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A non-conforming 3D spherical harmonic transport solver

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Abstract

A new 3D transport solver for the time-independent Boltzmann transport equation has been developed. This solver is based on the second-order even-parity form of the transport equation. The angular discretization is performed through the expansion of the angular neutron flux in spherical harmonics (P_N method). The novelty of this solver is the use of non-conforming finite elements for the spatial discretization. Such elements lead to a discontinuous flux approximation. This interface continuity requirement relaxation property is shared with mixed-dual formulations such as the ones based on Raviart-Thomas finite elements. Encouraging numerical results are presented.

KEYWORDS: neutronics core solver, even-parity neutron transport equation, P_N approximation, non-conforming finite elements

1. Introduction

A new 3D transport solver for the time-independent Boltzmann transport equation has been developed. This solver is based on the second-order even-parity form of the transport equation, obtained through the even/odd angular parity decomposition for the angular flux popularized by Vladimirov [1]. The angular discretization is performed through the expansion of the angular neutron flux in spherical harmonics, that is using the P_N method, whose main advantage over the simpler discrete ordinate (S_N) method lies in the absence of ray effects.

The combination of the even-parity transport equation with a P_N angular discretization is at the basis of well-known existing core solvers such as EVENT [2] and VARIANT [3] (this last solver uses a hybrid scheme with Lagrange multipliers). The novelty of the new solver we present is the use of non-conforming finite elements for the spatial discretization. By "non-conforming", we mean elements that allow interface discontinuities for the unknown, namely here the even-parity angular flux Ψ^+, leading to a discontinuous flux approximation. This interface continuity requirement relaxation property is shared with mixed-dual formulations such as the ones based on Raviart-Thomas finite elements. In fact, equivalences between mixed methods and non-conforming second-order methods can be established [4–6]. The flexibility and parallelization capabilities of the non-conforming finite elements have been proved useful in other fields [7, 8].

After briefly reviewing the even-parity transport equation in Section 2, we detail our non-conforming spatial discretization in Section 3. Then, we address the numerical solution scheme in Section 4, before presenting numerical results in Section 5. Note that the new solver presented here is currently restricted to Cartesian geometry.

2. Even-parity weak form equation

The even- and odd- (angular) parity decomposition for the angular flux [1] reads

$$\Psi(\boldsymbol{r},\boldsymbol{\Omega}) = \Psi^{+}(\boldsymbol{r},\boldsymbol{\Omega}) + \Psi^{-}(\boldsymbol{r},\boldsymbol{\Omega})$$

where

$$\Psi^{\pm}(\boldsymbol{r},\boldsymbol{\Omega}) = \frac{1}{2}\left(\Psi(\boldsymbol{r},\boldsymbol{\Omega}) \pm \Psi(\boldsymbol{r},-\boldsymbol{\Omega})\right).$$

With a similar decomposition for the source, one obtains the following coupled pair of first order equations for each energy group $g = 1 \ldots G$

$$\begin{aligned}
&\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\Psi_g^{-}(\boldsymbol{r},\boldsymbol{\Omega}) + \sigma^{g}(\boldsymbol{r})\Psi_g^{+}(\boldsymbol{r},\boldsymbol{\Omega}) \\
&\qquad = \sum_{n\ \text{even}}^{\infty}(2n+1)\,\sigma_{s,n}^{gg}(\boldsymbol{r})\int_S \Psi_g^{+}(\boldsymbol{r},\boldsymbol{\Omega}')P_n(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')d\boldsymbol{\Omega}' + s_g^{+}(\boldsymbol{r},\boldsymbol{\Omega}) \qquad (1)\\
&\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\Psi_g^{+}(\boldsymbol{r},\boldsymbol{\Omega}) + \sigma^{g}(\boldsymbol{r})\Psi_g^{-}(\boldsymbol{r},\boldsymbol{\Omega}) \\
&\qquad = \sum_{n\ \text{odd}}^{\infty}(2n+1)\,\sigma_{s,n}^{gg}(\boldsymbol{r})\int_S \Psi_g^{-}(\boldsymbol{r},\boldsymbol{\Omega}')P_n(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')d\boldsymbol{\Omega}' + s_g^{-}(\boldsymbol{r},\boldsymbol{\Omega}) \qquad (2)
\end{aligned}$$

where $\sigma^{g}(\boldsymbol{r})$ and $\sigma_{s,n}^{gg}(\boldsymbol{r})$ are the total and scattering cross-section within group g (expanded in Legendre polynomials P_n), and where the source terms $s_g^{\pm}(\boldsymbol{r},\boldsymbol{\Omega})$ contain the fission and inter-group scattering source terms, as well as any prescribed external neutron source.

