On classical and modern approximations for neutron transport in a unified framework

Matthias Schlottbom

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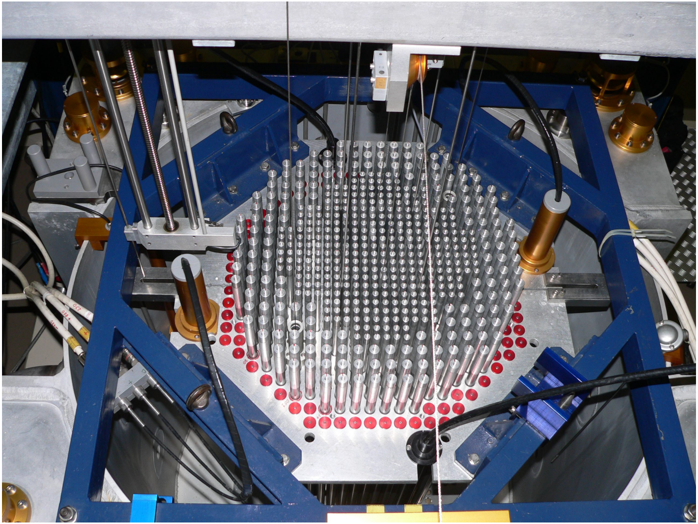
UNIVERSITY OF TWENTE.

Outline

Motivating examples

Nuclear reactors



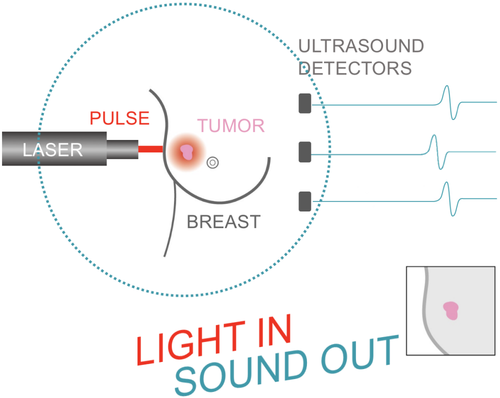
Core of reactor CROCUS (EPFL); picture from wikipedia

Motivating examples

Biomedical imaging

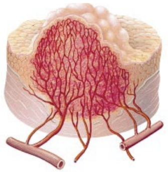
PHOTOACOUSTIC BREAST IMAGING

(ILLUSTRATIONS MADE BY SJOUKJE SCHOUSTRA – BMPI GROUP (TWENTE))



Folkman, 1996

angiogenesis

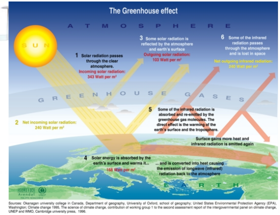


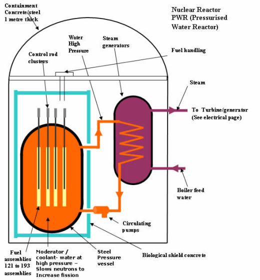
PHOTOACOUSTIC EFFECT

- LIGHT ABSORPTION
- TEMPERATURE RISE
- EXPANSION
- PRESSURE RISE
- ULTRASOUND WAVE
- SIGNALS
- RECONSTRUCTION

Further applications

- radiation therapy: [Larsen '97, Frank et al 2008]
- gas & oil reservoir exploration: [Meng et al 2017]
- LED lighting: [Leung, Lagendijk, Mosk, Vos et al 2014]
- climate simulation: [Thomas et al '99]
- ...





Angular density

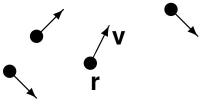
The angular density $\phi(t, \mathbf{r}, \mathbf{v})$: $\phi(t, \mathbf{r}, \mathbf{v})\, d\mathbf{r}\, d\mathbf{v}$ is equal to the expected number of neutrons in the volume element $d\mathbf{r}$ about $\mathbf{r}$, with velocities in $d\mathbf{v}$ about $\mathbf{v}$ at time t.

Energy dependent density: $\rho(t, \mathbf{r}, |\mathbf{v}|) = \int_{\mathbb{S}^2} \phi(t, \mathbf{r}, |\mathbf{v}|\mathbf{s})\, \mathrm{d}\mathbf{s}$

Total amount of neutrons at r and t: $\int_0^\infty \rho(t, \mathbf{r}, |\mathbf{v}|)|\mathbf{v}|^2\, \mathrm{d}|\mathbf{v}|$

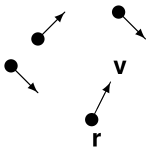
Flux: $j(t, \mathbf{r}, \mathbf{v}) \cdot \mathbf{n}\, dA\, d\mathbf{v}\, dt$ number of neutrons in $d\mathbf{v}$ about $\mathbf{v}$ which cross a small area dA in time dt.

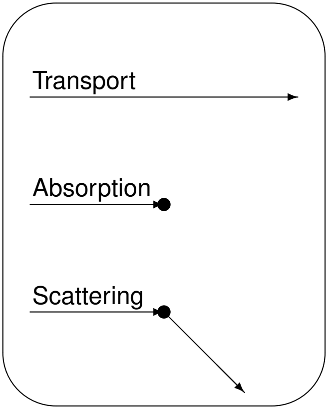
Angular current: $j(t, \mathbf{r}, \mathbf{v}) = \mathbf{v}\phi(t, \mathbf{r}, \mathbf{v})$



Particle model for neutron transport

Angular density $\phi(t, \mathbf{r}, \mathbf{v})$ for $\mathbf{r}, \mathbf{v} \in \mathbb{R}^3$, $\mathbf{v} \neq 0$





Assumptions:

- No interactions between particles
- Stationary and isotropic medium
- Particles travel along straight lines between scattering events (neutral particles)
- Relevant physical processes: transport, (different types of) scattering

Balance law for the change of neutrons

Change dN of number of neutrons in dt with velocity $d\mathbf{v}$ about $\mathbf{v}$ in a volume $\mathcal{R}$ with surface $\partial\mathcal{R}$ about $\mathbf{r}$:

$$dN = d\mathbf{v}\, dt \int_{\mathcal{R}} \frac{\partial \phi(t, \mathbf{r}, \mathbf{v})}{\partial t}\, d\mathbf{r}.$$

Balance relation for dN

$dN = -$ (a) net number flowing out of $\partial\mathcal{R}$ in dt

$-$ (b) number of neutrons suffering collisions in $\mathcal{R}$ in dt

$+$ (c) number of secondaries of velocity $\mathbf{v}$ produced in $\mathcal{R}$ in dt by collisions

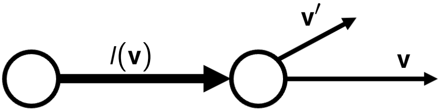
$+$ (d) number of neutrons of velocity $\mathbf{v}$ produced in $\mathcal{R}$ in dt by sources.

