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Localized Reduced Basis for Neutron Diffusion

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Eigenvalue Problem – Strong Formulation

Consider the neutron diffusion generalized eigenvalue problem:

Find the dominant eigen-couple $\phi : \Omega \rightarrow \mathbb{R}$, $k_{\text{eff}} \in \mathbb{R}^+$, with $\|\phi\|_{L^2(\Omega)} = 1$, such that

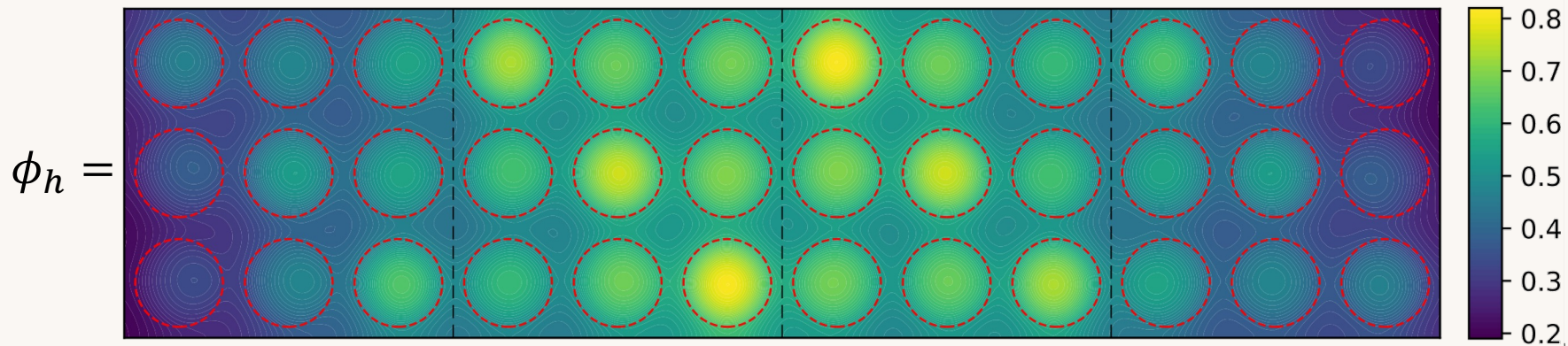
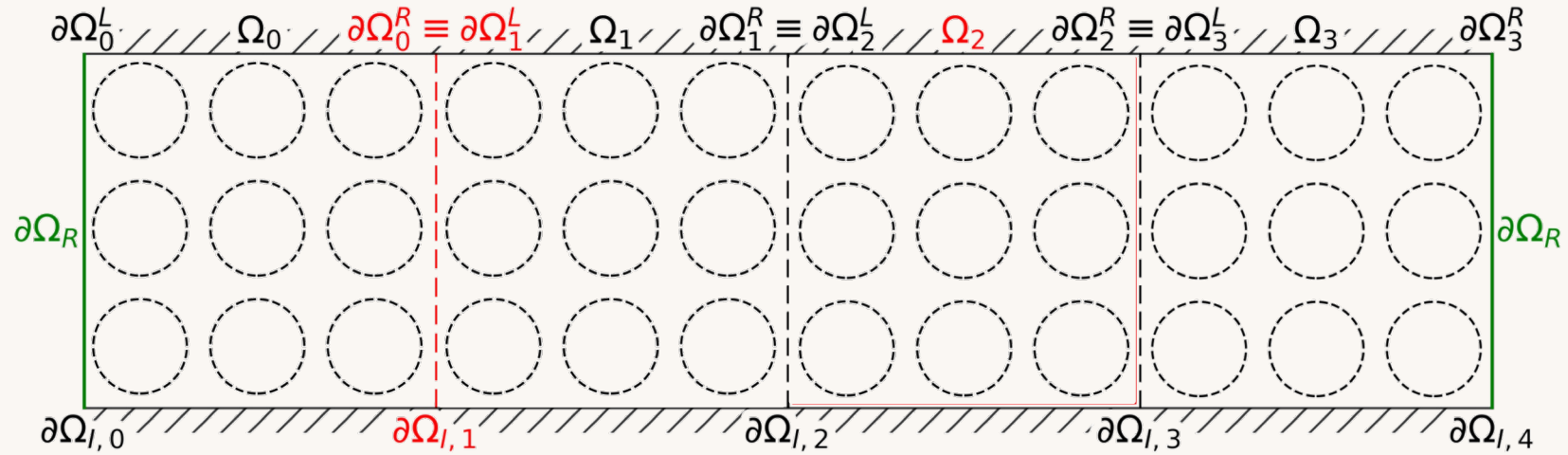
$$\begin{cases} -\nabla \cdot (D_c \nabla \phi) + \Sigma_a \phi = 1/k_{\text{eff}} \Sigma_f \phi & \text{in } \Omega, \\ -D_c \nabla \phi \cdot \mathbf{n} = \varrho \phi & \text{on } \partial\Omega_R, \\ -D_c \nabla \phi \cdot \mathbf{n} = 0 & \text{on } \partial\Omega_N, \end{cases}$$

