Adaptive FEM for second order formulations of the neutron transport problem

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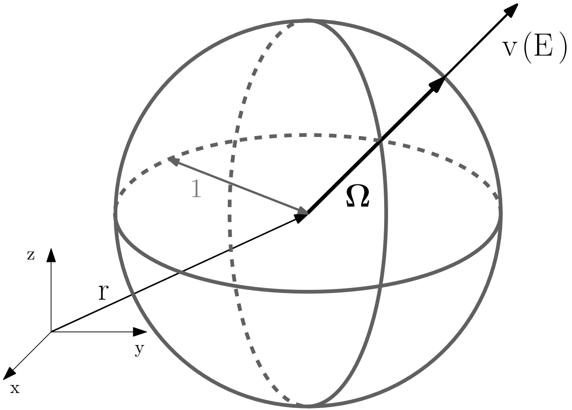
Overview

1. Neutron transport
2. Second order formulations
3. Multidimensional SP_N model
4. Adaptive FE solution

Phase space

$$X := \{(\mathbf{x}, \mathbf{\Omega}, E) : \ \mathbf{x} \in V \subset \mathbb{R}^3, \mathbf{\Omega} \in S_2, E \in [E_m, E_M]\}$$



- V ... bounded convex domain with smooth ∂V

Steady state neutron transport equation

... in the domain V occupied by an isotropic medium

$$\boldsymbol{\Omega}\cdot\nabla\psi(\mathbf{x},\boldsymbol{\Omega},E)+\sigma_t(\mathbf{x},E)\psi(\mathbf{x},\boldsymbol{\Omega},E)=$$
$$=\int_{E_m}^{E_M}\int_{S_2}\kappa(\mathbf{x},\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}',E\leftarrow E')\psi(\mathbf{x},\boldsymbol{\Omega}',E')\,\mathrm{d}\boldsymbol{\Omega}'\,\mathrm{d}E'+q(\mathbf{x},\boldsymbol{\Omega},E)$$

- ψ ... angular neutron flux density
- σ_t ... total cross section (all neutron-nuclei interactions)
- q ... volumetric neutron sources
- κ ... scattering + neutron multiplication processes (fission)

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$$= \int_{E_m}^{E_M} \int_{S_2} \kappa(\mathbf{x}, \mathbf{\Omega} \cdot \mathbf{\Omega}', E \leftarrow E') \psi(\mathbf{x}, \mathbf{\Omega}', E') \, \mathrm{d}\mathbf{\Omega}' \, \mathrm{d}E' + q(\mathbf{x}, \mathbf{\Omega}, E)$$

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- ν ... yield of fission neutrons with energy E

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$$T\psi(\mathbf{x},\mathbf{\Omega},E) = q(\mathbf{x},\mathbf{\Omega},E), \quad T = A + \Sigma_t - K$$

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Steady state neutron transport equation

... on the boundary ∂V

Define:

$$\partial X^{\pm} := \{(\mathbf{x}, \mathbf{\Omega}, E) \in \partial V \times S_2 \times [E_m, E_M], \text{ s.t. } \mathbf{\Omega} \cdot \mathbf{n}(\mathbf{x}) \gtrless 0\}$$

- Vacuum in $\mathbb{R}^3 \setminus \overline{X}$:

$$\psi|_{\partial X^-} = 0$$

- Specular reflection at boundary (plane of symmetry)

$$\psi(\mathbf{x}, \mathbf{\Omega}, E) = \psi(\mathbf{x}, \mathbf{\Omega}_R, E), \quad (\mathbf{x}, \mathbf{\Omega}, E) \in |_{\partial X^-}, \quad \mathbf{\Omega}_R = \mathbf{\Omega} - 2\mathbf{n}(\mathbf{\Omega} \cdot \mathbf{n})$$

Overview

Multigroup approximation of energetic dependence

- Let $[E_m, E_M] = [E^G, E^{G-1}] \cup \ldots \cup [E^g, E^{g-1}] \cup \ldots \cup [E^2, E^1]$ and with quantities averaged over each interval (*group*) solve

$$\begin{cases} T^G\{\psi^g(\mathbf{x}, \mathbf{\Omega})\} = \{q^g(\mathbf{x}, \mathbf{\Omega})\}, & \mathbf{x} \in V \\ \psi^g(\mathbf{x}, \mathbf{\Omega}) = 0, & \mathbf{x} \in \partial V,\ \mathbf{\Omega} \cdot \mathbf{n} < 0,\ g = 1, \ldots, G \end{cases}$$

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$$T^G\{\psi^g(\mathbf{x}, \mathbf{\Omega})\} \equiv \left\{ (A + \Sigma_r^g)\,\psi^g(\mathbf{x}, \mathbf{\Omega}) + \sum_{g'=1, g' \neq g}^{G} K^{gg'} \psi^{g'}(\mathbf{x}, \mathbf{\Omega}) \right\}$$

$$\Sigma_r^g = \sigma_t^g(\mathbf{x}) - \int_{S_2} \kappa^{g \leftarrow g}(\mathbf{x}, \mathbf{\Omega} \cdot \mathbf{\Omega}')\,\mathrm{d}\mathbf{\Omega}', \quad K^{gg'} = \int_{S_2} \kappa^{g \leftarrow g'}(\mathbf{x}, \mathbf{\Omega} \cdot \mathbf{\Omega}')\,\mathrm{d}\mathbf{\Omega}'$$

