}' + Q(\mathbf{x}, \boldsymbol{\Omega}, t), \tag{1}$$

where $\psi(\mathbf{x}, \boldsymbol{\Omega}, t)$ is the unknown function angular flux, $\mathbf{x}$ is the position, $\boldsymbol{\Omega}$ is the particle direction, t is time, Σ_s is the isotropic scattering cross section, Σ_t is the total cross section ($\Sigma_t = \Sigma_s + \Sigma_a$, where Σ_a is the absorption cross section), v is the neutron speed, which we set to $v = 1$ for convenience, and Q is the independent or external source ($Q = 0$ in the sequel).

This formulation is basis for a time-dependent problem. We can either seek for a time-dependent solution, or in some cases the basic goal is to find a steady (stationary) solution and the time-dependent solution has just the role of an iterative process.

The sought function is a function of spatial variables, angular variables and time (function of 6 variables). We distinguish discretization of direction (for example: P_N, S_N approximation), space and time.

3 The P_N approximation

This approximation is based on expanding the angular flux $\psi(\boldsymbol{\Omega})$ as a linear combination of the spherical harmonics as $\psi(\mathbf{x}, \boldsymbol{\Omega}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \psi_l^m(\mathbf{x}, t) Y_l^m(\boldsymbol{\Omega})$ [1]. This expansion is exact, but in order to make practical use of it, the series must be truncated. The P_N approximation is based on the assumption that all $\psi_l^m = 0$ for $l > N$. Then we solve a system of partial differential equations for the moments ψ_l^m.

The P_N equations can be written in the matrix form, in two dimensions as

$$\mathbf{q}_t + \mathbf{A}_x \mathbf{q}_x + \mathbf{A}_y \mathbf{q}_y = \mathbf{S}\mathbf{q} \tag{2}$$

and in one dimension as

$$\mathbf{q}_t + \mathbf{A}\mathbf{q}_x = \mathbf{S}\mathbf{q}, \tag{3}$$

where $\mathbf{q}$ is vector of the unknown moments ψ_l and ψ_l^m respectively. Matrices $\mathbf{A}, \mathbf{A}_x, \mathbf{A}_y$ (for their particular form see [1]) are diagonalizable, thus we are dealing with non-homogeneous linear hyperbolic systems of partial differential equations.

The basic goal is to construct an efficient solver applicable to both stationary and time-dependent problems with arbitrary geometry.

4 Spatial discretization

Up-to-date numerical methods for solving hyperbolic partial differential equations are various types of the finite volume method (FVM) – such as upwind methods, central methods, based on many approximate Riemann solvers (Roe, HLL, HLLE...) and different reconstruction methods (TVD, ENO, WENO), several limiter functions etc. Next we have novel methods such as Residual Distribution Schemes (RDS), Streamline Upwind Petrov–Galerkin method (SUPG) or Discontinuous Galerkin Finite Element Method (DGFEM).

We will discuss the Finite Volume Method and the Residual Distribution Schemes.

4.1 Finite volume method

We focus on analysing one-dimensional problems. Multidimensional problems will be treated simply as multiple, independent, one-dimensional problems. But this approach can cause problems and it means an important drawback of this method.

We begin by dividing the x axis into cells $\mathcal{C}_i = \langle x_{i-1/2}, x_{i+1/2} \rangle$ (see Fig. 1) with uniform widths $\Delta x = x_{i+1/2} - x_{i-1/2}$ and edges at $x_{i+1/2}$. We introduce space-averaged data in cell i at time t as

$$\mathbf{q}_i(t) = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{q}(x, t) \mathrm{d}x. \tag{4}$$