(a) net number flowing out of S in dt

Apply divergence theorem and definition of angular current:

$$
\begin{aligned}
\text{(a)} &= d\mathbf{v}\,dt \int_{\partial\mathcal{R}} j(t,\mathbf{r},\mathbf{v})\cdot\mathbf{n}\,d\sigma && \text{(Definition flux)}\\
&= d\mathbf{v}\,dt \int_{\mathcal{R}} \operatorname{div}_{\mathbf{r}}(j(t,\mathbf{r},\mathbf{v}))\,d\mathbf{r} && \text{(Gauss)}\\
&= d\mathbf{v}\,dt \int_{\mathcal{R}} \operatorname{div}_{\mathbf{r}}(\mathbf{v}\phi(t,\mathbf{r},\mathbf{v}))\,d\mathbf{r} && \text{(Definition angular current)}\\
&= d\mathbf{v}\,dt \int_{\mathcal{R}} \mathbf{v}\cdot\nabla_{\mathbf{r}}\phi(t,\mathbf{r},\mathbf{v}))\,d\mathbf{r} && (\operatorname{div}_{\mathbf{r}}(\mathbf{v})=0)
\end{aligned}
$$

(b) number of neutrons suffering collisions in V in dt



Frequency of collisions: $l(\mathbf{v})$ denotes the *mean free path* between collisions of neutrons of velocity $\mathbf{v}$, i.e., on average $|\mathbf{v}|/l$ collisions per second.

Collision rate: $\frac{|\mathbf{v}|}{l(\mathbf{r},\mathbf{v})}\phi(t,\mathbf{r},\mathbf{v})\,d\mathbf{r}\,d\mathbf{v}$

(b)$= \frac{|\mathbf{v}|}{l(\mathbf{r},\mathbf{v})}\phi(t,\mathbf{r},\mathbf{v})\,d\mathbf{r}\,d\mathbf{v}\,dt$

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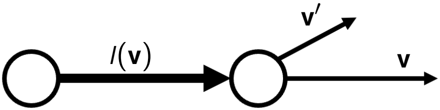

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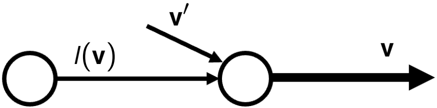
Macroscopic cross section: $\sigma(\mathbf{r},\mathbf{v}) = l^{-1}(\mathbf{r},\mathbf{v})$.

Types of collisions: elastic, inelastic scattering, radiative capture, fission:

$$\sigma = \sigma_s + \sigma_{in} + \sigma_a + \sigma_f.$$

(c) number of secondaries of velocity $\mathbf{v}$ produced in V in dt by collisions



$|\mathbf{v}'|\sigma(\mathbf{r},\mathbf{v}' \to \mathbf{v})\phi(t,\mathbf{r},\mathbf{v}')\,d\mathbf{v}'\,d\mathbf{r}\,dt =$ probable number of neutrons in $d\mathbf{r}$ at $\mathbf{r}$ emitted *into* $d\mathbf{v}$ at $\mathbf{v}$ in time dt about t due to collisions induced by neutrons of velocity in $d\mathbf{v}'$ at $\mathbf{v}'$.

$$(c) = d\mathbf{r}\,dt \int_{\mathbb{R}^3} \sigma(\mathbf{r},\mathbf{v}' \to \mathbf{v})\phi(t,\mathbf{r},\mathbf{v}')\,d\mathbf{v}'.$$

Balance relation: (neglecting delay)

$$\sigma_s(\mathbf{r},\mathbf{v}') + \sigma_{in}(\mathbf{r},\mathbf{v}') + \nu\sigma_f(\mathbf{r},\mathbf{v}') = \int_{\mathbb{R}^3} \sigma(\mathbf{r},\mathbf{v}' \to \mathbf{v})\,d\mathbf{v}$$

with ν number of neutrons produced due to fission.

The neutron transport equation

$$\frac{1}{|\mathbf{v}|}\frac{\partial\phi(t,\mathbf{r},\mathbf{v})}{\partial t}+\underbrace{\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi(t,\mathbf{r},\mathbf{v})}_{=\text{(a), transport}}+\underbrace{\sigma(\mathbf{r},\mathbf{v})\phi(t,\mathbf{r},\mathbf{v})}_{=\text{(b), out-collision}}$$

$$=\underbrace{\int_{\mathbb{R}^3}\sigma(\mathbf{r},\mathbf{v}'\to\mathbf{v})\phi(t,\mathbf{r},\mathbf{v}')\,d\mathbf{v}'}_{\text{c), secondaries}}+\underbrace{q(t,\mathbf{r},\mathbf{v})}_{\text{(d), sources}}$$

for $(\mathbf{r},\mathbf{v})\in\mathbb{R}^3\times\mathbb{R}^3$ with $\mathbf{s}=\mathbf{v}/|\mathbf{v}|\in\mathbb{S}^2$.

Notation:

$\phi(t,\mathbf{r},\mathbf{v})$ angular density

$\sigma(\mathbf{r},\mathbf{v})\geq 0$ macroscopic cross section

$\sigma(\mathbf{r},\mathbf{v}'\to\mathbf{v})$ scattering cross section

[Davison '57] [Case & Zweifel '67] [Duderstadt & Martin]

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Solution theory: [Dautray & Lions, vol. 6, Chapter XXI]

[Davison '57] [Case & Zweifel '67] [Duderstadt & Martin]

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for $(\mathbf{r},\mathbf{v})\in\mathbb{R}^3\times\mathbb{R}^3$ with $\mathbf{s}=\mathbf{v}/|\mathbf{v}|\in\mathbb{S}^2$.

Observations and challenges

- No regeneration $\sigma(\mathbf{r},\mathbf{v}'\to\mathbf{v})=0$: Family of ODEs for $\mathbf{v}\in\mathbb{R}^3$
- Low regularity of solutions (depending on q)
- Case $\sigma(\mathbf{r},\mathbf{v}'\to\mathbf{v})>0$: Non-trivial coupling. No analytic closed-form solution
- High-dimensional: $\dim(\mathbb{R}\times\mathbb{R}^3\times\mathbb{R}^3)=7$.

[Davison '57] [Case & Zweifel '67] [Duderstadt & Martin]

The stationary neutron transport equation

$$\underbrace{\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi(\mathbf{r},\mathbf{v})}_{=\text{(a), transport}}+\underbrace{\sigma(\mathbf{r},\mathbf{v})\phi(\mathbf{r},\mathbf{v})}_{=\text{(b), out-collision}}=\underbrace{\int_V \sigma(\mathbf{r},\mathbf{v}'\to\mathbf{v})\phi(\mathbf{r},\mathbf{v}')\,d\mathbf{v}'}_{\text{c), secondaries}}+\underbrace{q(\mathbf{r},\mathbf{v})}_{\text{(d), sources}}$$

for $(\mathbf{r},\mathbf{v})\in\mathbb{R}^3\times\mathbb{R}^3$ with $\mathbf{s}=\mathbf{v}/|\mathbf{v}|\in\mathbb{S}^2$.

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for $(\mathbf{r},\mathbf{s}) \in \mathbb{R}^3 \times \mathbb{S}^2$.

Assumptions:

- One velocity $\mathbf{v} = \mathbf{s} \in \mathbb{S}^2$.
- No fission, nor inelastic scattering, i.e., consider radiative absorption and elastic scattering

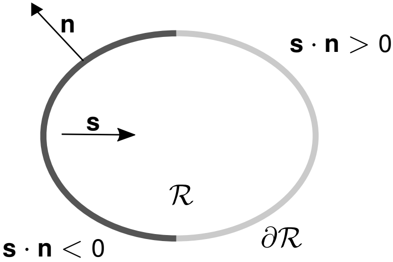
$$\sigma(\mathbf{r}) = \sigma_a(\mathbf{r}) + \sigma_s(\mathbf{r})$$

- Rotational invariance $\sigma(\mathbf{r},\mathbf{v}' \to \mathbf{v}) = \sigma_s(\mathbf{r})k(\mathbf{s}'\cdot\mathbf{s})$
- Often isotropic scattering $k(\mathbf{s}'\cdot\mathbf{s}) = 1/|\mathbb{S}^2|$.

