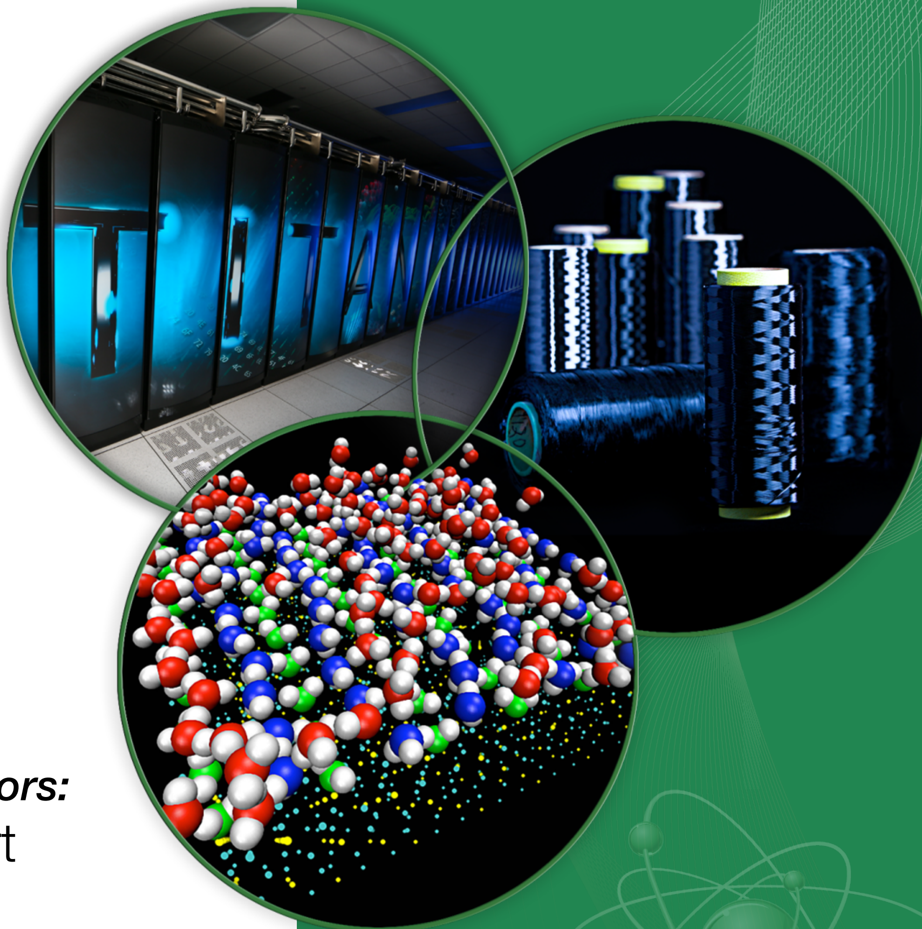
A first strike at an OpenACC C++ Monte Carlo code



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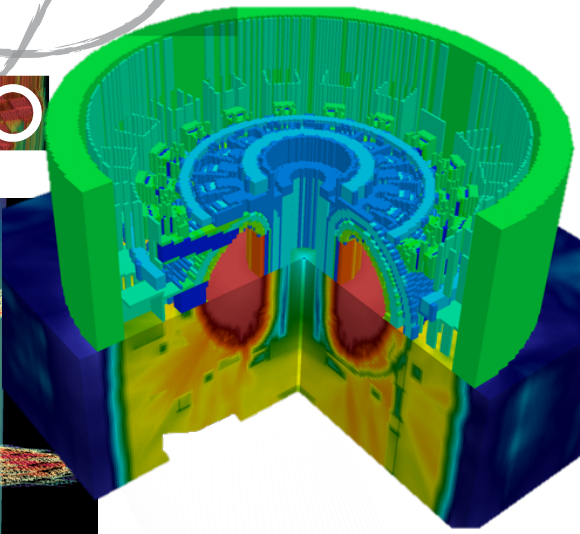
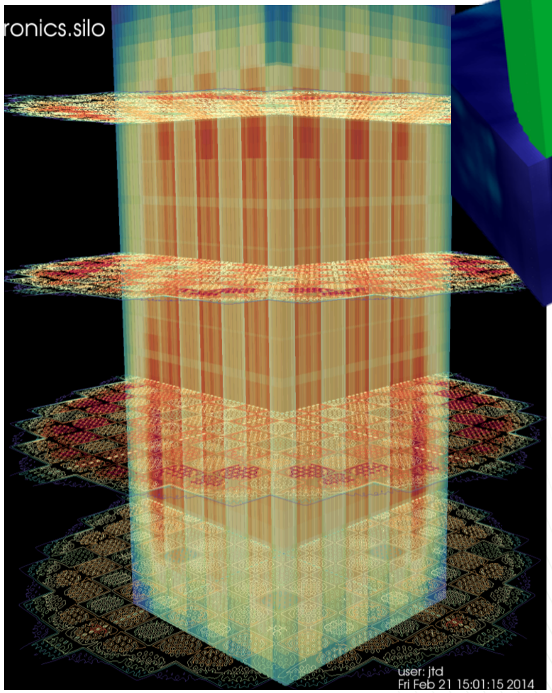
The codes