where:

- $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$ is a compact and decomposable Lipschitz domain
- $\partial\Omega = \partial\Omega_R \cup \partial\Omega_N$, $\partial\Omega_R \cap \partial\Omega_N = \emptyset$ is the outer boundary of the domain
- $D_c, \Sigma_a, \Sigma_f : \Omega \rightarrow \mathbb{R}^+$ are heterogeneous material properties (with $D_c, \Sigma_a \geq 0$)
- $\varrho : \partial\Omega_R \rightarrow \mathbb{R}^+$ is the Robin boundary coefficient, or albedo
- $\mathbf{n} \in \mathcal{S}^{d-1}$ is the outward unit normal to the outer boundary



Reference Problem



$$k_{\text{eff}} = 0.9905$$

$$N_h = 23,248$$



Eigenvalue Problem – Weak Formulation

For a conforming finite-dimensional function space $\mathcal{V}_h(\Omega) \subset H^1(\Omega)$, the discrete weak form of (1) reads as follows: Find the dominant eigen-couple $\phi_h, k_{\text{eff}} \in \mathcal{V}_h(\Omega) \times \mathbb{R}^+$, with $\|\phi_h\|_{L^2(\Omega)} = 1$, such that

$$\int_{\Omega} D_c \nabla \phi_h \cdot \nabla \xi_h \, d\Omega + \int_{\Omega} \Sigma_a \phi_h \xi_h \, d\Omega + \int_{\partial\Omega_R} \varrho \phi_h \xi_h \, d\gamma = \frac{1}{k_{\text{eff}}} \int_{\Omega} \Sigma_f \phi_h \xi_h \, d\Omega, \quad \forall \xi_h \in \mathcal{V}_h(\Omega),$$

or alternatively, introducing bilinear forms $a^\Omega, b^\Omega : \mathcal{V}_h(\Omega) \times \mathcal{V}_h(\Omega) \rightarrow \mathbb{R}^+$:
Find the dominant eigen-couple $\phi_h, k_{\text{eff}} \in \mathcal{V}_h(\Omega) \times \mathbb{R}^+$, with $\|\phi_h\|_{L^2(\Omega)} = 1$, such that

$$b^\Omega(\phi_h, \xi_h) = k_{\text{eff}} a^\Omega(\phi_h, \xi_h), \quad \forall \xi_h \in \mathcal{V}_h(\Omega),$$

where for all $\eta_h, \xi_h \in \mathcal{V}_h(\Omega)$

$$a^\Omega(\eta_h, \xi_h) := \int_{\Omega} D_c \nabla \eta_h \cdot \nabla \xi_h \, d\Omega + \int_{\Omega} \Sigma_a \eta_h \xi_h \, d\Omega + \int_{\partial\Omega_R} \varrho \eta_h \xi_h \, d\gamma,$$