[Davison '57] [Case & Zweifel '67] [Duderstadt & Martin]

Neutron transport on bounded domains

Vacuum boundary conditions



Assumptions

- $\mathcal{R} \subset \mathbb{R}^3$ bounded convex domain
- $\mathrm{supp}(q) \subset \mathcal{R}$
- $\mathrm{supp}(\sigma_s) \subset \mathcal{R}$

Inflow boundary

$$\Gamma_- = \{(\mathbf{r}, \mathbf{s}) \in \partial\mathcal{R} \times \mathbb{S}^2 : \mathbf{s} \cdot \mathbf{n}(\mathbf{r}) < 0\}$$

$$\mathbf{s} \cdot \nabla_{\mathbf{r}}\phi + \sigma\phi = \sigma_s \int_{\mathbb{S}^2} k(\mathbf{s} \cdot \mathbf{s}')\phi(\cdot, \mathbf{s}')\, d\mathbf{s}' + q \quad \text{in } \mathcal{R} \times \mathbb{S}^2$$

$$\phi = 0 \quad \text{on } \Gamma_-$$

Remark: Inhomogeneous inflow conditions, periodic boundary conditions, reflection conditions, etc., can be modeled similarly.

Well-posedness of the stationary neutron transport equation

$$\mathbf{s} \cdot \nabla_{\mathbf{r}} \phi + \sigma \phi = \sigma_s \int_{\mathbb{S}^2} k(\mathbf{s} \cdot \mathbf{s}') \phi(\cdot, \mathbf{s}') \, d\mathbf{s}' + q \quad \text{in } \mathcal{R} \times \mathbb{S}^2$$

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Theorem Let $\sigma_a, \sigma_s \geq 0$, $q \in L^2(\mathcal{R} \times \mathbb{S}^2)$. Then the NTE has a unique solution $\phi \in L^2(\mathcal{R} \times \mathbb{S}^2)$ with

$$\|\mathbf{s} \cdot \nabla_{\mathbf{r}} \phi\|_{L^2} + \|\phi\|_{L^2} \leq C \|q\|_{L^2}.$$

[Case Zweifel '63] [Dautray Lions '93] [Agoshkov '98] [Bal Jollivet 2008] [Egger S 2013]

Well-posedness of the stationary neutron transport equation

$$\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi + \sigma\phi = \sigma_s \int_{\mathbb{S}^2} k(\mathbf{s}\cdot\mathbf{s}')\phi(\cdot,\mathbf{s}')\, d\mathbf{s}' + q \quad \text{in } \mathcal{R}\times\mathbb{S}^2$$
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$$\|\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi\|_{L^2} + \|\phi\|_{L^2} \leq C\|q\|_{L^2}.$$

Proof (idea) Consider the mapping $T : L^2 \to L^2$, $\phi^n \mapsto \phi^{n+1}$, defined by

$$\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi^{n+1} + \sigma\phi^{n+1} = \sigma_s K\phi^n + q \quad \text{in } \mathcal{R}\times\mathbb{S}^2$$
$$\phi^{n+1} = 0 \quad \text{on } \Gamma_-.$$

Verify conditions of Banach's fixed-point theorem.

[Case Zweifel '63] [Dautray Lions '93] [Agoshkov '98] [Bal Jollivet 2008] [Egger S 2013]

Slab geometry

$$\mathbf{r} = (x, y, z) \in \mathbb{R}^2 \times (0, Z)$$

$$\mathbf{s} = (\cos\varphi \sin\theta, \sin\varphi \sin\theta, \cos\theta)$$

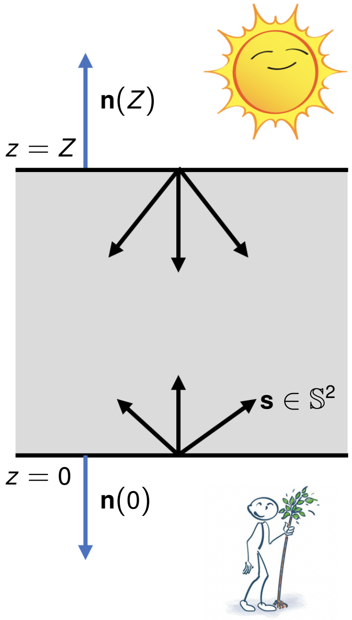
$$\mathbf{s} \cdot \mathbf{n}(Z) = \cos(\theta) =: \mu$$

$$\mathbf{s} \cdot \mathbf{n}(0) = -\mu$$

Assumption:

- $q(\mathbf{r}, \mathbf{s}) = q(z, \mu)$
- $\sigma = \sigma(z)$
- $k(\mathbf{s} \cdot \mathbf{s}') = 1/|\mathbb{S}^2|$
- $\phi = \phi(z, \mu)$

$$\Longrightarrow \quad \mathbf{s} \cdot \nabla_{\mathbf{r}} \phi = \mu \partial_z \phi$$

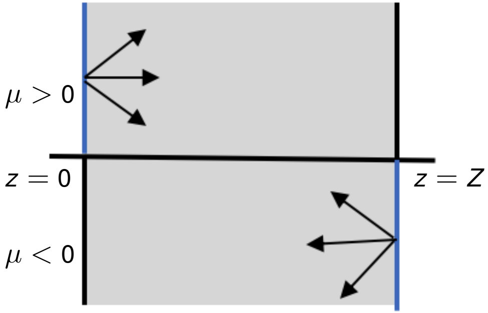


NTE in slab geometry

$$\mu \partial_z \phi + \sigma \phi = \frac{\sigma_s}{2} \int_{-1}^{1} \phi(\cdot, \mu')\, \mathrm{d}\mu' + q \quad \text{in } (0, Z) \times (-1, 1)$$

$$\phi(0, \mu) = g_0(\mu) \qquad \mu > 0$$

$$\phi(Z, \mu) = g_Z(\mu) \qquad \mu < 0$$



The P_L-approximation

Legendre polynomial expansion

$$\phi(z,\mu) = \sum_{\ell=0}^{\infty} \phi_\ell(z) P_\ell(\mu)$$

[Davison '57][Case Zweifel '67] [Modest 2003]

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Recurrence relations

$$(2\ell+1)\mu P_\ell = (\ell+1)P_{\ell+1} + \ell P_{\ell-1}$$

Neutron transport equation

$$\mu\partial_z\phi + \sigma\phi = \frac{\sigma_s}{2}\int_{-1}^{1}\phi(\cdot,\mu')\,\mathrm{d}\mu' + q$$

becomes an infinite coupled system

$$\frac{\ell+1}{2\ell+1}\partial_z\phi_{\ell+1} + \frac{\ell}{2\ell+1}\partial_z\phi_{\ell-1} + \sigma\phi_\ell = \frac{\sigma_s}{2}\phi_0\delta_{0,\ell} + q_\ell.$$

[Davison '57][Case Zweifel '67] [Modest 2003]

The P_L-approximation

Truncated Legendre polynomial expansion

$$\phi(z,\mu) = \sum_{\ell=0}^{\infty} \phi_\ell(z) P_\ell(\mu) \approx \sum_{\ell=0}^{L} \phi_\ell(z) P_\ell(\mu).$$

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Truncate system, by setting $\phi_\ell = 0$ for $\ell > L$.