The following equation is a consequence of the more general integral form of (3):

$$\frac{\partial \mathbf{q}_i}{\partial t} + \frac{\mathbf{F}_{i+1/2} - \mathbf{F}_{i-1/2}}{\Delta x} = \mathbf{S}\mathbf{q}_i. \tag{5}$$
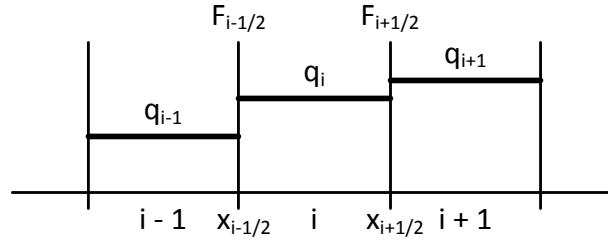
Fig. 1: *Notation of cells, cell averages and fluxes on interfaces in FVM.*

Here $\mathbf{F}_{i\pm1/2}$ denote the numerical fluxes at the cell boundaries, which we express using the Roe-type Riemann solver (the exact solution of the Riemann problem for the related linear homogeneous problem) as

$$\mathbf{F}_{i+1/2} = \frac{1}{2}\mathbf{A}(\mathbf{q}_l + \mathbf{q}_r) - \frac{1}{2}|\mathbf{A}|(\mathbf{q}_r - \mathbf{q}_l), \tag{6}$$

where $|\mathbf{A}| = \sum_k \mathbf{r}_k |\lambda_k| \mathbf{l}_k$ (λ_k are the eigenvalues of the matrix $\mathbf{A}$ from Eq. (3), $\mathbf{r}_k$ and $\mathbf{l}_k$ the right and left eigenvectors) and $\mathbf{q}_l$, $\mathbf{q}_r$ is obtained using the values of $\mathbf{Q}_i$ "to the left" and "to the right" of the cell i ($\mathbf{Q}_i \approx \mathbf{q}_i$).

If we at the interface $i+1/2$ naturally set $\mathbf{q}_l = \mathbf{Q}_i$ a $\mathbf{q}_r = \mathbf{Q}_{i+1}$, we get a method that is first order accurate in space. To get a higher-order method we reconstruct the approximate solution using linear interpolation within a cell to have a better estimate of the solution at the cell boundary. We seek to prevent the introduction of artificial oscillations into the solution, hence a nonlinear method must be used to calculate the slope within a cell to achieve better than first order accuracy. This is a statement of Godunov's Theorem. For example, the Van Leer's method and the minmod method can be used [3].

As we already mentioned, the multidimensional finite volume method is based on multiple one-dimensional problems, which brings some drawbacks, such as significant numerical diffusion, inability to tackle the real multidimensionality (no physical reasoning), wide stencil of the higher order schemes, rectangular mesh – disadvantage for problems with arbitrary geometry.

For the time integration we can use both the explicit and implicit Euler method, in this contribution just the explicit method was used. Another option are the TVD Runge–Kutta methods (suitable for computing the time-dependent solutions).

4.2 Residual distribution schemes

The residual distribution schemes have been developed on ideas borrowed from both the finite volume and finite element approaches and have become an attractive alternative to either one. The compact discretization stencil allows for the development of efficient implicit iterative solution strategies and for an easy parallelisation [2].

4.2.1 One–dimensional case

Consider scalar conservation law with source term $q_t + [f(q)]_x = s(q, x, t)$.

The solution is approximated by a continuous piecewise linear function $q(x, t) \approx \sum_i q_i(t) N_i(x)$, where $q_i(t)$ is the value of q at node i, and N_i the linear shape function equal to unity at x_i and equal to zero outside the interval $\langle x_{i-1}, x_{i+1} \rangle$ (see Fig. 2).
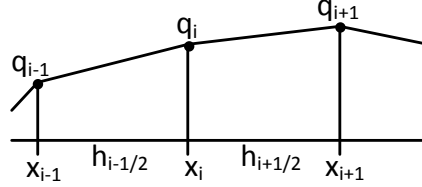

Fig. 2: *Data representation for RDS, using P1 elements.*

We define the cell residual as

$$\phi^{i+\frac{1}{2}} = \int_{x_i}^{x_{i+1}} (f_x - s)\mathrm{d}x = f_{i+1} - f_i - \frac{s_i + s_{i+1}}{2} h_{i+\frac{1}{2}}. \tag{7}$$