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- Can be used to define a Gauss-Seidel type iterative scheme

$$(A^g + \Sigma_r^g)\,\Psi_{i+1}^g = \sum_{g'\leq g-1} K^{gg'}\Psi_{i+1}^{g'} + \sum_{g'\geq g+1} K^{gg'}\Psi_i^{g'} + q^g$$

- In each iteration – one-speed transport problem, where only the advection term A^g spoils self-adjointness

Selected second order formulations

S. Kaplan and J. A. Davis
Canonical and Involutory Transformations of the Variational Problems of Transport Theory. *Nucl. Sci. Eng.*, 28(1967), pp. 166-176.

J. E. Morel and J. M. McGhee
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$\Rightarrow$ complicated, strongly coupled system of 2^{nd} order PDEs

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Standard Galerkin approximation of $\psi(\cdot, \mathbf{\Omega}, \cdot)$ in the subspace of $L^2(S_2)$ spanned by the spherical harmonic functions Y_n^m

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- Insert into NTE, simplify the scattering kernel κ by using

$$\sigma_s(\mathbf{x}, \mathbf{\Omega} \cdot \mathbf{\Omega}', E \leftarrow E') \approx \sum_{k=0}^{K} \frac{2k+1}{4\pi} \sigma_{sk}(\mathbf{x}, E \leftarrow E') P_k(\mathbf{\Omega}' \cdot \mathbf{\Omega})$$

(P_k Legendre polynomial of degree k)

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$\Rightarrow$ P_N system with an attractive form in the following cases:

1. $N = 1$: $\longrightarrow$ diffusion equation
2. $1D$, any N: $\longrightarrow$ system of weakly coupled diffusion eqns.

Case 1: Diffusion approximation

- $\psi(\mathbf{x},\mathbf{\Omega},E) \approx \frac{1}{4\pi}\left[\phi(\mathbf{x},E) + 3\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{x},E)\right], \;\; \phi \equiv \phi_0^0, \; \mathbf{J} = \mathbf{J}\left(\phi_1^{-1}, \phi_1^0, \phi_1^1\right)$
- Set $N = L = 1$ and neglect the $n = 1$ moment of q
- Assume a multigroup approximation s.t.

$$\sum_{g'} \sigma_{s1}^{g\leftarrow g'} \mathbf{J}^{g'} = \sum_{g'} \sigma_{s1}^{g'\leftarrow g} \mathbf{J}^{g} \equiv \sigma_{s1}^{g} \mathbf{J}^{g} \qquad \text{(E.T.)}$$

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- For vacuum b.c.

$$\begin{cases} T_d^G\{\phi^g\} = \{q_0^g\}, & \text{in}\, V \\ B_d^g \phi^g = 0, & \text{on } \partial V, \qquad g = 1,\ldots,G \end{cases}$$

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$$T_d^G\{\phi^g\} \equiv \left\{ \left(A_d^g + \Sigma_r^g\right) \phi^g - \sum_{g' \neq g} K_d^{gg'} \phi^{g'} \right\}$$

$$A_d^g = -\nabla \cdot D^g \nabla, \quad D^g = \frac{1}{3(\sigma_t^g - \sigma_{s1}^g)}, \quad B_d^g \phi^g = 2D^g \nabla \phi^g \cdot \mathbf{n} + \phi^g$$

$$\Sigma_r^g = \sigma_t^g - \sigma_{s0}^{g \leftarrow g} - \nu \sigma_f^{g \leftarrow g}, \; K_d^{gg'} = \sigma_{s0}^{g \leftarrow g'} + \nu \sigma_f^{g \leftarrow g'}$$

Case 1: Diffusion approximation, vacuum b.c.

Weak formulation

- Assume $\{q_0^g\} \equiv \mathbf{q} \in \mathbb{L}^2(V) := \left[L^2(V)\right]^G$
- Let $\mathbb{H}^1(V) := \left[H^1(V)\right]^G$, $\mathbb{H}_0^1(V) := \left[H_0^1(V)\right]^G$

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- Find $\{\psi^g\} \equiv \mathbf{u} \in \mathbb{H}^1(V): \quad a(\mathbf{u},\mathbf{v}) = q(\mathbf{v}), \quad \forall \mathbf{v} \in \mathbb{H}_0^1(V)$

$$a(\mathbf{u},\mathbf{v}) := \int_V (\mathbf{D}\nabla\mathbf{u}) : \nabla\mathbf{v} + (\mathbf{\Sigma}_r - \mathbf{K}_d)\mathbf{u}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + \frac{1}{2}\int_{\partial V} \mathbf{u}\cdot\mathbf{v}\,\mathrm{d}s$$

$$q(\mathbf{v}) = \int_V \mathbf{q}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x}\,, \quad (\mathbf{D}\nabla\mathbf{u}) : \nabla\mathbf{v} = \sum_{g,i} D^g \frac{\partial \mathbf{u}^g}{\partial \mathbf{x}_i}\frac{\partial \mathbf{v}^g}{\partial \mathbf{x}_i}$$

