# PhD Defense: Finite Elements with Discontiguous Support for Energy Discretization in Particle Transport


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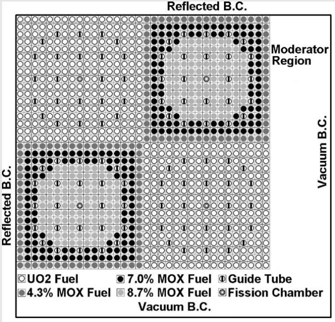
# Outline

1. Introduction and Motivation
2. Method
   - A finite element in energy
   - Researching and inventing our way out of problems
3. Results
   - A neutron time-of-flight problem
   - A reactor problem with comparisons to MCNP
4. Conclusions
   - . . . and continuations

# We desire accurate and inexpensive quantities of interest (QOI) for neutron problems, which requires accurate and efficient simulation of neutron transport

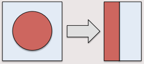
## Reactor applications

QOI: Pin powers, criticality eigenvalue



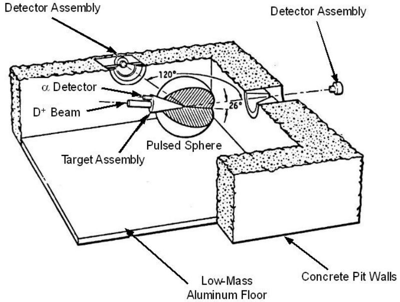

M.A. Smith *et al.*, *Prog. in Nuclear Energy*, Vol. 45, 2004

Simplified reactor problems



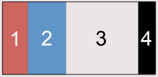
## Time-dependent neutronics problems

QOI: Detector response in time




R.J. Procassini, M.S. McKinley, LLNL-PROC-453212, SNA+MC2010

Simplified TOF problem



# Problem: How to discretize the energy variable accurately without requiring an $\mathcal{O}(10,000)$ energy unknown count?

**This research tackles a long-standing issue in neutron transport through a series of "problem-research-solution" cycles**

Our solution: Divide in "solution space" instead of energy space using our **Finite-Element**-with-Discontiguous Support (FEDS) method

# The linear Boltzmann transport equation describes the interaction of radiation quanta with their environment

## The neutron transport equation

(radiative transfer equation is similar; no material motion or neutron-neutron interactions are considered; $q_{\text{coll}}$ term includes fission)

$$\left[\frac{1}{v(E)}\partial_t + \mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E,t)\right]\psi(\mathbf{r},E,\mathbf{\Omega},t) = q_{\text{coll}}(\mathbf{r},E,\mathbf{\Omega},t) + q_{\text{ext}}(\mathbf{r},E,\mathbf{\Omega},t)$$

$$q_{\text{coll}}(\mathbf{r},E,\mathbf{\Omega},t) = \sum_i N_i(\mathbf{r},t)\int_{4\pi}\mathrm{d}\Omega'\int_0^\infty \mathrm{d}E'\,\sigma_{s,i}(E'\to E,\mathbf{\Omega}'\cdot\mathbf{\Omega},T(\mathbf{r},t))\,\psi(\mathbf{r},E',\mathbf{\Omega}',t)$$

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$$\text{Total cross section} = \Sigma_t(\mathbf{r},E,t) = \sum_i N_i(\mathbf{r},t)\,\sigma_{t,i}(E,T(\mathbf{r},t))$$

$$\text{Solution (``Scalar flux'')} = \phi(\mathbf{r},E,t) = \int_{4\pi}\mathrm{d}\Omega\,\psi(\mathbf{r},E,\mathbf{\Omega},t)$$

$$\text{Quantities of interest (QOI)} = R_{i,n} \propto \int_{\Delta t_n}\mathrm{d}t\int_{V_i}\mathrm{d}^3r\int_0^\infty \mathrm{d}E\,\phi(\mathbf{r},E,t)\,\Sigma_x(\mathbf{r},E,t)$$

$$\text{or} \propto \int_{\Delta t_n}\mathrm{d}t\int_{S_i}\mathrm{d}^2r\int_0^\infty \mathrm{d}E\int_{\hat{\mathbf{n}}\cdot\mathbf{\Omega}>0}\mathrm{d}\Omega\,(\hat{\mathbf{n}}\cdot\mathbf{\Omega})\,\psi(\mathbf{r},E,\mathbf{\Omega},t)$$

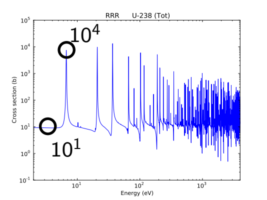
# Problem: The solution is strongly impacted by resonances in the material cross sections (XS)

## Reactor problems

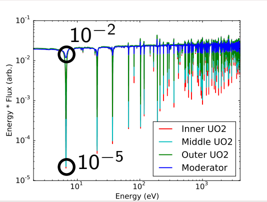
$$\left[E\phi\right]_{\text{outside of fuel}} \simeq 1$$

$$\left[E\phi\right]_{\text{inside of fuel}} \simeq 1/\Sigma_t(E)$$

$\sigma_t(E)$ for U-238 in the resonance range




Flux in the resonance range

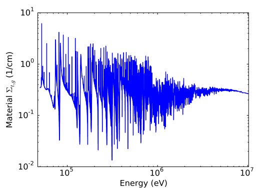



## Time-of-flight (TOF) problems

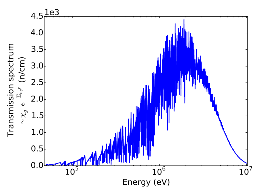
$$\text{Absorption} \propto \chi(E)\left(1 - e^{-\Sigma_t(E)X}\right)$$

$$\text{Transmission} \propto \chi(E)\, e^{-\Sigma_t(E)X}$$

$\Sigma_t(E)$ for natural iron




Transmission spectrum



# MG solution: Discretize in energy by grouping together particles with similar energies

This multigroup (MG) approach averages material parameters within each group

## The neutron transport equation

$$\left[\frac{1}{v(E)}\partial_t + \mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E,t)\right]\psi(\mathbf{r},E,\mathbf{\Omega},t) = q_{\text{scat}}(\mathbf{r},E,\mathbf{\Omega},t) + q_{\text{ext}}(\mathbf{r},E,\mathbf{\Omega},t)$$

