# An efficient mass-conservative and bound-preserving limiting technique and its application on the neutron transport equations

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Jean-Luc Guermond[1], Zuodong Wang[2]

Texas A&M University[1]
Eastern Institute of Technology, Ningbo[2]

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Highly-contrasted coefficients

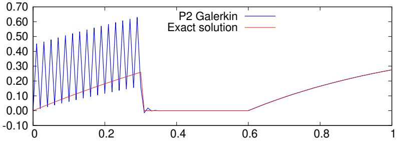
- Physically meaningful numerical solution:
  bound-preserving, mass-conservative, ...

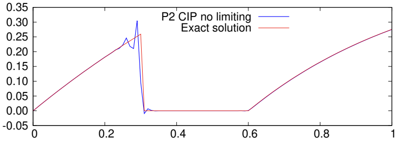
# Common challenges

- Physically meaningful numerical solution:
  bound-preserving, mass-conservative, ...

- Well-captured shocks and singularities:
  correct wave speed, as small as possible oscillation, ...

# Example


P2 Galerkin
Exact solution
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
-0.10
0
0.2
0.4
0.6
0.8
1


P2 CIP no limiting
Exact solution
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
0
0.2
0.4
0.6
0.8
1

# PDE model

Find $\Psi : D \times S^2 \to \mathbb{R}^+$ s.t.

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with non-negative inflow BC,
total and scattering cross sections $\sigma^t \geq \sigma^s \geq 0$ (can vary on $D$),
absorption section $\sigma^a = \sigma^t - \sigma^s \geq 0$.

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- Key properties:
  - > Positivity-preserving: $\Psi(\boldsymbol{x}, \Omega) \geq 0$

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  - $|\sigma^s| \to \infty \Rightarrow$ diffusion limit $\Psi^0$

## Short literature review

- $S_N$ for angular discretization

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- Main challenge: find a method with
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| | $\Psi \geq 0$ | AP | high-order | no osc. | conserv. | fast post-proc. |
|---|---|---|---|---|---|---|
| dG(0) + modif. | ✓ | ✓ | ✗ | ✓ | ✓ | - |
| dG(p) | ✗ | ✓ | ✓ | ✗ | ✓ | - |
| dG(p) + optim. | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ |
| cG | ✗ | ✓ | ✓ | ✗ | ✓ | - |
| cG + $h\Delta\Psi$ + rescaling | ✓ | ✓ | ✗ | ✓ | ✗ | - |

References: [Chandrasekhar, 50], [Larsen, Morel, Miller, 87], [Gosse, Toscani, 02], [Guermond, Kanschat, 10], [Buet, Després, Frank, 12], [Guermond, Popov, Ragusa, 20], [Yee, Olivier, Haut, Holec, Tomov, Maginot, 20]

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➤ oscillation-free ➤ conservative ➤ fast (linear complexity)

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A two-step post-process:

1. Local limiting: temper oscillation
   - > loop on all dofs:
   - > apply local limiter based on mass redistribution
2. Global limiting: impose global a priori bounds
   - > apply global limiter based on cut-off technique

$$\Omega \cdot \nabla_{\boldsymbol{x}} u + \sigma u = q \qquad \text{in } D \subset \mathbb{R}^d$$

with suitable BC, fixed $\Omega \in \mathbb{R}^d$, $d = 1, 2, 3$, $\sigma, q \geq 0$

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Solution method:

- stabilized high-order numerical method (e.g., edge stabilization/CIP [Burman, Hansbo, 04]) $\Rightarrow \{u_i\}_{i \in \mathcal{V}}$;

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  - estimate local bounds $\Rightarrow \{(u_i^{\max}, u_i^{\min})\}_{i \in \mathcal{V}}$
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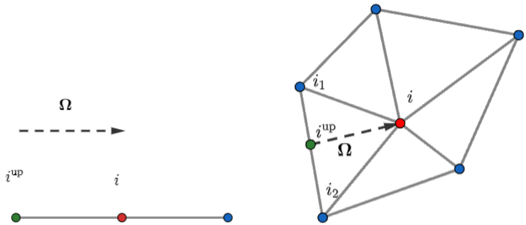
  - > estimate local bounds $\Rightarrow \{(u_i^{\max}, u_i^{\min})\}_{i \in \mathcal{V}}$
  - > apply local limiter $\Rightarrow \{\tilde{u}_i\}_{i \in \mathcal{V}}$
- Global limiting to guarantee positivity $\Rightarrow \{u_i^+\}_{i \in \mathcal{V}}$