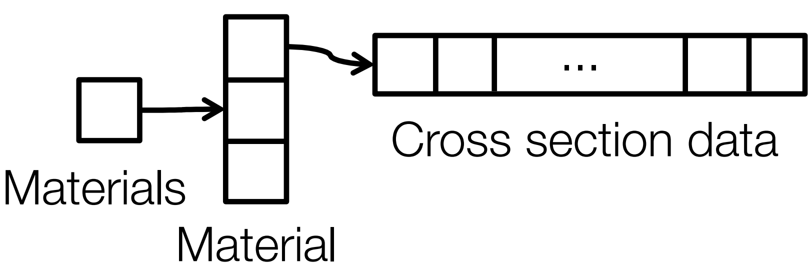
- Exnihilo: radiation transport framework
  - Multi-application (fusion, fission, detectors, homeland security)
  - Export controlled
- Profugus mini-app:
  - Written for algorithmic and HPC development
  - Limited capability
  - Reduced complexity

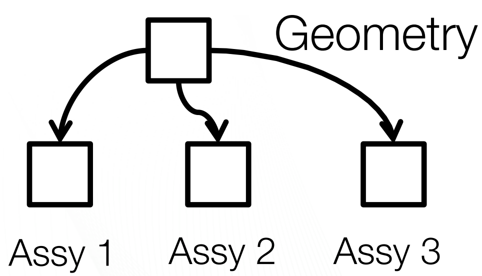




Introduction to the code environment

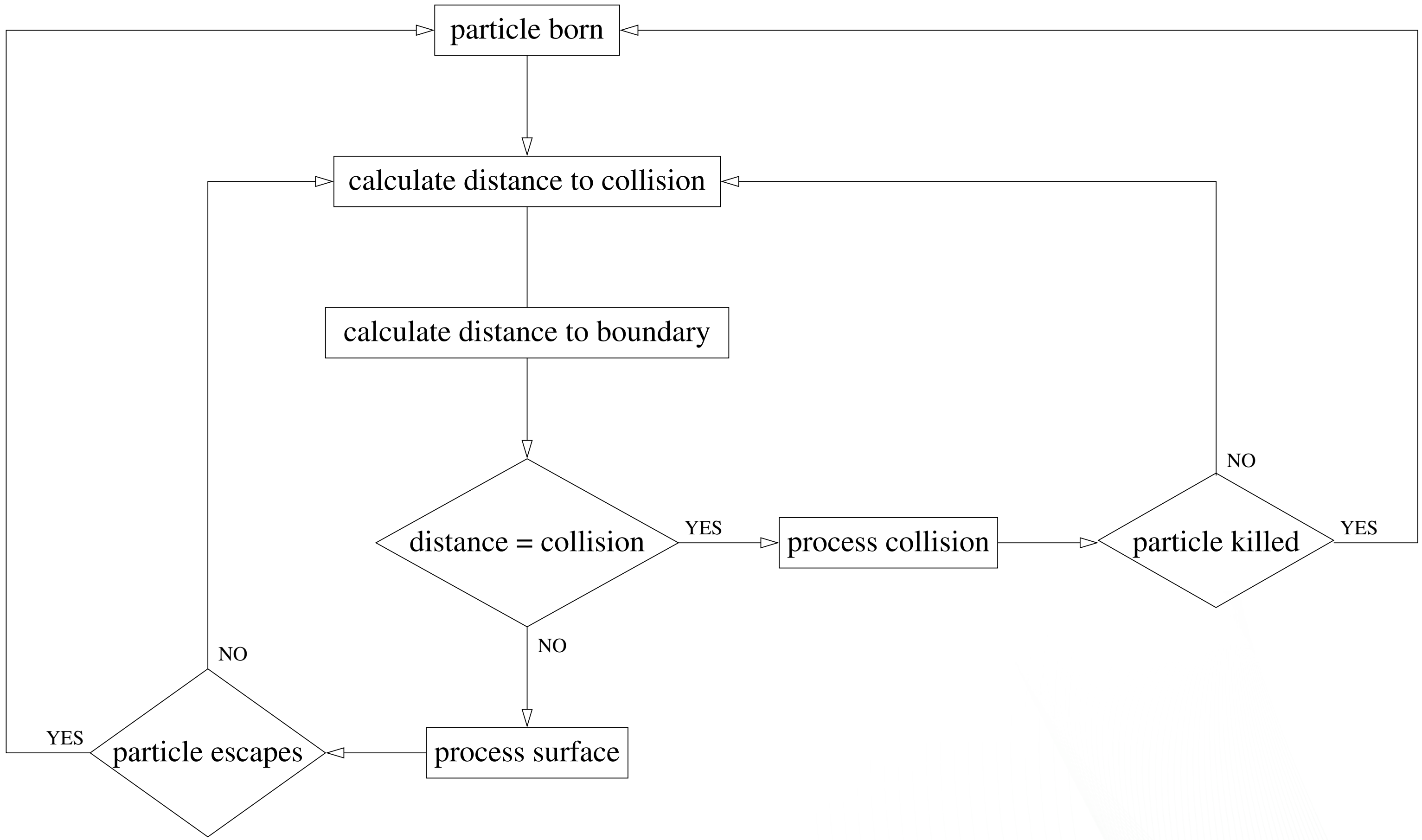
- C++11: unordered maps, `auto`, lambdas, etc.
- TPLs: Trilinos, HDF5
- Data structures are not POD, have irregular shape
  - Many distinct objects, dynamically sized vectors, shared pointers, etc. trade convenience for poorer data locality
  - Examples: particle, geometry cell, material attributes