## The MG neutron transport equation

$$\left[\frac{1}{v_g}\partial_t + \mathbf{\Omega}\cdot\nabla + \Sigma_{t,i,g}(t)\right]\psi_g(\mathbf{r},\mathbf{\Omega},t) = q_{\text{scat},g}(\mathbf{r},\mathbf{\Omega},t) + q_{\text{ext},g}(\mathbf{r},\mathbf{\Omega},t)$$

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$$\Sigma_{t,i,g}(t) \equiv \frac{\int_{\Delta E_g} \mathrm{d}E\, f_i(E)\,\Sigma_t(\mathbf{r}\in V_i,E,t)}{\int_{\Delta E_g} \mathrm{d}E\, f_i(E)}$$

$$\psi_g(\mathbf{r},\mathbf{\Omega},t) \simeq \int_{\Delta E_g} \mathrm{d}E\,\psi(\mathbf{r},E,\mathbf{\Omega},t) \quad \text{if} \quad f_i(E)\simeq\psi(\mathbf{r},E,\mathbf{\Omega},t) \quad \text{or} \quad \Delta E_g \text{ is small}$$

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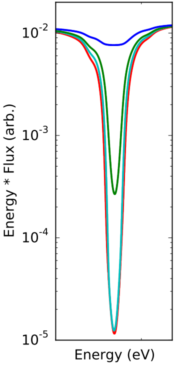
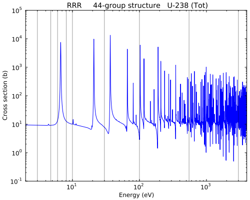
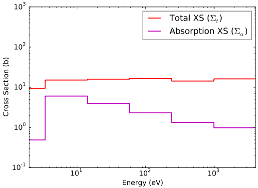
# Problem: We cannot afford to resolve cross sections in energy space and the solution is not separable in energy



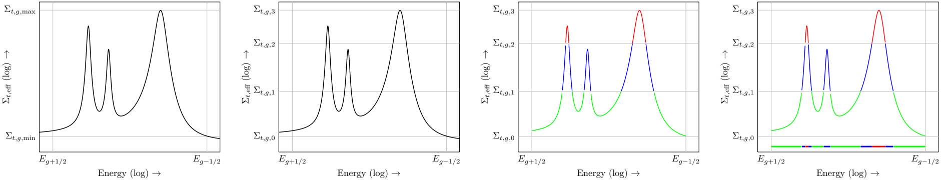

## Usually impractical to make $\Delta E_g$ small wrt to resonance widths (top)

- There are many resonances: $\mathcal{O}(1,000) - \mathcal{O}(10,000)$
- We must resolve a multiscale 7-D phase space $(\mathbf{r}, E, \mathbf{\Omega}, t)$

## $f_i(E) \not\simeq \psi(\mathbf{r}, E, \mathbf{\Omega}, t)$ due to self-shielding effects (left)

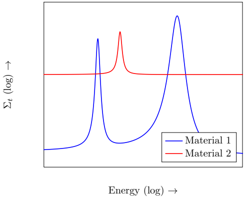
- The spectrum changes within a material region and in angle
- We can preserve bulk reaction rates if
  $$\int_{V_i} \mathrm{d}^3 r \int_{4\pi} \mathrm{d}\Omega \int_{\Delta E_g} \mathrm{d}E \left[ f_i(E) - \psi(\mathbf{r}, E, \mathbf{\Omega}, t) \right] \simeq \text{small}$$
- Above does not work for quantities such as leakage

# MB solution: Resonance resolution at low unknown count requires discretizing cross section space




## Problem: Solution depends on more than one total XS

- The MB family discretizes total XS space through banding (top)
- $[\boldsymbol{\Omega}\cdot\nabla+\Sigma_t(\mathbf{r},E,t)]\,\psi(\mathbf{r},E,\boldsymbol{\Omega},t)=q(\mathbf{r},E,\boldsymbol{\Omega},t)$
    - Solution depends on $\Sigma_t$ not any $\sigma_t$
    - Solution depends on the source, $q$, which is not smooth in energy (scattering resonances)
    - Solution depends on upstream $\Sigma_t$ and $q$
- Banding does not work when multiple resonant materials / nuclides are simultaneously considered (right)



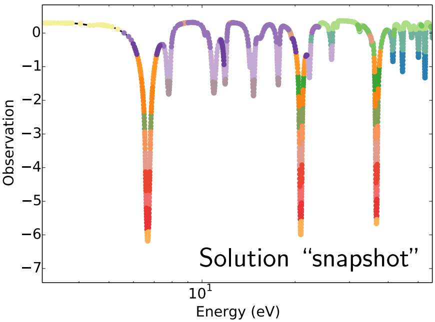
# Outline

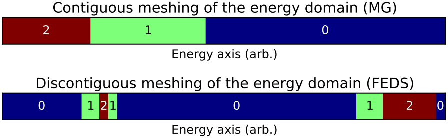
## Up Next

- A high-level overview of FEDs
- Details of FEDS

# FEDS solution: Our new method overcomes the drawbacks of MG and MB

- We **divide in solution space**, not energy or XS space (top)
- Our method is **defined in energy space** (bottom)
- We naturally **handle multiple resonant inputs** (minimize the spectral variance in each energy unknown over all snapshots)
- Our method often **achieves $\mathcal{O}\left(10^{-4}\right)$ relative accuracy with $\mathcal{O}\,(200)$ energy unknowns**
- **Less sensitive to weighting spectrum**, $f_i(E)$, for XS condensation than is MG



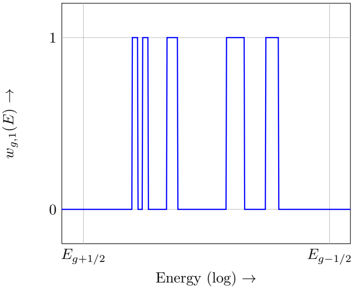



# Our method is the Finite-Element with Discontiguous Support (FEDS) method

FEDS is a Petrov-Galerkin finite element method in energy

## This is our *only* approximation

$$\psi_{\text{exact}}(\mathbf{r}, E, \mathbf{\Omega}, t) \simeq \psi_{\text{FEDS}}(\mathbf{r}, E, \mathbf{\Omega}, t) \equiv \sum_k b_k(\mathbf{r}, E)\psi_k(\mathbf{r}, \mathbf{\Omega}, t),$$




## Our weight functions (left)

$$w_k(E) = \begin{cases} 1 & \text{if } E \in \mathbb{E}_k, \\ 0 & \text{otherwise,} \end{cases}$$

## Our basis functions

$$b_k(\mathbf{r} \in V_i, E) = \begin{cases} C_{i,k}\, f_i(E) & E \in \mathbb{E}_k, \\ 0 & \text{otherwise,} \end{cases}$$

where the $f_i(E)$ are approximate solution spectra (usually from simpler calculations) and $C_{i,k} = \frac{1}{\int_{\mathbb{E}_k} \mathrm{d}E\, f_i(E)}$.

