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Topologically Optimal Nuclear Core Designs using Deterministic Neutronics

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THE NEW OUTLOOK



Overview

- Motivation
 - Additive manufacturing viable for nuclear
 - Implication: nearly arbitrary reactor geometries
- How to make use of arbitrary reactor geometry
 - PDE-constrained optimization (define the problem)
 - Numerical techniques (solve the problem)
- Some preliminary results
 - pin cell
 - graphite pile

What is manufacturable in nuclear?

- The paper [1] by Terrani et. al. establishes arbitrarily shaped TRISO-based fuel matrices as part of a reactor designer's toolbelt
- Benefits:
 - embedded burnable poisons
 - embedded sensors
 - shaped coolant channels
- **How much further can we push the neutronics with arbitrary geometry?**

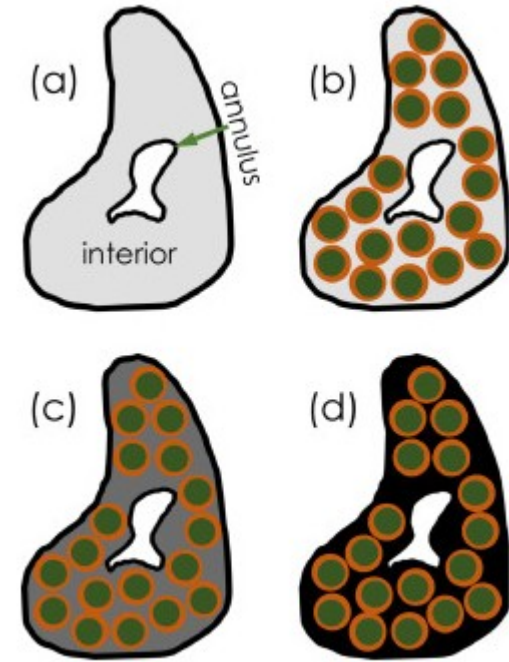


Fig: From [1], fuel shell can be printed, filled with TRISO, matrix powder poured, and lastly sintered

How to take advantage of arbitrary shape

- Field of PDE-constrained optimization fairly mature today [2], techniques for solid mechanics available in CAD software e.g. Autodesk Inventor

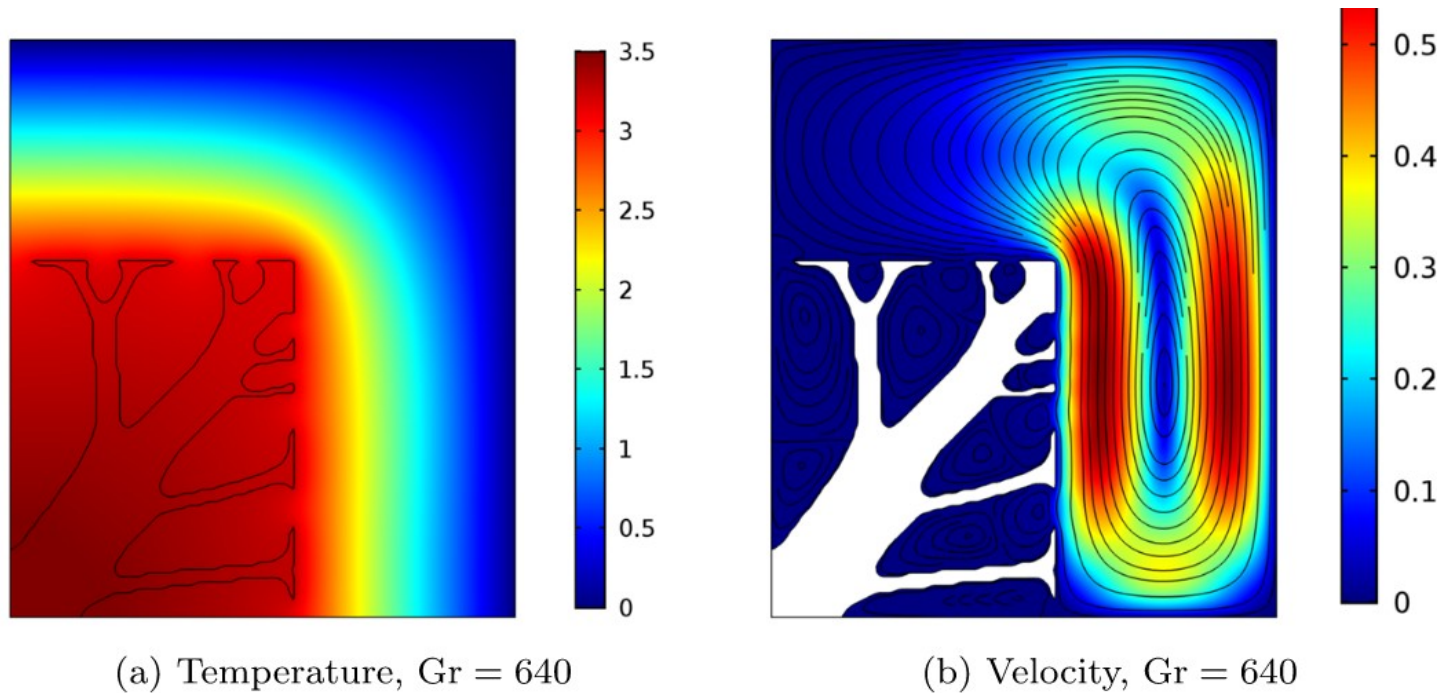


Fig: from [3], Navier-Stokes coupled with heat conduction used to minimize average temperature at region of heat flux application (bottom left area)

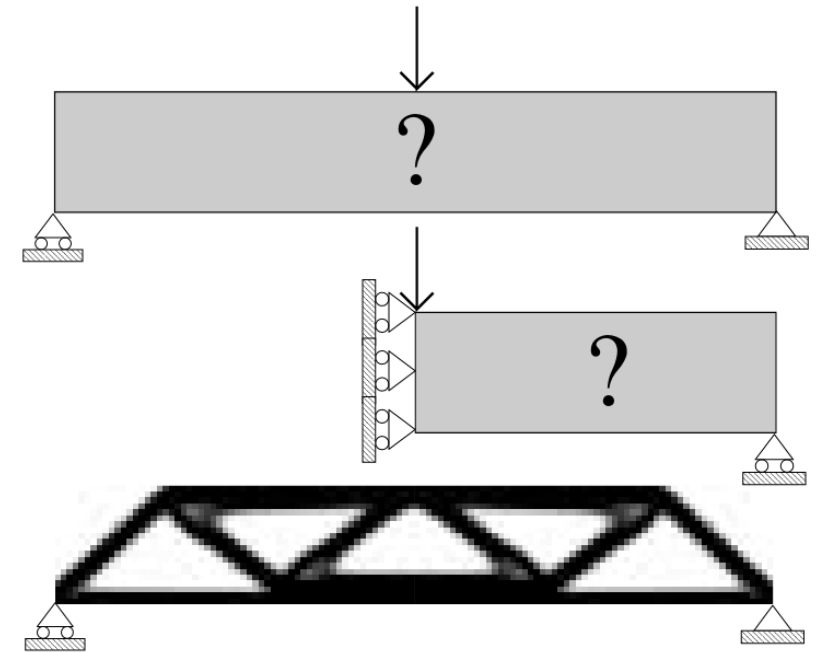


Fig: from [4], unknown area represented by “?”, voxelized, symmetry BC applied, and final solution for minimal compliance