[Davison '57][Case Zweifel '67] [Modest 2003]

The P_L-approximation

boundary conditions

P_L**-equations.** For $0 \leq \ell \leq L$:

$$\frac{\ell+1}{2\ell+1}\partial_z\phi_{\ell+1} + \frac{\ell}{2\ell+1}\partial_z\phi_{\ell-1} + \sigma\phi_\ell = \frac{\sigma_s}{2}\phi_0\delta_{0,\ell} + q_\ell.$$

Truncation condition $\phi_\ell = 0$ for all $\ell > L$; and $\phi_{-1} = 0$.

Typical choices of **boundary conditions**, $z_b \in \{0, Z\}$, L odd:

$$\int (\phi(z_b,\mu) - g_{z_b}(\mu))\mu^\ell \, \mathrm{d}\mu = 0, \quad \ell = 1, 3, \ldots, L \qquad \textbf{(Marshak)}$$

$$\phi(z_b,\mu_n) = g_{z_b}(\mu_n), \quad n = 1, 2, \ldots, (L+1)/2, \qquad \textbf{(Mark)}$$

$\rightsquigarrow$ strong coupling of ϕ_ℓ.

[Davison '57][Case Zweifel '67] [Modest 2003]

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$\rightsquigarrow$ strong coupling of ϕ_ℓ.

Which are the correct ones? How to generalize to multi-d?

[Davison '57][Case Zweifel '67] [Modest 2003]

Discrete ordinates methods: Wick-Chandrasekhar

Gauss-Legendre quadrature ($N \geq 2$ even)

$$\int_{-1}^{1} \phi(z,\mu)\,\mathrm{d}\mu \approx \sum_{i=1}^{N} \omega_i \phi(z,\mu_i).$$

[Case Zweifel '67]

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$$\int_{-1}^{1} \phi(z,\mu)\,\mathrm{d}\mu \approx \sum_{i=1}^{N} \omega_i \phi(z,\mu_i).$$

Introduce $\phi_n(z) \approx \phi(z,\mu_n)$ and evaluate NTE in μ_n, $n = 1,\ldots,N$:

$$\mu_n \partial_z \phi_n + \sigma \phi_n = \frac{\sigma_s}{2} \sum_{i=1}^{N} \omega_i \phi_i + q_n \quad \text{in } (0,Z)$$

System of N ODEs for the N functions ϕ_n.

[Case Zweifel '67]

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System of N ODEs for the N functions ϕ_n.

Boundary conditions:

$$\begin{aligned} \phi_n(0) &= g_0(\mu_n) \quad \text{for } \mu_n > 0 \\ \phi_n(Z) &= g_Z(\mu_n) \quad \text{for } \mu_n < 0 \end{aligned}$$

[Case Zweifel '67]

Discrete ordinates methods: Wick-Chandrasekhar

Gauss-Legendre quadrature ($N \geq 2$ even)

$$\int_{-1}^{1} \phi(z,\mu)\,\mathrm{d}\mu \approx \sum_{i=1}^{N} \omega_i \phi(z,\mu_i).$$

Introduce $\phi_n(z) \approx \phi(z,\mu_n)$ and evaluate NTE in μ_n, $n = 1,\ldots,N$:

$$\mu_n \partial_z \phi_n + \sigma \phi_n = \frac{\sigma_s}{2} \sum_{i=1}^{N} \omega_i \phi_i + q_n \quad \text{in } (0,Z)$$

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This method is equivalent to the P_{N-1}-approximation (with Mark b.c.).

[Case Zweifel '67]

Discrete ordinates method

Approximate $\phi(z,\mu)$ with discontinuous, piecewise constant functions

$$\phi(z,\mu) \approx \phi_n(z), \quad \mu_{n-1} \leq \mu \leq \mu_n,\ 1 \leq n \leq N.$$

Integrate NTE over (μ_{n-1}, μ_n):

$$\frac{\mu_n + \mu_{n-1}}{2}\partial_z\phi_n + \sigma\phi_n = \frac{\sigma_s}{2}\sum_{i=1}^{N}\omega_i\phi_i + q_n.$$

- Partition $-1 = \mu_0 < \mu_1 < \ldots < \mu_N = 1$ arbitrary
- System of ODEs for ϕ_n

[Reed, Hill '73] [Lesaint, Raviart '74] [Kanschat et al 2012, 2014]

Summary of classical semidiscretizations

P_L **method**

- global approximation in angle μ
- scattering is diagonalized
- dense coupling due to boundary conditions
- multi-d: spherical harmonics
- boundary conditions for multi-d ?

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Aim: Recover semi-discretizations from one framework

Advantage: Unified analysis, (perhaps) simplified implementation, and more.

Even-odd splitting

Even-odd parities

$$\phi^{\pm}(z,\mu) = \frac{1}{2}(\phi(z,\mu) \pm \phi(z,-\mu))$$

Observations

- $\phi = \phi^+ + \phi^-$ is an L^2-orthogonal splitting
- Parity transformation

$$\mu\partial_z\phi^+ \text{ is odd}, \qquad \bar{\phi}(z,\mu) := \frac{1}{2}\int_{-1}^{1}\phi(z,\mu')\,d\mu' \quad \text{is even.}$$

Projection of the NTE onto even-odd functions:

$$\begin{aligned} \mu\partial_z\phi^- + \sigma\phi^+ &= \sigma_s\bar{\phi}^+ + q^+ \quad &&\text{in } (0,Z)\times(-1,1) \\ \mu\partial_z\phi^+ + \sigma\phi^- &= q^- &&\text{in } (0,Z)\times(-1,1). \end{aligned}$$

[Vladimirov '61]

Derivation of a variational principle

Multiply

$$\mu \partial_z \phi^- + \sigma \phi^+ = \sigma_s \bar{\phi}^+ + q^+$$

with ψ^+ and integrate over $(0, Z) \times (-1, 1)$:

$$(\mu \partial_z \phi^-, \psi^+) + (\mu \partial_z \phi^+, \psi^-) + (\sigma \phi, \psi) = (\sigma_s \bar{\phi}, \psi^+) + (q^+, \psi^+)$$

[Egger S 2012, Palii S 2020]

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Integration-by-parts:

$$(\mu\partial_z\phi^-, \psi^+) = -(\phi^-, \mu\partial_z\psi^+) + \int_{-1}^{1} \mu\, \phi^-(\cdot, \mu)\psi^+(\cdot, \mu)\Big|_0^Z \,\mathrm{d}\mu$$

[Egger S 2012, Palii S 2020]

Derivation of a variational principle

Multiply

$$\mu \partial_z \phi^- + \sigma \phi^+ = \sigma_s \bar{\phi}^+ + q^+$$

with ψ^+ and integrate over $(0, Z) \times (-1, 1)$:

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Integration-by-parts:

$$(\mu \partial_z \phi^-, \psi^+) = -(\phi^-, \mu \partial_z \psi^+) + \int_{-1}^{1} \mu \, \phi^-(\cdot, \mu) \psi^+(\cdot, \mu) \Big|_0^Z \, \mathrm{d}\mu$$