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- We assumed the E.T. condition (otherwise $\mathbf{D} \neq \mathrm{diag}\{D^g\}$)
- For symmetry of $a(\mathbf{u},\mathbf{v})$, we also need symmetric $\mathbf{K}_d$ (i.e. multigroup G-S iterations)
- Under the subcriticality conditions, $a(\mathbf{u},\mathbf{v})$ is bounded and coercive

Case 2: 1D P_N equations

- Use azimuth-independent SHF – Legendre polynomials
- Neglect the $n \geq 1$ moments of q (isotropic sources)

$$\frac{n+1}{2n+1}\frac{\mathrm{d}\phi_{n+1}^{g}}{\mathrm{d}z} + \frac{n}{2n+1}\frac{\mathrm{d}\phi_{n-1}^{g}}{\mathrm{d}z} + \Sigma_r^g \phi_n^g = q_n^{gg'}, \quad n = 0, \dots, N$$

$$q_0^{gg'} = \sum_{g' \neq g} K_d^{gg'} \phi^{g'} + q_0^g, \quad q_n^{gg'} = \sum_{g' \neq g} \sigma_{sn}^{g \leftarrow g'} \phi_n^{g'}, \ n \geq 1$$

$$\Sigma_{rn}^g = \sigma_t^g - \sigma_{sn}^{g \leftarrow g} - \delta_{n0} \nu \sigma_f^{g \leftarrow g}, \quad \phi^g \equiv \phi_0^g$$

- $N = 1$ with the E.T. condition $\Rightarrow$ 1D diffusion equation

Case 2: 1D P_3 equations

- For $N = 3$, assume the standard closure $\frac{\mathrm{d}\phi_4^g}{\mathrm{d}z} \equiv 0$

$$
\begin{aligned}
\frac{\mathrm{d}\phi_1^g(z)}{\mathrm{d}z} + \Sigma_{r0}^g(z)\phi_0^g(z) &= q_0^{gg'}(z) \\
\frac{2}{3}\frac{\mathrm{d}\phi_2^g(z)}{\mathrm{d}z} + \frac{1}{3}\frac{\mathrm{d}\phi_0^g(z)}{\mathrm{d}z} + \Sigma_{r1}^g(z)\phi_1^g(z) &= q_1^{gg'}(z) \\
\frac{3}{5}\frac{\mathrm{d}\phi_3^g(z)}{\mathrm{d}z} + \frac{2}{5}\frac{\mathrm{d}\phi_1^g(z)}{\mathrm{d}z} + \Sigma_{r2}^g(z)\phi_2^g(z) &= q_2^{gg'}(z) \\
\frac{3}{7}\frac{\mathrm{d}\phi_2^g(z)}{\mathrm{d}z} + \Sigma_{r3}^g(z)\phi_3^g(z) &= q_3^{gg'}(z)
\end{aligned}
$$

- Vacuum b.c.

$$
\begin{aligned}
\frac{\phi_0^g(z_B)}{4} \pm \frac{\phi_1^g(z_B)}{2} + \frac{5\phi_2^g(z_B)}{16} &= 0 \\
-\frac{\phi_0^g(z_B)}{16} \pm \frac{\phi_3^g(z_B)}{2} + \frac{5\phi_2^g(z_B)}{16} &= 0
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SP_3 equations

- Analogously to the diffusion approximation, assume

$$\sum_{g'} \sigma_{sn}^{g \leftarrow g'} \phi_n^{g'} = \sum_{g'} \sigma_{sn}^{g' \leftarrow g} \phi_n^{g} \equiv \sigma_{sn}^{g} \phi_n^{g}, \quad n \geq 1, \qquad \text{(E.T.')}$$

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- Then $q_n^{gg'}$ involves ϕ_n^g instead of all $\phi_n^{g'}$ and can be moved to l.h.s.
- The P_3 equations can now be manipulated as in the diff. case

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left[D_1^g \frac{\mathrm{d}\Phi_0^g}{\mathrm{d}z}\right] + \widetilde{\Sigma}_{r0}^g \Phi_0^g - 2\widetilde{\Sigma}_{r0}^g \Phi_2^g = \widetilde{Q}_0^{gg'}(\phi^{g'})$$

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left[D_3^g \frac{\mathrm{d}\Phi_2^g}{\mathrm{d}z}\right] + \left[\frac{4}{3}\widetilde{\Sigma}_{r0}^g + \frac{5}{3}\widetilde{\Sigma}_{r2}^g\right]\Phi_2^g - \frac{2}{3}\widetilde{\Sigma}_{r0}^g \Phi_0^g = -\frac{2}{3}\widetilde{Q}_0^{gg'}(\phi^{g'})$$

$$\Phi_0^g = \phi_0^g + 2\phi_2^g, \quad \Phi_2^g = 3\phi_2^g, \quad \phi^g \equiv \phi_0^g = \Phi_0^g - \tfrac{2}{3}\Phi_2^g$$

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- The P_3 equations can now be manipulated as in the diff. case