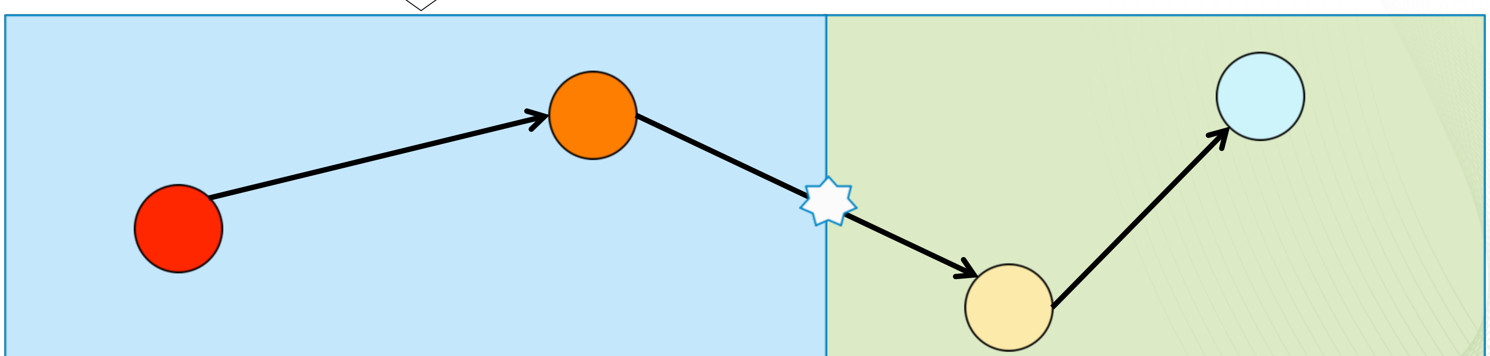




- Production environment: Chester (OLCF cluster)
  - PGI 14.7.0 (a few months old)
  - CUDA 5.5 (more than 2 years old)