Based on method of characteristics [Lathrop, 69];
$\sigma = const$ for simplicity

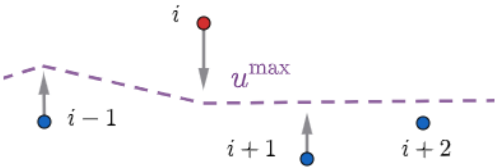
$$\begin{cases} \Omega \cdot \nabla_{\boldsymbol{x}} u + \sigma u = q \\ u|_{\partial D^-} = u^{\text{up}} \end{cases} \Leftrightarrow u(x) = u^{\text{up}} e^{\frac{\sigma}{|\Omega|}|x^{\text{up}} - x|} + \int_{x^{\text{up}}}^{x} \frac{q}{|\Omega|} e^{\frac{\sigma}{|\Omega|} s} \, \mathrm{d}s$$




- Upwinding node $i^{\text{up}}$ defined using local dof stencil $\mathcal{I}(i)$
- Maximizing/minimizing $q \Rightarrow$ local bound

Main steps (repeat a few times):

- loop on all dofs $i \in \mathcal{V}$:
  1. compute $\{u_i^{\max}, u_i^{\min}\}$
  2. apply local limiter on each dof $i \in \mathcal{V}$
     - ⋆ $u_i > u_i^{\max} \Rightarrow$ decrease $u_i$, increase $\{u_j\}_{j\in\mathcal{I}(i)}$
     - ⋆ $u_i < u_i^{\min} \Rightarrow$ increase $u_i$, decrease $\{u_j\}_{j\in\mathcal{I}(i)}$



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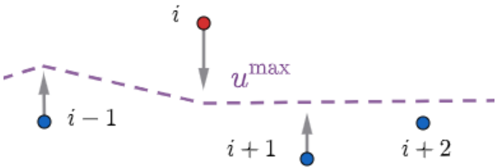
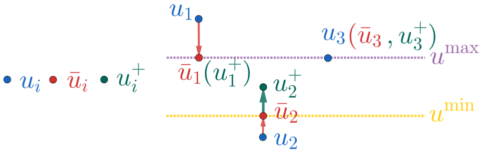



- Locally mass conservative
- Converging in a few number of iterations on all dofs

Main steps:

- set lower/upper bound to $u^{\min}$, $u^{\max}$;
- cut-off $\Rightarrow \{\bar{u}_i\}_{i\in\mathcal{V}}$;
- small modification on dofs based on $\sum_{i\in\mathcal{V}} m_i u_i \Rightarrow \{u_i^+\}_{i\in\mathcal{V}}$.



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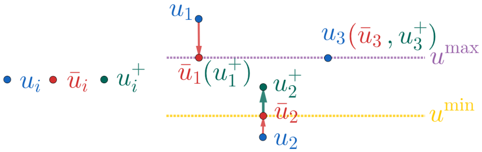
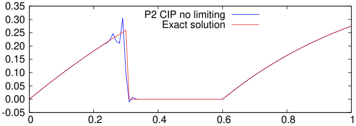


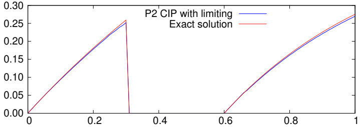

**Lemma (properties of global limiter)**

$u^{\min} \leq u_i^+ \leq u^{\max}, \qquad \sum_{i\in\mathcal{V}} m_i u_i^+ = \sum_{i\in\mathcal{V}} m_i u_i$

- $\Omega = 1$, $D = (0, 1)$, $u(0) = 0$, $q = O(1)$
  highly-contrasted $\sigma$ between 1 and $10^3$
- Simulation with $h \approx 2 \times 10^{-2}$, $\mathbb{P}_2$