The nodal equation for node i is then formed by distributing the cell residual to the two nodes of the cell. Gathering the contributions of the two elements at node i we obtain for the steady state equation $\beta_i^{i-\frac{1}{2}} \phi^{i-\frac{1}{2}} + \beta_i^{i+\frac{1}{2}} \phi^{i+\frac{1}{2}} = 0$ where the distribution coefficients β sum to one for a given cell (conservativity condition), $\beta_i^{i+\frac{1}{2}} + \beta_{i+1}^{i+\frac{1}{2}} = 1$. The coefficients β can be specified so as to satisfy certain properties of monotonicity and accuracy in the solution, while maintaining the compact stencil. We formally define the distributed residuals as $\phi_i^{i-\frac{1}{2}} = \beta_i^{i-\frac{1}{2}} \phi^{i-\frac{1}{2}}$.

Time discretization For the higher order time-accurate time-dependent solution it is mandatory to use the consistent time discretization (for details see [2]). For the steady solution it is common to use the inconsistent time discretization (here using the explicit Euler method)

$$q_i^{n+1} = q_i^n - \frac{\Delta t}{h_i} \left(\beta_i^{i-\frac{1}{2}} \phi^{i-\frac{1}{2}} + \beta_i^{i+\frac{1}{2}} \phi^{i+\frac{1}{2}} \right), \tag{8}$$

where $h_i = \frac{1}{2}(h_{i-\frac{1}{2}} + h_{i+\frac{1}{2}})$ is the volume of the median dual cell surrounding node i.

4.2.2 Two–dimensional case for systems

Consider the system of conservation laws $\mathbf{q}_t + \nabla \cdot \mathbf{F} = \mathbf{0}$ to be solved on an arbitrary triangulation of the domain. The solution is approximated by a continuous function, varying linearly over each triangle, $\mathbf{q}(x, y, t) \approx \sum_i \mathbf{q}_i(t) N_i(x, y)$. The residual in triangle T is defined as

$$\Phi^T = -\iint_T \mathbf{q}_t \mathrm{d}x = \oint_{\partial T} \mathbf{F} \cdot \vec{\mathrm{d}n}_{ext}. \tag{9}$$

174

The Residual Distribution method consists of distributing fractions of this residual to the surrounding nodes. Starting from the inconsistent formulation and an Euler explicit time integration, we obtain the following update scheme

$$\mathbf{q}_i^{n+1} = \mathbf{q}_i^n - \frac{\Delta t}{S_i} \sum_T \beta_i^T \Phi^T = \mathbf{q}_i^n - \frac{\Delta t}{S_i} \sum_T \Phi_i^T, \tag{10}$$

where S_i is the area of the median dual cell around node i, i. e. 1/3 of the area of all triangles meeting at node i (see Fig. 3). The residual Φ^T is now a vector, while the β_i^T have become distribution matrices.
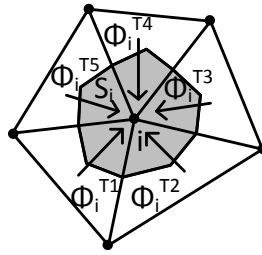

Fig. 3: *Node i and median dual cell S_i, with surrounding cells and updates Φ_i^T.*

5 Results and conclusion

For clarity and brevity and regarding to the extent of this text, we used $q_t + 0.5q_x + 0.5q_y = -0.1q$ (a "special case" of (2)) as a simple test equation with initial condition a unit pulse in the center of the square domain. For the P_N system the results would be analogous.

The test domain consists of 49×49 cells, $\Delta x = \Delta y = 0.32$ (FVM), for the RDS we used the Delaunay triangulation for the centres of the cells. The time interval is $T = 8$ and the time step $\Delta t = 0.25$.