The weak form is obtained by multiplying equation (1) by a test function $\tilde{\Psi}^{+}$, integrating over space and angle, and applying the divergence theorem. Then, expressing Ψ^{-} in terms of Ψ^{+} using (1), using the addition theorem for spherical harmonics, and introducing an operator G acting on any suitable f as

$$G\,f(\boldsymbol{\Omega}) = \sum_{n\ \text{odd}}^{\infty}\sum_{m=-n}^{n}(\sigma(\boldsymbol{r}) - \sigma_{s,n}(\boldsymbol{r}))^{-1}Y_{n,m}(\boldsymbol{\Omega})\int_S f(\boldsymbol{\Omega}')\,Y_{n,m}(\boldsymbol{\Omega}')d\boldsymbol{\Omega}',$$

we obtain (see also [2])

$$\begin{aligned}
&\int_S d\Omega\int_V dV\,\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\tilde{\Psi}^{+}\,\left\{Gs^{-} - G(\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\Psi^{+})\right\} \\
&+\int_S d\Omega\int_{\partial V_{vac}} d\Gamma\,|\boldsymbol{\Omega}\cdot\boldsymbol{n}|\tilde{\Psi}^{+}\Psi^{+} + \int_S d\Omega\int_V dV\sigma\tilde{\Psi}^{+}\Psi^{+} \\
&-\int_S d\Omega\int_V dV\tilde{\Psi}^{+}\Big(\sum_{n\ \text{even}}^{\infty}(2n+1)\,\sigma_{s,n}\int_S \Psi^{+}P_n d\boldsymbol{\Omega}'\Big) = \int_S d\Omega\int_V dV\;s^{+}\;\tilde{\Psi}^{+}
\end{aligned}$$

where we dropped the group indices for simplicity, and where ∂V_{vac} is the part of the boundary where vacuum conditions are imposed. As for reflected boundary condition, they are treated by canceling appropriate coefficients in the flux spherical harmonic expansion.

3. Non-conforming spatial discretization

The spatial discretization is based on a simple non-conforming finite element denoted by NC_4 (non-conforming element with 4 nodes) in 2D and by NC_6 in 3D.

In 2D, the NC_4 element is rectangular-shaped with nodes (here in their finite element interpretation) placed in the middle of each side. The basis $\{1, x, y, xy\}$ is not unisolvent with such node positioning, and the spatial basis to use is then $\{1, x, y, x^2 - y^2\}$. In our code, we used the following basis functions:

$$\frac{1 - 2y + y^2 - x^2}{4}, \frac{1 - 2x + x^2 - y^2}{4}, \frac{1 + 2x + x^2 - y^2}{4}, \frac{1 + 2y + y^2 - x^2}{4}.$$

Note that the NC_4 element can be obtained by rotating the usual lowest-order Lagrangian element, and is therefore known as the "rotated Q_1" element in the numerical analysis community. It was tested long ago by Lautard [9] on the diffusion equation, and more recently used by Rannacher and Turek [10] for the Stokes problem. The choice of the NC_4 element among various non-conforming elements was motivated by an earlier study by the author [11]. This study (empirically) demonstrated that the NC_4 element provides an enhanced accuracy compared to the usual lowest-order Lagrangian element at a reasonable cost. Such property was showed even though the NC_4 element does not pass the "patch test" [12], that is the continuity of the mean value of Ψ^+ is not guaranteed across element interfaces.