(a) Galerkin + CIP




(b) Galerkin + CIP + limiting

- $\Omega = (1,0)$, $D = (0,1)^2$, $q = O(1)$
  highly-contrasted $\sigma$ between $1$ and $10^3$

| $\mathbb{P}_1$ | | | $\mathbb{P}_2$ | | | $\mathbb{P}_3$ | | |
|---|---|---|---|---|---|---|---|---|
| $I$ | $L^1$-Err | rate | $I$ | $L^1$-Err | rate | $I$ | $L^1$-Err | rate |
| 961 | 5.08E-02 | – | 1681 | 2.32E-02 | – | 961 | 4.12E-02 | – |
| 3721 | 2.34E-02 | 1.15 | 6561 | 1.04E-02 | 1.18 | 3721 | 1.96E-02 | 1.10 |
| 14641 | 9.62E-03 | 1.30 | 25921 | 3.74E-03 | 1.49 | 14641 | 7.08E-03 | 1.49 |
| 58081 | 3.18E-03 | 1.61 | 103041 | 1.09E-03 | 1.79 | 58081 | 1.71E-03 | 2.06 |
| 231361 | 8.28E-04 | 1.95 | 410881 | 4.64E-04 | 1.23 | 231361 | 4.18E-04 | 2.04 |

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1. Discretization:
   - angular: discrete ordinate/$S_N$:
     quadrature $\{\Omega_k, \mu_k\}_{k \in K}$ on unit sphere

$$\Omega \cdot \nabla_{\boldsymbol{x}} \Psi + \sigma^t \Psi = \frac{\sigma^s}{4\pi} \int_{S^2} \Psi + q$$

Main steps:

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   - space: Galerkin + CIP (numerically AP)

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   - space: Galerkin + CIP (numerically AP)
   - numerical solution: $\{\Psi_{k,h}\}_{k \in K}$, dofs $\{\Psi_{k,i}\}_{k \in K, i \in \mathcal{V}}$

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2. Source iteration (on $n$):
   - $\Omega_k \cdot \nabla_{\boldsymbol{x}} \Psi_{k,h}^{n+1} + \sigma^t \Psi_{k,h}^{n+1} = \frac{\sigma^s}{4\pi} \sum_l \mu_l \Psi_{l,h}^n + q := q^n$

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   - > local bounds estimator $\Rightarrow \{(\Psi_{k,i}^{\max}, \Psi_{k,i}^{\min})\}_{k,i}$ using $q^n$
     local limiting $\Rightarrow \{\tilde{\Psi}_{k,i}^{n+1}\}_{k,i}$

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   local limiting $\Rightarrow \{\tilde{\Psi}_{k,i}^{n+1}\}_{k,i}$
   > global limiting with $(\Psi^{\min}, \Psi^{\max}) = (0, +\infty) \Rightarrow \{\Psi_{k,i}^{n+1,+}\}_{k,i}$

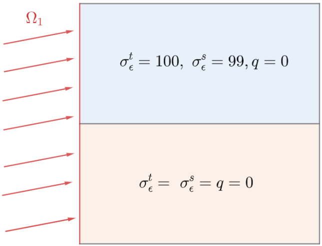
- $\sigma^t = \sigma^s = \varepsilon^{-1}$, $q = 2\varepsilon\pi^2 \sin(\pi x)\sin(\pi y)/3$, zero BC, $\psi^0 = \lim_{\varepsilon\to 0} \Psi = \sin(\pi x)\sin(\pi y)$
- $\mathbb{P}_1$, $h \gg \varepsilon$, $\bar{\Psi}_h$ as average of $\Psi_{k,h}$ over $k$
- convergence $\|\bar{\Psi}_h - \psi^0\|$ in $L^2$- and $H^1$-norms

Table 6.2: Diffusion limit. Convergence test with respect to the mesh-size and $\epsilon$.