$$b^\Omega(\eta_h, \xi_h) := \int_{\Omega} \Sigma_f \eta_h \xi_h \, d\Omega.$$



Eigenvalue Problem – Variational Formulation

The same generalized eigenvalue problem can alternatively be written in variational form as

$$(\phi_h, k_{\text{eff}}) = \arg \max_{\substack{\eta_h \in \mathcal{V}_h(\Omega) \\ \|\eta_h\|_{L^2(\Omega)}=1}} \frac{b^\Omega(\eta_h, \eta_h)}{a^\Omega(\eta_h, \eta_h)}.$$

With this work, we aim at solving this problem on a local reduced basis space $\mathcal{V}_\varepsilon(\Omega) = \bigoplus_{i=1}^{N_D} \mathcal{V}_{\varepsilon,i}(\Omega) \subset \mathcal{V}_h(\Omega)$ exploiting the decomposability of the global domain. For the construction of $\mathcal{V}_\varepsilon(\Omega)$, we proceed assuming

1. ϕ_h, k_{eff} are both known
2. k_{eff} is known, ϕ_h is unknown
3. ϕ_h, k_{eff} are both unknown



Domain Decomposition

We assume the global domain Ω can be decomposed in $N_D \in \mathbb{N}$ non-overlapping subdomains Ω_i , such that

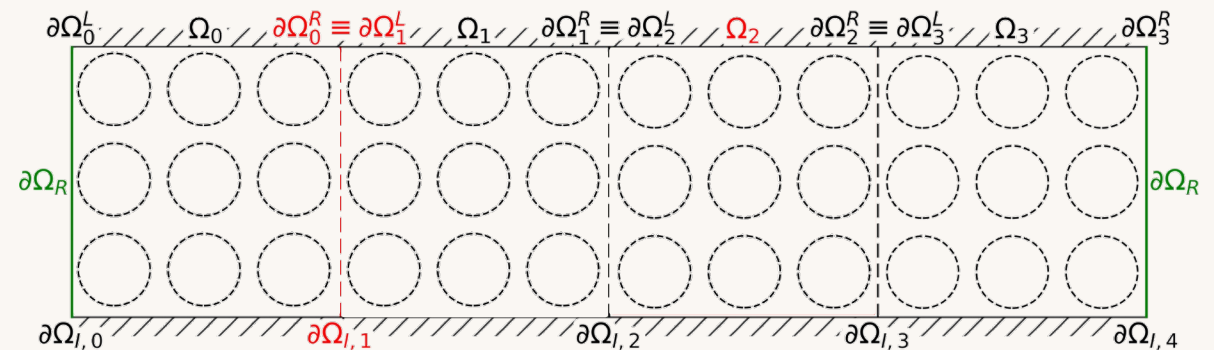
$$\Omega = \bigcup_{i=1}^{N_D} \Omega_i, \quad \text{with} \quad \partial\Omega_i \cap \partial\Omega_j = \emptyset \quad \text{for all } i, j \in \{1, \dots, N_D\}.$$

For every subdomain Ω_i , we define an oversampling region $\Omega_i \subset \Omega_i^+ \subset \Omega$, such that $\partial\bar{\Omega}_i^+ \cap \partial\bar{\Omega}_i = \partial\bar{\Omega}_i \setminus \partial\Omega$.