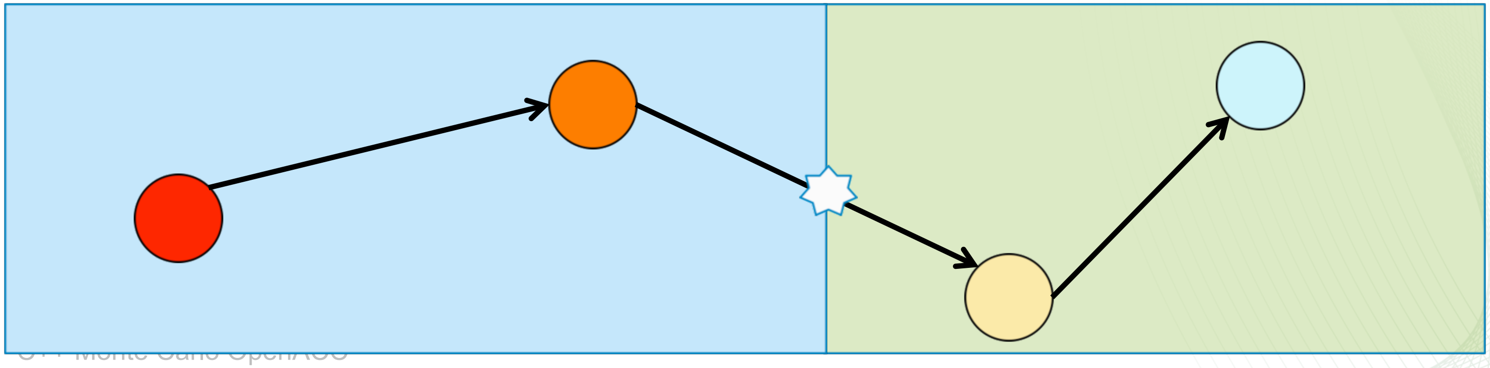
Introduction to Monte Carlo for neutronics