Key observation: $\mu \mapsto \mu \phi^-(\cdot, \mu) \psi^+(\cdot, \mu)$ is even.

$$\int_{-1}^{1} \mu \phi^-(Z, \mu) \psi^+(Z, \mu) \, \mathrm{d}\mu = 2 \int_{-1}^{0} \mu \phi^-(Z, \mu) \psi^+(Z, \mu) \, \mathrm{d}\mu$$

$$= 2 \int_{-1}^{0} \mu (g_Z(\mu) - \phi^+(Z, \mu)) \psi^+(Z, \mu) \, \mathrm{d}\mu$$

[Egger S 2012, Palii S 2020]

Summary: Variational principle for the NTE

Find $\phi = \phi^+ + \phi^- \in \mathbb{W}^+ \oplus \mathbb{V}^-$ such that

$$b(\phi, \psi) = k(\phi, \psi) + \ell(\psi) \qquad \forall \psi = \psi^+ + \psi^- \in \mathbb{W}^+ \oplus \mathbb{V}^- \tag{1}$$

where

$$\begin{aligned}
b(\phi, \psi) &= \langle |\mu| \phi^+, \psi^+ \rangle_\Gamma - (\phi^-, \mu \partial_z \psi^+) + (\mu \partial_z \phi^+, \psi^-) + (\sigma \phi, \psi), \\
k(\phi, \psi) &= (\sigma_s \bar{\phi}, \psi), \\
\ell(\psi) &= (q, \psi) + 2 \langle |\mu| g, \psi^+ \rangle_{\Gamma_-} \\
\mathbb{V} &:= L^2((0, Z) \times (-1, 1)) \\
\mathbb{W}^+ &:= \{\psi \in \mathbb{V}^+ : \mu \partial_z \psi \in \mathbb{V}\}
\end{aligned}$$

Remarks

- Boundary conditions are incorporated naturally
- Equation (1) is well-posed for $\sigma_a \geq \gamma > 0$ [Palii & S, 2020]
- For bounded $\mathcal{R}$, well-posedness holds for $\sigma_a \geq 0$ [Egger & S, 2012].

Galerkin approximation

Let $\mathbb{W}_h^+ \subset \mathbb{W}^+$ and $\mathbb{V}_h^- \subset \mathbb{V}^-$ be finite dimensional spaces.

Galerkin formulation. Find $\phi_h = \phi_h^+ + \phi_h^- \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$ such that

$$b(\phi_h, \psi_h) = k(\phi_h, \psi_h) + \ell(\psi_h)$$

for all $\psi_h \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$

Theorem. If $\sigma^{-1}\mu\partial_z\mathbb{W}_h^+ \subset \mathbb{V}_h^-$ and $\sigma_a \geq \gamma > 0$, then the Galerkin problem is well-posed and

$$\|\mu\partial_z(\phi^+ - \phi_h^+)\|_{L^2} + \|\phi - \phi_h\|_{L^2} \leq C \inf \|\mu\partial_z(\phi^+ - \psi_h^+)\|_{L^2} + \|\phi - \psi_h\|_{L^2}$$

where the infimum is taken over all $\psi_h \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$.

[Egger S (2012)] [Palii S (2020)]

FEM + Legendre expansion: FEM-P_L method

Partition $(0,Z)$ into J intervals: $0 = z_0 < z_1 < \ldots < z_J = Z$.

Piecewise polynomials on $(0,Z)$

$$\mathbb{P}_k(0,Z) = \{v : \ v_{|(z_{j-1},z_j)} \text{ is a polynomial of degree } k)\}$$
$$\mathbb{P}_k^c(0,Z) = \{v \in \mathbb{P}_k(0,Z) : \ v \text{ is continuous}\}$$

Basis for $\mathbb{P}_1^c$: $\varphi_j \in \mathbb{P}_1^c$ satisfying $\varphi_j(z_i) = \delta_{i,j}$.

Basis for $\mathbb{P}_0$: $\chi_n \in \mathbb{P}_0$ satisfying $\chi_n(z) = \delta_{n,m}$ for $z \in (z_{m-1}, z_m)$.

Approximations, for L odd and $k=1$,

$$\phi_{L,J}^+(z,\mu) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c_{j,\ell}^+ \varphi_j(z) P_{2\ell}(\mu),$$

$$\phi_{L,J}^-(z,\mu) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=1}^{J} c_{j,\ell}^- \chi_j(z) P_{2\ell+1}(\mu).$$

Remark: For L odd, σ pcw. constant, the compatibility condition $\sigma^{-1}\mu\partial_z \mathbb{W}_h^+ \subset \mathbb{V}_h^-$ holds.

Towards a linear system

Insert approximations

$$\phi^+_{L,J}(z,\mu) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell}\varphi_j(z)P_{2\ell}(\mu),$$

$$\phi^-_{L,J}(z,\mu) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=1}^{J} c^-_{j,\ell}\chi_j(z)P_{2\ell+1}(\mu),$$

into **Galerkin problem**

$$b(\phi^+_{L,J} + \phi^-_{L,J}, \psi) = k(\phi^+_{L,J} + \phi^-_{L,J}, \psi) + \ell(\psi)$$

where $\psi = \varphi_i P_{2k}$ or $\psi = \chi_i P_{2k+1}$ ranges over all basis functions.
Each basis function ψ yields a row of a linear system

$$\mathbf{Sc} = \mathbf{f}$$

for the unknown coefficients $\mathbf{c}$.

Implementational details

for the term $(\mu\partial_z\phi^+_{L,J}, \psi^-)$

We compute for $\psi^- = \chi_n P_{2k+1}$

$$(\mu\partial_z\phi^+_{L,J}, \psi^-) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \int_{-1}^{1} \int_0^Z \partial_z\varphi_j \mu P_{2\ell} \chi_n P_{2k+1} \,\mathrm{d}z\,\mathrm{d}\mu$$

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$$= \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \left(\underbrace{\int_0^Z \partial_z\varphi_j \chi_n \,\mathrm{d}z}_{=\mathbf{D}_{j,n}} \right) \left(\underbrace{\int_{-1}^{1} \mu P_{2\ell}(\mu) P_{2k+1}(\mu)\,\mathrm{d}\mu}_{=\mathbf{P}_{k,\ell}} \right).$$

Implementational details

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Identify $\phi^+_{L,J}$ with its coefficient matrix $\mathbf{C}^+ = (c^+_{j,\ell})_{j,\ell}$. Then we can write

$$(\mu\partial_z\phi^+_{L,J,1}, \psi^-) = (\mathbf{D}\mathbf{C}^+\mathbf{P}^T)_{n,k}.$$

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$$= \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \Bigg(\underbrace{\int_0^Z \partial_z\varphi_j \chi_n \,\mathrm{d}z}_{=\mathbf{D}_{j,n}}\Bigg) \Bigg(\underbrace{\int_{-1}^{1} \mu P_{2\ell}(\mu) P_{2k+1}(\mu)\,\mathrm{d}\mu}_{=\mathbf{P}_{k,\ell}}\Bigg).$$

Identify $\phi^+_{L,J}$ with its coefficient matrix $\mathbf{C}^+ = (c^+_{j,\ell})_{j,\ell}$. Then we can write

$$(\mu\partial_z\phi^+_{L,J,1}, \psi^-) = (\mathbf{D}\mathbf{C}^+\mathbf{P}^T)_{n,k}.$$