In 3D, the NC_4 element naturally extends to the NC_6 element, i.e., a rectangular parallelepiped with a node in the middle of each face. An unisolvent basis is then given (among others) by $\{1, x, y, z, x^2 - y^2, x^2 - z^2\}$, and the basis functions used in our code read as follows:

$$\frac{1}{6} - \frac{z}{2} + \frac{-x^2 - y^2 + 2z^2}{6}, \frac{1}{6} - \frac{y}{2} + \frac{-x^2 + 2y^2 - z^2}{6}, \frac{1}{6} - \frac{x}{2} + \frac{2x^2 - y^2 - z^2}{6},$$
$$\frac{1}{6} + \frac{x}{2} + \frac{2x^2 - y^2 - z^2}{6}, \frac{1}{6} + \frac{y}{2} + \frac{-x^2 + 2y^2 - z^2}{6}, \frac{1}{6} + \frac{z}{2} + \frac{-x^2 - y^2 + 2z^2}{6}.$$

4. Numerical solution method

Let us now have a look at the numerical solution method. For the outer iteration, a classical power iteration method with Chebyshev acceleration was used. For the inner iteration, an iterative preconditioned conjugate gradient was implemented. Various preconditioning strategies were investigated: diagonal, forward-backward Gauss-Seidel, and incomplete Cholesky (IC) factorization with or without fill-in [13]. The best numerical results, presented in the next section, were obtained using the IC factorization without fill-in. Note that the spatio-angular matrices to be preconditioned are symmetric positive definite but not diagonally dominant nor M-matrices, which makes their preconditioning challenging. Indeed, the positivity of the pivots in the incomplete factorization, and thus the applicability of the IC method, is not guaranteed for such matrices. (This is by the way also the case when usual Lagrangian elements are used.) It appears that in all our test calculations (see Section 5), the IC factorization with no fill-in did not break down. This was not the case with additional fill-in and furthermore, even in the absence of breakdown, the increase in preconditioner quality obtained with additional fill-in could not offset the additional time spent in building this preconditioner. Finally, preconditioning using modified IC factorizations (i.e., with diagonal compensation of the dropped elements) still need to be investigated. This will be hopefully done before the conference.

5. Numerical results

The new solver was tested on the 3D Takeda 1 benchmark [14] consisting in a small LWR core with (case 1) or without (case 2) inserted control rods. Note that this benchmark contains low-density regions, which makes simplified transport approximations (SP_N) inappropriate. The new P_N solver results were compared to reference results [15] as well as to the discrete ordinate (S_N) solver CRONOS/PRIAM in order to compare CPU times. The S_N solver was used with the lowest two rectangular Lagragian finite elements, namely LL_4 (linear Lagrangian element with 4 nodes) and PL_9, (parabolic Lagrangian element with 9 nodes) coupled to a linear approximation in the third direction. For all calculations, a 25×25 mesh on a quarter core was used. Table 1 presents k_{eff} results demonstrating the proper convergence of the new non-conforming solver. We notice that the new solver provides a P_3 result faster than what CRONOS/PRIAM requires for the basic S_4-LL_4 calculation. Table 2 displays the average flux errors in the three zones (core, reflector and void/rod). We observe that the agreement with the reference solution is slightly better for the P_3 non-conforming solver than for the S_4-LL_4 solver.

	CASE 1 (rods out)			CASE 2 (rods in)		
	Reference results					
Monte-Carlo	$k_{eff} = 0.9778 \pm 46$ pcm			$k_{eff} = 0.9623 \pm 48$ pcm		
P_N	$k_{eff} = 0.9766 \pm 58$ pcm			$k_{eff} = 0.9630 \pm 78$ pcm		
S_8	$k_{eff} = 0.9772 \pm 7$ pcm			$k_{eff} = 0.9624 \pm 19$ pcm		
	k_{eff}	CPU time (s)	# ext. iter.	k_{eff}	CPU time (s)	# ext. iter.
	CRONOS/PRIAM S_N results					
S_4, LL_4	0.97641	508	91	0.96322	179	30
S_8, LL_4	0.97699	1668	93	0.96324	563	30
S_4, PL_9	0.97676	4900	127	0.96294	1466	31
	Non-conforming P_N results					
P_1	0.92876	16	15	0.93229	6	10
P_3	0.97247	202	14	0.96121	113-123	16
P_5	0.97555	1600-2000	15	0.96222	1100-1250	24
P_7	0.97633	$\sim$ 7,329	15	0.96241	$\sim$ 4750	32
P_9	0.97664	$\sim$ 20,000	15	0.96247	$\sim$ 14,000	45

Table 1: k_{eff} results for the Takeda 1 benchmark

The new non-conforming P_N solver is still currently under development, and optimizations can be envisioned. Up-to-date results will be presented at the conference. Finally, the 2-D OECD benchmark [16] with C5 MOX fuel assemblies and 7-group energy discretization is currently being used to further assess the accuracy of the new solver. The corresponding numerical results will also be presented at the conference.