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left[D_1^g \frac{\mathrm{d}\Phi_0^g}{\mathrm{d}z}\right] + \widetilde{\Sigma}_{r0}^g \Phi_0^g - 2\widetilde{\Sigma}_{r0}^g \Phi_2^g = \widetilde{Q}_0^{gg'}(\phi^{g'})$$

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left[D_3^g \frac{\mathrm{d}\Phi_2^g}{\mathrm{d}z}\right] + \left[\frac{4}{3}\widetilde{\Sigma}_{r0}^g + \frac{5}{3}\widetilde{\Sigma}_{r2}^g\right]\Phi_2^g - \frac{2}{3}\widetilde{\Sigma}_{r0}^g \Phi_0^g = -\frac{2}{3}\widetilde{Q}_0^{gg'}(\phi^{g'})$$

$$\Phi_0^g = \phi_0^g + 2\phi_2^g, \quad \Phi_2^g = 3\phi_2^g, \quad \phi^g \equiv \phi_0^g = \Phi_0^g - \tfrac{2}{3}\Phi_2^g$$

$$\widetilde{\Sigma}_{rn}^g = \sigma_t^g - \sigma_{sn}^g - \delta_{n0}\nu\sigma_f^{g \leftarrow g}, \quad D_1^g = \tfrac{1}{3}\left(\widetilde{\Sigma}_{r1}^g\right)^{-1}, \; D_3^g = \tfrac{1}{7}\left(\widetilde{\Sigma}_{r3}^g\right)^{-1}$$

$$\widetilde{Q}_0^{gg'} = \sum_{g' \neq g} K_d^{gg'} \phi^{g'} + q_0^g$$

Overview

Extension of SP_N into 3D

- Since 1960's, the usual practice has been to replace $\frac{\mathrm{d}}{\mathrm{d}z}$ by ∇, $\nabla\cdot$ or $\nabla\cdot\mathbf{n}$ (in the b.c. equations)
- 1990's – asymptotic and boundary layer analysis showed that the transport solution satisfies the SP_N equations to increasing orders of an ε characterizing the "diffusivity" of the medium
- See [Brantley00] for references and also for a variational characterization of the SP_3 equations

P. S. Brantley and E. W. Larsen
The Simplified P_3 Approximation. *Nucl. Sci. Eng.*, 134(2000), pp. 1-21.

New way of getting to the 3D SP_N equations

Use the *Maxwell-Cartesian surface spherical harmonics* instead of Y_n^m

n	$\mathbb{Y}^n(\mathbf{\Omega}) \propto$	$\mathbb{P}^{(n)}(\mathbf{\Omega})$
0	1	1
1	$\Omega_z,\ \Omega_x \pm i\Omega_y$	$\Omega_x,\ \Omega_y,\ \Omega_z$
2	$\Omega_z^2 - \frac{1}{3},\ \Omega_z(\Omega_x \pm i\Omega_y),$ $(\Omega_x \pm i\Omega_y)^2$	$\Omega_x^2 - \frac{1}{3},\ \Omega_y^2 - \frac{1}{3},\ \Omega_z^2 - \frac{1}{3},$ $\Omega_x\Omega_y,\ \Omega_x\Omega_z,\ \Omega_y\Omega_z$

$$\mathbf{\Omega} = \begin{bmatrix} \Omega_x \\ \Omega_y \\ \Omega_z \end{bmatrix} = \begin{bmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{bmatrix}$$

J. Applequist
Maxwell-Cartesian Spherical Harmonics in Multipole Potentials and Atomic Orbitals. *Theor. Chem. Acc.*, 107(2002), pp. 103-115

Some properties of the MC SHF

$\mathbb{P}^{(n)} = \{\mathbb{P}^{(n)}_{\alpha_1,\ldots,\alpha_n}\}$, $\alpha_i \in \{1,2,3\}$ is a real tensor of rank n which

- shares some important properties with the tesseral SHF
  - addition theorem (to simplify the scattering kernel in NTE)
  - orthogonality for different orders m, n:

$$\int_{S_2} \mathbb{P}^{(n)}(\boldsymbol{\Omega}) \otimes \mathbb{P}^{(m)}(\boldsymbol{\Omega})\,\mathrm{d}\boldsymbol{\Omega} = \mathbb{O}^{m+n}$$

  - recurrence rule analogous to Legendre polynomials ([Coppa10])

$$\mathbb{P}^{(n+1)}(\boldsymbol{\Omega}) = \left[\boldsymbol{\Omega} \otimes \mathbb{P}^{(n)}(\boldsymbol{\Omega}) - \frac{n^2}{4n^2-1}\mathbb{I} \otimes \mathbb{P}^{(n-1)}(\boldsymbol{\Omega})\right]_{\mathrm{sym}}, \; n = 1,2,\ldots$$

G. Coppa
Deduction of a Symmetric Tensor Formulation of the P_N Method for the Linear Transport Equation. *Prog. Nucl. Energy*, 52(2010), pp. 747-752

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- differs in being
  - *totally symmetric* – invariant under any permutation $\mathcal{P}(\{\alpha_i\})$
  - *traceless* – $\mathbb{P}^{(n)}_{\beta\beta\alpha_3,\ldots,\alpha_n} = \mathbb{O}^{n-2}$ (Einstein summation convention)