# We derive a weak form of the transport equation

## We begin with the continuous-energy neutron transport equation

$$\mathbf{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \mathbf{\Omega}) + \Sigma_t(\mathbf{r}, E)\psi(\mathbf{r}, E, \mathbf{\Omega}) = \frac{1}{4\pi} \int_0^\infty \mathrm{d}E' \Sigma_s(\mathbf{r}, E' \to E)\phi(\mathbf{r}, E') + \frac{\chi(\mathbf{r}, E)}{4\pi\, k_{\text{eff}}} \int_0^\infty \mathrm{d}E' \nu\Sigma_f(\mathbf{r}, E')\phi(\mathbf{r}, E')$$

## We test the transport equation against the weight functions and expand the fluxes into their basis function representations

$$\vdots$$

## After algebraic manipulation we get what looks like a standard MG formulation

$$\mathbf{\Omega} \cdot \nabla \psi_k(\mathbf{r}, \mathbf{\Omega}) + \Sigma_{t,k,i}\psi_k(\mathbf{r}, \mathbf{\Omega}) = \frac{1}{4\pi} \sum_{k'} \Sigma_{s,k' \to k,i}\phi_{k'}(\mathbf{r}) + \frac{\chi_{k,i}}{4\pi\, k_{\text{eff}}} \sum_{k'} \nu\Sigma_{f,k',i}\phi_{k'}(\mathbf{r})$$

# The FE definitions give us expressions for the cross sections and unknowns

**Cross sections are now averaged over discontinuous energy domains instead of continuous ones**

$$\Sigma_{t,k,i} \equiv \int_0^\infty \mathrm{d}E\, b_k(\mathbf{r}, E)\, \overline{\Sigma}_{t,i}(E),$$

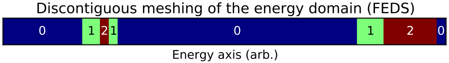
$$\chi_{k,i} \equiv \int_0^\infty \mathrm{d}E\, w_k(E)\, \overline{\chi}_i(E),$$

$$\Sigma_{s,k'\to k,i} \equiv \int_0^\infty \mathrm{d}E'\, b_{k'}(\mathbf{r}, E') \int_0^\infty \mathrm{d}E\, w_k(E)\, \overline{\Sigma}_{s,i}(E' \to E),$$

$$\psi_k(\mathbf{r}, \boldsymbol{\Omega}, t) \equiv \int_0^\infty \mathrm{d}E\, w_k(E)\, \psi(\mathbf{r}, E, \boldsymbol{\Omega}, t),$$

$w_k(E)$ and $b_k(\mathbf{r}, E)$ are nonzero only for $E \in \mathbb{E}_k$,

The $\mathbb{E}_k$ are discontiguous energy ranges (*e.g.*, see below)



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# Problem: How to discretize the energy variable accurately without requiring an $\mathcal{O}(10,000)$ energy unknown count?

**This research tackles a long-standing issue in neutron transport through a series of problem-research-solution cycles**

Our solution: Divide in solution space instead of energy space using our **Finite-Element**-with-Discontiguous Support (FEDS) method

I How to determine the energy mesh ($\mathbb{E}_k$)?

II How to determine the condensing spectrum ( $f_i(E)$ )?

III How to assess the method?

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I How to determine the energy mesh ($\mathbb{E}_k$)?
1. How do we divide in solution space when there is more than one spectrum?
   Minimize a projection error to the coarse grid
2. How do we form accurate spectra for the minimization problem?
   Take advantage of decades of transport and MG work
3. How do we solve this minimization problem efficiently?
   Use clustering algorithms from machine learning
4. How do we solve our discrete transport equation in energy?
   Employ traditional MG solvers

II How to determine the condensing spectrum ( $f_i(E)$ )?

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I How to determine the energy mesh ($\mathbb{E}_k \Leftrightarrow w_k(E)$, the FE weight functions)?

II How to determine the condensing spectrum ( $f_i(E)$ )?

1. How do we treat resonance-scale energy behavior of the solution accurately?
   Take advantage of decades of MG work
2. How do we treat long-range energy behavior of the solution accurately?
   Nested energy mesh with an outer level of coarse groups
3. How do we apportion energy unknowns among the coarse groups?
   Apportion based on relative variance within a coarse group

III How to assess the method?

*Reactor problem*

$$\phi_\infty(E) \simeq \frac{1}{E} \; \frac{1}{\Sigma_t(E)}$$

*TOF problem*

$$\phi_{\text{transmission}}(E) \simeq \chi(E) \; e^{-\Sigma_t(E)X}$$

$$t_{\text{arrival}} \propto \frac{1}{v(E)}$$

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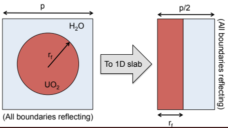
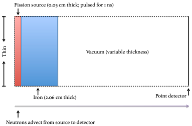
III How to assess the method?

- Compare to an optimal MG competitor whose energy mesh comes from a contiguous partitioning solution of the minimization problem
- Compare to continuous-energy Monte Carlo for simple reactor problems (left)
- Compare to an analytic solution for a time-dependent problem where the $1/v$ term becomes important (right)



# We travel through a series of problem-research-solution cycles

I Determining the energy mesh

1. Dividing in solution space with more than one spectrum
2. Forming accurate spectra for the minimization problem
3. Solving this minimization problem efficiently
4. Solving our discrete transport equation in energy

II Determining the condensing spectrum

III Testing the method

# Problem: How do we divide in solution space for multiple resonant snapshots

## Research: Applied mathematics

### Before performing the minimization

1. Determine a hyperfine group structure that resolves all desired resonances
   $\{E_{g\pm 1/2}\}$, $g = 1, \ldots, G$
2. Obtain $P$ representative high-resolution snapshots of the solution on the hyperfine structure
   $\phi_{g,p}$, $p = 1, \ldots, P$
3. Choose a final number of energy elements, $N_e$
   Elements indexed by $e = 1, \ldots, N_e$

### Solution: The minimization problem

1. Guess $\mathbb{S}_e$, the set of hyperfine groups that belong to element $e$
   Each group, $g$, belongs to exactly one element, $e$
2. Average the spectra in energy over each element for each material
   $\bar{\phi}_{e,p} = \mathrm{mean}_{g \in \mathbb{S}_e}(\phi_{g,p})$
3. Compute a metric of variance over all elements and snapshots
   $F = \sum_p \sum_e \sum_{g \in \mathbb{S}_e} \left|\phi_{g,p} - \bar{\phi}_{e,p}\right|^2$
4. Choose element definitions that minimize $F$
   $\mathbb{S}_e = \mathrm{argmin}\, F$

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Discontiguous meshing of the energy domain (FEDS)


Energy axis (arb.)

