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Assessment of the performance of the spectral element method applied to neutron transport problems

A. Barbarino [a], S. Dulla [a,*], E.H. Mund [b], P. Ravetto [a]

[a] *Dipartimento Energia, Politecnico di Torino, I-10129 Torino, Italy*
[b] *Service de Métrologie Nucléaire, Université Libre de Bruxelles, B-1050 Bruxelles, Belgium*

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ABSTRACT

The spectral element method can be used to deal with the spatial operators of neutron transport problems with high efficiency, as shown recently in the framework of the second-order A_N transport approximation. The results highlight interesting computational features and show the appeal of the scheme for reactor physics applications. In this paper we investigate the numerical performance of the method in detail. In order to carry out an accurate monitoring of the error behavior to levels close to numerical round-off, we use benchmark problems with known analytical solutions, or with manufactured solutions. Manufactured solutions can easily be obtained for source-injected problems, by tailoring the external neutron source and the boundary conditions to a pre-established analytical solution for a given system. The results presented prove the effectiveness of the method and the high level of accuracy that can be attained.

1. Introduction

In a previous paper (Barbarino et al., 2013) the spectral element method (SEM) was applied to the solution of neutron transport problems in the A_N space second-order formulation, which is particularly suitable to be treated by SEM. The results presented showed that accurate solutions can be attained for some benchmark configurations and interesting features were highlighted. Hence, the method looks promising for applications to neutronic calculations in nuclear systems.

In this paper, the numerical performance of the method is investigated in detail. In order to carry out an accurate monitoring of the behavior of the error up to levels close to numerical round-off, it is necessary to have an exact reference solution. Exact benchmarks are available either through fully analytical solutions (Ganapol, 2008) or through a manufactured solution process. Manufactured solutions can be easily obtained for source-injected neutron transport problems, by tailoring the external neutron source and the boundary conditions to a pre-established analytical neutron distribution in a given system (Warsa et al., 2010). In the present work, manufactured and analytical solutions are derived and the performance of SEM is assessed by direct comparisons and error studies.

While in the previous work the SEM approach was applied to two-dimensional configurations with the A_N model, in this work we focus the attention on the comparison of the performance of the method also when applied to standard approximations, such as spherical harmonics and discrete ordinate formulations of the transport problem. This allows a more consistent evaluation of the error, eliminating differences associated to the angular treatment adopted and focusing on the error introduced by the spatial discretization schemes only. For this purpose, we consider the one-speed transport equation in plane geometry with isotropic scattering and a general anisotropic source:

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\int_{-1}^{+1} d\mu' \psi(x,\mu') + S(x,\mu), \qquad (1)$$

with $(x,\mu) \in \mathcal{D} := (a,b) \times [-1,+1]$. The unknown $\psi(x,\mu)$ is the neutron angular flux and $S(x,\mu)$ is a prescribed anisotropic neutron source. In what follows, the cross sections $\Sigma_s(x)$ and $\Sigma_t(x)$ are assumed to be piecewise constant functions. Eq. (1) must be supplemented with boundary conditions. Vacuum conditions are assumed at the boundaries of the spatial domain:

$$\psi(a,\mu) = 0, \quad \forall \mu \in [0,1]; \qquad \psi(b,\mu) = 0, \quad \forall \mu \in [-1,0]. \qquad (2)$$

Discrete ordinate and spherical harmonics equations are then derived for Eq. (1), in a form suitable to be handled by SEM.

Furthermore, using the exact Green function for the transport equation in the infinite homogeneous medium, analytical reference solutions may also be generated. Such solutions are used as

* Corresponding author. Tel.: +39 0110904416; fax: +39 0110904499.
E-mail addresses: andrea.barbarino@polito.it (A. Barbarino), sandra.dulla@polito.it (S. Dulla), emund@ulb.be (E.H. Mund), piero.ravetto@polito.it (P. Ravetto).

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benchmarks by direct comparison with the results of the application of the spectral element method.