G. Coppa
Deduction of a Symmetric Tensor Formulation of the P_N Method for the Linear Transport Equation. *Prog. Nucl. Energy*, 52(2010), pp. 747-752

MC P_N approximation (one-speed)

- *n-fold contraction* $(n \leq m)$

$$\mathbb{C}^{(m-n)}_{\alpha_{n+1},\dots,\alpha_m} = \mathbb{A}^{(n)} \underset{n}{\cdot} \mathbb{B}^{(m)} := \mathbb{A}^{(n)}_{\alpha_1,\dots,\alpha_n} \mathbb{B}^{(m)}_{\alpha_n,\dots,\alpha_1} \quad \text{(Einstein summ.)}$$

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- Use the expansion

$$\psi(\mathbf{x},\mathbf{\Omega}) \approx \sum_{n=0}^{N} \psi^{(n)}(\mathbf{x}) \underset{n}{\cdot} \mathbb{P}^{(n)}(\mathbf{\Omega}), \quad \psi^{(n)}(\mathbf{x}) = \int_{S_2} \psi(\mathbf{x},\mathbf{\Omega}) \otimes \mathbb{P}^{(n)}(\mathbf{\Omega}) \,\mathrm{d}\mathbf{\Omega}$$

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- Require vanishing projection of the NTE residual

$$\sum_{n=0}^{N} \left[\int_{S_2} \left[T\psi(\mathbf{x},\mathbf{\Omega}) - q(\mathbf{x},\mathbf{\Omega}) \right] \otimes \mathbb{P}^{(n)}(\mathbf{\Omega}) \,\mathrm{d}\mathbf{\Omega} \right] \underset{n}{\cdot} \mathbb{P}^{(n)}(\mathbf{\Omega}) = 0$$

and utilize the properties of $\mathbb{P}^{(n)}$

MC P_N approximation (one-speed)

$$\Rightarrow \qquad \sum_{n=0}^{N} \mathbb{R}^{(n)}(\mathbf{x}) \underset{n}{\cdot} \mathbb{P}^{(n)}(\mathbf{\Omega}) = 0 \qquad (*)$$

- Components of $\mathbb{P}^{(n)}(\mathbf{\Omega})$ are not entirely linearly independent (there exist linearly independent subsets with $2n+1$ components)
- But: $\mathbb{P}^{(n)}(\mathbf{\Omega}) = \mathscr{D}^{(n)} \underbrace{(\mathbf{\Omega} \otimes \cdots \otimes \mathbf{\Omega})}_{n \text{ times}} = \mathscr{D}^{(n)}(\mathbf{\Omega}^n)$
  - Operator $\mathscr{D}^{(n)}$ transforms a totally symmetric tensor into a totally symmetric traceless one
- Apply the *detracer exchange theorem* ([Applequist02]) to $(*)$

$$\Rightarrow \qquad \sum_{n=0}^{N} \mathscr{D}^{(n)} \left(\left[\mathbb{R}^{(n)}(\mathbf{x}) \right]_{\text{sym}} \right) \underset{n}{\cdot} \mathbf{\Omega}^n = 0,$$

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$$\Rightarrow \qquad \mathscr{D}^{(n)}\left(\left[\mathbb{R}^{(n)}(\mathbf{x})\right]_{\text{sym}}\right) = 0, \quad n = 0, \dots, N$$

MC P_3 approximation (one-speed)

- With $\phi^{(n)} := \frac{1}{2n+1}\psi^{(n)}$, we obtain

$$\nabla \cdot \phi^{(1)} + \Sigma_{r0}\phi^{(0)} = q^{(0)}$$

$$\frac{2}{3}\nabla \cdot \phi^{(2)} + \frac{1}{3}\left[\nabla \otimes \phi^{(0)}\right]_{\text{sym}} + \Sigma_{r1}\phi^{(1)} = q^{(1)}$$

$$\frac{3}{5}\nabla \cdot \phi^{(3)} + \frac{3}{5}\left[\nabla \otimes \phi^{(1)}\right]_{\text{sym}} - \frac{1}{5}\left[\mathbb{I} \otimes \nabla \cdot \phi^{(1)}\right]_{\text{sym}} + \Sigma_{r2}\phi^{(2)} = q^{(2)}$$

$$\frac{5}{7}\left[\nabla \otimes \phi^{(2)}\right]_{\text{sym}} - \frac{2}{7}\left[\mathbb{I} \otimes \nabla \cdot \phi^{(2)}\right]_{\text{sym}} + \Sigma_{r3}\phi^{(3)} = q^{(3)}$$

MC SP_3 approximation (one-speed)

- Assuming isotropic sources and locally 1D solution

$$\nabla \cdot \phi_1 + \Sigma_{r0}\phi_0 = q_0$$
$$\tfrac{2}{3}\nabla\phi_2 + \tfrac{1}{3}\nabla\phi_0 + \Sigma_{r1}\boldsymbol{\phi}_1 = 0$$
$$\tfrac{3}{5}\nabla \cdot \boldsymbol{\phi}_3 + \tfrac{2}{5}\nabla \cdot \boldsymbol{\phi}_1 + \Sigma_{r2}\phi_2 = 0$$
$$\tfrac{3}{7}\nabla\phi_2 + \Sigma_{r3}\boldsymbol{\phi}_3 = 0$$

- May be manipulated into a 3D analogue of the 1D P_3 eqns.

$$-\nabla \cdot D_1^g \nabla \Phi_0^g + \widetilde{\Sigma}_{r0}^g \Phi_0^g - 2\widetilde{\Sigma}_{r0}^g \Phi_2^g = \widetilde{Q}_0^{gg'}(\phi^{g'})$$
$$-\nabla \cdot D_3^g \nabla \Phi_2^g + \left[\frac{4}{3}\widetilde{\Sigma}_{r0}^g + \frac{5}{3}\widetilde{\Sigma}_{r2}^g\right]\Phi_2^g - \frac{2}{3}\widetilde{\Sigma}_{r0}^g \Phi_0^g = -\frac{2}{3}\widetilde{Q}_0^{gg'}(\phi^{g'})$$
$$\Phi_0^g = \phi_0^g + 2\phi_2^g, \quad \Phi_2^g = 3\phi_2^g, \quad \phi^g \equiv \phi_0^g = \Phi_0^g - \tfrac{2}{3}\Phi_2^g$$

MC P_3 approximation (one-speed)

- Assuming isotropic sources and isotropic scattering

$$\begin{aligned}
\nabla \cdot \phi^{(1)} + \Sigma_{r0}\phi^{(0)} &= q^{(0)} \\
\tfrac{2}{3}\nabla \cdot \phi^{(2)} + \tfrac{1}{3}\left[\nabla \otimes \phi^{(0)}\right]_{\mathrm{sym}} + \Sigma_t \phi^{(1)} &= 0 \\
\tfrac{3}{5}\nabla \cdot \phi^{(3)} + \tfrac{3}{5}\left[\nabla \otimes \phi^{(1)}\right]_{\mathrm{sym}} - \tfrac{1}{5}\left[\mathbb{I} \otimes \nabla \cdot \phi^{(1)}\right]_{\mathrm{sym}} + \Sigma_t \phi^{(2)} &= 0 \\
\tfrac{5}{7}\left[\nabla \otimes \phi^{(2)}\right]_{\mathrm{sym}} - \tfrac{2}{7}\left[\mathbb{I} \otimes \nabla \cdot \phi^{(2)}\right]_{\mathrm{sym}} + \Sigma_t \phi^{(3)} &= 0
\end{aligned}$$

- Using the tracelessness property, contracting with $\Sigma_t^{-1}\nabla \otimes \Sigma_t^{-1}\nabla$

$$\frac{3}{35\Sigma_t^3}\nabla^4\phi + \frac{11}{21\Sigma_t^2}\nabla^2(q_0 - \Sigma_{r0}\phi) - \frac{1}{3\Sigma_t}\nabla^2\phi = q_0 - \Sigma_{r0}\phi$$

Overview

Variational approximation

- Extension of the multigroup weak formulation into $\left[\mathbb{H}^1(V)\right]^{\frac{N+1}{2}G}$

$$\mathbf{u} = [\Phi_0^1, \ldots, \Phi_0^G, \Phi_2^1, \ldots, \Phi_2^G, \ldots, \Phi_{2m}^g, \ldots, \Phi_{(N+1)/2}^G],$$

$$\mathbb{D} = \mathrm{diag}\left\{\mathbf{D}_{2m+1}\right\} \text{ (with E.T.)}, \quad \text{etc.}$$

- Very different spatial variation of different g, n components
  $\Rightarrow$ take advantage of efficient multimesh discretization ([Solin10])

- Implementation in the *hp*-FEM library Hermes
  - *hp*-adaptivity based on a difference between a reference solution $\mathbf{u}_{\mathrm{ref}} = \mathbf{u}_{h/2,p+1}$ and its projection onto a coarse space $\mathbf{u}_{h,p}$
  - *h*-adaptivity using an analogous technique, or alternatively a Kelly-based error indicator

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P. Solin et al.
Monolithic Discretization of Linear Thermoelasticity Problems via Adaptive Multimesh hp-FEM. *J. Comput. Appl. Math 234 (2010)*

hp-adaptive solution

- We have for the error on element K

$$
\begin{aligned}
\|\mathbf{u}-\mathbf{u}_{hp}\|_K^2 &\leq \frac{C_\mathrm{c}}{C_\mathrm{e}}\left(\|\mathbf{u}-\mathbf{u}_{h/2,p+1}\|_K^2+\|\mathbf{u}_{h/2,p+1}-\mathbf{u}_{h,p}\|_K^2\right)\\
&\approx \frac{C_\mathrm{c}}{C_\mathrm{e}}\|\mathbf{u}_{h/2,p+1}-\mathbf{u}_{h,p}\|_K^2\\
&\equiv \frac{C_\mathrm{c}}{C_\mathrm{e}}\sum_{g,n}\tilde{\eta}_n^g
\end{aligned}
$$