Furthermore, we define the outer and inner boundaries

$$\partial\bar{\Omega}_{i,O} = \partial\bar{\Omega}_i \cap \partial\Omega, \quad \text{and} \quad \partial\bar{\Omega}_{i,I} = \partial\bar{\Omega}_i \setminus \partial\Omega,$$

$$\partial\bar{\Omega}_{i,O}^+ = \partial\bar{\Omega}_i^+ \cap \partial\Omega, \quad \text{and} \quad \partial\bar{\Omega}_{i,I}^+ = \partial\bar{\Omega}_i^+ \setminus \partial\Omega.$$





Local Bilinear Forms

For any subdomain $\Omega_\star \subset \Omega$, we define $a^{\Omega_\star}, b^{\Omega_\star}: \mathcal{V}_h(\Omega_\star) \times \mathcal{V}_h(\Omega_\star) \rightarrow \mathbb{R}$ such that

$$a^{\Omega_\star}(\varphi_h, \zeta_h) := \int_{\Omega_\star} D_c \nabla \varphi_h \cdot \nabla \zeta_h \, d\Omega + \int_{\Omega_\star} \Sigma_a \varphi_h \zeta_h \, d\Omega + \int_{\partial\Omega_R \cap \partial\bar{\Omega}_\star} \varrho \varphi_h \zeta_h \, d\gamma, \quad \forall \varphi_h, \zeta_h \in \mathcal{V}_h(\Omega_\star),$$

$$b^{\Omega_\star}(\varphi_h, \zeta_h) := \int_{\Omega_\star} \Sigma_f \varphi_h \zeta_h \, d\Omega, \quad \forall \varphi_h, \zeta_h \in \mathcal{V}_h(\Omega_\star).$$

As long as the coefficients are $\Sigma_f \geq 0$, and $D_c, \Sigma_a > 0$, we have that

$$a^{\Omega_\star} > 0,$$

$$b^{\Omega_\star} \geq 0.$$



Bounding the Eigenvalue

The global eigenvalue k_{eff} can be bounded from above and from below relying on the eigenvalues of problems defined only on the subdomains Ω_i , and Ω_i^+ . Specifically, we define

- 1) the local eigenvalue problem with **zero Neumann** boundary conditions defined as follows:
Find the dominant eigen-couple $\phi_h^{N,i}, k_{\text{eff}}^{N,i} \in \mathcal{V}_h(\Omega_i) \times \mathbb{R}^+$, with $\|\phi_h\|_{L^2(\Omega_i)} = 1$, such that

$$b^{\Omega_i}(\phi_h^{N,i}, \zeta_h) = k_{\text{eff}}^{N,i} a^{\Omega_i}(\phi_h^{N,i}, \zeta_h), \quad \forall \zeta_h \in \mathcal{V}_h(\Omega_i),$$

- 2) the local eigenvalue problem with **zero Dirichlet** boundary condition defined as follows:
Find the dominant eigen-couple $\phi_h^{D,i}, k_{\text{eff}}^{D,i} \in \mathcal{V}_h^0(\Omega_i^+) \times \mathbb{R}^+$, with $\|\phi_h^{D,i}\|_{L^2(\Omega_i^+)} = 1$, such that

$$b^{\Omega_i^+}(\phi_h^{D,i}, \varphi_h) = k_{\text{eff}}^{D,i} a^{\Omega_i^+}(\phi_h^{D,i}, \varphi_h), \quad \forall \varphi_h \in \mathcal{V}_h^0(\Omega_i^+),$$

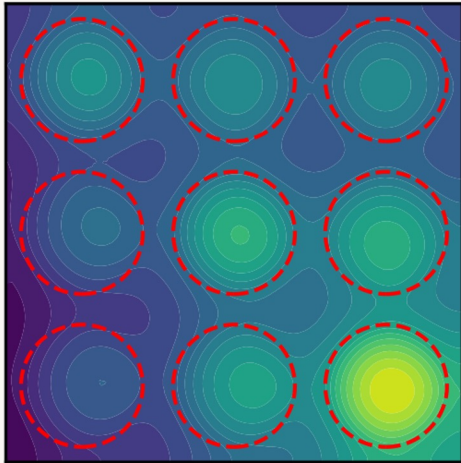
where $\mathcal{V}_h^0(\Omega_i^+) := \{\zeta_h \in \mathcal{V}_h(\Omega_i^+) \mid \mathcal{J}_{\Omega_i \rightarrow \partial\bar{\Omega}_{i,l}^+} \zeta_h = 0\}$. With these, we can prove that

$$\underline{k}_{\text{eff}} = \max_{0 \leq i \leq N_D} k_{\text{eff}}^{D,i} < k_{\text{eff}} \leq \max_{0 \leq i \leq N_D} k_{\text{eff}}^{N,i} = \bar{k}_{\text{eff}}$$