Previous work in nuclear engineering

- Chabod and coworkers [6]
 - Centers on use of MCNP PERT cards to get objective function gradients with respect to nuclide densities
 - Quite computationally expensive (~1000x overhead by my estimate!)
 - **1000s of optimization variables**
- Sobes and coworkers [7]
 - Build machine learning model that predicts outcome of coupled neutronics/thermal-hydraulics as function of geometry
 - Parameter space must be fairly small to train the model (**~20 optimization variables**)

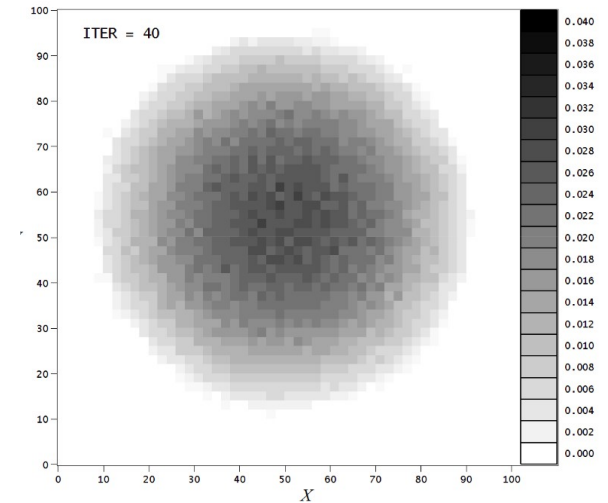


Fig: Optimization result from [6]

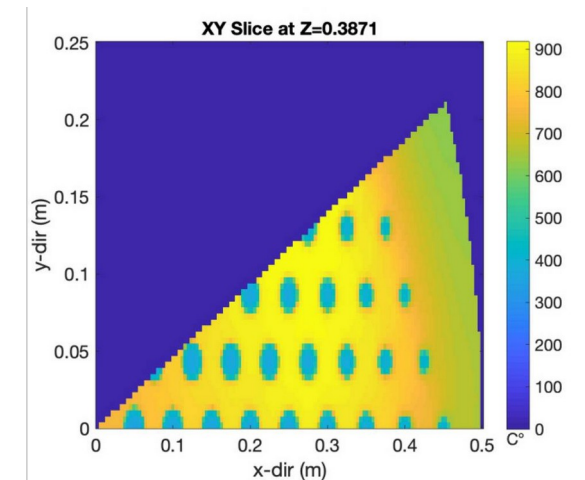


Fig: Optimization result from [7]

Applying PDE-constrained optimization to neutronics

- **Option 1:** start from rigorous statement of Karush-Kuhn-Tucker conditions in Banach space, solve numerically. See [5]
- **Option 2:** define an objective function, get gradients via perturbation theory, iterate on our design (*much* more intuitive, but less flexible)
- That being said, let's solve the simplest possible topology optimization problem relevant to reactor design:

Material is graphite if
 $\alpha=0$, or natural
enriched uranium
dioxide if $\alpha=1$

Steady-state neutron
transport equation with
isotropic scattering

$$\max_{\alpha(r) \in A} k_{\text{eff}}$$

$$\text{s.t.} \quad \hat{\Omega} \cdot \nabla \varphi + \Sigma_t(\alpha(r))\varphi =$$

$$\frac{1}{4\pi} \Sigma_s(\alpha(r))\phi + \frac{1}{4\pi k_{\text{eff}}} \chi \otimes \nu \Sigma_f(\alpha(r))\phi$$

$$\Sigma_x(\alpha) = \Sigma_{x,\text{graphite}}(1 - \alpha) + \Sigma_{x,\text{fuel}}\alpha$$

Applying PDE-constrained optimization to neutronics

- For sensitivity, rather than using a true “gradient”, we can get what I call an “integrated gradient” from the classic reactivity perturbation formula:

$$\Delta\rho \approx \frac{\int_V \phi^* \cdot \left(\frac{1}{k_{\text{eff}}} \delta(\chi \otimes \nu \Sigma_f) - \delta \Sigma_t + \delta \Sigma_s \right) \phi}{\int_V \phi^* \cdot \frac{1}{k_{\text{eff}}} \chi \otimes \Sigma_f \phi}$$

$$-\hat{\Omega} \cdot \nabla \varphi^* + \Sigma_t(\alpha(r)) \varphi^* = \frac{1}{4\pi} \Sigma_s(\alpha(r))^T \varphi^* + \frac{1}{4\pi k_{\text{eff}}} \nu \Sigma_f(\alpha(r)) \otimes \chi \varphi^*$$

- Loop over each mesh cell, compute “what if” reactivity change if the material were changed from fuel to moderator or vice versa
- To limit the step size (gradients are only a linearization of a nonlinear objective function as a function of the control variables), only allow a certain maximum amount of volume to change at each iteration

Applying PDE-constrained optimization to neutronics

- The previously described procedure can be written as the **much** simpler optimization problem below, after calculating the adjoint flux in the current configuration

$$\begin{aligned} \max_{I(r) \in A} \quad & \int_V I(r) \Delta \rho_{\text{flipflop}}(r) \\ \text{s.t.} \quad & \int_V I(r) = a \end{aligned}$$