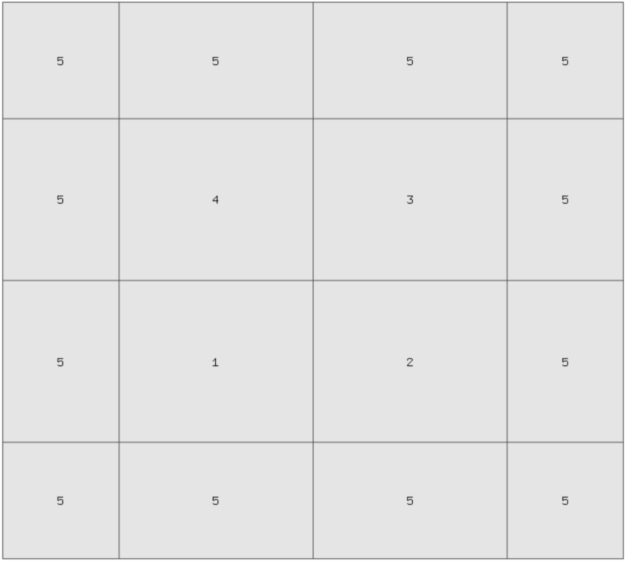
- Since the quantity of primary interest is the scalar (group-g) flux $\phi_0^g = \Phi_0^g - \frac{2}{3}\Phi_2^g + \frac{8}{15}\Phi_4^g - \frac{128}{315}\Phi_6^g + \ldots = \sum_{2m} F_m\Phi_m^g$, the element-wise error indicator is given by the components

$$\tilde{\eta}_n^g = F_{2m}^2\|\Phi^g_{m,h/2,p+1} - \Phi^g_{m,h/2,p+1}\|^2$$

- Refine elements with largest η_n^g (taking all meshes into account) until the given fraction of total error is processed (possibly anisotropically)

