Computational methods and software development

in nuclear engineering research

R. N. Slaybaugh
Univ. of Cal. Berkeley

BIDS Tea
4 December 2014

What Are We Sovling?

I study how to solve the steady state, neutral particle Boltzmann transport equation more efficiently:

$$[\hat{\Omega}\cdot\nabla+\Sigma(\vec{r},E)]\psi(\vec{r},\hat{\Omega},E)=q(\vec{r},\hat{\Omega},E)+\int_0^\infty dE'\int_{4\pi}d\hat{\Omega}'\,\Sigma_s(\vec{r},E'\rightarrow E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega}',E')$$

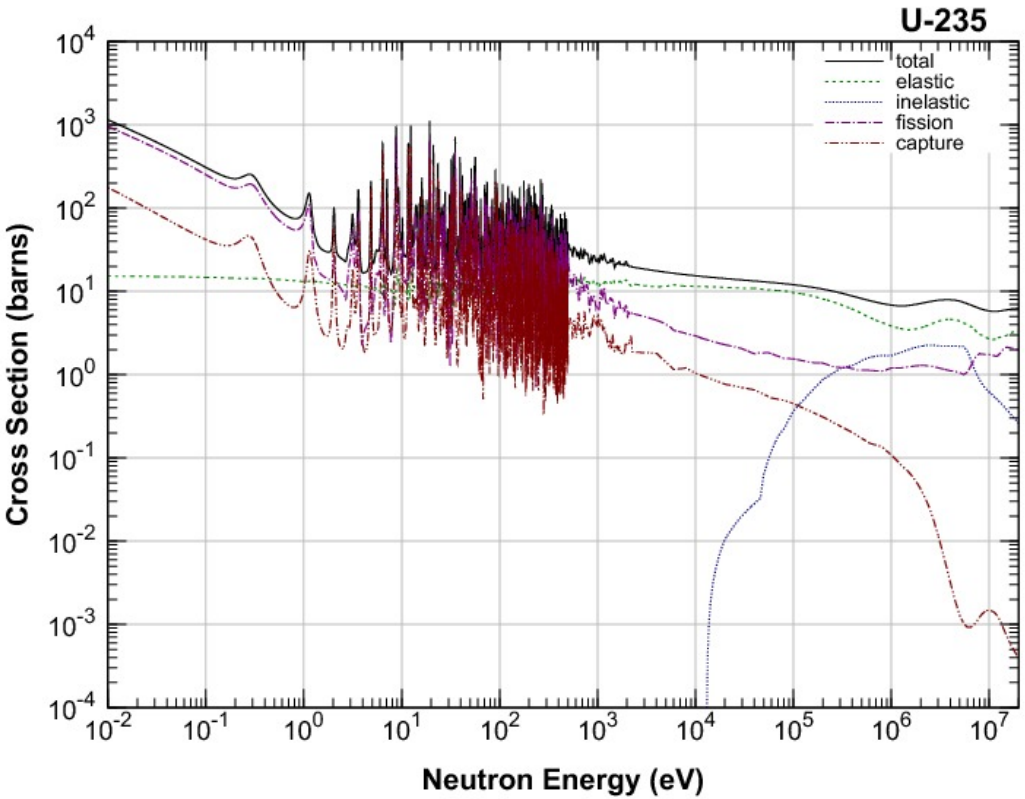
Discretize, then convert to operator form:

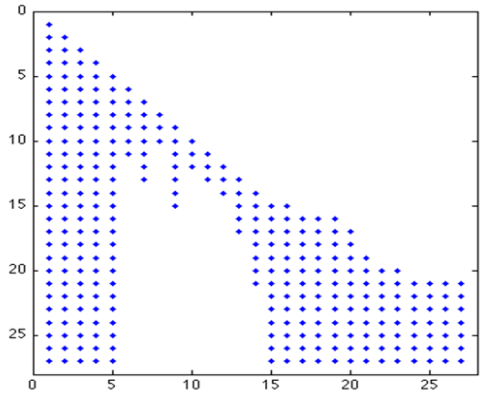
$$\begin{aligned}\mathbf{L}\psi&=\mathbf{MS}\phi+\mathbf{Q}\\ \phi&=\mathbf{D}\psi\\ \underbrace{(\mathbf{I}-\mathbf{DL}^{-1}\mathbf{MS})}_{\mathbf{A}}\phi&=q\end{aligned}$$