Upper Bound

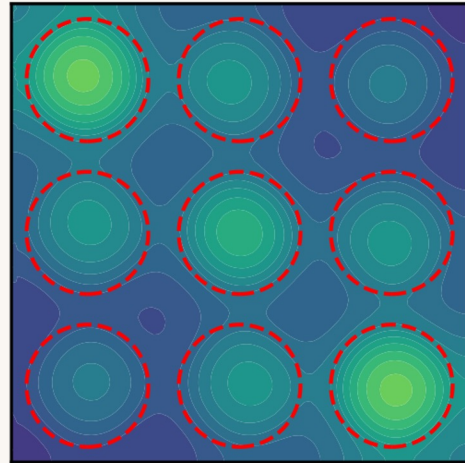


$\phi_h^{N,1}$



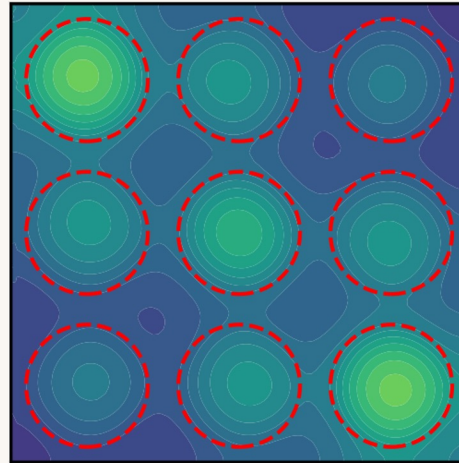
$$k_{\text{eff}}^{N,1} = 0.9776$$

$\phi_h^{N,2}$



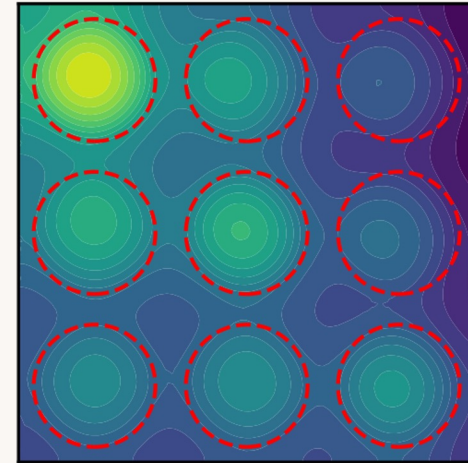
$$k_{\text{eff}}^{N,2} = 1.0063$$

$\phi_h^{N,3}$



$$k_{\text{eff}}^{N,3} = 1.0063$$

$\phi_h^{N,4}$



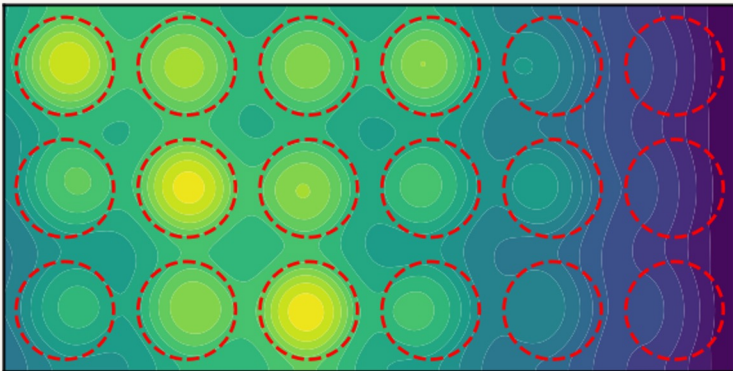
$$k_{\text{eff}}^{N,4} = 0.9776$$

$$k_{\text{eff}} = 0.9905 \leq 1.0063 = \max_{0 \leq i \leq N_D} k_{\text{eff}}^{N,i}$$