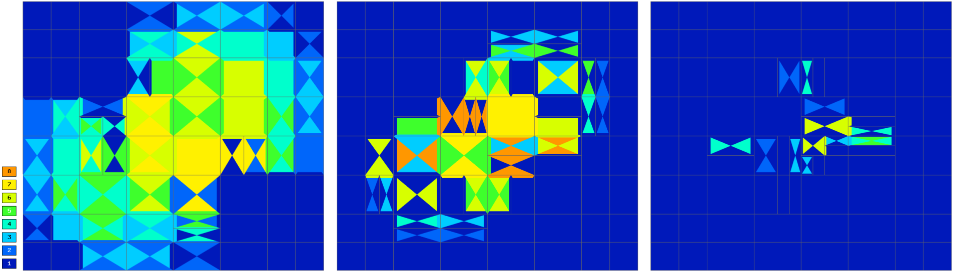
IAEA EIR-2 Benchmark

Geometry



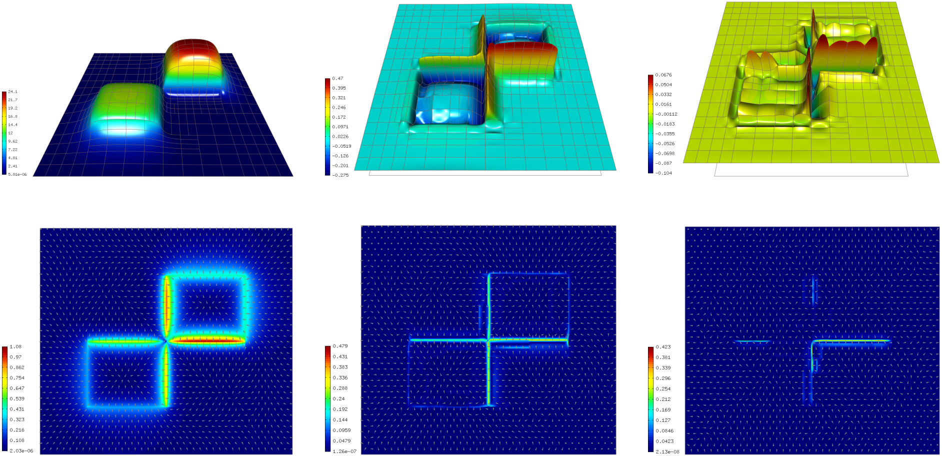
IAEA EIR-2 Benchmark

hp-FEM SP_5 solution



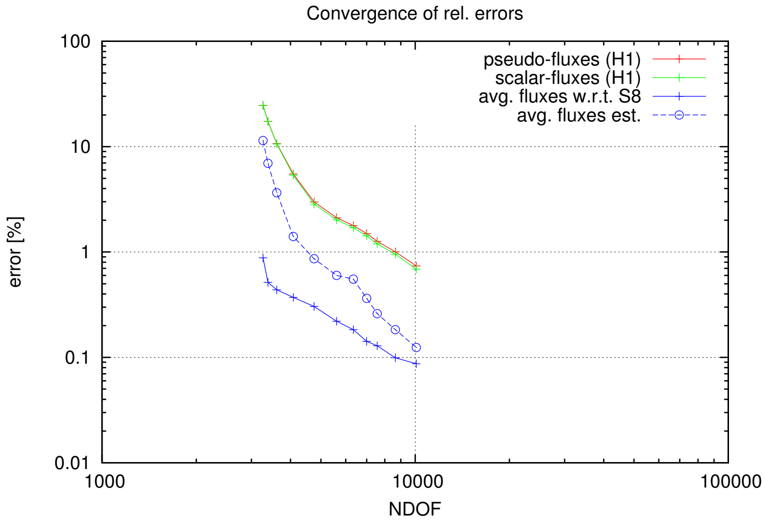
IAEA EIR-2 Benchmark

hp-FEM SP_5 solution



IAEA EIR-2 Benchmark

hp-adaptivity convergence



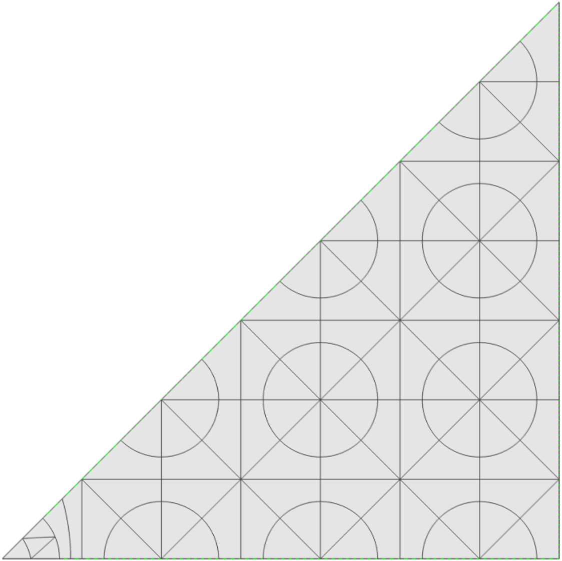
Rel. errors [%] of average scalar flux in regions $i = 1, \dots, 5$ w.r.t. S_8

i	SP_1	SP_3	SP_5	SP_7
1	0.81	0.14	0.09	0.09
2	5.23	0.86	0.39	0.45
3	0.90	0.17	0.08	0.10
4	3.86	0.83	0.51	0.56
5	0.83	0.08	0.07	0.10
t_{CPU} [s]	18	53	155	162

Ciolini et al.
Simplified P_N and A_N Methods in Neutron Transport.
Progr. Nucl. Energy, 40(2002), pp. 237-264

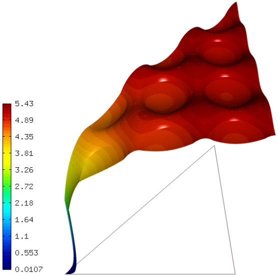
7x7 PWR Assembly

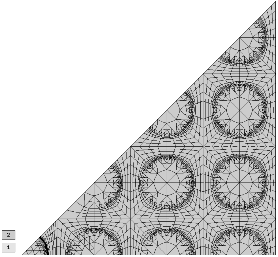
Geometry

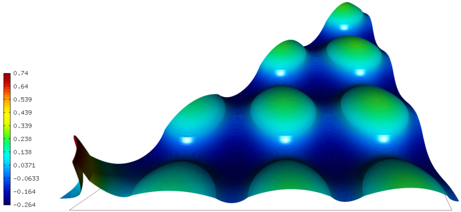


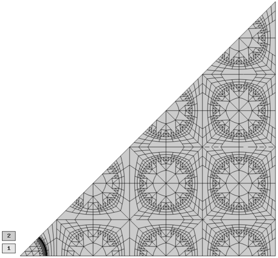
7x7 PWR Assembly

h-FEM (Kelly) SP_3 solution

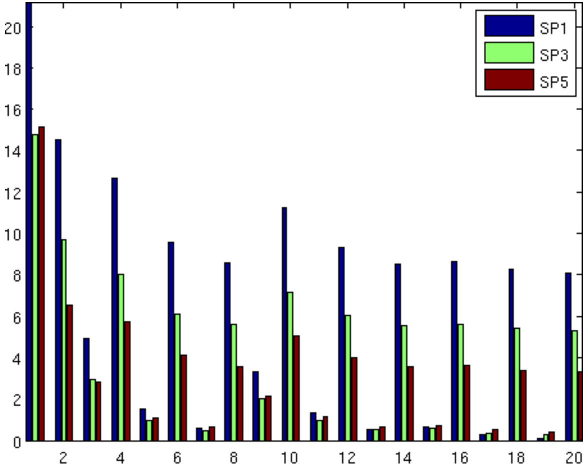








Rel. errors [%] of average scalar flux in regions $i = 1, \dots, 20$ w.r.t. a collision probabilities solution by the DRAGON code (École Polytechnique Montréal)



Summary and outlook

- Very efficient numerical methods can be used to solve the second order forms of the NTE
- Accuracy of the cheapest diffusion approximation may be improved with a reasonably low performance hit by the SP_N model
- Multigroup, $N, L \leq 9$, fixed-source/eigenvalue SP_N framework implemented in Hermes
- Use of the Maxwell-Cartesian SHF provides some new insight into the structure of the angular approximation

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- Assessment of higher N approximations

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Thank you for your attention.