2. The spectral element method applied to the second-order form of the transport equation

The even and odd parity fluxes, denoted by $\psi^{+}(x,\mu)$ and $\psi^{-}(x,\mu)$, respectively, are introduced as:

$$\psi^{\pm}(x,\mu) = \frac{1}{2}[\psi(x,\mu) \pm \psi(x,-\mu)], \tag{3}$$

while the total flux is given by:

$$\phi(x) = 2\int_0^{+1} d\mu\psi^{+}(x,\mu). \tag{4}$$

Using the standard procedure (Lewis and Miller, 1993), by writing Eq. (1) for μ and $-\mu$, adding and subtracting the resulting equations and eliminating the odd parity flux, one obtains a second-order form of the equation for $\psi^{+}(x,\mu)$:

$$-\mu^2\frac{\partial}{\partial x}\left(\frac{1}{\Sigma_t(x)}\frac{\partial\psi^{+}(x,\mu)}{\partial x}\right) + \Sigma_t(x)\psi^{+}(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + Q(x,\mu), \tag{5}$$

with

$$Q(x,\mu) = S^{+}(x,\mu) - \frac{\mu}{\Sigma_t(x)}\frac{\partial S^{-}}{\partial x}(x,\mu), \tag{6}$$

where the even and odd parity sources, S^{+} and S^{-}, are defined as in Eq. (3). Assuming that no emission from the external source is taking place on the boundary, i.e. $S(a,\mu) = S(b,\mu) = 0$, one can easily show using Eq. (3) that the vacuum boundary conditions for $\psi^{+}(x,\mu)$ take the following Robin-type form:

$$\begin{aligned}
&\mu\frac{\partial\psi^{+}}{\partial x}(a,\mu) - \Sigma_t(a)\psi^{+}(a,\mu) = 0, \qquad \forall\mu\in[0,1],\\
&\mu\frac{\partial\psi^{+}}{\partial x}(b,\mu) + \Sigma_t(b)\psi^{+}(b,\mu) = 0, \qquad \forall\mu\in[-1,0].
\end{aligned} \tag{7}$$

Eqs. (5)–(7) constitute the basic formulation of the transport problem.

The angular treatment can be dealt with adopting the spherical harmonics approach, that amounts to an expansion in terms of Legendre polynomials in plane geometry, thus leading to a set of coupled equations for the even moments of the flux. The development of a spectral element approach to the spherical harmonics equations has been carried out in full detail by Mund (2011). Alternatively, the discrete ordinate method can be applied by discretization of the angular variable coupled to the Gauss–Legendre quadrature scheme over the half range $\mu\in[0,1]$. In the following, the discrete ordinate spectral element formulation is derived. The spatial domain is supposed to be made of subdomains in which nuclear data are constant.

2.1. The discrete ordinate model

A discrete ordinate model can be derived easily from the second-order transport equation, Eq. (5) with boundary conditions given by Eq. (7), assuming piecewise constant cross sections. For brevity, it is useful to set the following definitions:

$$\varphi_\ell(x) := \psi^{+}(x,\mu_\ell) \quad \text{and} \quad Q_\ell(x) := Q(x,\mu_\ell). \tag{8}$$

Choosing a set of N symmetric angular directions $\{\mu_\ell\}_{\ell=1}^{N}$, one can write Eq. (5) for each direction $\mu_\ell > 0$, obtaining the following system of coupled differential equations for each homogeneous subdomain:

$$-\frac{\mu_\ell^2}{\Sigma_t}\frac{d^2\varphi_\ell(x)}{dx^2} + \Sigma_t\varphi_\ell(x) = \frac{\Sigma_s}{2}\phi(x) + Q_\ell(x), \qquad \ell = 1,\ldots,N/2. \tag{9}$$

Recalling Eq. (7), at the boundary points a and b one can write:

$$\begin{aligned}
&\mu_\ell\frac{d\varphi_\ell}{dx}(a) - \Sigma_t(a)\varphi_\ell(a) = 0,\\
&\mu_\ell\frac{d\varphi_\ell}{dx}(b) + \Sigma_t(b)\varphi_\ell(b) = 0, \qquad \ell = 1,\ldots,N/2.
\end{aligned} \tag{10}$$

Interface conditions need also to be imposed at points x_∂ between two different homogeneous subdomains:

$$\begin{aligned}
&\varphi_\ell(x_\partial^-) = \varphi_\ell(x_\partial^+)\\
&\frac{1}{\Sigma_t(x_\partial^-)}\frac{d\varphi_\ell(x_\partial^-)}{dx} = \frac{1}{\Sigma_t(x_\partial^+)}\frac{d\varphi_\ell(x_\partial^+)}{dx}, \qquad \ell = 1,\ldots,N/2.
\end{aligned} \tag{11}$$