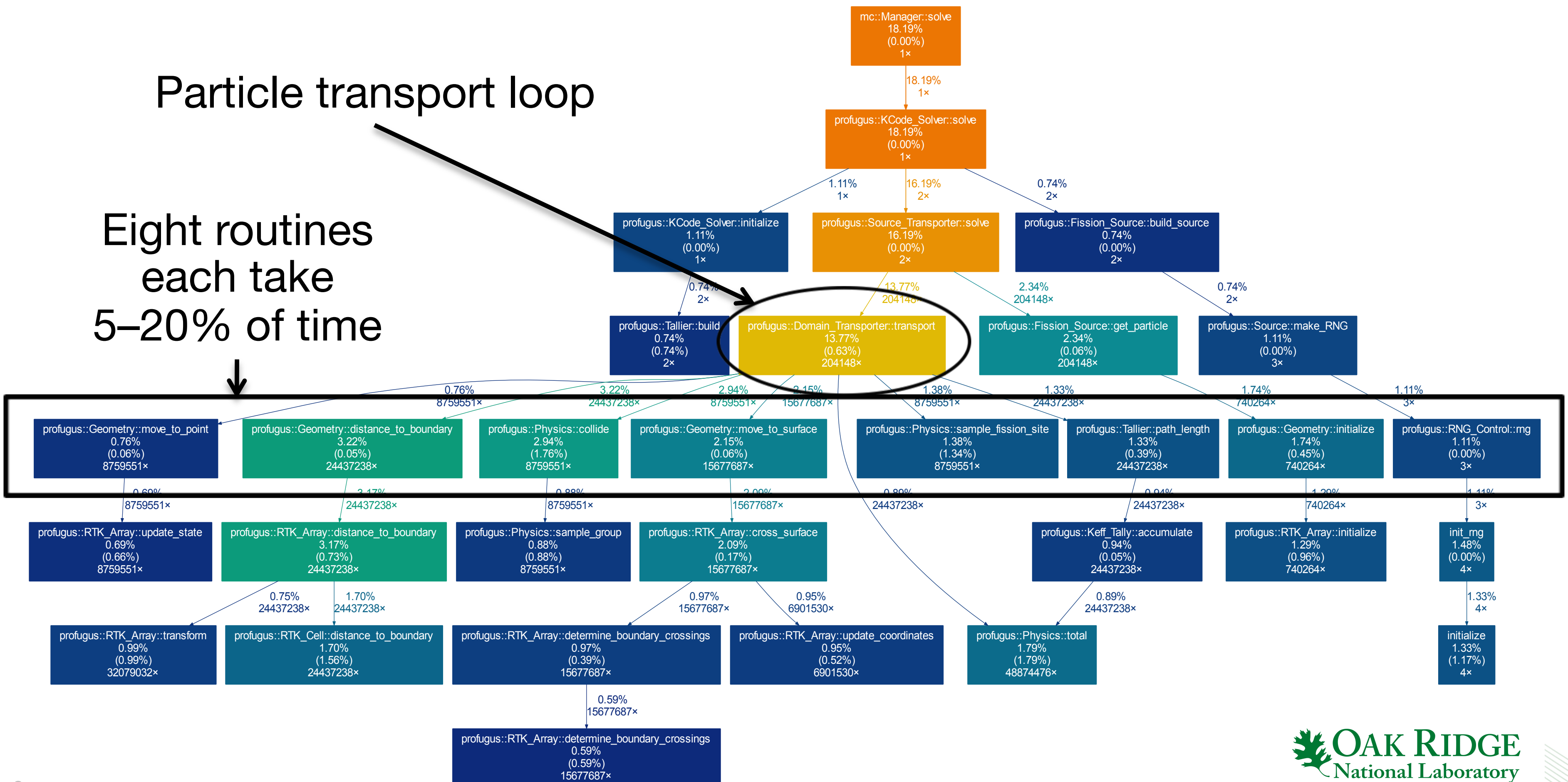
Algorithmic challenges

- Inherently stochastic process
  - Fast, long-period random number sampling required
  - Highly divergent code paths between loops
  - There is no fixed-length nested “`for` loop” to parallelize
- Complex data structures built to mirror physical processes
  - Indirection, dynamic allocation, irregular data shapes
  - There is no homogeneous multi-dimensional array of data



Initial timing profile

- Ran a semi-realistic reactor assembly problem
- No compute-intensive bottlenecks to offload



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The initial plan

- Rewrite classes for on-device execution
  - Geometry, Physics, Particle, Transporter
- Put CPU-intensive routines on the GPU
  - Particle geometry tracking
  - Cross section sampling and collisions
  - Tallying
- Run a simplified reactor assembly problem
- Get new timing profile using GPUs

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The immediate derailing of the initial plan

- Adding `-acc` flag broke our code
  - No OpenACC (or other) pragmas even being used
  - Unintelligible errors emitted from a standard library include inside Trilinos
  - Split OpenACC-dependent code into a subpackage that uses that flag, preventing its propagation elsewhere
- At least a day of team effort with Nvidia/PGI to get a C++ class with multiple vectors compiling

The final plan

- Attempt to write an adapter class to flatten CPU classes into data structures suitable for OpenACC
- Write a simple random number generator
- Write a simple brick mesh ray tracer that can be parallelized with OpenACC
- Write simple OpenACC-enabled multigroup physics with data access and collisions

What *actually* was accomplished

- 23 PGI compiler bug reports
  - PGI is the only compiler to support both OpenACC and C++11
  - We were probably the first group to use both in a production environment
- Primitive multigroup physics on the GPU
  - Driven through unit tests, reproduced CPU results
- Successfully ray-traced particles on brick mesh on the GPU
  - 20X faster if all particles do the same thing
  - 15X faster with divergence

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C++ suggestions for OpenACC

- Separate compilation units for ACC code
  - Inline keyword gives the compilers trouble; always write in .cc files
  - Include as few headers as possible (no Trilinos) to avoid compiler errors from non-ACC code and to reduce compiler time
- CPU data management with `std::vector`, then copy address to raw pointer for OpenACC
- Complexity hidden by ACC means more mysteries:
  - Do not rely on thread-private data

```
84, Accelerator restriction: scalar variable live-out from loop: seed
98, Loop carried scalar dependence for 'seed' at line 104
```

  - Issues with reduction operations on scalars
  - Do not use “const” class member data

Positive takeaways

- Learned basics of OpenACC and how it can be used in a C++ environment
- Better understanding of the heterogeneous architecture and how it relates to OpenACC directives (prior knowledge of CUDA is helpful)
- For very simplified and specific MC problems, we may be able to achieve speedup and the ability to run full problems on the GPU using Profugus (with a lot of rewriting)

Negative takeaways

- Existing MC algorithms are fundamentally incompatible with OpenACC-type usage
  - Monte Carlo does not have nested, fixed-length loops
  - Memory-managed objects cannot be accelerated
- C++, PGI, and OpenACC do not currently get along
  - Two weeks preparation to compile with PGI on Titan
  - C++11 incompatible with installed Cray compiler wrapper
  - Profiling tool issues with the code
  - Mystery compiler errors when turning on `-acc` on PGI
- No OpenACC libraries yet
  - We had write a simple pseudorandom number generator
  - No microkernels or algorithms for sorting, binary search

Concluding comments

- Hackathon was critical to kick-starting our investigation into Monte Carlo on the GPU
  - Resources: the compiler experts are there to help you
  - Time: you have a solid week to work in a focused environment with one task at hand
  - Perspective: you are not the only team struggling!
- OpenACC feasibility for C++
  - `#pragma` is not very pragmatic (inherently incompatible with C++ features): appropriate for Fortran
  - Compiler and environment are very difficult to get working
- Our next step: Kokkos as template-based abstraction layer

Acknowledgements

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- And thanks to Fernanda and OLCF for making the Hackathon happen!

Profugus:
http://ornl-cees.github.io/Profugus/

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