Furthermore, the matrix $\mathbf{D}\mathbf{C}^+\mathbf{P}^T$ can be identified with a vector

$$(\mathbf{P} \otimes \mathbf{D})\mathbf{c}^+.$$

Implementational details continued

the remaining terms

The term $(\sigma\phi^{+}_{L,J},\psi^{+}) = \int_{-1}^{1}\int_{0}^{Z}\sigma(z)\phi^{+}_{L,J}(z,\mu)\psi^{+}(z,\mu)\,\mathrm{d}z\,\mathrm{d}\mu$ becomes

$$(\mathbf{I}\otimes\mathbf{M}(\sigma)^{+})\mathbf{c}^{+} \quad \text{with } (\mathbf{M}(\sigma)^{+})_{i,j} = \int_{0}^{Z}\sigma\varphi_i\varphi_j\,\mathrm{d}z.$$

Implementational details continued

the remaining terms

The term $(\sigma\phi^+_{L,J}, \psi^+) = \int_{-1}^1 \int_0^Z \sigma(z)\phi^+_{L,J}(z,\mu)\psi^+(z,\mu)\,\mathrm{d}z\,\mathrm{d}\mu$ becomes

$$(\mathbf{I} \otimes \mathbf{M}(\sigma)^+)\mathbf{c}^+ \quad \text{with } (\mathbf{M}(\sigma)^+)_{i,j} = \int_0^Z \sigma\varphi_i\varphi_j\,\mathrm{d}z.$$

The term $(\sigma_s\bar{\phi}^+_{L,J}, \psi^+)$ becomes $(\mathrm{diag}(1,0,\dots,0) \otimes \mathbf{M}(\sigma_s)^+)\mathbf{c}^+$.

Implementational details continued

the remaining terms

The term $(\sigma\phi^+_{L,J},\psi^+) = \int_{-1}^1\int_0^Z \sigma(z)\phi^+_{L,J}(z,\mu)\psi^+(z,\mu)\,\mathrm{d}z\,\mathrm{d}\mu$ becomes

$$(\mathbf{I}\otimes\mathbf{M}(\sigma)^+)\mathbf{c}^+ \quad \text{with } (\mathbf{M}(\sigma)^+)_{i,j} = \int_0^Z \sigma\varphi_i\varphi_j\,\mathrm{d}z.$$

The term $(\sigma_s\bar{\phi}^+_{L,J},\psi^+)$ becomes $(\mathrm{diag}(1,0,\ldots,0)\otimes\mathbf{M}(\sigma_s)^+)\mathbf{c}^+$.

The term $\langle|\mu|\phi^+_{L,J},\psi^+\rangle_{\Gamma_-}$ becomes $(\mathbf{B}\otimes\mathrm{diag}(1,0,\ldots,0,1))\mathbf{c}^+$

$$\text{with } (\mathbf{B})_{\ell,k} = \int_{-1}^1 P_{2\ell}(\mu)P_{2k}(\mu)|\mu|\,d\mu = 2\int_0^1 P_{2\ell}(\mu)P_{2k}(\mu)\mu\,d\mu.$$

Note that **B** is a dense matrix.

Discrete system for P_L method

Solve

$$\begin{pmatrix} \mathbf{R} + \mathbf{A}^+ & -\mathbf{P}^T \otimes \mathbf{D}^T \\ \mathbf{P} \otimes \mathbf{D} & \mathbf{A}^- \end{pmatrix} \begin{pmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{pmatrix} = \begin{pmatrix} \mathbf{q}^+ \\ \mathbf{q}^- \end{pmatrix}$$

with

$$\mathbf{R} = \mathbf{B} \otimes \mathrm{diag}(1, 0, \dots, 0, 1), \qquad \text{'boundary' matrix}$$

$$\mathbf{A}^+ = \mathbf{I} \otimes \mathbf{M}(\sigma)^+ \otimes -\mathrm{diag}(1, 0, \dots, 0) \otimes \mathbf{M}(\sigma_s)^+, \quad \text{'attenuation' matrix}$$

$$\mathbf{A}^- = \mathbf{I} \otimes \mathbf{M}(\sigma)^-, \quad \text{'attenuation' matrix}$$

Take away. Use Kronecker structure!

- Assembling matrices for spatial and angular parts separately, tremendously simplifies the implementation!
- Storing the factors instead of the Kronecker product reduces memory requirements!

Notes on solving the discrete system

The discrete system

$$\begin{pmatrix} \mathbf{R} + \mathbf{A}^{+} & -\mathbf{P}^{T} \otimes \mathbf{D}^{T} \\ \mathbf{P} \otimes \mathbf{D} & \mathbf{A}^{-} \end{pmatrix} \begin{pmatrix} \mathbf{c}^{+} \\ \mathbf{c}^{-} \end{pmatrix} = \begin{pmatrix} \mathbf{q}^{+} \\ \mathbf{q}^{-} \end{pmatrix}$$

is equivalent to

$$\begin{aligned} (\mathbf{R} + \mathbf{A}^{+})\mathbf{c}^{+} - (\mathbf{P} \otimes \mathbf{D})^{T}\mathbf{c}^{-} &= \mathbf{q}^{+} \\ (\mathbf{P} \otimes \mathbf{D})\mathbf{c}^{+} + \mathbf{A}^{-}\mathbf{c}^{-} &= \mathbf{q}^{-}. \end{aligned}$$

Observation: $\mathbf{A}^{-} = \mathbf{I} \otimes \mathbf{M}(\sigma)^{-}$ is a diagonal matrix. Setting $\mathbf{C} = (\mathbf{M}(\sigma)^{-})^{-1}$, elimination of $\mathbf{c}^{-}$ yields the **Schur complement:**

$$\left(\mathbf{R} + \mathbf{A}^{+} + (\mathbf{P}^{T}\mathbf{P} \otimes \mathbf{D}^{T}\mathbf{C}\mathbf{D})\right)\mathbf{c}^{+} = \mathbf{q}^{+} + (\mathbf{P} \otimes \mathbf{C}\mathbf{D})^{T}\mathbf{q}^{-}.$$

Once $\mathbf{c}^{+}$ is obtained, we can solve for $\mathbf{c}^{-}$.

Properties of the Schur complement

$$\left(\mathbf{R} + \mathbf{A}^{+} + \left(\mathbf{P}^{T}\mathbf{P} \otimes \mathbf{D}^{T}\mathbf{C}\mathbf{D}\right)\right)\mathbf{c}^{+} = \mathbf{q}^{+} + \left(\mathbf{P} \otimes \mathbf{C}\mathbf{D}\right)^{T}\mathbf{q}^{-}.$$

- symmetric, positive definite
- sparse matrix (except for **B** in $\mathbf{R} = \mathbf{B} \otimes \mathrm{diag}(1, 0, \ldots, 0, 1)$)
- system size is about halved (compared to the full system for $(\mathbf{c}^{+}, \mathbf{c}^{-})$).