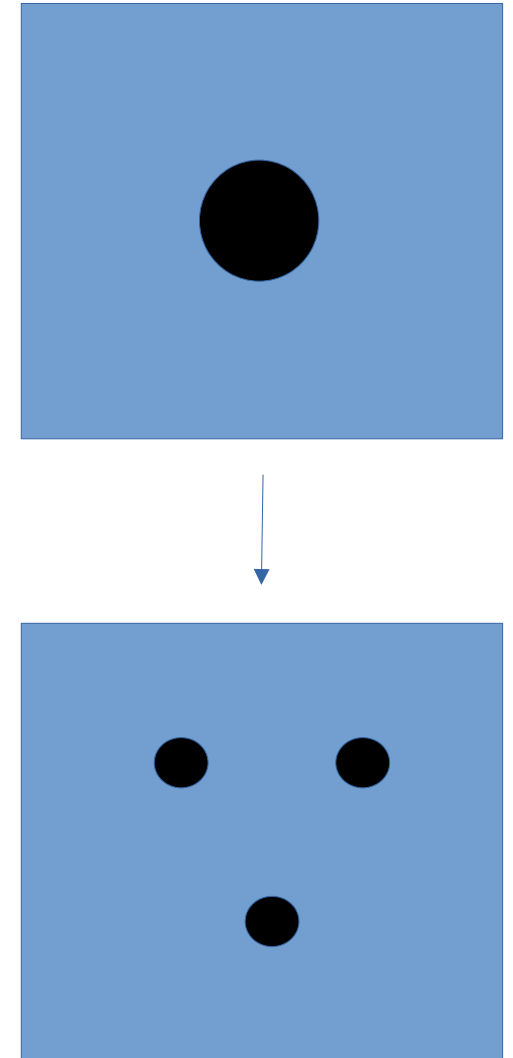
$$\Delta \rho_{\text{flipflop}}(r) = \frac{\phi^* \cdot \delta T(\alpha(r)) \phi}{\int_V \phi^* \cdot \frac{1}{k_{\text{eff}}} \chi \otimes \Sigma_f \phi}$$

$$\begin{aligned} \delta T(\alpha(r)) = \frac{1}{k_{\text{eff}}} \big(\chi \otimes \nu \Sigma_f (1 - \alpha(r)) - \chi \otimes \nu \Sigma_f (\alpha(r)) \big) - \\ \Sigma_t (1 - \alpha(r)) + \Sigma_t (\alpha(r)) + \Sigma_s (1 - \alpha(r)) - \Sigma_s (\alpha(r)) \end{aligned}$$

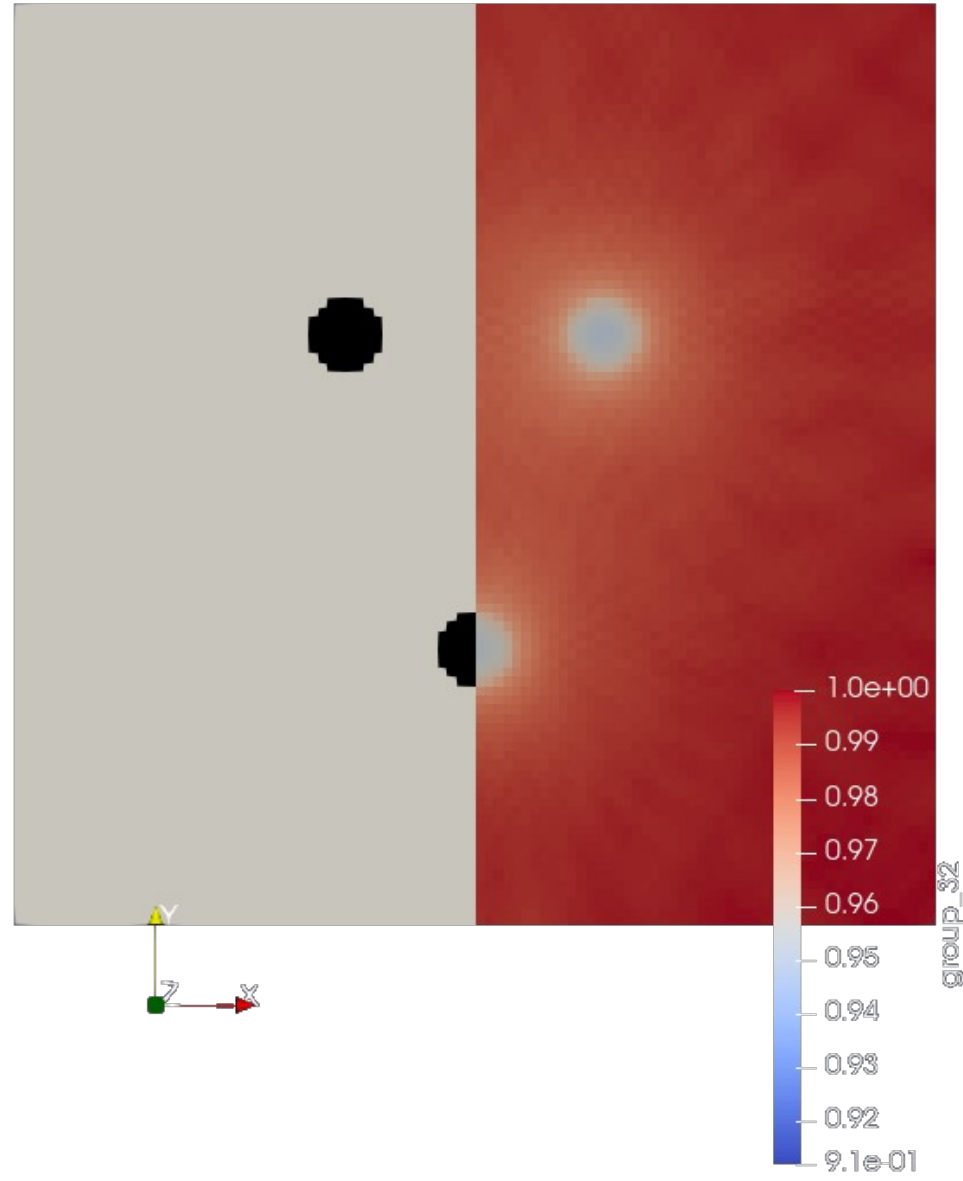
- Flip all mesh cells to the other material if $I(r)=1$

Example problem: graphite pile pin cell

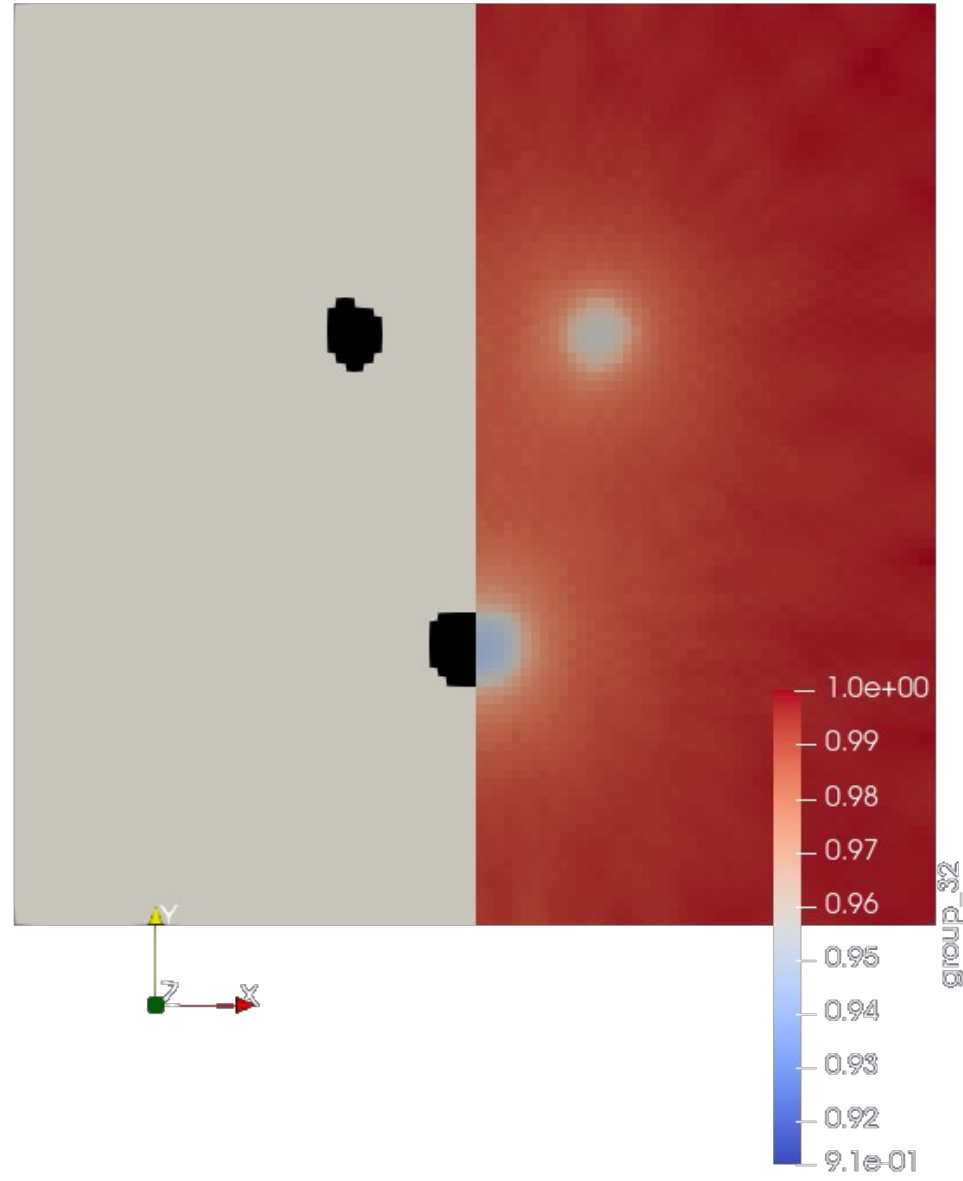
- Generated transport-corrected 33 group constants with OpenMC [8] for
 - cylindrical uranium dioxide pin
 - natural enrichment
 - optimal radius for k
 - embedded in graphite 5x5 cm square lattice
 - neglect changes in resonance self shielding
- Discretized shape using 100x100 square mesh
- Deterministic neutronics solve using a modified version of MOCKingbird [10]
- Test: since we know that resonance absorption is reduced by lumping the fuel, **will our algorithm re-lump the fuel if we split it up?**



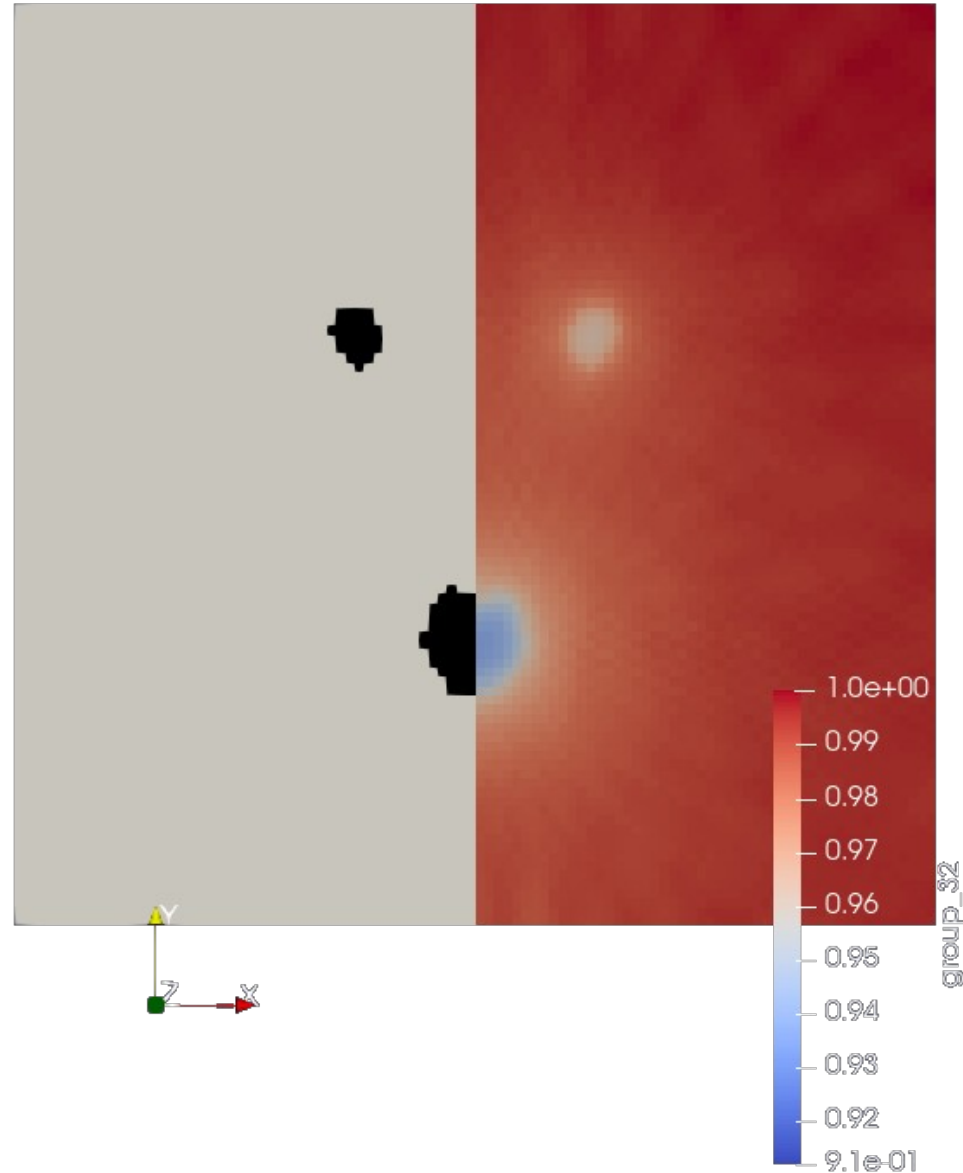
Iteration=0, $k=1.0283$



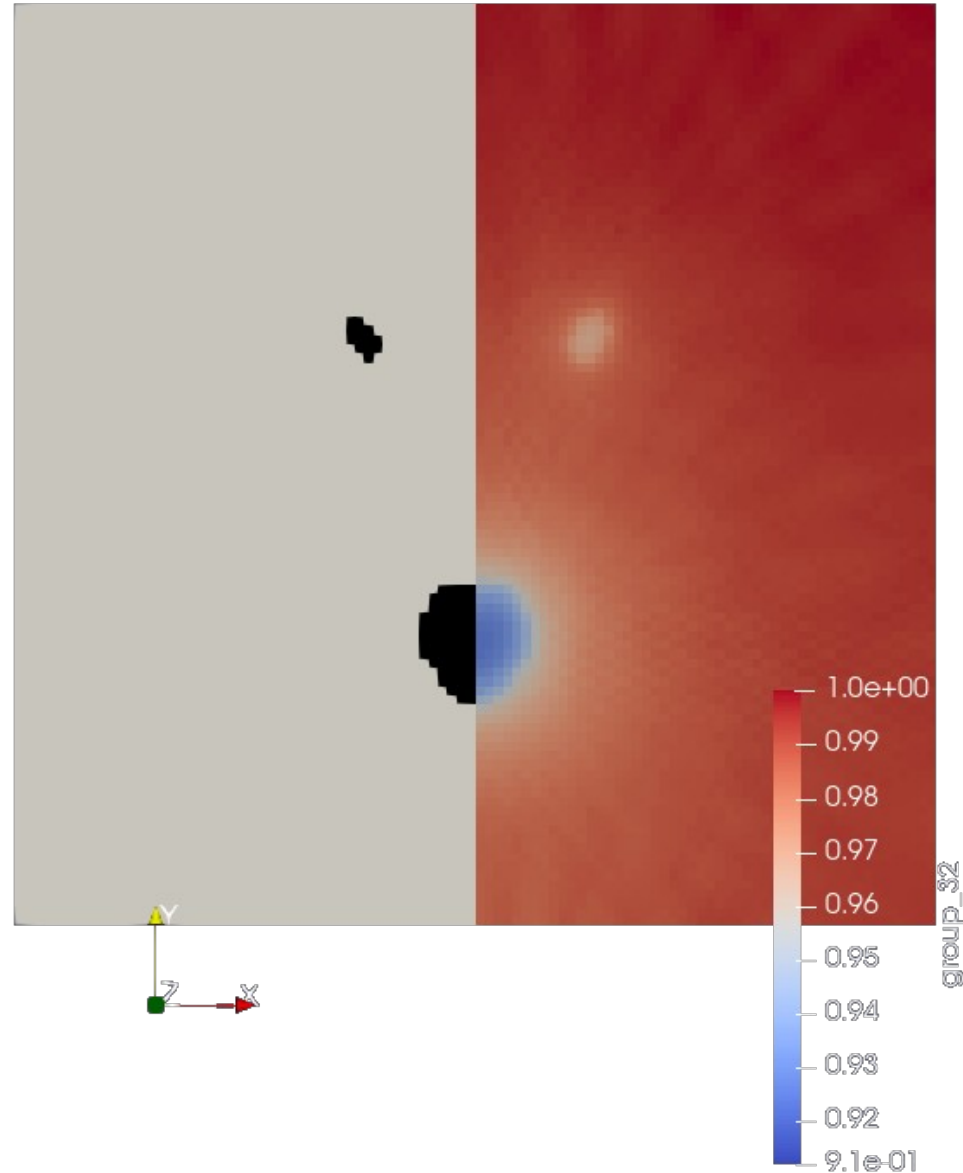
Iteration=5, $k=1.0284$



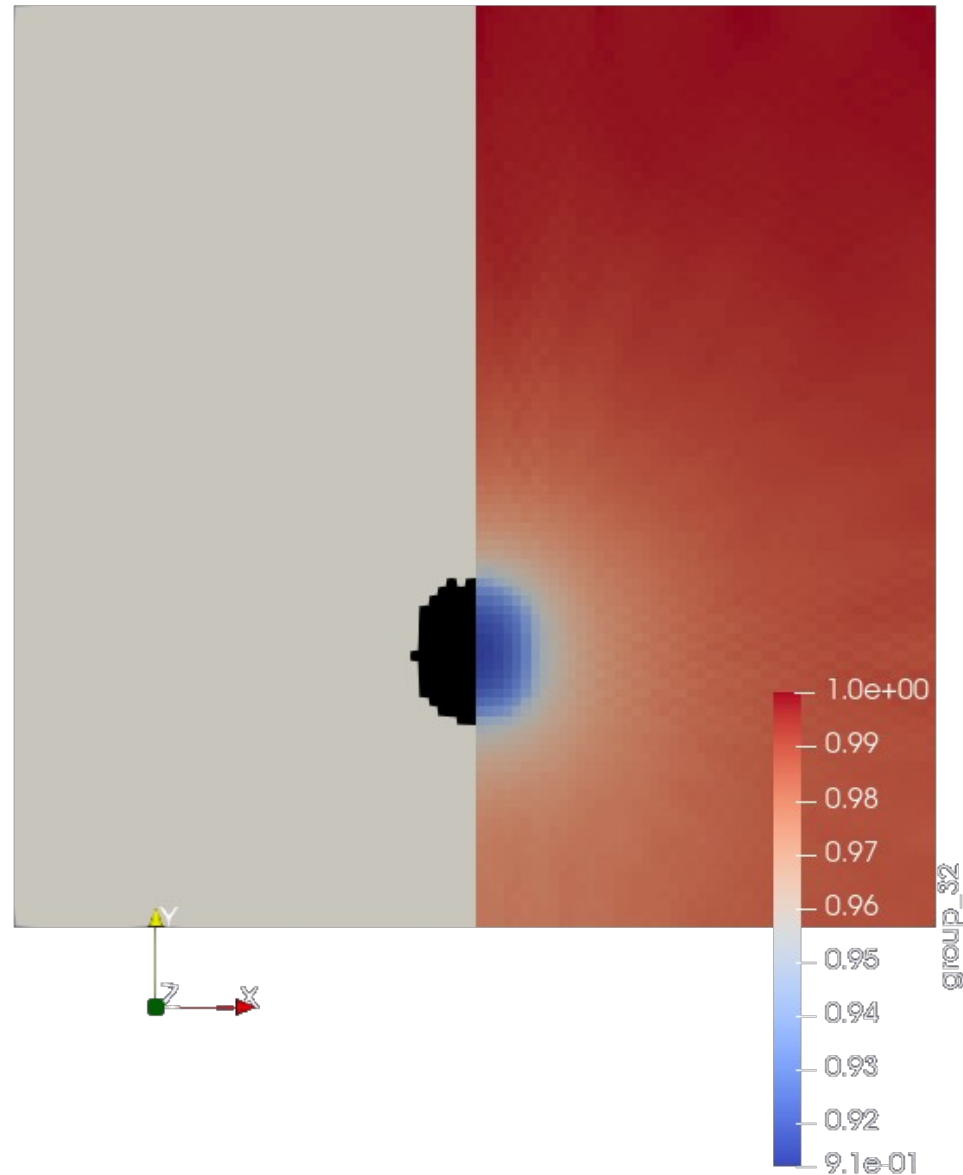
Iteration=10, $k=1.0286$



Iteration=15, $k=1.0290$



Iteration=20, $k=1.0298$



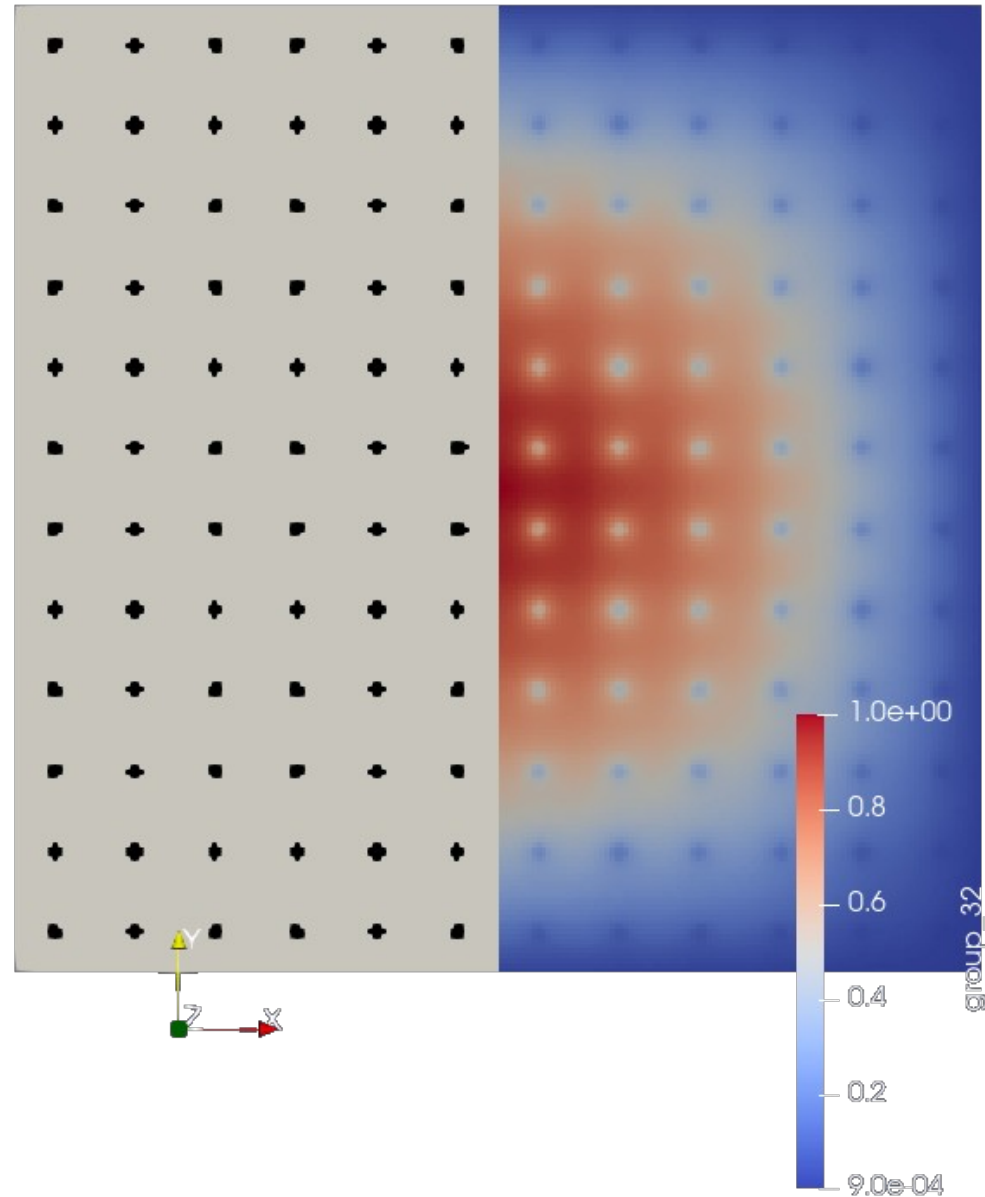
Example problem: MIT graphite pile

- Use group constants from pin cell problem
- Discretized 2D shape (axially infinite approximation) using 200x200 square mesh
- Vacuum BCs make for a far more interesting situation