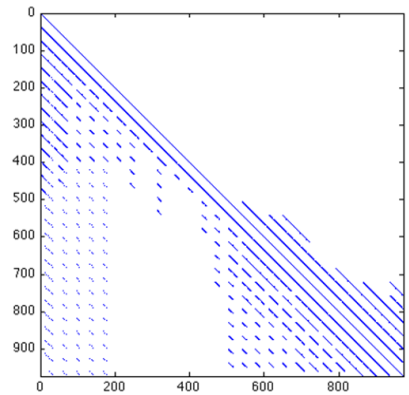
Linear Algebra now runs the show...

What Drives the Challenges and Solutions?

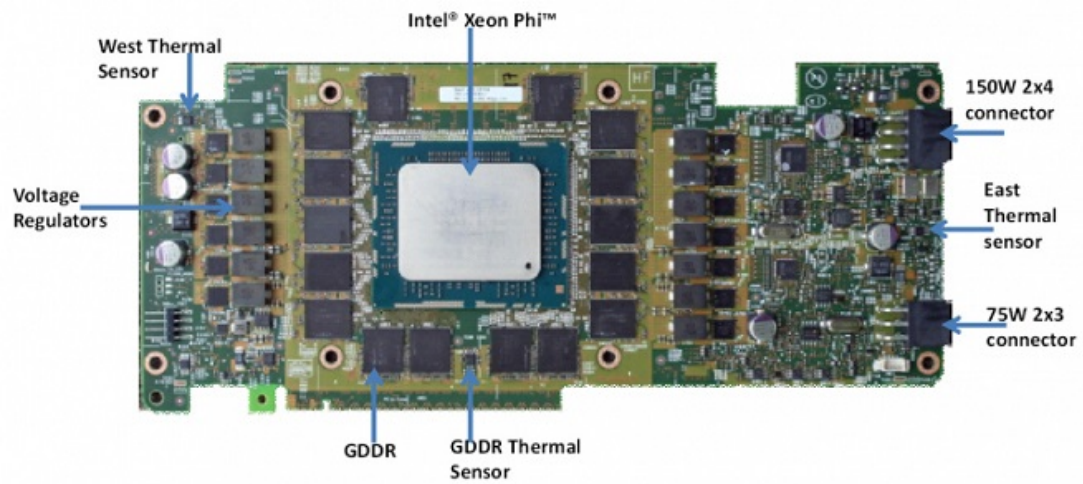
Properties of the matrix govern solution behavior





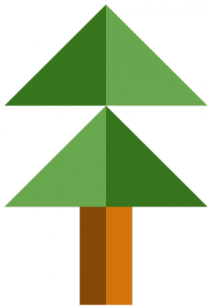


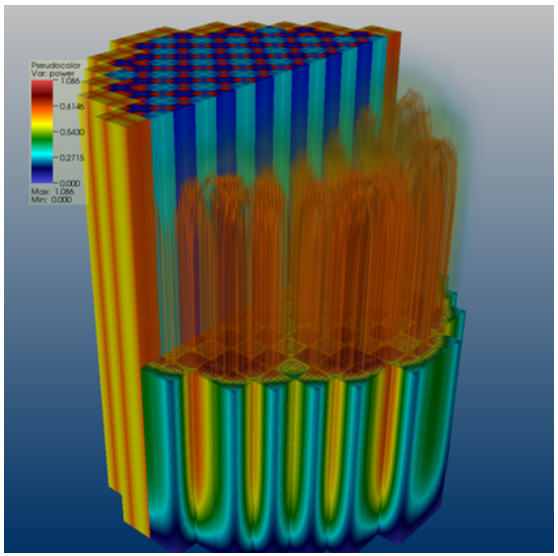
What Drives the Challenges and Solutions?



Architecture influences algorithm choices and data management

Research, Tools, Applications





`PyNE` Goals:

- be more productive (don't reinvent the wheel!)
- have the best solvers
- have a clear and useful API
- write really great code
- teach the next generation

It is permissively licensed (2-clause BSD)

It supports both a C++ and a Python API