From the Residual Distribution Schemes we chose the N (Narrow) scheme with $\phi_i^{T,N} = -\frac{k_i^+}{\sum_j k_j^+} \sum_j k_j^- (u_i^n - u_j^n)$ (monotone linear first order) and the LDA (Low Diffusion A) scheme with $\beta_i^{LDA} = \frac{k_i^+}{\sum_j k_j^+}$ (linear second order). The scalars k_i, termed the inflow parameters, defined as $k_i = \frac{1}{2}\vec{\lambda}\cdot\vec{n}_i$, allows to distinguish between inflow and outflow faces, and upstream and downstream nodes of the triangle. The vectors $\vec{n}_i$ are defined as the interior normals to the triangle, scaled by their respective lengths, $\vec{\lambda}$ is the vector of advection coefficients (see [2] for details).

At the figures 4 and 5 we can see results of the first-order Finite Volume Method and of the N scheme and LDA scheme. According to their theoretical properties, the LDA scheme gives most accurate results, however not keeping the solution positive. The positivity requirement is satisfied by the N scheme.

For the future work we want to focus on blending these two schemes together to gain better accuracy in smooth regions while maintaining positivity in transient areas. Another objective is to see the PDE as a whole, define a space-time residual and introduce the space-time Residual Distribution Schemes.
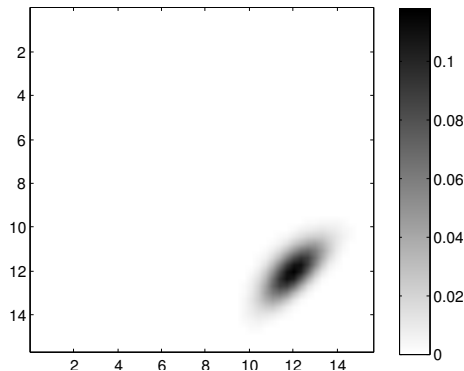

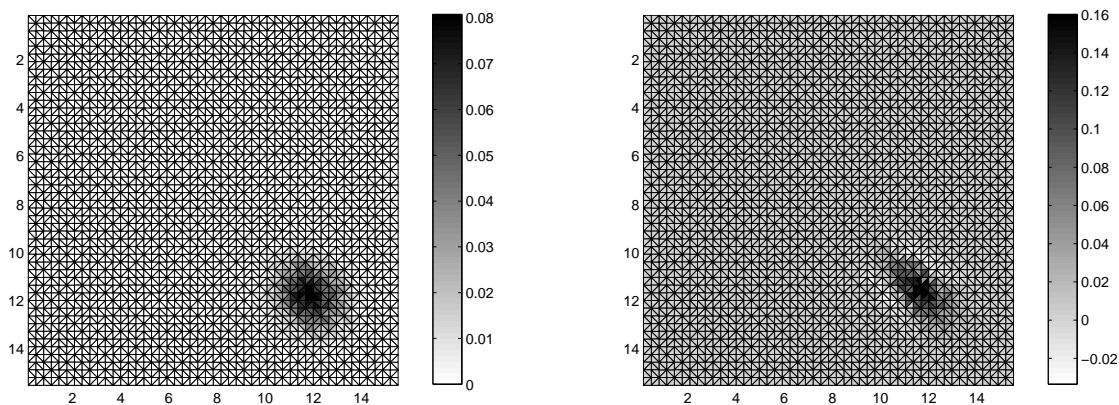**Fig. 4:** *Result of the Finite Volume Method.*

Fig. 5: *Result of the N (left) and LDA (right) scheme (RDS).*

References

[1] Brunner, T.: *Riemann solvers for time-dependent transport based on the maximum entropy and spherical harmonics closures.* Ph.D. thesis, The University of Michigan, 2000.

[2] Deconinck H., Ricchiuto M., and Sermeus K.: Introduction to residual distribution schemes and comparison with stabilized finite elements. In: H. Deconinck (Ed.), *33rd VKI Lecture Series CFD.* Von Karman Institute, Sint-Genesius-Rode, 2003.

[3] LeVeque, R.: *Finite volume methods for hyperbolic problems.* 1. edition, Cambridge University Press, Cambridge, 2002.