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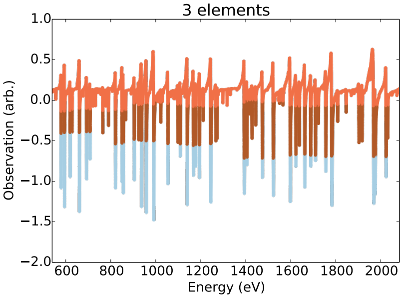
4. Choose element definitions that minimize $F$
   $\mathbb{S}_e = \mathrm{argmin}\, F$

# Problem: How do we obtain accurate snapshots for the minimization problem

## Research: Integral form of the transport equation, physics of downscattering




### Solution: Infinite-medium calculations

Snapshots are spectra that come from solving:

$$\left(\Sigma_e + \Sigma_{t,g}\right)\phi_{g,p} = q_{\mathrm{scat},g,p}\left(\phi_{g',p}\right) + q_{\mathrm{ext},g,p}$$

This is one simple way to generate high-resolution snapshots

FEDS is insensitive to this choice

Minimization problem uses these $\phi_{g,p}$:

$$\mathbb{S}_e = \mathrm{argmin} \sum_p \sum_e \sum_{g \in \mathbb{S}_e} \left|\phi_{g,p} - \bar{\phi}_{e,p}\right|^2$$

Mesh is encoded in the $\mathbb{S}_e$ (left)

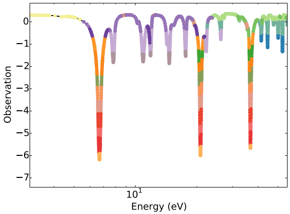
# Problem: How do we solve the minimization problem

## Research: Clustering algorithms from machine learning

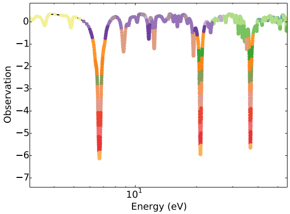
### Solution: Clustering algorithms solve the minimization problem approximately

- Minimization problem: $\mathbb{S}_e = \operatorname{argmin} \sum_p \sum_e \sum_{g \in \mathbb{S}_e} |\phi_{g,p} - \bar{\phi}_{e,p}|^2,\ e = 1, \ldots, N_e$
- We use **hierarchical agglomeration** (accurate, not stochastic, medium cost)
  - Starts with all hyper-fine groups in their own cluster ($\mathbb{S}_e^0 = \{g\},\ e = 1, \ldots, G$)
  - In each stage, it combines the two closest clusters into one new cluster ($\mathbb{S}_{\text{new}}^{n+1} = \mathbb{S}_{e_1}^n \cup \mathbb{S}_{e_2}^n$)
- Creates elements with minimal variance over all the snapshots
- Efficient implementation in `scikit-learn`, a Python module
- Other notable algorithms include Birch, K-Means, and Mini-Batch-K-Means

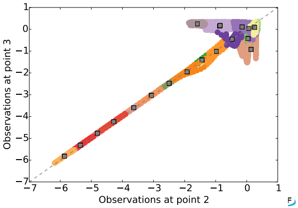
Snapshot of MOX spectrum:




Snapshot of $UO_2$ spectrum:




Clustering algorithm view:

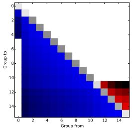


# Problem: How do we solve the FEDS neutron transport equation

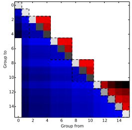
## Research: Finite element methods, iterative methods, sweeps

Scattering matrices

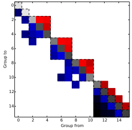
MG H-1:



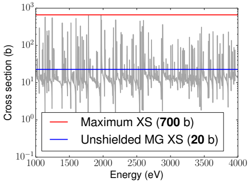

FEDS H-1:



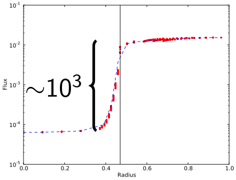

FEDS Pu-239:




Unresolved MG does not preserve large XS:




Large XS may introduce boundary layers:




### Solution: FEDS can use existing MG transport solvers

- Code thinks it is solving MG
- Caveat 1: Iterative methods
  FEDS introduces effective upscattering (left)
- Caveat 2: Spatial discretizations
  FEDS **resolves** large XS that introduce boundary layers (middle)

# We travel through a series of problem-research-solution cycles

I Determining the energy mesh

II Determining the condensing spectrum

1. Treating resonance-scale energy behavior of the solution
2. Treating long-range energy behavior of the solution
3. Apportioning energy unknowns among the coarse groups

III Testing the method

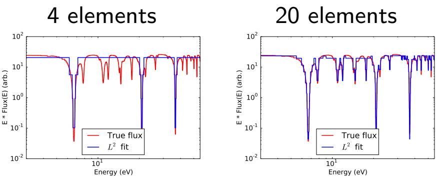
# Problem: How do we choose accurate and insensitive basis functions to capture local resonance effects

Research: Physics of streaming and downscattering, equivalence theory

## Solution, Part 1: FEDS

- Minimization problem yields elements that can adapt to the behavior of the solution-like spectra
- As energy unknowns are increased, fit improves (right)

$L^2$ fit of the spectra by the elements:




## Solution, Part 2: Reduced-geometry, high-energy-resolution calculations

- Basis function shape should match material-average solution shape (not be flat, as above)
- We use infinite-medium-equivalent calculations for the basis functions:
- $\left[\Sigma_{e,i} + \Sigma_{t,i}(E)\right] f_i(E) = \sum_{k \in \text{matl.}\, i} \left[\frac{N_k}{1-\alpha_k} \int_E^{E/\alpha_k} \mathrm{d}E' \, \frac{f_i(E')\sigma_{s,k}(E')}{E'}\right] + q_{\text{ext},i}(E)$
- $\Sigma_{e,i} \sim \mathrm{SA}_i/(4V_i)$ captures geometry information of real problem

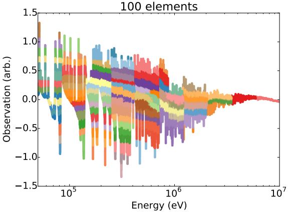
# Problem: How do we choose accurate and insensitive basis functions to capture long-range energy behavior

Research: Physics of streaming and downscattering, MB methods

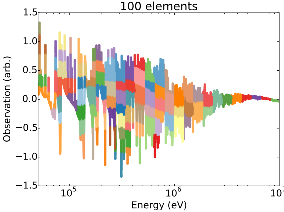
## Solution: Use coarse groups

- Large energy elements are inaccurate
- Restrict each element to live in one coarse group
- Balance coarse groups and, $r$, the average number of elements per coarse group (below)
- $r = 1$ is equal-lethargy-spaced MG

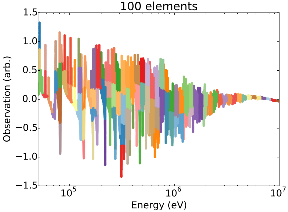
10 coarse groups ($r = 10$)




25 coarse groups ($r = 4$)




50 coarse groups ($r = 2$)

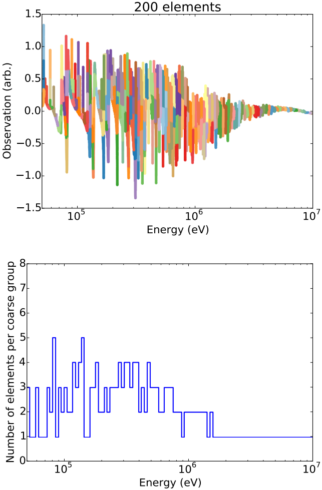


# Problem: How do we automatically apportion energy unknowns among the coarse groups?

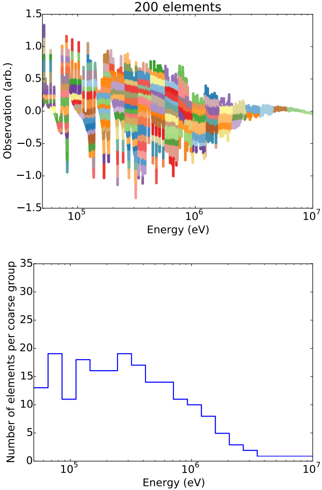
Research: Applied mathematics, the minimization problem

Solution: Proportionally to the relative standard deviation of the spectra within a coarse group

## 100 coarse groups ($r = 2$)




## 20 coarse groups ($r = 10$)



# We travel through a series of problem-research-solution cycles

I Determining the energy mesh

II Determining the condensing spectrum

III Assessing the method

- Comparing to a MG competitor
- Comparing to an analytic solution for a streaming-dominated time-dependent problem where the $1/v$ term becomes important
- Comparing to a continuous-energy Monte Carlo solution for reactor problems

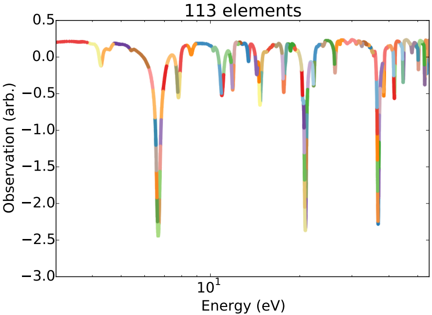
# Problem: How do we compare against an optimal MG method?

Research: The minimization problem

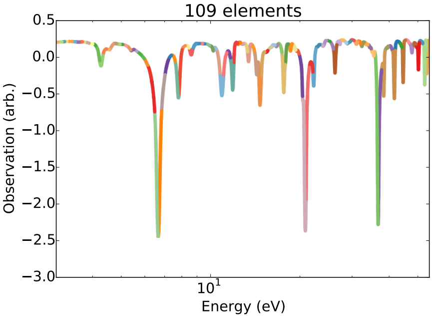
Solution: Solve the minimization problem with contiguous clustering

## Low-energy RRR (resolved)

Adaptive MG




Standard MG



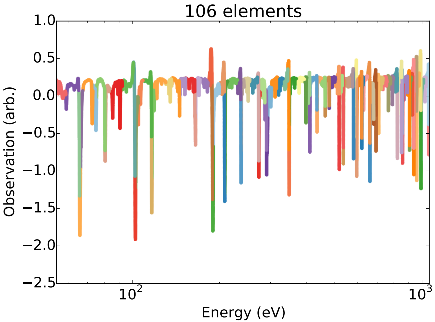
# Problem: How do we compare against an optimal MG method?

Research: The minimization problem

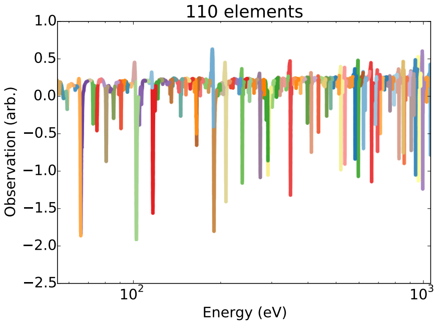
Solution: Solve the minimization problem with contiguous clustering

## Medium-energy RRR (unresolved)

### Adaptive MG

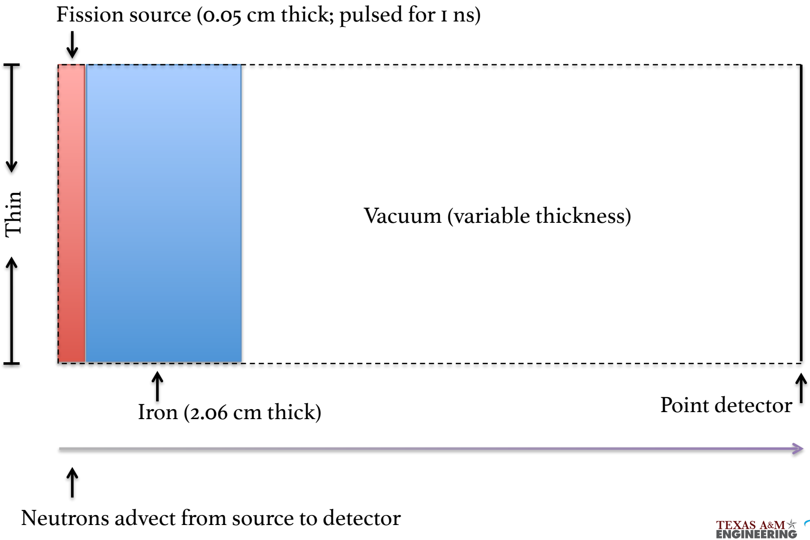



### Standard MG



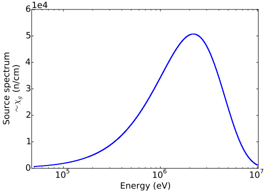
# We investigated a time-dependent neutron pulsed-source problem with analytic solution in space-time each energy element

## Simplified such that all neutrons move in $+\hat{x}$ and do not scatter



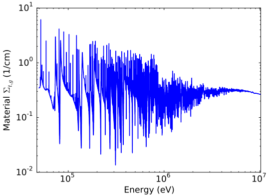
# We investigated a time-dependent neutron pulsed-source problem with analytic solution in space-time each energy element

Fission spectrum



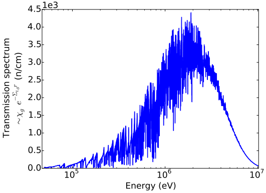

$+$

Iron cross section




$=$

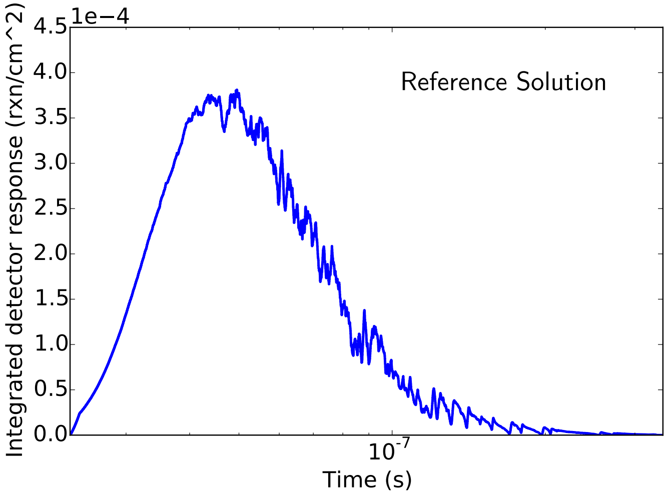
Transmission spectrum




(Abscissae: energy)

# We investigated a time-dependent neutron pulsed-source problem with analytic solution in space-time each energy element

Detector response at 1 m (abscissa: time $[t \propto E^{-1/2}]$)



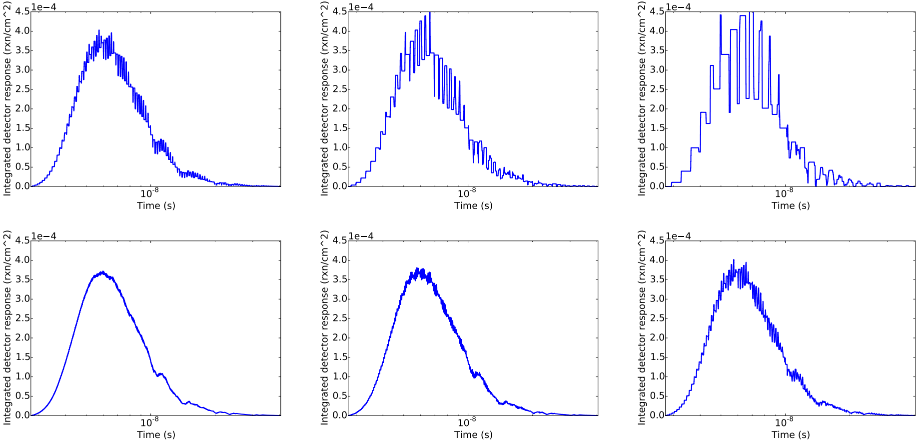
# TOF results — Detector response at 10 cm with 10,000 time bins

**Top** row: **100** total energy elements

**Bottom** row: **400** total energy elements

$r =$ (number of total energy elements) / (number of coarse groups)

Standard MG ($r = 1$) | FEDS ($r = 2$) | FEDS ($r = 4$)



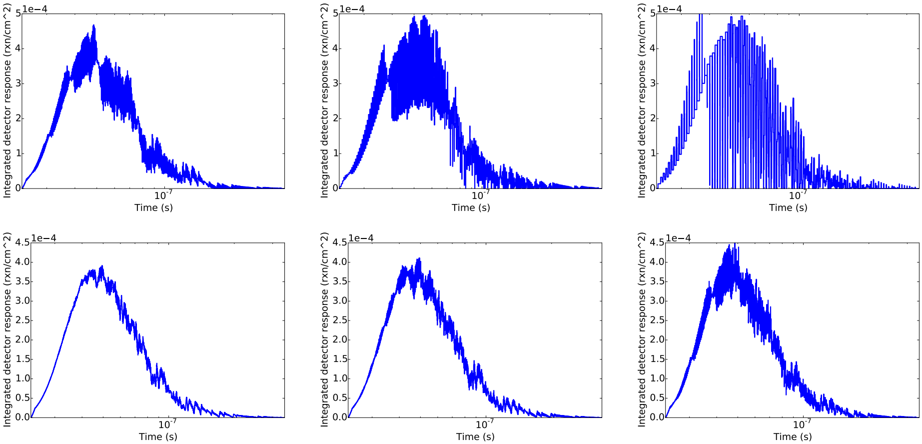
# TOF results — Detector response at 1 m with 10,000 time bins

Top row: **400** total energy elements

Bottom row: **1600** total energy elements

$r$ = (number of total energy elements) / (number of coarse groups)

Standard MG ($r = 1$) | FEDS ($r = 2$) | FEDS ($r = 4$)