Lower Bound

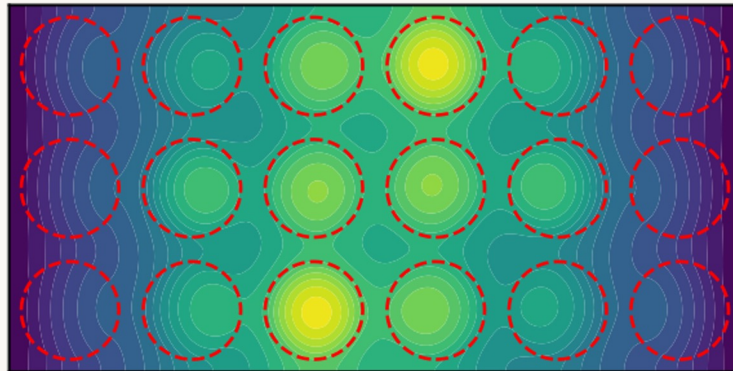


$\phi_h^{D,1}$



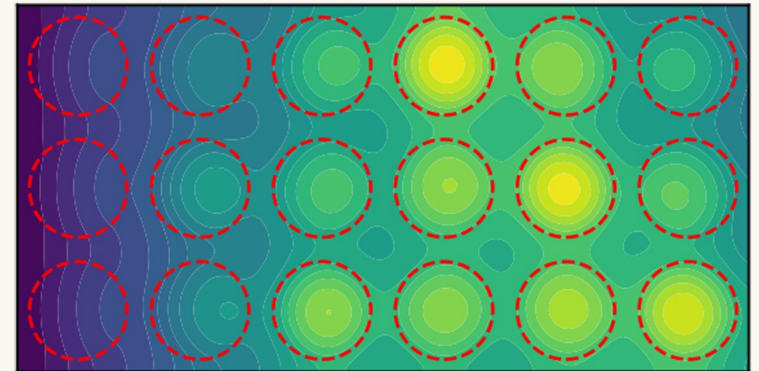
$$k_{\text{eff}}^{D,1} = 0.9556$$

$\phi_h^{D,2}$



$$k_{\text{eff}}^{D,2} = 0.9207$$

$\phi_h^{D,3}$



$$k_{\text{eff}}^{D,3} = 0.9556$$

$$\max_{0 \leq i \leq N_D} k_{\text{eff}}^{D,i} = 0.9556 \geq 0.9905 = k_{\text{eff}}$$

...contact me for the complete presentation





Relevant Literature

For drafting these notes, we were inspired by the following works:

- [1] *Y. Efendiev, J. Galvis, T. Y. Hou, Generalized multiscale finite element methods (GMsFEM)*
Journal of computational physics, 2013
- [2] *P. Henning, A. Målqvist, Localized orthogonal decomposition techniques for boundary value problems,*
SIAM Journal on Scientific Computing, 2014
- [3] *A. Abdulle, E. Weinan, B. Engquist, E. Vanden-Eijnden, The heterogeneous multiscale method,*
Acta Numerica, 2012
- [4] *D. B. P. Huynh, D. J. Knezevic, A. T. Patera, A static condensation reduced basis element method:
approximation and a posteriori error estimation,* Mathematical Modelling and Numerical Analysis, 2013
- [5] *K. Smetana, A. T. Patera, Optimal local approximation spaces for component-based static
condensation procedures,* SIAM Journal on Scientific Computing, 2016



THANK YOU

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