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From Local to Global: Multiscale Localized Reduced Basis Methods for Neutron Transport

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Motivation

Setting:

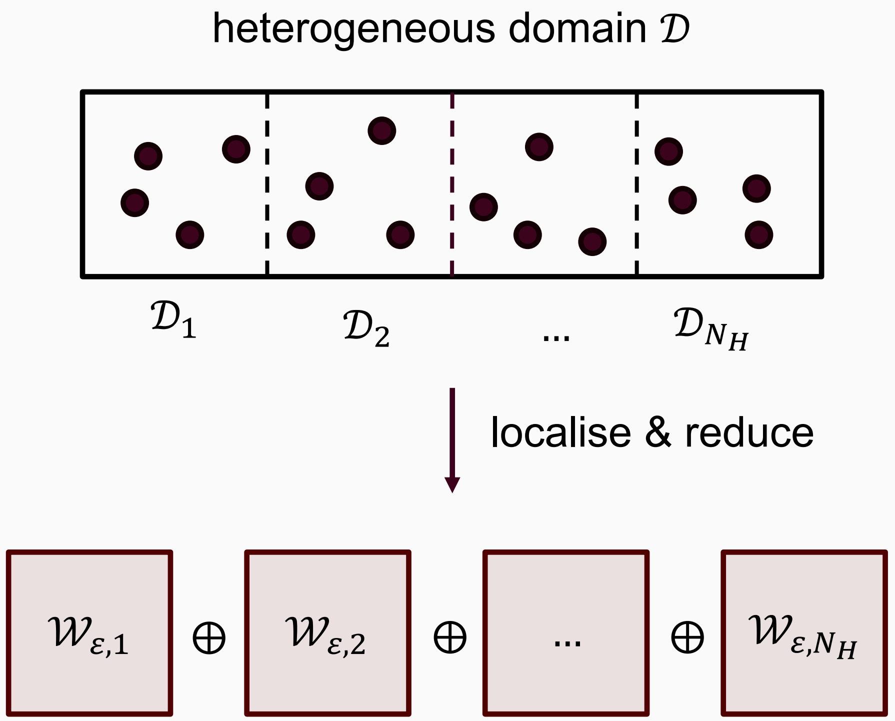
Stationary neutron transport on domains with many small inclusions or, in general, with parametrized heterogeneities.

Target:

Many-query problems where geometry and cross sections vary independently per subdomain: a large dimensional parameter space in which *global* reduced basis is inefficient

Idea:

Build low-dimensional local spaces per subdomain, coupled through the DG numerical flux, i.e., build localized reduced bases (LRB).

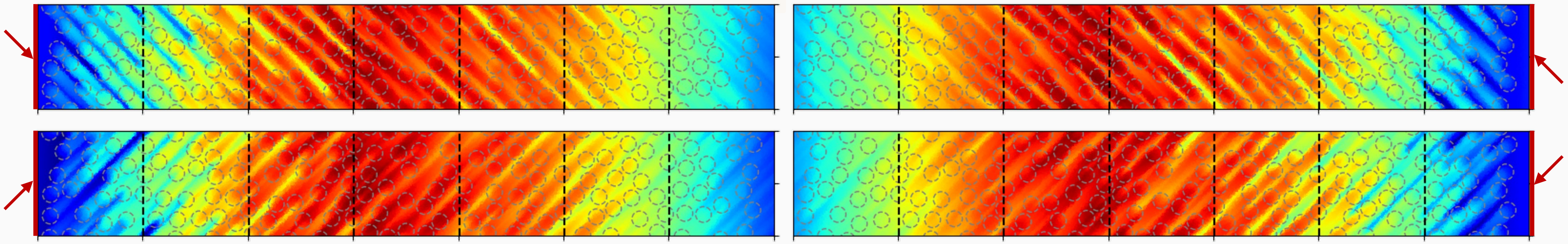


The Neutron Transport Problem

Mono-energetic, steady state, heterogeneous (possibly multiplying) medium on the phase space $\mathcal{D}\times\mathcal{S}^2$, with inflow/outflow split $\boldsymbol{\partial}^{\pm}\mathcal{D}$ and inflow data $\Psi(\mathbf{x},\boldsymbol{\Omega}) = \Psi^{\mathrm{inc}}(\mathbf{x},\boldsymbol{\Omega})$ on $\boldsymbol{\partial}^{-}\mathcal{D}$

$$\underbrace{\boldsymbol{\Omega}\cdot\nabla_{\mathbf{x}}\Psi}_{\text{streaming}} + \underbrace{\sigma_t\Psi}_{\text{removal}} - \underbrace{\frac{\sigma_s+\nu\sigma_f}{4\pi}\int_{\mathcal{S}^2}\Psi\,\mathrm{d}\boldsymbol{\Omega}'}_{\text{scattering + fission}} = \underbrace{\frac{Q}{4\pi}}_{\text{source}}$$

$\partial_1^-\mathcal{D}$ $\mathcal{D}\times\boldsymbol{\Omega}_1 = \mathcal{D}\times(1/\sqrt{3},-1/\sqrt{3},\pm1/\sqrt{3})$ $\mathcal{D}\times\boldsymbol{\Omega}_3 = \mathcal{D}\times(-1/\sqrt{3},1/\sqrt{3},\pm1/\sqrt{3})$ $\partial_2^-\mathcal{D}$



$\partial_2^-\mathcal{D}$ $\mathcal{D}\times\boldsymbol{\Omega}_2 = \mathcal{D}\times(1/\sqrt{3},1/\sqrt{3},\pm1/\sqrt{3})$ $\mathcal{D}\times\boldsymbol{\Omega}_4 = \mathcal{D}\times(-1/\sqrt{3},-1/\sqrt{3},\pm1/\sqrt{3})$ $\partial_4^-\mathcal{D}$

High-fidelity Model: Discrete Ordinates in Angle

Replace the angular variable by a quadrature on $\mathcal{S}^2$: $\{(\mathbf{\Omega}_{\mathrm{d}}, \omega_{\mathrm{d}})\}_{\mathrm{d}=1}^{N_\Omega}$, $\sum_{\mathrm{d}=1}^{N_\Omega} \omega_{\mathrm{d}} = 4\pi$ employing N_Ω discrete ordinates. For example, level symmetric or Lebedev.