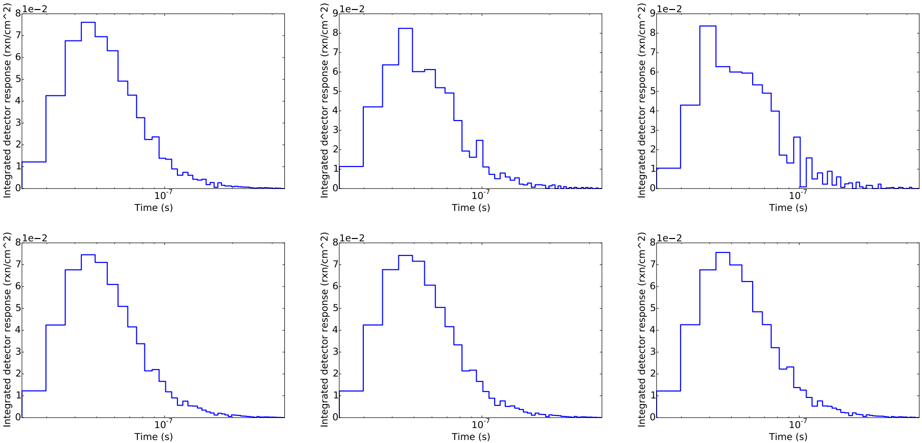
# TOF results — Detector response at 1 m with 50 time bins

Top row: **100** total energy elements

Bottom row: **400** total energy elements

$r$ = (number of total energy elements) / (number of coarse groups)

Standard MG ($r = 1$) | FEDS ($r = 2$) | FEDS ($r = 4$)

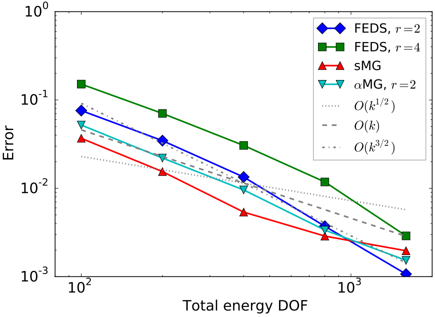


# TOF results — Convergence rates for fixed ratios

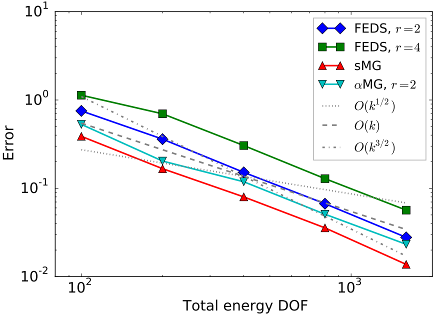
## Detector Response Error

$$\text{Error} \sim \sqrt{\frac{\sum_b \left|\text{ref}_b - \text{feds}_b\right|^2}{\sum_b \left|\text{ref}_b\right|^2}}$$

$r$ = (number of total energy elements) / (number of coarse groups)




**10 cm**, 10,000 time bins




**1 m**, 10,000 time bins

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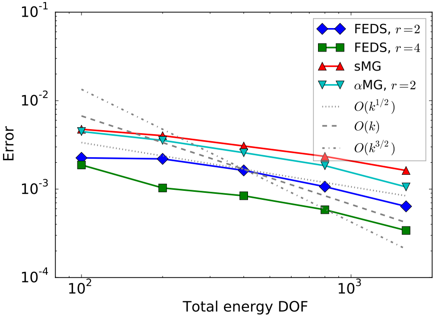
# TOF results — Convergence rates for fixed ratios

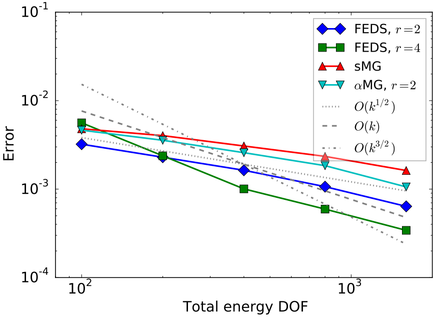
## Cumulative Detector Response Error

$$\text{Error} \sim \sqrt{\frac{\sum_b \left| \sum_{b' \leq b} (\text{ref}_{b'} - \text{feds}_{b'}) \right|^2}{\sum_b \left| \sum_{b' \leq b} \text{ref}_{b'} \right|^2}}$$

$r$ = (number of total energy elements) / (number of coarse groups)

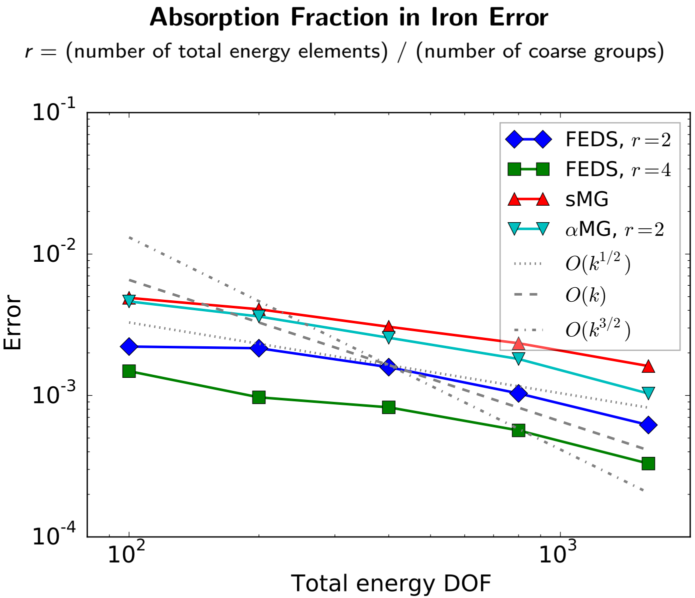



**10 cm**, 10,000 time bins




**1 m**, 10,000 time bins

# TOF results — Convergence rates for fixed ratios

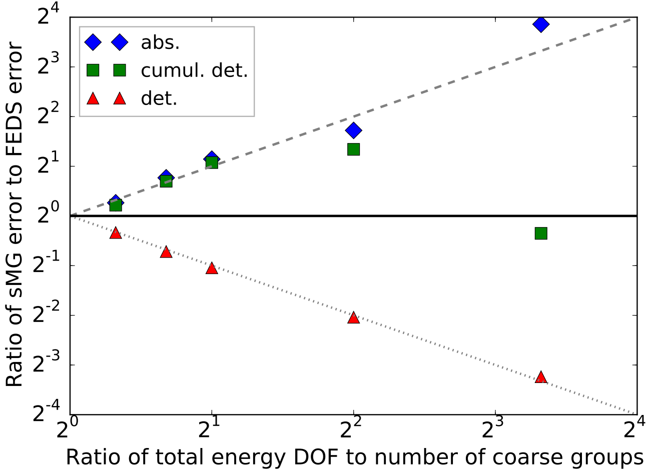


# TOF results — Convergence rates for *varying* ratios

## FEDS

10 cm, 10,000 time bins, 100 total energy unknowns

Ratio of standard MG error to FEDS error (higher is better)