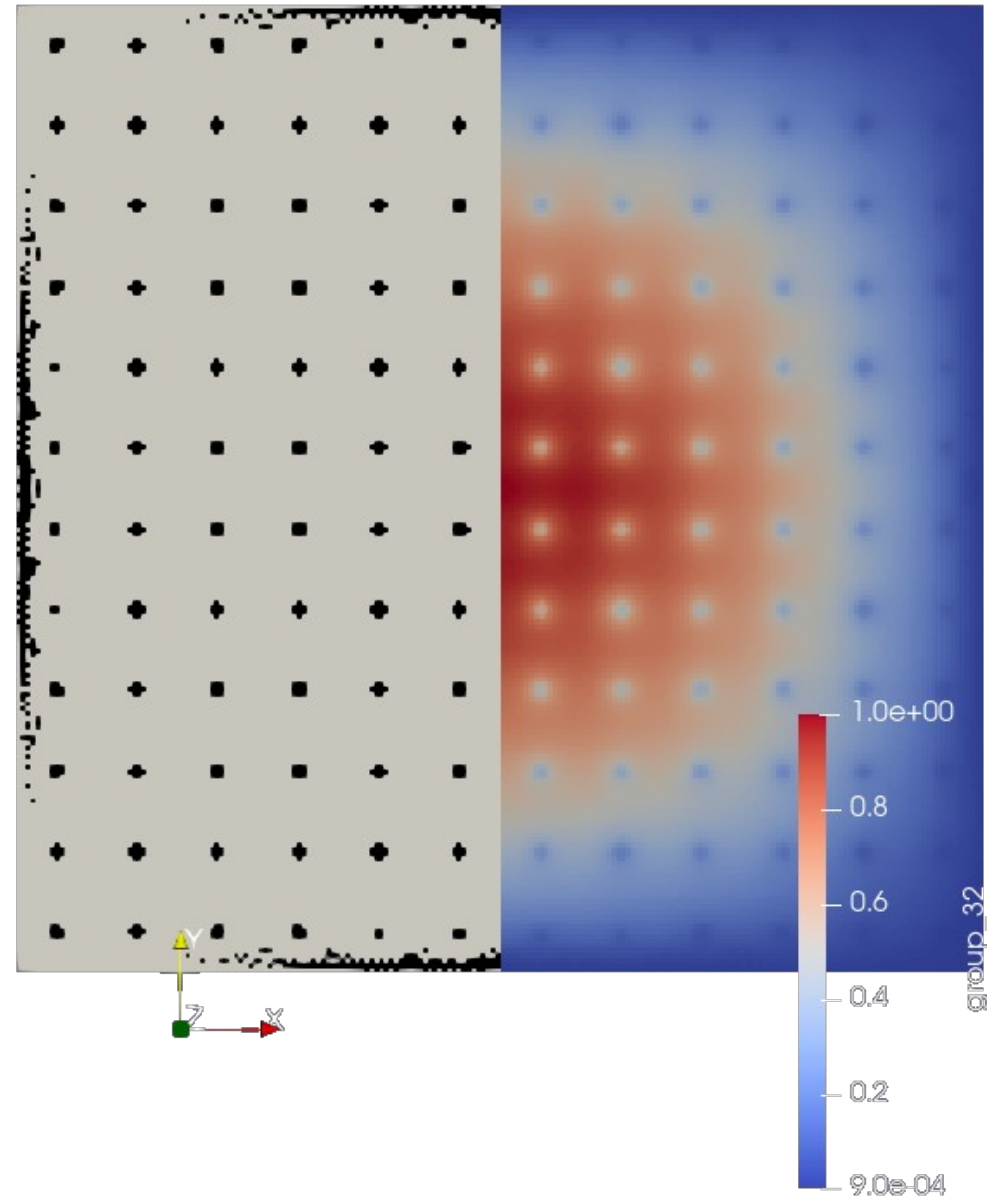


Fig: MIT graphite pile shown in [10]

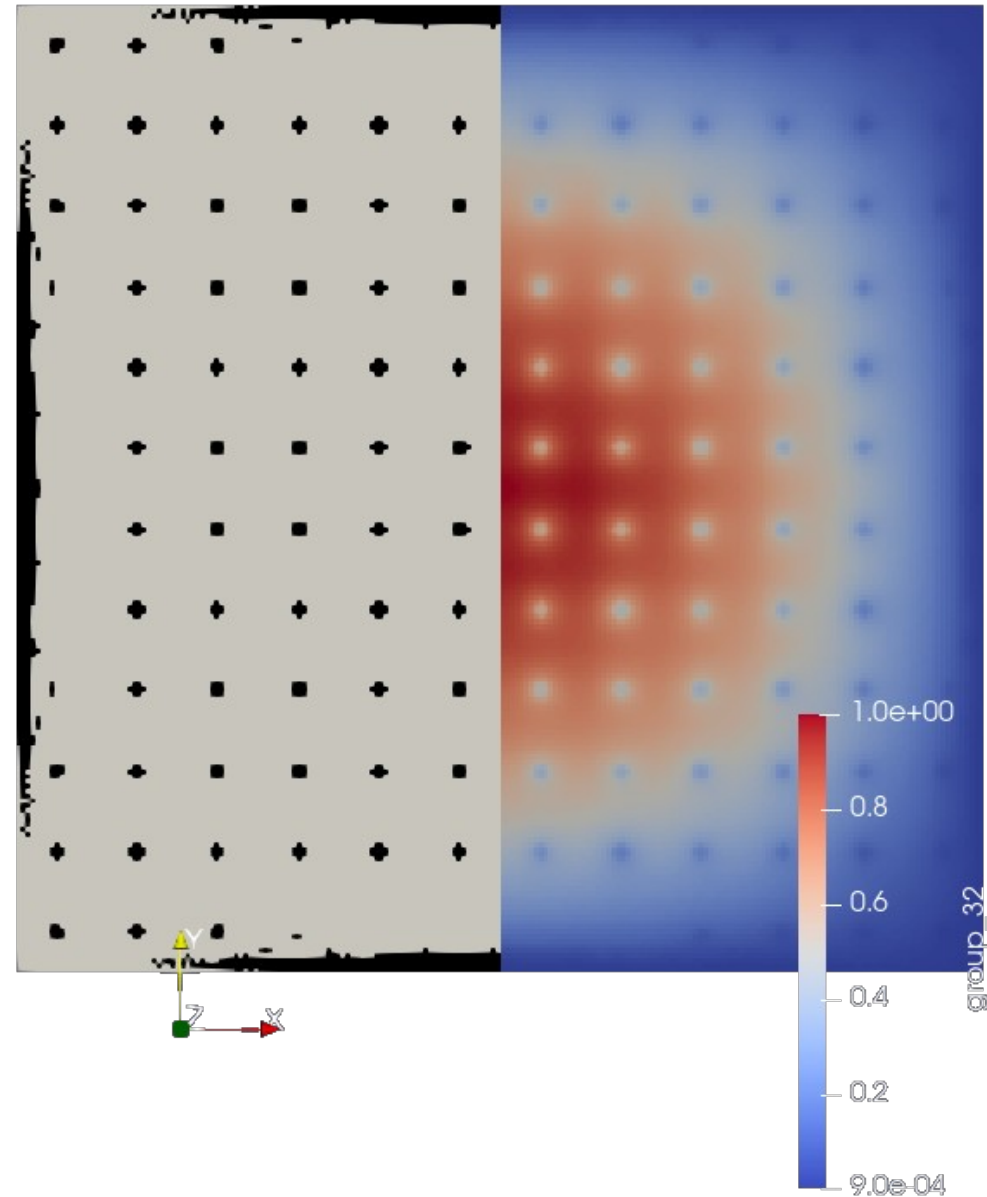
Iteration=0, $k=0.7972$



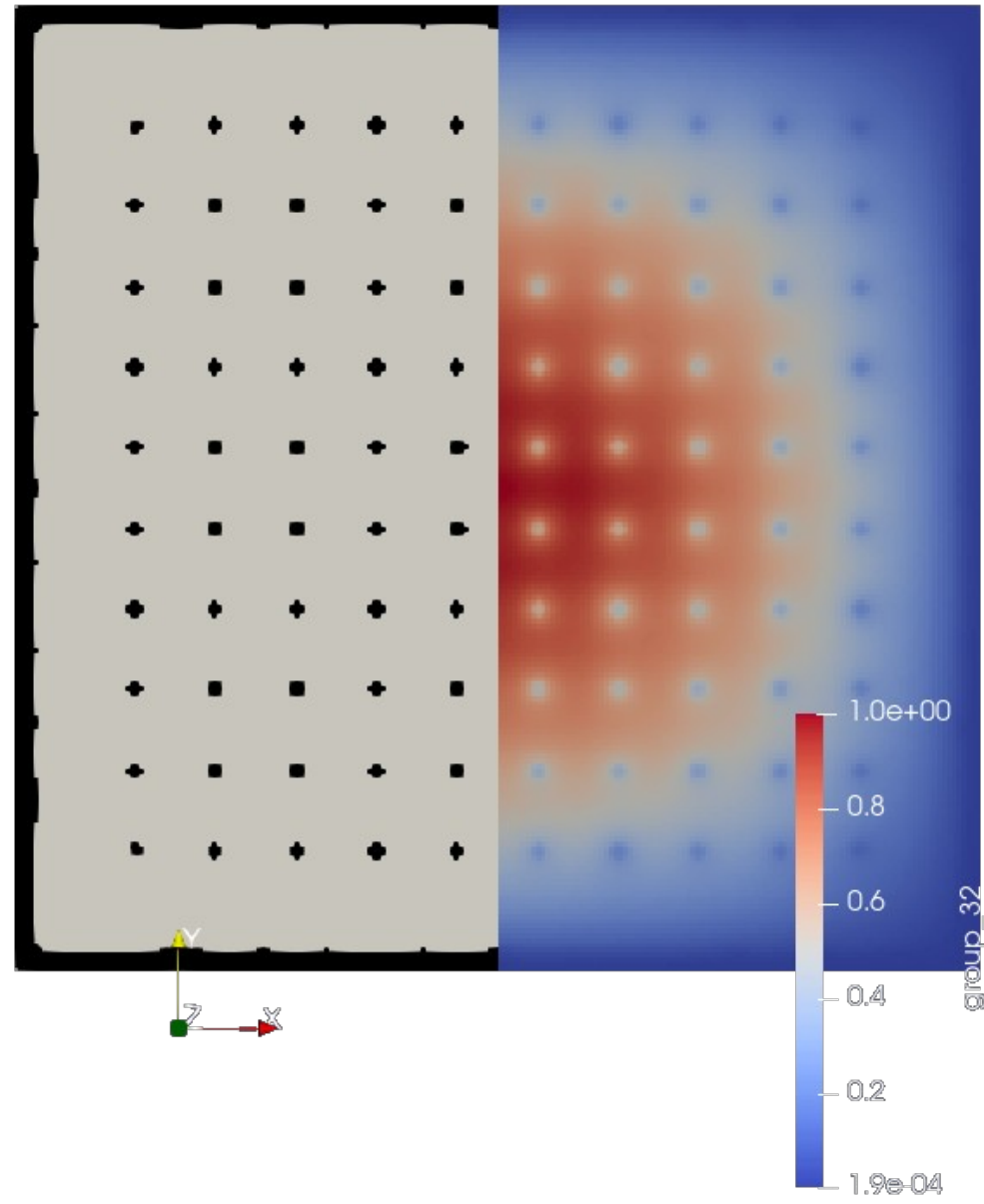
Iteration=100, $k=0.8006$



Iteration=200, $k=0.8025$



Iteration=400, $k=0.8031$



Conclusions

- Algorithm suitable for large-scale topology optimization of nuclear reactor geometries presented
- Use of deterministic neutronics greatly accelerates time to solution in exchange for modeling error
- Techniques to include other quantities in objective function using generalized perturbation theory to be presented at some point in the future
 - Fuel volume, peaking factors, etc
- Coupled multiphysics is a possibility in the future using general PDE-constrained optimization theory
- **~1000 pcm gain in reactivity possible on MIT graphite pile without changing geometric envelope or fuel composition**

Thanks

Any questions?

References

- [1] K. A. TERRANI et al. “Architecture and Properties of TCR Fuel Form”. In: Journal of Nuclear Materials 547 (Apr. 15, 2021)
- [2] O. SIGMUND and K. MAUTE. “Topology Optimization Approaches”. In: Structural and Multidisciplinary Optimization 48.6 (Dec. 2013)
- [3] Asmussen, J., et al. “A “poor man’s” approach to topology optimization of natural convection problems”. Structural and Multidisciplinary Optimization. (Jan. 2019)
- [4] Sigmund, O.: A 99 Line Topology Optimization Code Written in MATLAB. Structural and Multidisciplinary Optimization 21
- [5] J. C. D. LOS REYES. Numerical PDE-Constrained Optimization. 2015th edition. Cham Heidelberg: Springer, Mar. 5, 2015.
- [6] S. CHABOD. “A Topology Optimization Procedure for Assisting the Design of Nuclear Components”. In: Journal of Nuclear Engineering 2.2 (2 June 2021).
- [7] V. SOBES et al. “AI-based Design of a Nuclear Reactor Core”. In: Scientific Reports 11.1 (1 Oct. 4, 2021)
- [8] P. K. ROMANO et al. “OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development”. In: Annals of Nuclear Energy. SNA + MC 2013. (Aug. 1, 2015)
- [9] D. R. GASTON et al. “Method of Characteristics for 3D, Full-Core Neutron Transport on Unstructured Mesh”. In: Nuclear Technology 207. (July 3, 2021)
- [10] <https://news.mit.edu/2017/75th-anniversary-first-nuclear-fission-reactor-mit-re-enacts-seminal-experiment-1204>