The angular collocation turns the integro-differential equation into a coupled system of *advection-reaction* partial differential equations, one per direction:

$$\mathbf{\Omega}_{\mathrm{d}} \cdot \nabla_{\mathbf{x}} \Psi_{\mathrm{d}} + \sigma_t \Psi_{\mathrm{d}} - \frac{\sigma_s + \nu\sigma_f}{4\pi} \Phi = \frac{Q}{4\pi}, \qquad \Phi = \sum_{\mathrm{d}'=1}^{N_\Omega} \omega_{\mathrm{d}'} \Psi_{\mathrm{d}'}$$

- each equation has a constant transport direction $\mathbf{\Omega}_{\mathrm{d}}$
- directions couple through the scattering term $\Phi = \sum_{\mathrm{d}'=1}^{N_\Omega} \omega_{\mathrm{d}'} \Psi_{\mathrm{d}'}$

High-fidelity Model: Upwind DG in Space

Discretization in space uses a broken piecewise-affine space $\mathcal{W}_h = \mathcal{V}_h(\mathcal{D})^{N_\Omega}$ on a mesh $\mathcal{T}_h$ resolving the material interfaces. Here we assume $\mathcal{V}_h(\mathcal{D}) = \{\varphi \in L^2(\mathcal{D}) : \varphi|_K \in \mathbb{P}^{\mathrm{n}}(K)\ \forall K \in \mathcal{T}_h\}$ and $\dim \mathcal{V}_h(\mathcal{D}) = N_h \ \longrightarrow \mathcal{N} = N_\Omega N_h$

Employing a stable upwind DG scheme allows to naturally handle $\sigma_t, \sigma_s, \sigma_f$ and Q with parametric dependencies and discontinuities across interfaces. The upwind numerical flux is defined by

$$\hat{\mathrm{u}}_{\mathrm{d}} = \begin{cases} \mathrm{u}_d|_E \ , & \boldsymbol{\Omega}_{\mathrm{d}} \cdot \mathbf{n}_E \geq 0 \qquad \text{outflow: own value,} \\ \mathrm{u}_d|_{E'} \, , & \boldsymbol{\Omega}_{\mathrm{d}} \cdot \mathbf{n}_E < 0 \qquad \text{inflow: upwind neighbor,} \\ 0 \, , & \boldsymbol{\Omega}_{\mathrm{d}} \cdot \mathbf{n}_E < 0 \qquad \text{inflow: physical boundary} \end{cases}$$

where E is the current element/subdomain, E' its neighbor across the face, and $\mathbf{n}_E$ the outward normal.

Discrete Weak Formulation

The discrete weak problem can be written in terms of linear and bilinear forms, introducing ℓ_h and $a_h = t_h - b_h$. Here $t_h, b_h\colon \mathcal{W}_h \times \mathcal{W}_h \to \mathbb{R}$ are the *transport* and the *scattering-fission* bilinear forms, defined by

$$t_h(\mathbf{u},\mathbf{v}) = \sum_{\mathrm{d}=1}^{N_\Omega} \omega_\mathrm{d} \sum_{K\in\mathcal{T}_h} \int_K \sigma_t \mathrm{u}_\mathrm{d} \mathrm{v}_\mathrm{d} d\mathbf{x} - \int_K \mathrm{u}_\mathrm{d}(\mathbf{\Omega}_\mathrm{d} \cdot \nabla_\mathbf{x} \mathrm{v}_\mathrm{d}) d\mathbf{x} + \int_{\partial K} (\mathbf{\Omega}_\mathrm{d} \cdot \mathbf{n}_E) \hat{\mathrm{u}}_\mathrm{d} \mathrm{v}_\mathrm{d} dS(\mathbf{x})$$

$$b_h(\mathbf{u},\mathbf{v}) = \int_\mathcal{D} \frac{\sigma_s + \nu\sigma_f}{4\pi} \Phi_\mathrm{u} \Phi_\mathrm{v} d\mathbf{x}, \qquad \Phi_\mathrm{u} = \sum_{\mathrm{d}'=1}^{N_\Omega} \omega_{\mathrm{d}'} \mathrm{u}_{\mathrm{d}'},\ \ \Phi_\mathrm{v} = \sum_{\mathrm{d}'=1}^{N_\Omega} \omega_{\mathrm{d}'} \mathrm{v}_{\mathrm{d}'}$$

and $\ell_h\colon \mathcal{W}_h \to \mathbb{R}$ is the *load* functional, including the source and the prescribed inflow terms

$$\ell_h(\mathbf{v}) = \sum_{\mathrm{d}=1}^{N_\Omega} \omega_\mathrm{d} \int_\mathcal{D} \frac{Q}{4\pi} \mathrm{v}_\mathrm{d} dx + \sum_{\mathrm{d}=1}^{N_\Omega} \omega_\mathrm{d} \int_{\partial_\mathrm{d}^- \mathcal{D}} |\mathbf{\Omega}_\mathrm{d} \cdot \mathbf{n}_E| \Psi^{\mathrm{inc}} \mathrm{v}_\mathrm{d} dS(\mathbf{x}), \qquad \partial_\mathrm{d}^- \mathcal{D} = \{\mathbf{x} \in \partial\mathcal{D} |\ \mathbf{\Omega}_\mathrm{d} \cdot \mathbf{n}_E(\mathbf{x}) < 0\}$$

Full order Sn-DG problem:

Find $\mathbf{\Psi}_h = \{\Psi_{h,\mathrm{d}}\}_{\mathrm{d}=1}^{N_\Omega} \in \mathcal{W}_h$ such that $a_h(\mathbf{\Psi}_h, \mathbf{v}_h) = \ell_h(\mathbf{v}_h)$ for all $\mathbf{v}_h \in \mathcal{W}_h$.