If the directions are chosen as the nodes of a suitable quadrature formula, the scalar flux can be written as:

$$\phi(x) := 2\sum_{\ell=1}^{N/2} w_\ell\varphi_\ell(x), \tag{12}$$

where $\{w_\ell\}_{\ell=1}^{N}$ is the set of quadrature weights. Note that, for the even parity approach, we need to use only half of the nodes and weights of a quadrature set to evaluate the total flux, since $\psi^{+}(x,\mu) = \psi^{+}(x,-\mu)$.

Using a compact matrix notation, the set of $N/2$ ordinary differential equations given in Eq. (9) and the two boundary conditions given in Eq. (10) become for each homogeneous subdomain:

$$-\frac{1}{\Sigma_t}\mathbf{D}\frac{d^2\boldsymbol{\varphi}}{dx^2} + \Sigma_t\boldsymbol{\varphi}(x) = \Sigma_s\mathbf{W}\boldsymbol{\varphi}(x) + \mathbf{Q}(x), \tag{13}$$

and

$$\mathbf{D}^{1/2}\frac{d\boldsymbol{\varphi}}{dx}(a) - \Sigma_t(a)\boldsymbol{\varphi}(a) = \mathbf{0}, \tag{14}$$

$$\mathbf{D}^{1/2}\frac{d\boldsymbol{\varphi}}{dx}(b) + \Sigma_t(b)\boldsymbol{\varphi}(b) = \mathbf{0}, \tag{15}$$

with $\boldsymbol{\varphi}(x) := \{\varphi_1(x),\ldots,\varphi_{N/2}\}^T$ and $\mathbf{Q}(x) := \{Q_1(x),\ldots,Q_{N/2}(x)\}^T$. The $(N/2)\times(N/2)$ diagonal matrix $\mathbf{D}$ has the non-zero elements equal to μ_ℓ^2, while $\mathbf{W}$ contains $N/2$ identical rows with one Gaussian quadrature weight w_ℓ per column. Matrix $\mathbf{D}^{1/2}$ is clearly diagonal with non-zero elements equal to μ_ℓ. As for the spherical harmonics equations, the transport model is thus reduced again to a set of coupled second-order differential equations.

2.2. Spectral elements applied to the discrete ordinate equations

The spectral element approach can be applied along the same line established previously (Barbarino et al., 2013). Let $\theta(x)\in(H^1(a,b))^{N/2}$ denote any suitable $N/2$-dimensional test vector. We take the inner product of Eq. (13) by $\theta(x)$ which, after integration by parts and application of the boundary conditions, Eq. (10), yields:

$$\begin{aligned}
&\int_a^b dx\left[\frac{1}{\Sigma_t(x)}\left(\mathbf{D}\frac{d\boldsymbol{\varphi}}{dx}\right)\cdot\frac{d\boldsymbol{\theta}}{dx} + \Sigma_t(x)\boldsymbol{\varphi}(x)\cdot\boldsymbol{\theta}(x)\right] + \mathbf{D}^{1/2}\boldsymbol{\varphi}(a)\cdot\boldsymbol{\theta}(a)\\
&\quad + \mathbf{D}^{1/2}\boldsymbol{\varphi}(b)\cdot\boldsymbol{\theta}(b) = \int_a^b dx[\Sigma_s(x)(\mathbf{W}\boldsymbol{\varphi}(x))\cdot\boldsymbol{\theta}(x) + \mathbf{Q}(x)\cdot\boldsymbol{\theta}(x)].
\end{aligned} \tag{16}$$

Then we partition the space domain $\mathcal{D}_x$ into E adjacent elements $\mathcal{D}_x^e$ $(e = 1,\ldots,E)$ and inside each element we select a Gauss–Lobatto–Legendre (GLL) quadrature grid χ_k^e with its associated Lagrange interpolation polynomials of degree $(K+1)$. By this process we build a $(EK+1)$-dimensional subspace of $H^1(a,b)$, say V_{EK+1}. For each element e, the even parity unknown fluxes can be written as: