Core Loading Pattern Optimization of a Tie-Tube NTP Reactor using a Simulated Annealing Algorithm and Nodal Diffusion

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Agenda

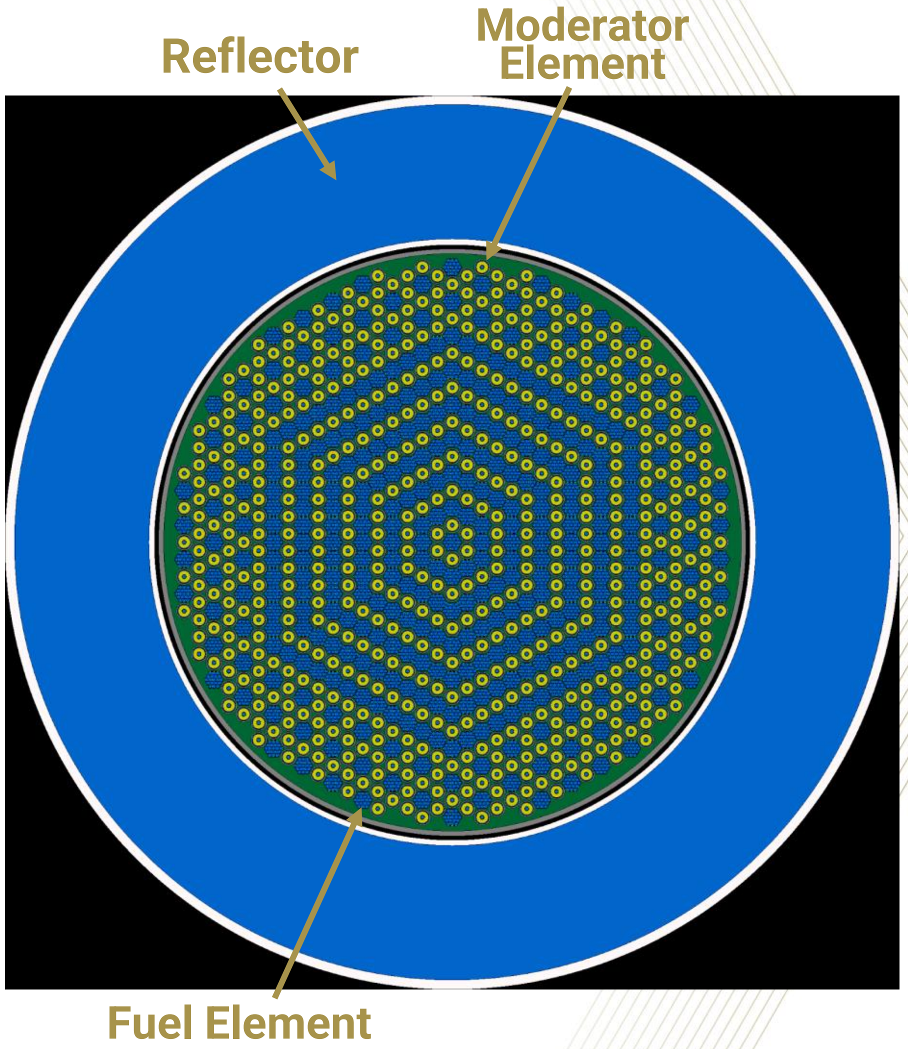
1. **Motivations and Design Space**
   - Hexagonal tie-tube moderated nuclear thermal propulsion (NTP) reactor
2. **Codes and Methods**
   - SERPENT/DYN3D
   - Cross-section generation
   - Assembly discontinuity factors (ADFs)
3. **Simulated Annealing Algorithm**
   - Coupled input file generator
4. **Sensitivity Results**
   - Variable acceptance criterion
5. **Conclusions and Acknowledgements**

Motivations

- **Key drawback of high accuracy Monte Carlo nuclear software tools (e.g., MCNP, SERPENT, etc.) is the computational burden to receive acceptable statistics**
  - Uses stochastic methods to solve the complex transport equation
  - Bulk reactor sensitivities typically requires use of an HPC
- **Diffusion theory greatly simplifies the process with non-trivial assumptions to significantly reduce the lead time for 2D and 3D test cases**
- **For NTP reactor designs, high operational temperature and power result in significant radial power peaking**
  - PP minimization is preferable for:
    - Optimization of specific impulse (Isp)
    - Maintaining temperature limits of the fuel material
- **This effort uses a Simulated Annealing (SA) optimization algorithm to vary the core loading pattern using power peaking as an objective function**

Reference Reactor Design

- Pewee-based hexagonal fuel and moderator elements surrounded by an annular reflector region
  - Fuel: Uranium nitride (UN) CERamic METallic (CERMET)
    - High-assay low-enriched uranium (HALEU) loading, 19.75 wt%
  - Moderator: Tie-tube with zirconium hydride moderator (ZrHx)
  - Reflector: Beryllium oxide (BeO), control drums emitted
- Metal matrix material choice in the CERMET fuel is axially variant based on a defined "split height" [1]
  - Top of core, or "cold region", uses molybdenum
  - Bottom of core, or "hot region", uses moly-tungsten (Mo-30W)
  - Split height is the length ratio of the hot region to the total active core
- Core loading patterns can be varied using constant and variable moderator to fuel element (ME/FE) ratios



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Codes and Methods

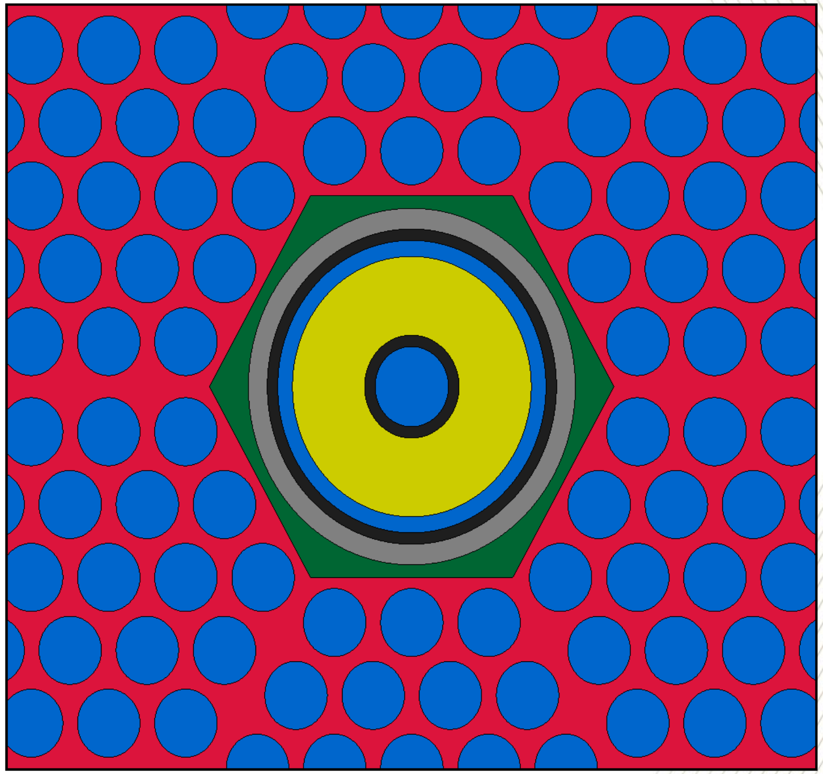
- Monte Carlo – SERPENT [6]
  - Responsible for reference solution (compare with DYN3D results)
  - Generation of few-group macroscopic cross-sections (for DYN3D)
  - Main expected outputs from the code are:
    - Power profiles, multiplication factors, cross-sections

- Nodal Diffusion – DYN3D [7]
  - Computationally inexpensive
  - Few-group cross-sections generated in Serpent will serve as DYN3D inputs
  - Cross-section wrapper will be used to process into required format
  - DYN3D will be used to obtain the steady-state neutronic solution

Cross-Section Generation

- DYN3D and other nodal diffusion software **<u>do not</u>** require material definitions
  - Nodal-averaged cross-sections
- Multigroup cross-sections are generated in SERPENT using a supercell infinite lattice
  - Material of choice is surrounded by six equivalent 19 channel Pewee-based fuel elements
  - Central reflector, tie-tube, and fuel element
- Hot and cold fuel choices are modeled separately
  - Axial fuel variation imperative for 3-D model
- Benchmark of group binning structure shows 2-group structure to be best for this effort
  - Also investigated 8-group and B1 leakage-corrected cross-sections

Fuel/Moderator Element Supercell Lattice



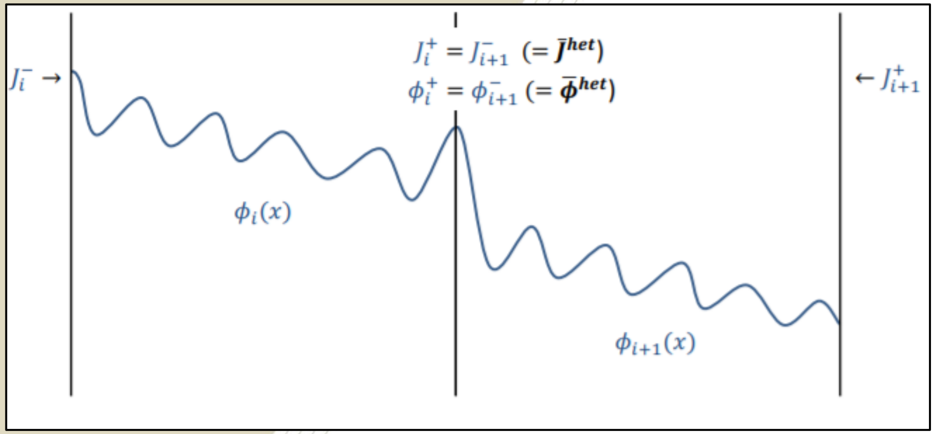
Assembly Discontinuity Factors (ADFs)

- Predominately found in highly heterogenous fuel assemblies, such as light water reactor (LWR) analyses, to improve nodal diffusion software fidelity
  - Minimal documented use cases in advanced terrestrial or space reactor designs
- Serves as the ratio between the heterogenous and homogeneous energy-dependent flux distributions at a material or nodal interface

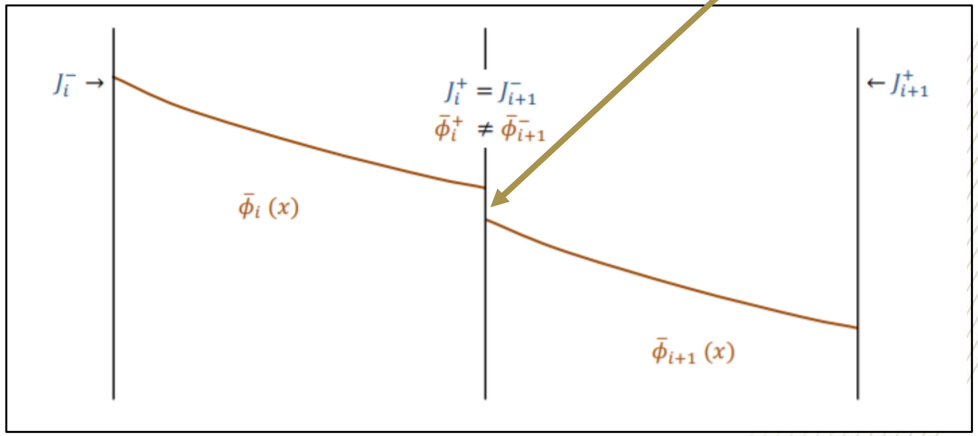
$$ADF_{i,g} = \frac{\phi_{i,g}^{het}}{\phi_{i,g}^{hom}}$$

Interface Discontinuity

[2]



Heterogeneous Flux Distribution

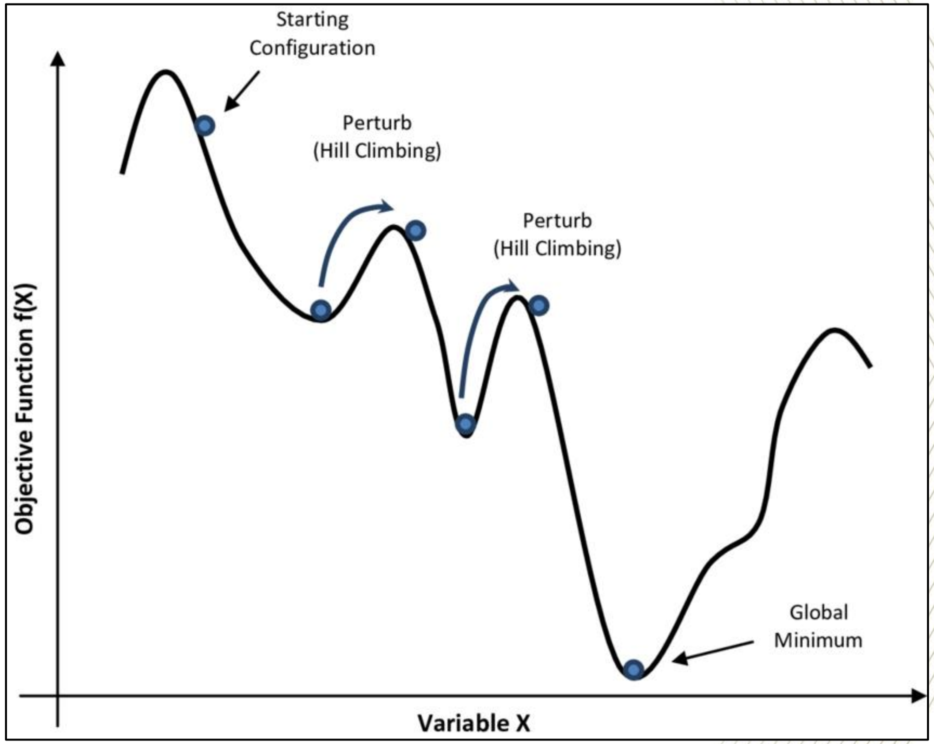


[2]

Homogeneous Flux Distribution

Simulated Annealing Algorithm

- Machine learning optimization scheme to avoid getting trapped local extrema
  - Accepts worse cases using probability
  - Relies on small perturbations to an initial configuration
- Based on an initially defined objective function (power peaking, keff, etc.)
  - This study focuses on power peaking
  - Future efforts can look at variable objective functions
- SA algorithm is applied in DYN3D to efficiently simulate a thousands of reactor designs
  - 60-degree symmetrical wedge
  - Hexagonal node lattice



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Simulated Annealing Algorithm

1. User-defined initial reference core converted to a 60-degree wedge equivalent
   - Apply node-specific cross-sections
2. Simulate this reference core in DYN3D and post-process the radial power peaking (PP0)
3. Swap a randomly picked fuel and moderator element to create a new perturbed geometry
4. Simulate the new core in DYN3D to find the new radial PP (PP1)
5. Determine the acceptance of this perturbed core:
   - If PP1 < PP0, accept the perturbed core as the reference core
   - If PP1 > PP0, calculate the annealing probability based on:

$$p_{sa} = exp(-\frac{k_a}{T_0} * (PP_1 - PP_0))$$

   - Randomly generate a number between 0 and 1. If P_{sa} is larger, then accept this "worse" case
6. If the perturbed core is accepted, then consider this geometry as the new reference core

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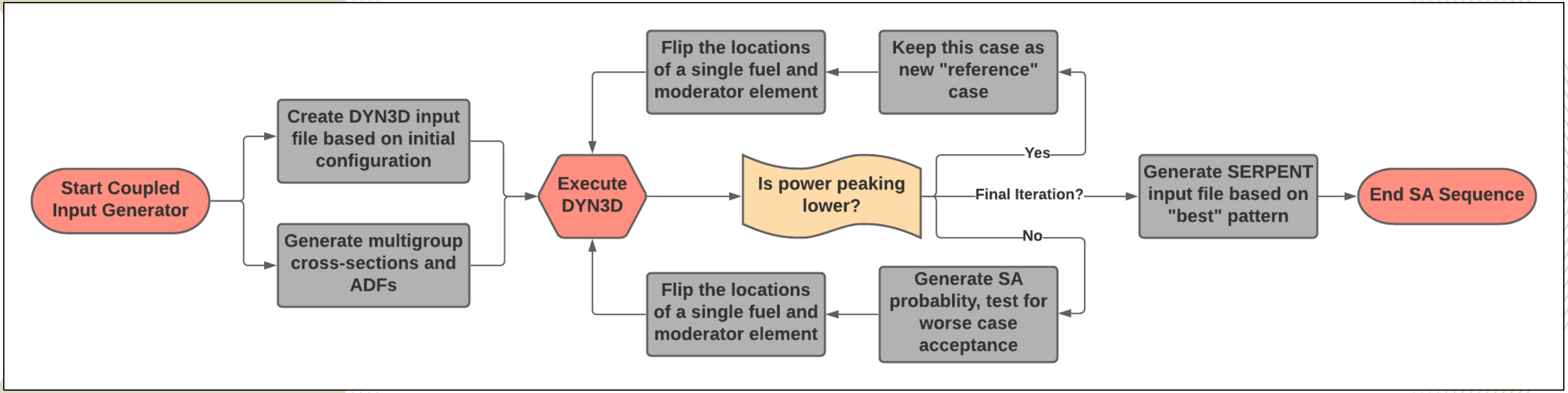
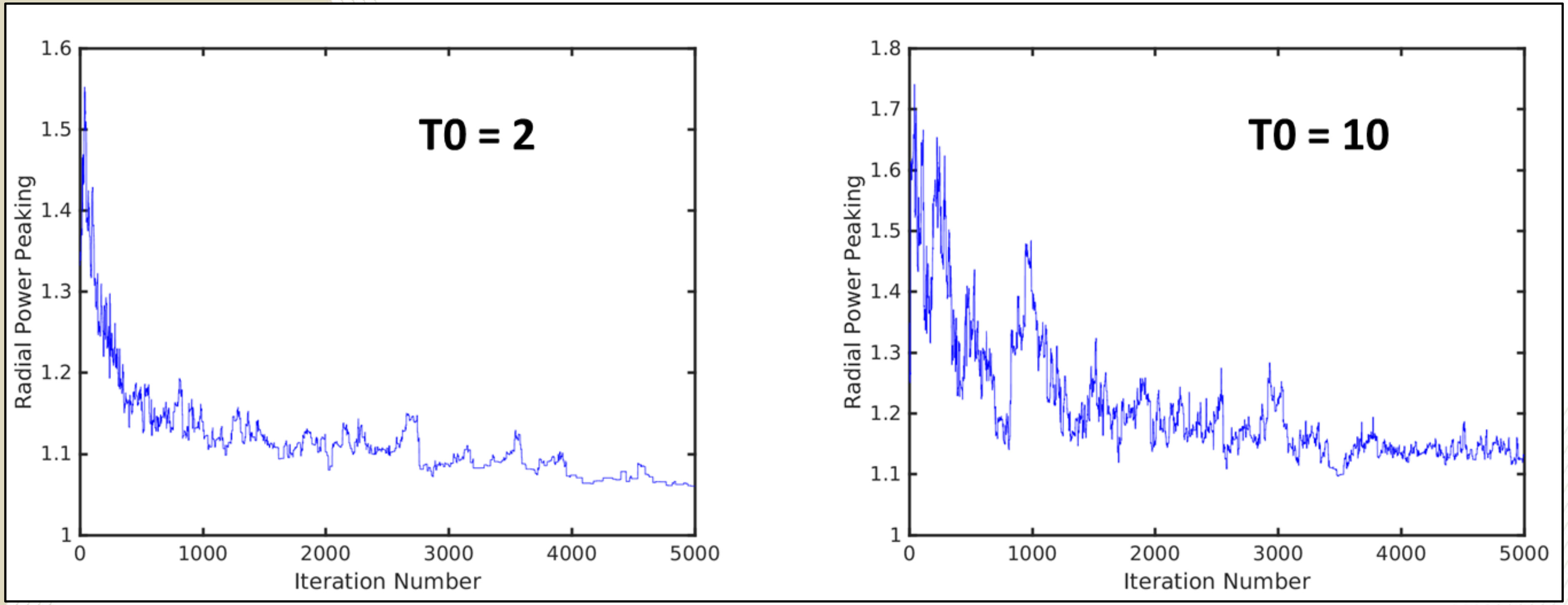
Coupled Input File Generator



Variable Acceptance Criterion

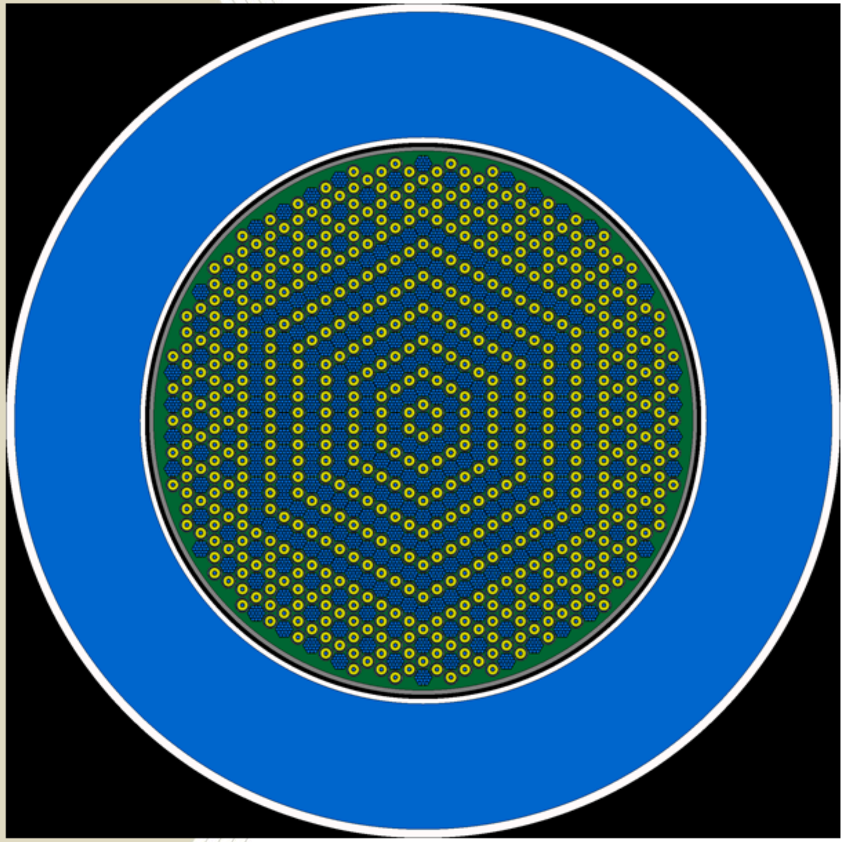
- Constituents of the SA probability equation are varied to determine their impact on the algorithm outputs
  - Five annealing temperatures (T_0): 2, 4, 6, 8, 10
  - Three maximum acceptance criterion (%): 50, 70, 90
- 15 total cases, 75000 random core geometries simulated
  - ~5 seconds per simulation