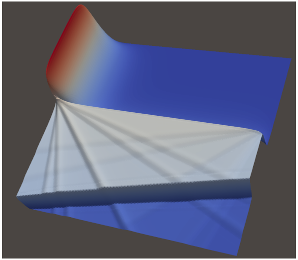
| $\epsilon$ | I | rel($\|\boldsymbol{e}\|_{L^2}$) | rate | rel($\|\nabla\boldsymbol{e}\|_{L^2}$) | rate |
|---|---|---|---|---|---|
| $10^{-3}$ | 140 | 3.48E-02 | – | 7.57E-02 | – |
| | 507 | 5.19E-03 | 2.96 | 1.91E-02 | 2.14 |
| | 1927 | 2.35E-03 | 1.18 | 5.88E-03 | 1.77 |
| | 7545 | 2.91E-03 | -.31 | 2.32E-03 | 1.36 |
| | 29870 | 3.05E-03 | -.07 | 1.44E-03 | 0.69 |
| $10^{-4}$ | 140 | 1.52E-02 | – | 3.92E-02 | – |
| | 507 | 3.39E-03 | 2.33 | 1.20E-02 | 1.84 |
| | 1927 | 6.35E-04 | 2.51 | 4.23E-03 | 1.56 |
| | 7545 | 1.82E-04 | 1.83 | 1.19E-03 | 1.86 |
| | 29870 | 2.70E-04 | -.57 | 3.14E-04 | 1.93 |

| $\epsilon$ | I | rel($\|\boldsymbol{e}\|_{L^2}$) | rate | rel($\|\nabla\boldsymbol{e}\|_{L^2}$) | rate |
|---|---|---|---|---|---|
| $10^{-5}$ | 140 | 1.25E-02 | – | 2.24E-02 | – |
| | 507 | 3.16E-03 | 2.13 | 6.98E-03 | 1.81 |
| | 1927 | 7.66E-04 | 2.12 | 2.65E-03 | 1.45 |
| | 7545 | 1.70E-04 | 2.21 | 7.11E-04 | 1.93 |
| | 29870 | 2.81E-05 | 2.62 | 2.38E-04 | 1.59 |
| $10^{-6}$ | 140 | 1.23E-02 | – | 1.95E-02 | – |
| | 507 | 3.14E-03 | 2.12 | 5.75E-03 | 1.90 |
| | 1927 | 7.84E-04 | 2.08 | 1.98E-03 | 1.60 |
| | 7545 | 1.92E-04 | 2.06 | 7.06E-04 | 1.51 |
| | 29870 | 4.59E-05 | 2.08 | 2.35E-04 | 1.60 |

- $\Psi(\boldsymbol{x},\Omega) = \begin{cases} 1 & \text{if } \boldsymbol{n}(\boldsymbol{x})\cdot\Omega < 0 \text{ and } \Omega = \Omega_1 \\ 0 & \text{otherwise} \end{cases}$
- $h \approx 2.6 \times 10^{-3}$, $\max_{\boldsymbol{x}\in D} \sigma^s \approx 10^2$, $S_6$ (few angulars)

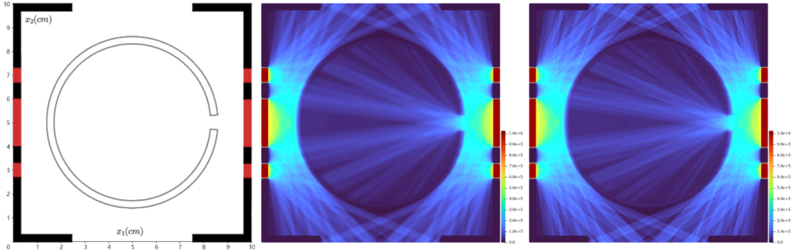



(a) geometry & parameters



(b) $\mathbb{P}_1$, $\bar{\Psi}_h$

Figure 6.7: Hohlraum problem. Left: geometry of the problem. Center, scalar flux, $\overline{\psi}_h$, $\mathbb{P}_1$, 682261 grid points, $S_{12}$ quadrature. Right, scalar flux, $\overline{\psi}_h$, $\mathbb{P}_3$, 864754 grid points, $S_{12}$ quadrature.



Thank you for your attention