From Global to Local

The passage from *global* to *local* is obtained replacing the global high-fidelity space $\mathcal{W}_h$, with the direct a sum of local reduced basis spaces

$$\mathcal{W}_\varepsilon = \bigoplus_{i=1}^{N_H} \mathcal{W}_{\varepsilon,i} \subset \mathcal{W}_h \qquad \dim \mathcal{W}_\varepsilon = \sum_{i=1}^{N_H} \dim \mathcal{W}_{\varepsilon,i} = \sum_{i=1}^{N_H} N_{\varepsilon,i} \ll \mathcal{N}$$

- each $\mathcal{W}_{\varepsilon,i}$ must capture the transport dynamics, the local heterogeneities and the coupling to neighbors
- coupling between subdomains happens through the upwind flux only, making the reduced problem an exact Galerkin restriction of the high-fidelity scheme

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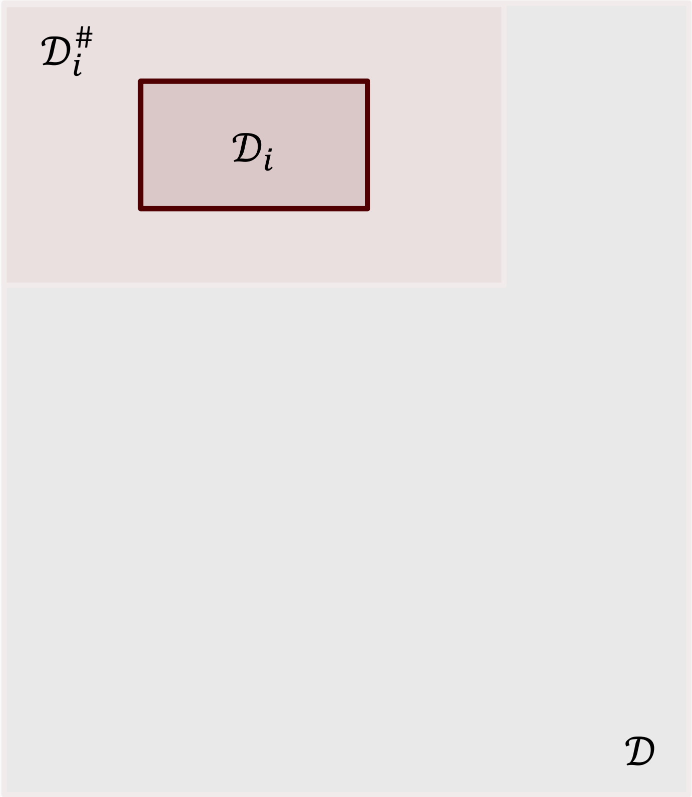
Two questions

(i) How do we construct good approximation spaces? **(ii)** Can we certify the error?

The *optimal local approximation* theory from Babuška–Lipton and Smetana–Patera is adopted to a *non-self-adjoint, non-coercive* transport setting.

Coarse Decomposition and Oversampling

- given the non-overlapping coarse partition $\{\mathcal{D}_i\}_{i=1}^{N_H}$, the oversampling regions $\mathcal{D} \supset \mathcal{D}_i^{\#} \supset \mathcal{D}_i$ are selected to buffer the artificial boundary effects



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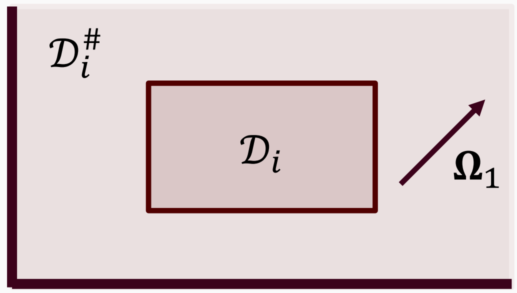
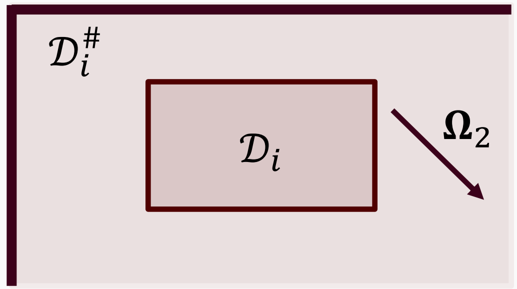
- inflow boundaries are *per ordinate,* rotating with $\mathbf{\Omega}_{\mathrm{d}}$, specifically, $\partial_{\mathrm{d}}^{-} E = \{\mathbf{x} \in \partial E \mid \mathbf{\Omega}_{\mathrm{d}} \cdot \mathbf{n}_E(\mathbf{x}) < 0\}$



$\mathbf{\Omega}_1 = (1/\sqrt{3}, 1/\sqrt{3})$: inflow = left + bottom



$\mathbf{\Omega}_2 = (1/\sqrt{3}, -1/\sqrt{3})$: inflow = left + top

— inflow boundary $\partial_{\mathrm{d}}^{-} \mathcal{D}_i^{\#}$

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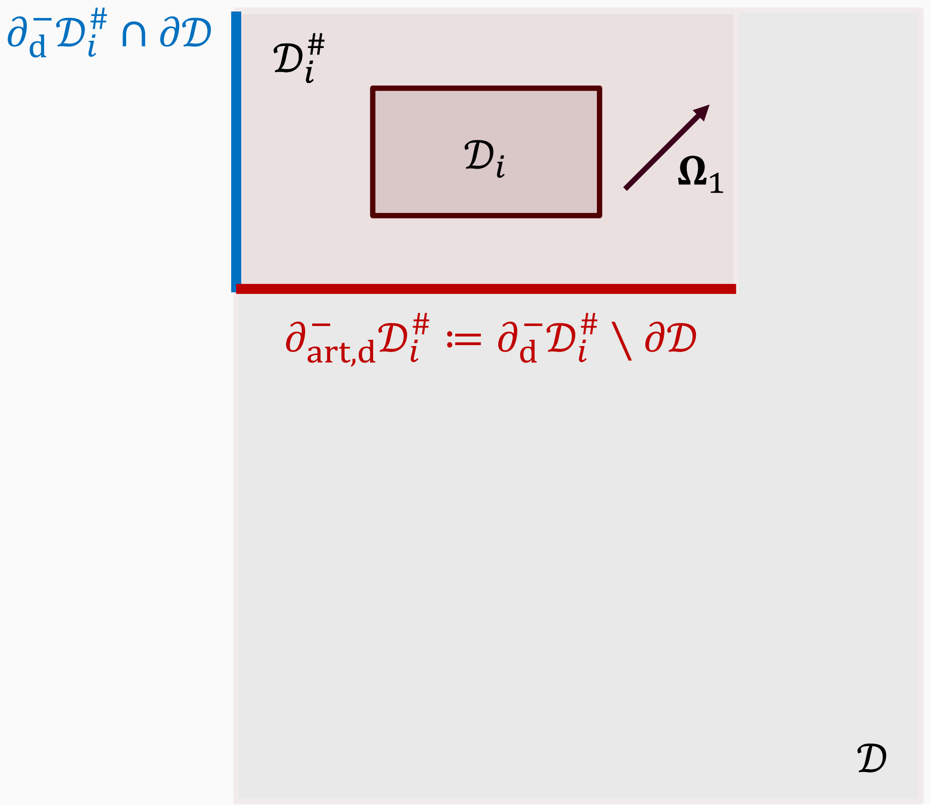
- inflow boundaries of $\mathcal{D}_i^\#$ split into *physical* b. (on $\partial\mathcal{D}$), carrying the boundary data Ψ^inc, and *artificial* b. ($\boldsymbol{\partial}_\mathrm{art}^-\mathcal{D}_i^\#$), carrying transmission data



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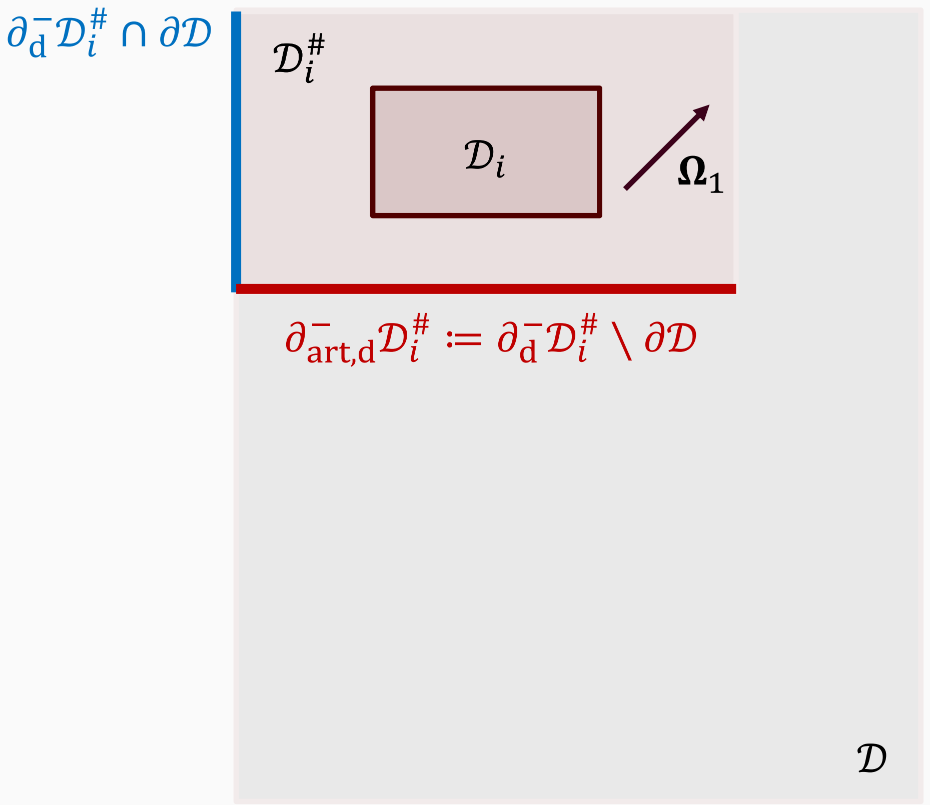
Finally, we introduce the transport-weighted inflow-trace inner product:

$$(\mathbf{u}, \mathbf{v})_{\boldsymbol{\partial}_{\mathrm{art}}^{-} E} = \sum_{\mathrm{d}=1}^{N_\Omega} \omega_{\mathrm{d}} \int_{\partial_{\mathrm{d}}^{-} E} |\mathbf{\Omega}_{\mathrm{d}} \cdot \mathbf{n}_E| \, \mathrm{u}_{\mathrm{d}} \mathrm{v}_{\mathrm{d}} dS(\mathbf{x})$$



The Local Transfer Operators

Consider the homogenous local lift $\boldsymbol{\Psi}_{h,i}^{\text{hom}} \in \mathcal{W}_h(\mathcal{D}_i^{\#})$ mapping the inflow-trace $\boldsymbol{\delta} \in \mathcal{W}_h(\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i^{\#})$ to a space-angle state defined on the full oversampling region. The state solves the following Sn–DG problem:

$$-\int_K \Psi_{h,i,\text{d}}^{\text{hom}}\, \boldsymbol{\Omega}_\text{d} \cdot \nabla_{\mathbf{x}} \zeta_h d\mathbf{x} + \int_{\partial K} (\boldsymbol{\Omega}_\text{d} \cdot \mathbf{n}_K)\, \widehat{\Psi}_{h,i,\text{d}}^{\text{hom}}\, \zeta_h dS(\mathbf{x}) + \int_K \sigma_t\, \Psi_{h,i,\text{d}}^{\text{hom}} \zeta_h d\mathbf{x} - \int_K \frac{\sigma_s - \nu\sigma_f}{4\pi}\, \Phi_{h,i}^{\text{hom}} \zeta_h d\mathbf{x} = 0,$$

with $\Phi_{h,i}^{\text{hom}} = \sum_{\text{d}=1}^{N_\Omega} \omega_\text{d} \Psi_{h,i,\text{d}}^{\text{hom}}$, zero source, zero physical inflow, and $\boldsymbol{\Psi}_{h,i}^{\text{hom}}|_{\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i^{\#}} = \boldsymbol{\delta}$.

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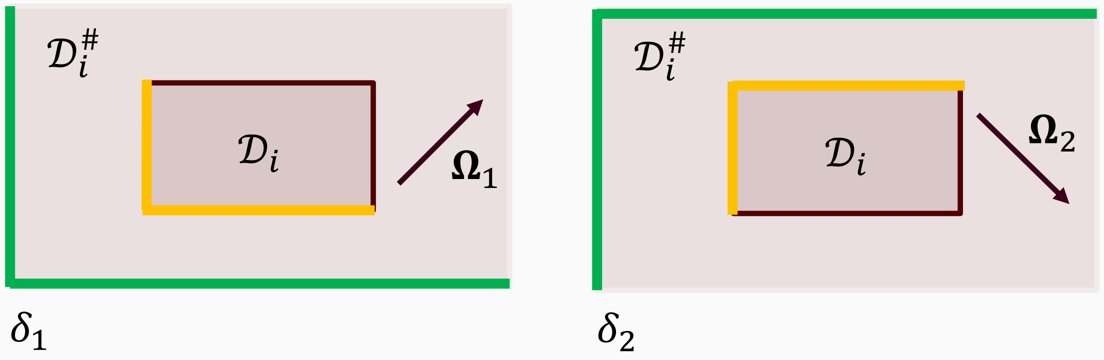
Boundary transfer map: $\mathcal{G}_i$

$\mathcal{G}_i \boldsymbol{\delta} = \boldsymbol{\Psi}_{h,i}^{\text{hom}}|_{\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i}$ (inflow trace on the target)



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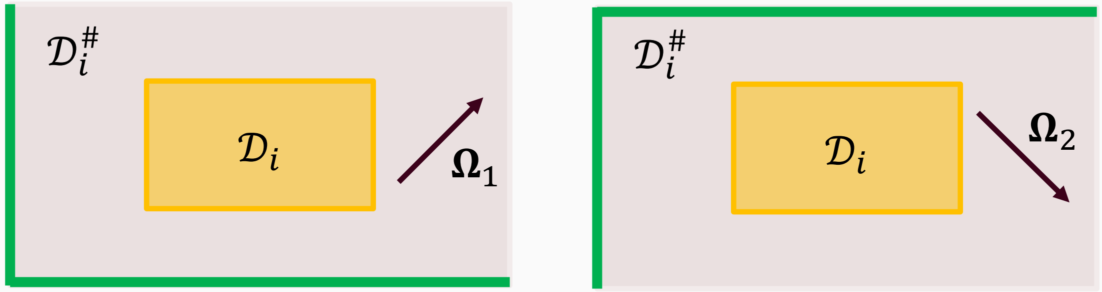

δ_1 δ_2

Volume transfer map: $\mathcal{H}_i$

$\mathcal{H}_i\boldsymbol{\delta} = \boldsymbol{\Psi}^{\text{hom}}_{h,i}|_{\mathcal{D}_i}$ (angular flux inside $\mathcal{D}_i$)

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The spectrum of $\mathcal{G}_i$ is analyzed to extract optimal boundary modes; $\mathcal{H}_i$ is used to transport them into the volume.

Optimal Local Approximation Spaces

The worst-case boundary transfer error on a boundary space $\tilde{\mathcal{U}}$ is:

$$d_{\mathcal{G}_i}(\tilde{\mathcal{U}}) = \sup_{\boldsymbol{\delta}\neq 0} \inf_{\boldsymbol{u}\in\tilde{\mathcal{U}}} \frac{\|\mathcal{G}_i\boldsymbol{\delta} - \boldsymbol{u}\|_{\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i}}{\|\boldsymbol{\delta}\|_{\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i^{\#}}}.$$

The Kolmogorov-optimal space minimizing this distance is spanned by the dominant transfer modes obtained from the singular value decomposition of $\mathcal{G}_i$ or, equivalently, from the eigenvalue problem for $\mathcal{G}_i^*\mathcal{G}_i$

$$\left(\mathcal{G}_i\boldsymbol{\delta}_{i,j}, \mathcal{G}_i\boldsymbol{\eta}\right)_{\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i} = \lambda_{i,j}\left(\boldsymbol{\delta}_{i,j}, \boldsymbol{\eta}\right)_{\boldsymbol{\partial}_{\text{art}}^{-}\mathcal{D}_i^{\#}}, \qquad \lambda_{i,1} \geq \cdots \geq \lambda_{i,j} \geq \cdots \geq 0,$$

the optimal error is given by $\sqrt{\lambda_{i,N_{\varepsilon,i}+1}}$, i.e., the first discarded singular value.

Homogenous modes

$\boldsymbol{\chi}_{i,j}^{\text{hom}} = \mathcal{H}_i\boldsymbol{\delta}_{i,j}$ maps the boundary modes to the homogeneous volume basis functions.

Randomized Construction

- The exact singular value decomposition would require one local transport solve per artificial boundary DoF, most of which are discharged.
- Instead, use a randomized range finder (Halko–Martinsson–Topp, Buhr–Smetana)

Algorithm (target dimension N, oversampling p, $S = N + p$)

1. draw S Gaussian random inflow samples $\boldsymbol{\delta}^{(s)}$
2. compute one forward solve for each: $\boldsymbol{\beta}^{(s)} = \mathcal{G}_i \boldsymbol{\delta}^{(s)}$, $\boldsymbol{\chi}^{(s)} = \mathcal{H}_i \boldsymbol{\delta}^{(s)}$
3. eigen-decompose the $S{\times}S$ Gram matrix $G_{s,\ell} = \left(\boldsymbol{\beta}^{(s)}, \boldsymbol{\beta}^{(\ell)}\right)_{\boldsymbol{\partial}_{\mathrm{art}}^{-}\mathcal{D}_i}$
4. assemble nearly-optimal boundary and volume modes

The cost of the algorithm is of S solves instead of $\dim \mathcal{W}_h(\boldsymbol{\partial}_{\mathrm{art}}^{-}\mathcal{D}_i^{\#})$. It produces near optimal solutions with high probability.

Source and Physical Inflow: Particular Modes

- Homogeneous modes described so far carry only *inter-subdomain transmission.*
- We still need the response to the volumetric source Q and to the physical inflow Ψ^{inc}.

For this purpose, consider the Sn-DG problem:

$$-\int_K \Psi_{h,i,\mathrm{d}}^{\mathrm{par}}\, \mathbf{\Omega}_\mathrm{d} \cdot \nabla_\mathbf{x} \zeta_h d\mathbf{x} + \int_{\partial K} (\mathbf{\Omega}_\mathrm{d} \cdot \mathbf{n}_K)\, \widehat{\Psi}_{h,i,\mathrm{d}}^{\mathrm{par}}\, \zeta_h dS(\mathbf{x}) + \int_K \sigma_t\, \Psi_{h,i,\mathrm{d}}^{\mathrm{par}} \zeta_h d\mathbf{x} - \int_K \frac{\sigma_s - \nu\sigma_f}{4\pi}\, \Phi_{h,i}^{\mathrm{par}} \zeta_h d\mathbf{x}$$
$$= \int_K \frac{Q}{4\pi} \zeta_h d\mathbf{x} + \int_{\partial_\mathrm{d}^- \mathcal{D} \cap \partial K} |\mathbf{\Omega}_\mathrm{d} \cdot \mathbf{n}_E|\, \Psi^{\mathrm{inc}} \zeta_h dS(\mathbf{x}),$$

with $\Phi_{h,i}^{\mathrm{par}} = \sum_{\mathrm{d}=1}^{N_\Omega} \omega_\mathrm{d} \Psi_{h,i,\mathrm{d}}^{\mathrm{par}}$, and zero artificial inflow boundary conditions, i.e., $\mathbf{\Psi}_{h,i}^{\mathrm{par}}|_{\boldsymbol{\partial}_{\mathrm{art}}^- \mathcal{D}_i^\#} = \mathbf{0}$.

Particular data response mode

$\chi_i^{\mathrm{par}} = \mathbf{\Psi}_{h,i}^{\mathrm{par}}|_{\mathcal{D}_i}$ defines the local lift on $\mathcal{D}_i$ of the actual source and physical inflow data.

The Coarse-grid Reduced Problem

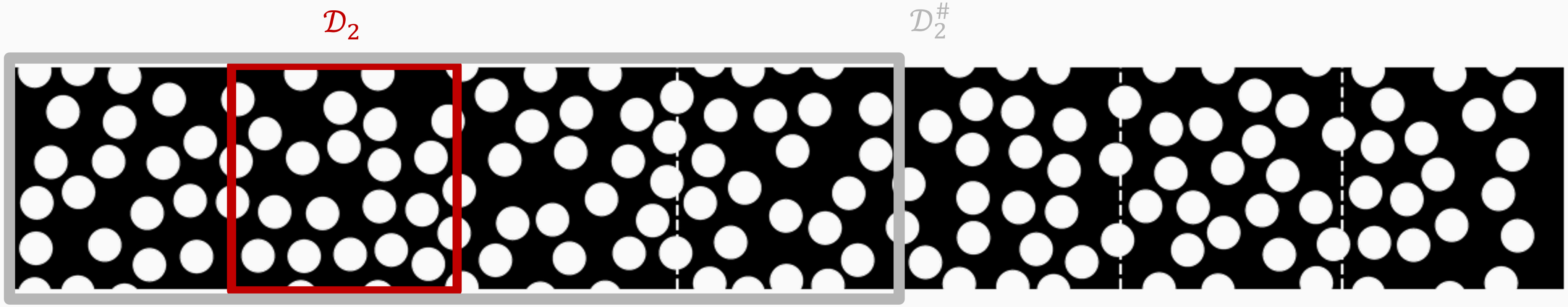
Assemble the local reduced spaces: $\mathcal{W}_{\varepsilon,i} = \mathrm{span}\{\chi_{i,j}^{\mathrm{hom}}\} \oplus \mathrm{span}\{\chi_i^{\mathrm{par}}\}$, for every $i \in N_H$.

Gluing together the local spaces gives $\mathcal{W}_\varepsilon \subset \mathcal{W}_h$. The reduced problem is therefore a Galerkin restriction of the full-order problem with the same a_h and ℓ_h:

Reduced problem

Find $\boldsymbol{\Psi}_\varepsilon = \{\Psi_{\varepsilon,\mathrm{d}}\}_{\mathrm{d}=1}^{N_\Omega} \in \mathcal{W}_\varepsilon$ such that $a_h(\boldsymbol{\Psi}_\varepsilon, \boldsymbol{\xi}) = \ell_h(\boldsymbol{\xi})$ for all $\boldsymbol{\xi} \in \mathcal{W}_\varepsilon$.

A Heterogenous Benchmark



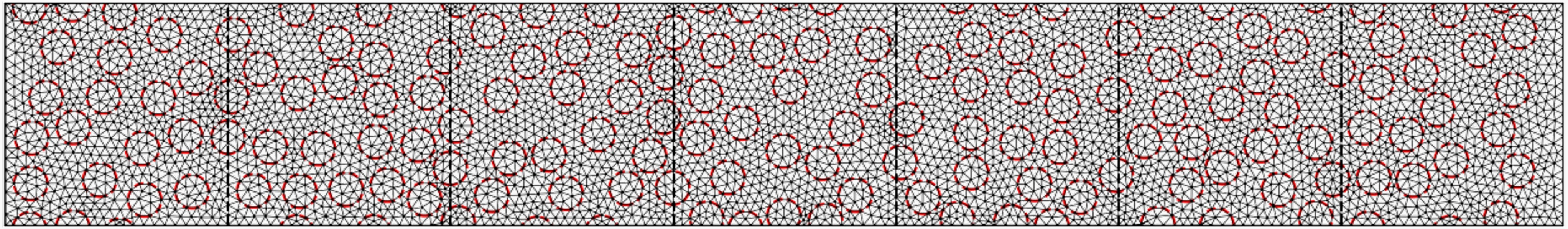
- $\mathcal{D}$=[0,7]×[0,1], N_H=7 unit subdomains with oversampling R=2
- 140 non overlapping, reactive, circular inclusions
- top and bottom boundaries are periodically identified
- constant inflow Ψ^{inc} on $\boldsymbol{\partial}^{-}\mathcal{D}$ and $Q = 0$
- $N_\Omega = 4$ directions, $N_{\mathbf{x}} = 91{,}284$ for a total of $\mathcal{N} = 365{,}136$

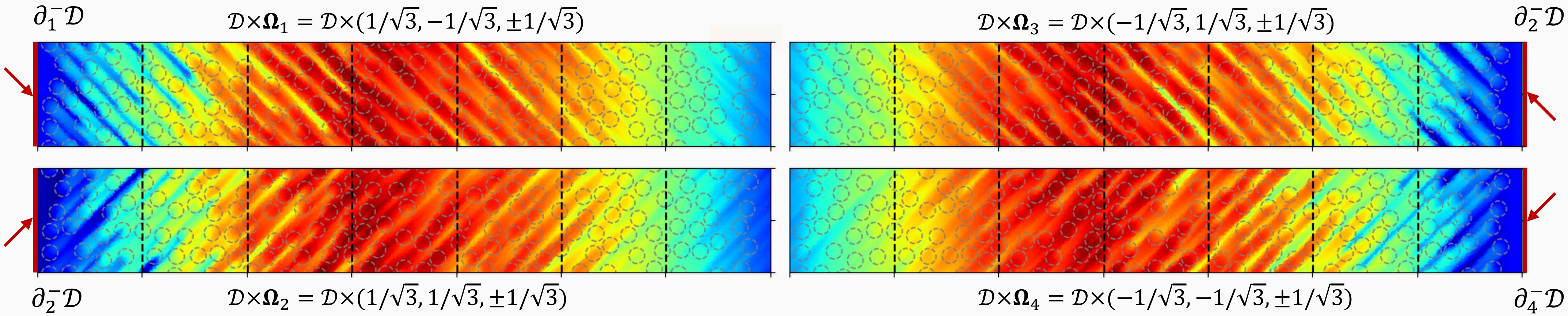
	background	inclusions
σ_t	0.1.	7.0
$\sigma_s + \nu\sigma_f$	0.0	7.2

inclusions are locally multiplying

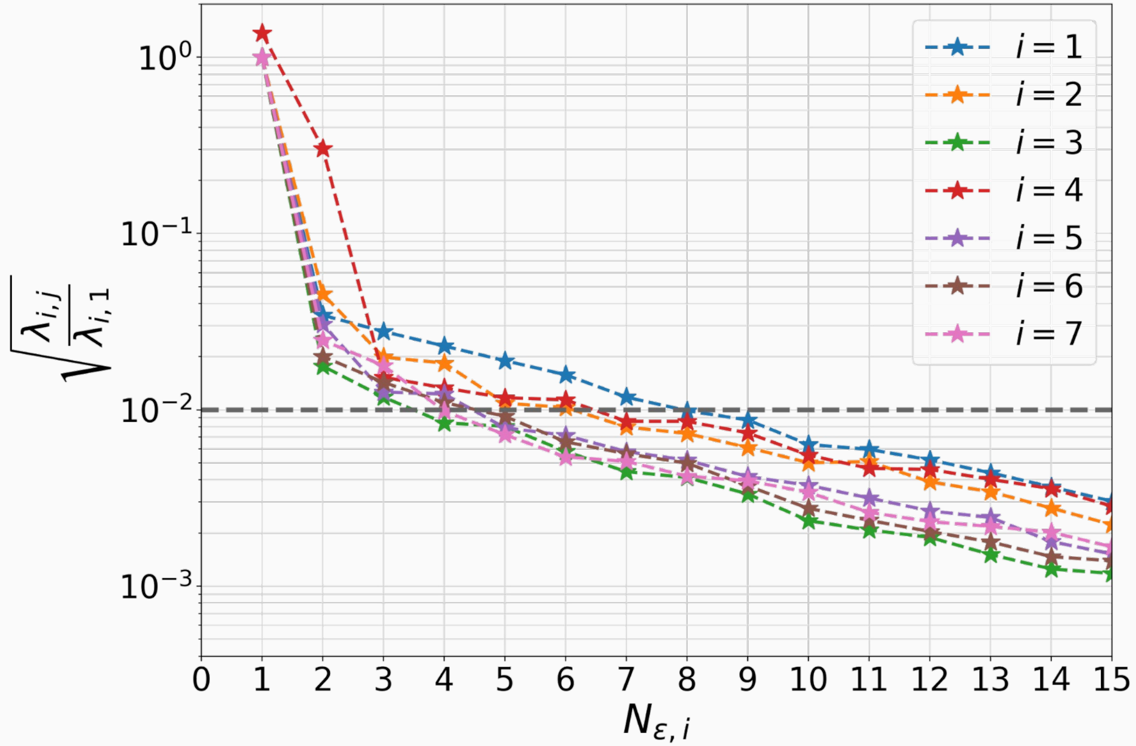
Full Order Reference Solution

fine DG triangulation resolving inclusions and coarse interface





Decay of the Local Transfer Spectra

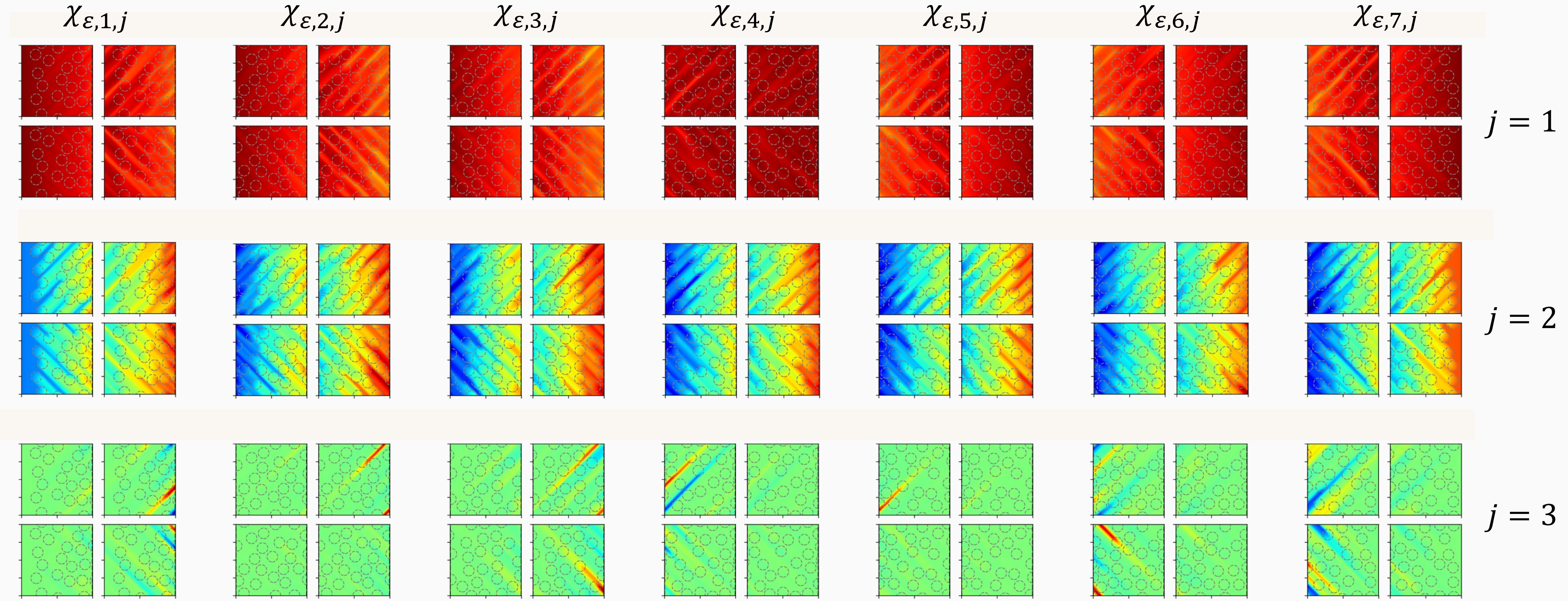


- singular values decay on all seven subdomains, few local mode suffice for an accurate reconstruction
- decay are slightly non uniform: more heterogenous and directional buffers decay more slowly

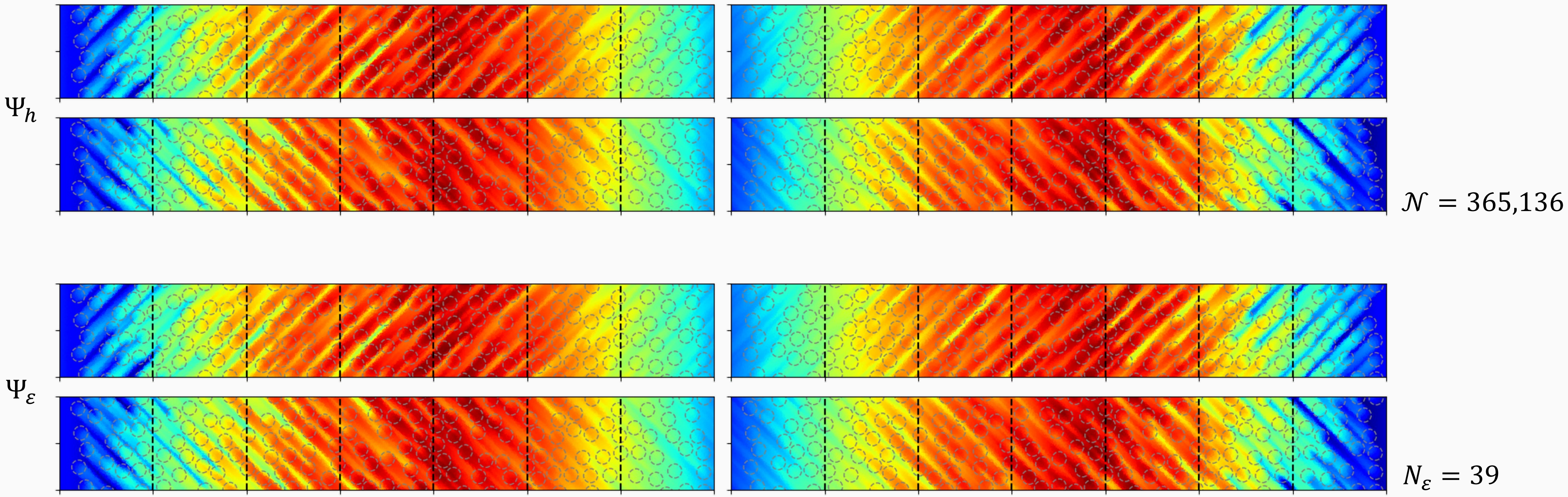
Working conjecture for the coercive regime

$$\sqrt{\lambda_{i,N_{\varepsilon,i}}} \lesssim e^{-\tau_i^{\min}} \rho_i(c)^{N_{\varepsilon,i}} + e^{-\frac{\alpha'\delta}{L_{\mathrm{diff}}}} e^{-\gamma N_{\varepsilon,i}^{1/(d-1)}}$$

Optimal Local Basis



Localized Reduced Basis Solution



relative error $= 1.9127 \times 10^{-4}$

$\times 661$ online speed-up

Summary and Outlook

What we have

- optimal local approximation expanded to non-coercive Sn-DG transport
- local spaces coupled purely by the upwind fluxes, and exact Galerkin restriction
- a priori (transfer spectra) and a posteriori (data + skeleton) error control
- benchmark with a clear transport spectra decay in strongly heterogeneous, locally multiplying media

Where we are going

- multi-group energy dependence
- parametric cross sections varying per subdomain
- parameter-robust local spaces via spectral-greedy
- model-free basis generation for random geometry

From local to global: modular reduced models for particle transport in random heterogeneous media.

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THANK YOU

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