$$p_{sa} = exp(-\frac{k_a}{T_0} * (PP_1 - PP_0))$$



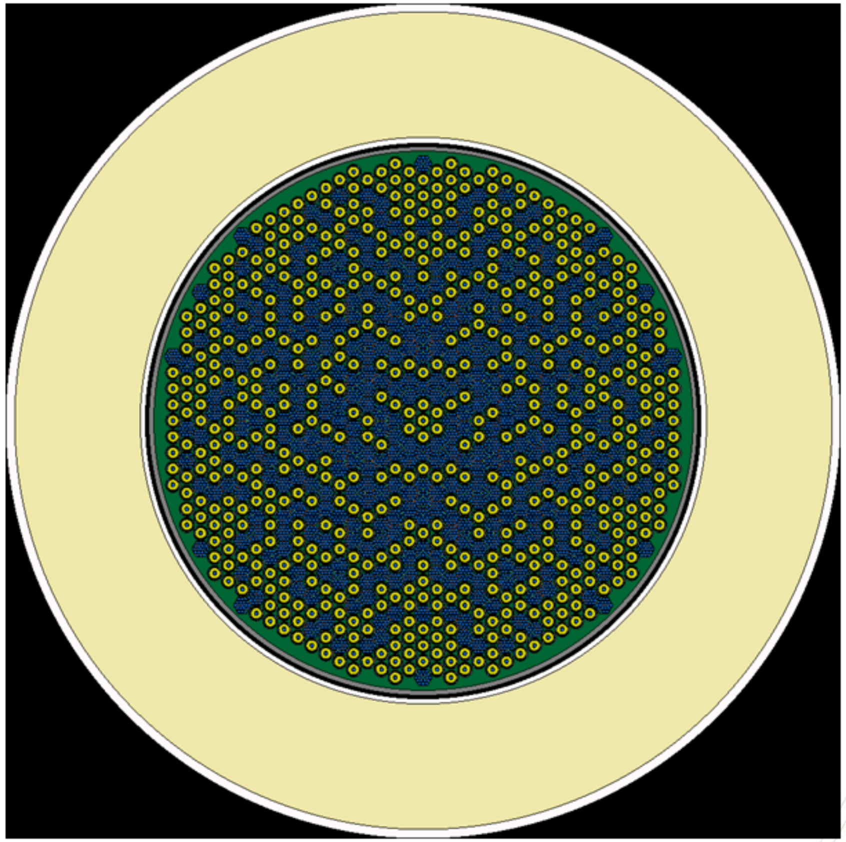
Core Loading Impact on Specific Impulse

Reference Core



Max Radial Power Peaking = 1.3322
Isp = 755.29

SA-derived Optimal Core



Max Radial Power Peaking = 1.0605
Isp = 848.09

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Final Remarks

Conclusions

- **Significant reduction of the radial power peaking increases the output performance (Isp) of the engine by more than 12%**
- Recommended future work could include:
  - Variable enrichment zoning
  - Impact of geometry fluctuations (length, radius, etc.) on criticality
  - Application to other active core configurations

Acknowledgements

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- 2020 Georgia Tech NTP Senior Design team for assisting me with the creation of necessary SERPENT post-processing
  - Andrew Nelson, Ben Adams, Jonathan Merritt, and Warren Erling

Questions?

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