	$(\frac{\Delta F}{F})_{core}$ (%)	$(\frac{\Delta F}{F})_{refl}$ (%)	$(\frac{\Delta F}{F})_{void/rod}$ (%)
CRONOS/PRIAM, S_4, LL_4			
Case 1 (rods out)			
group 1	-0.90	-0.76	-1.33
group 2	-0.67	-1.91	-5.21
Case 2 (rods in)			
group 1	-0.58	-0.35	-1.34
group 2	0.03	-1.23	0.02
Non-conforming, P_3			
Case 1 (rods out)			
group 1	-0.81	0.86	-0.09
group 2	-0.69	0.56	-3.27
Case 2 (rods in)			
group 1	-0.45	0.81	0.98
group 2	0.01	0.92	0.13

Table 2: Average flux errors (compared to the Monte-Carlo reference results [15])

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References

1) V. Vladimirov, Mathematical problems in the one-velocity theory of particle transport, Tech. rep., Atomic Energy of Canada Ltd., Ontario, translated from Transactions of the V.A. Steklov Mathematical Institute, **61**, 1961 (1963).

2) C. de Oliveira, An arbitrary geometry finite element method for multigroup neutron transport with anisotropic scattering, Progress in Nuclear Energy 18 (1/2) (1986) 227–236.

3) G. Palmiotti, E. Lewis, C. Carrico, VARIANT: VARIational Anisotropic Nodal Transport for multidimensional cartesian and hexagonal geometry calculations, Tech. Rep. ANL-95/40, Argonne National Laboratory (1995).

4) J. Hennart, A general family of nodal schemes, SIAM J. Sci. Stat. Comput. 7 (1) (1986) 264–286.

5) D. Arnold, F. Brezzi, Mixed and non conforming finite element methods: implementation, postprocessing and error estimates, Math.Mod.Numer.Anal. 19 (1) (1985) 7–32.

6) T. Arbogast, Z. Chen, On the implementation of mixed methods as nonconforming methods for second order elliptic problems, Math. Comp. 64 (1995) 943–972.

7) P. Kloucek, B. Li, M. Luskin, Analysis of a class of nonconforming finite elements for crystalline microstructures, Math. Comp. 65 (215) (1996) 1111–1135.

8) T. Ha, J. Santos, D. Sheen, Nonconforming finite element methods for the simulation of waves in viscoelastic solids, Comput. Methods Appl. Mech. Engrg. 191 (2002) 5647–5670.

9) J. Lautard, New finite element representation for 3D reactor calculations, in: Proc. of the Topical Meeting on Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems, Munchen, Germany, 1981.

10) R. Rannacher, S. Turek, Simple nonconforming quadrilateral stokes element, Numerical Methods for Partial Differential Equations 8 (1992) 97–111.

11) S. Van Criekingen, A non-conforming generalization of Raviart-Thomas elements to the spherical harmonic form of the even-parity neutron transport equation, Annals of nuclear energy To appear.

12) G. Strang, G. Fix, An Analysis of the Finite Element Method, Prentice-Hall, 1973.

13) Y. Saad, Iterative Methods for Sparse Linear Systems, SIAM, 2003.

14) T. Takeda, M. Tamitani, H. Unesaki, Proposal of 3D neutron transport benchmark, NEACRPA-953 rev.1, Department of nuclear engineering, Osaka University, Japan (1989).

15) T. Takeda, H. Ikeda, Final report on 3D neutron transport benchmark, department of nuclear engineering, Osaka University, Japan.

16) Benchmark on deterministic transport calculations without spatial homogenisation. a 2-D/3-D MOX fuel assembly benchmark, Vol. NEA/NSC/DOC(2003)16 of Nuclear Science, OECD, Nuclear Energy Agency, 2005.