Numerical example for P_L-method

Manufactured solution

$$\phi(z, \mu) = |\mu| e^{-\mu} e^{-z(1-z)}$$

Parameters

$$\sigma_a = 0.01, \quad \sigma_s = 2 + \sin(\pi z)/2, \quad z \in (0, 1)$$

Results

P_L with $J = 16\,384$			P_L with $L = 127$		
L	$\|\phi - \phi_h\|_{L^2}$	rate	J	$\|\phi - \phi_h\|_{L^2}$	rate
1	4.27e-01		2	5.91e-02	
3	4.51e-02	3.24	4	2.26e-02	1.39
7	1.94e-02	1.22	8	1.00e-02	1.17
15	6.56e-03	1.56	16	4.84e-03	1.05
31	2.25e-03	1.54	32	2.40e-03	1.01
63	7.84e-04	1.52	64	1.22e-03	0.98
127	2.74e-04	1.51	128	6.55e-04	0.90

Double Legendre expansion

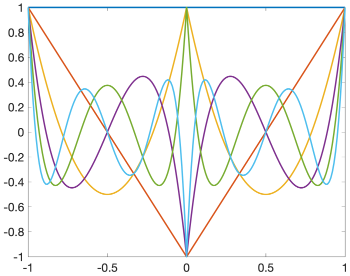
dP_L method

Treatment of z-variable as before.

Angular basis functions:

$$Q_\ell^+(\mu) = P_\ell(2|\mu| - 1)$$
$$Q_\ell^-(\mu) = \mathrm{sign}(\mu) P_\ell(2|\mu| - 1)$$

for $0 \leq \ell \leq L$.



Approximations

$$\phi^+_{L,J}(z,\mu) = \sum_{\ell=0}^{L} \sum_{j=0}^{J} c^+_{j,\ell} \varphi_j(z) Q^+_\ell(\mu),$$

$$\phi^-_{L,J}(z,\mu) = \sum_{\ell=0}^{L+1} \sum_{j=1}^{J} c^-_{j,\ell} \chi_j(z) Q^-_\ell(\mu).$$

Remark: For σ pcw. constant, the compatibility condition $\sigma^{-1}\mu\partial_z \mathbb{W}_h^+ \subset \mathbb{V}_h^-$ holds.

Towards a linear system

dP_L method

Insert approximations

$$\phi^+_{L,J}(z,\mu) = \sum_{\ell=0}^{L}\sum_{j=0}^{J} c^+_{j,\ell}\varphi_j(z)Q^+_\ell(\mu),$$
$$\phi^-_{L,J}(z,\mu) = \sum_{\ell=0}^{L+1}\sum_{j=1}^{J} c^-_{j,\ell}\chi_j(z)Q^-_\ell(\mu),$$

into **Galerkin problem**

$$b(\phi^+_{L,J} + I^-_{L,J}, \psi) = k(\phi^+_{L,J} + I^-_{L,J}, \psi) + \ell(\psi)$$

where $\psi = \varphi_i Q^+_k$ or $\psi = \chi_i Q^-_k$ ranges over all basis functions.
Each basis function ψ yields a row of a linear system

$$\mathbf{Sc} = \mathbf{f}$$

for the unknown coefficients $\mathbf{c}$.

Implementational details

for the term $(\mu\partial_z\phi^+_{L,J}, \psi^-)$ in dP_L method

We compute for $\psi^- = \chi_n Q_k^-$

$$(\mu\partial_z\phi^+_{L,J}, \psi^-) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \int_0^Z \partial_z\varphi_j\chi_n\, dz \qquad \underbrace{\int_{-1}^{1} \mu Q^+_\ell Q^-_k\, d\mu}$$

Implementational details

for the term $(\mu\partial_z\phi^+_{L,J}, \psi^-)$ in dP_L method

We compute for $\psi^- = \chi_n Q_k^-$

$$(\mu\partial_z\phi^+_{L,J}, \psi^-) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \int_0^Z \partial_z\varphi_j \chi_n \, dz \qquad \underbrace{\int_{-1}^{1} \mu Q^+_\ell Q^-_k \, d\mu}_{=\int_{-1}^{1} |\mu| P_\ell(2|\mu|-1) P_k(2|\mu|-1) d\mu}$$

Implementational details

for the term $(\mu\partial_z\phi^+_{L,J}, \psi^-)$ in dP_L method

We compute for $\psi^- = \chi_n Q_k^-$

$$(\mu\partial_z\phi^+_{L,J}, \psi^-) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \int_0^Z \partial_z\varphi_j \chi_n \, dz \qquad \underbrace{\int_{-1}^{1} \mu Q^+_\ell Q^-_k \, d\mu}_{=\int_{-1}^{1} |\mu| P_\ell(2|\mu|-1) P_k(2|\mu|-1) d\mu}$$

$$= \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \left(\underbrace{\int_0^Z \partial_z\varphi_j \chi_n \, dz}_{=\mathbf{D}_{j,n}} \right) \left(\underbrace{\int_{-1}^{1} \frac{\mu+1}{2} P_\ell(\mu) P_k(\mu) \, d\mu}_{=\mathbf{P}_{k,\ell}} \right).$$

Implementational details

for the term $(\mu\partial_z\phi^+_{L,J}, \psi^-)$ in dP_L method

We compute for $\psi^- = \chi_n Q^-_k$

$$(\mu\partial_z\phi^+_{L,J}, \psi^-) = \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \int_0^Z \partial_z\varphi_j\chi_n\, dz \qquad \underbrace{\int_{-1}^{1} \mu Q^+_\ell Q^-_k\, d\mu}_{=\int_{-1}^{1} |\mu| P_\ell(2|\mu|-1) P_k(2|\mu|-1) d\mu}$$

$$= \sum_{\ell=0}^{(L-1)/2} \sum_{j=0}^{J} c^+_{j,\ell} \left(\underbrace{\int_0^Z \partial_z\varphi_j\chi_n\, dz}_{=\mathbf{D}_{j,n}}\right)\left(\underbrace{\int_{-1}^{1} \frac{\mu+1}{2} P_\ell(\mu) P_k(\mu)\, d\mu}_{=\mathbf{P}_{k,\ell}}\right).$$

Identify $\phi^+_{L,J}$ with its coefficient matrix $\mathbf{C}^+ = (c^+_{j,\ell})_{j,\ell}$. Then we can write

$$(\mu\partial_z\phi^+_{L,J,1}, \psi^-) = (\mathbf{D}\mathbf{C}^+\mathbf{P}^T)_{n,k}.$$

Furthermore, the matrix $\mathbf{D}\mathbf{C}^+\mathbf{P}^T$ can be identified with a vector

$$(\mathbf{P} \otimes \mathbf{D})\mathbf{c}^+.$$

Implementational details continued

dP_L method

The term $(\sigma\phi, \psi) = \int_{-1}^{1} \int_0^Z \sigma(z)\phi(z,\mu)\psi(z,\mu)\, dz\, d\mu$ becomes

$$(\mathbf{M}(\sigma)^+ \otimes \mathbf{I})\mathbf{c}^+ \quad \text{with } (\mathbf{M}(\sigma)^+)_{i,j} = \int_0^Z \sigma\varphi_i\varphi_j\, dz.$$

The term $(\sigma_s\bar{\phi}, \psi)$ becomes

$$(\mathrm{diag}(1,0,\dots,0) \otimes \mathbf{M}(\sigma_s)^+)\mathbf{c}^+$$

The term $\langle|\mu|\phi^+, \psi^+\rangle_{\Gamma_-}$ becomes

$$(\mathbf{B} \otimes \mathrm{diag}(1,0,\dots,0,1))\mathbf{c}^+ \quad \text{with } (\mathbf{B})_{\ell,k} = \int_{-1}^{1} P_\ell(\mu)P_k(\mu)\frac{\mu+1}{2}\, d\mu$$

Remark: B is a sparse matrix.

Discrete system for dP_L method

Solve

$$\begin{pmatrix} \mathbf{R}+\mathbf{A}^{+} & -\mathbf{D}^{T}\otimes \mathbf{P}^{T} \\ \mathbf{D}\otimes \mathbf{P} & \mathbf{A}^{-} \end{pmatrix} \begin{pmatrix} \mathbf{c}^{+} \\ \mathbf{c}^{-} \end{pmatrix} = \begin{pmatrix} \mathbf{q}^{+} \\ \mathbf{q}^{-} \end{pmatrix}$$

with

$$\mathbf{R} = \mathbf{B}\otimes \mathrm{diag}(1,0,\dots,0,1), \qquad \text{'boundary' matrix}$$

$$\mathbf{A}^{+} = \mathbf{I}\otimes \mathbf{M}(\sigma)^{+} - \mathrm{diag}(1,0,\dots,0)\otimes \mathbf{M}(\sigma_s)^{+}, \quad \text{'attenuation' matrix}$$

$$\mathbf{A}^{-} = \mathbf{I}\otimes \mathbf{M}(\sigma)^{-}, \quad \text{'attenuation' matrix}$$

All matrices are sparse for the dP_L-method and isotropic scattering.

Take away. Use Kronecker structure!

- Assembling matrices for spatial and angular parts separately, tremendously simplifies the implementation!
- Storing the factors instead of the Kronecker product reduces memory requirements!

Numerical example for dP_L-method

Manufactured solution

$$\phi(z,\mu) = |\mu| e^{-\mu} e^{-z(1-z)}$$

Parameters

$$\sigma_a = 0.01, \quad \mu_s = 2 + \sin(\pi z)/2, \quad z \in (0,1)$$

Results

dP_L with $J = 16\,384$		dP_L with $L = 7$		
L	$\|\phi - \phi_h\|_{L^2}$	J	$\|\phi - \phi_h\|_{L^2}$	rate
1	1.05e-01	256	2.97e-04	1.00
2	1.29e-02	512	1.49e-04	1.00
3	1.40e-03	1024	7.44e-05	1.00
4	7.44e-05	2048	3.72e-05	1.00
5	7.54e-06	4096	1.86e-05	1.00
6	4.65e-06	8192	9.30e-06	1.00
7	4.65e-06	16384	4.65e-06	1.00

Piecewise constant expansions: *dG* method

Treatment of z-variable as before.

Partition $(-1,1)$: $-1 = \mu_{-N} < \ldots < \mu_N = 1$, such that $\mu_{-n} = -\mu_n$.

Basis for piecewise constants in angle

$\iota_k \in \mathbb{P}_0$ satisfying $\iota_n(\mu) = \delta_{n,m}$ for $\mu \in (\mu_{m-1}, \mu_m)$.

Angular basis functions for $1 \le n \le N$

$Q_n^+(\mu) = \iota_n(|\mu|)$

$Q_{n,\ell}^-(\mu) = \mathrm{sign}(\mu)\iota_n(|\mu|)P_\ell(2(|\mu| - \mu_{n+1/2}))$ for $\ell = 0, 1$.

Approximations

$$\phi_{N,J}^+(z,\mu) = \sum_{n=1}^{N}\sum_{j=0}^{J} c_{j,n}^+ \varphi_j(z) Q_n^+(\mu),$$

$$\phi_{N,J}^-(z,\mu) = \sum_{n=1}^{N}\sum_{\ell=0}^{1}\sum_{j=1}^{J} c_{j,n,\ell}^- \chi_j(z) Q_{n,\ell}^-(\mu).$$

Remark: For σ pcw. constant, the compatibility condition $\sigma^{-1}\mu\partial_z \mathbb{W}_h^+ \subset \mathbb{V}_h^-$ holds.

Discrete system for *dG* method

Solve

$$\begin{pmatrix} \mathbf{R} + \mathbf{A}^+ & -\mathbf{P}^T \otimes \mathbf{D}^T \\ \mathbf{P} \otimes \mathbf{D} & \mathbf{A}^- \end{pmatrix} \begin{pmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{pmatrix} = \begin{pmatrix} \mathbf{q}^+ \\ \mathbf{q}^- \end{pmatrix}$$

with

$$\mathbf{R} = \mathbf{B} \otimes \mathrm{diag}(1, 0, \dots, 0, 1), \qquad \text{'boundary' matrix}$$

$$\mathbf{A}^+ = \mathbf{N} \otimes \mathbf{M}(\sigma)^+ - \mathbf{K} \otimes \mathbf{M}(\sigma_s)^+, \quad \text{'attenuation' matrix}$$

$$\mathbf{A}^- = \mathbf{N} \otimes \mathbf{M}(\sigma)^-, \quad \text{'attenuation' matrix}$$

All matrices are sparse for the *dG*-method except the scattering part **K**.

Take away. Use Kronecker structure!

- Assembling matrices for spatial and angular parts separately, tremendously simplifies the implementation!
- Storing the factors instead of the Kronecker product reduces memory requirements!

For effective treatment of dense scattering part see [Dölz Palii S (2022)].

Numerical example for *dG*-method

Manufactured solution

$$\phi(z,\mu) = |\mu| e^{-\mu} e^{-z(1-z)}$$

Parameters

$$\sigma_a = 0.01, \quad \sigma_s = 2 + \sin(\pi z)/2, \quad z \in (0,1)$$

Results

dG with $J = 16\,384$			*dG* with $N = 128$		
N	$\|\phi - \phi_h\|_{L^2}$	rate	J	$\|\phi - \phi_h\|_{L^2}$	rate
2	4.23e-01		2	5.92e-02	
4	1.42e-01	1.57	4	2.28e-02	1.37
8	6.11e-02	1.22	8	1.06e-02	1.11
16	2.85e-02	1.10	16	5.89e-03	0.85
32	1.38e-02	1.05	32	4.13e-03	0.51
64	6.79e-03	1.02	64	3.57e-03	0.21
128	3.37e-03	1.01	128	3.42e-03	0.06

Take aways

Take away 1. Many classical approximations of radiative transfer (P_L, dP_L, discrete ordinates) can be formulated, analyzed and implemented in one framework.

Take away 2. Use Kronecker structure!

- Assembling matrices for spatial and angular parts separately, tremendously simplifies the implementation!
- Storing the factors instead of the Kronecker product reduces memory requirements!

Generalizations to 3D

P_L-method

- use spherical harmonics instead of Legendre polynomials.
- Transport and attenuation matrices sparse and Kronecker structure.
- Scattering matrix diagonal; for general scattering kernels $k(\mathbf{s} \cdot \mathbf{s}')$.
- but the boundary matrix coupling becomes more expensive (also no Kronecker product structure); cf. [Egger & S 2019] for a remedy using PMLs.

dP_L-method

- has no direct counterpart in general.

DG-method

- use pcw. constant functions on $\mathbb{S}^2$.
- Transport and boundary matrix are sparse and Kronecker structure.
- Scattering matrix is dense, but compression possible [Dahmen et al 2020, Dölz et al 2022].

Structure allows to assemble and apply matrices efficiently.