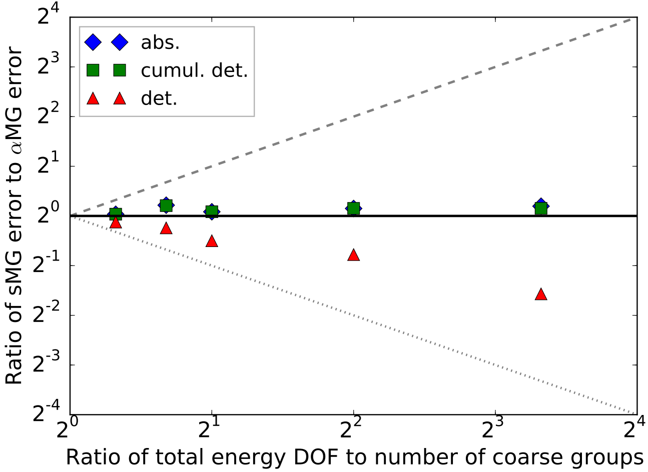


# TOF results — Convergence rates for *varying* ratios

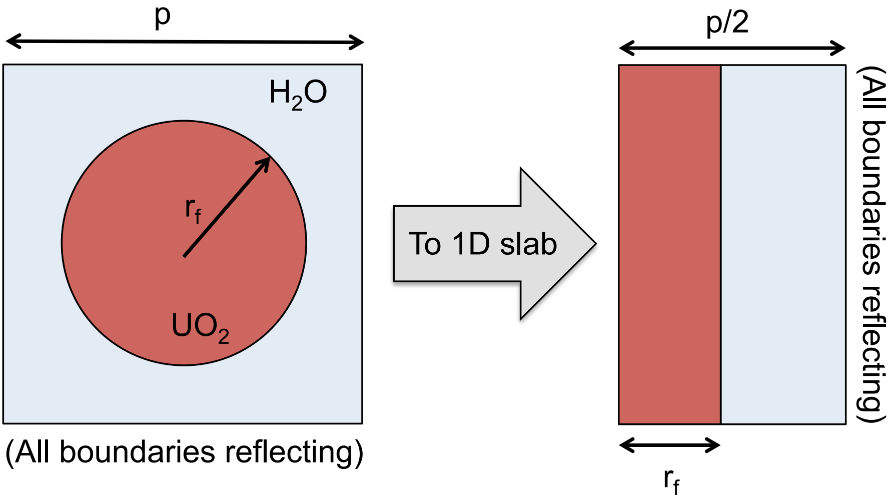
**Adaptive MG**

10 cm, 10,000 time bins, 100 total energy unknowns

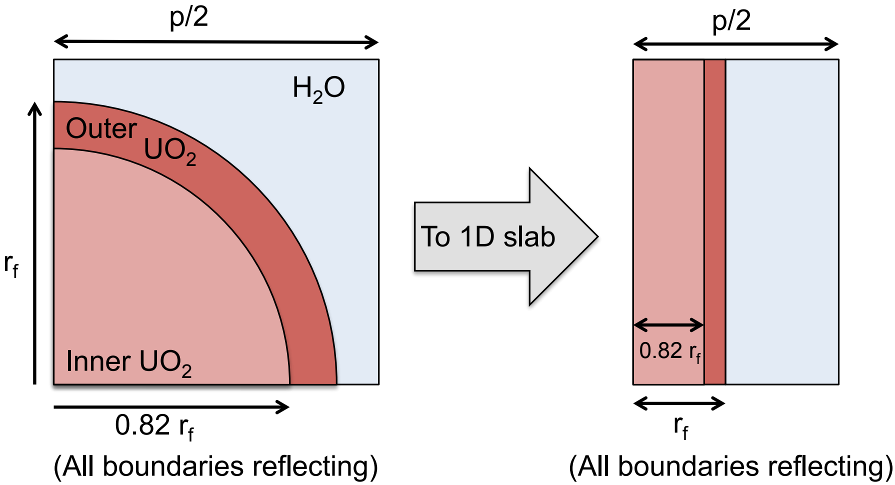
Ratio of standard MG error to FEDS error (higher is better)



# We investigated a slab pincell problem and made comparisons to continuous-energy MCNP with consistent cross sections



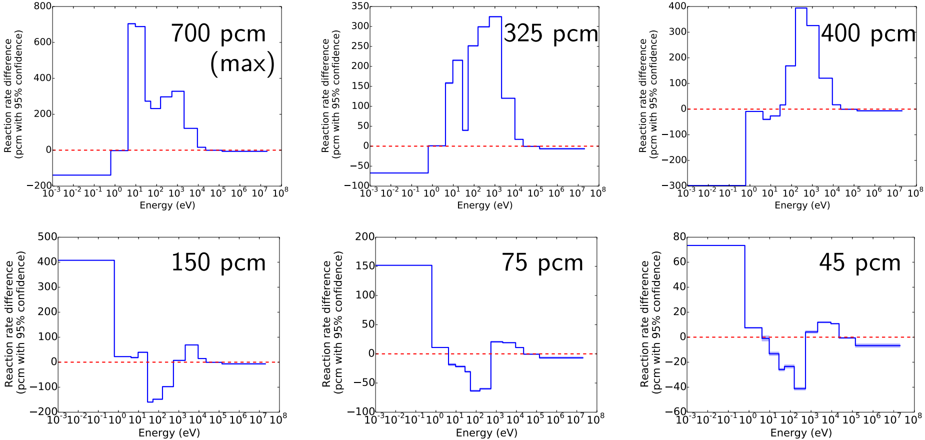
# We investigated a slab pincell problem and made comparisons to continuous-energy MCNP with consistent cross sections



# Slab vs MCNP results — U-238 absorption rate in the inner fuel errors

Top row: MG (SHEM boundaries)
Bottom row: FEDS

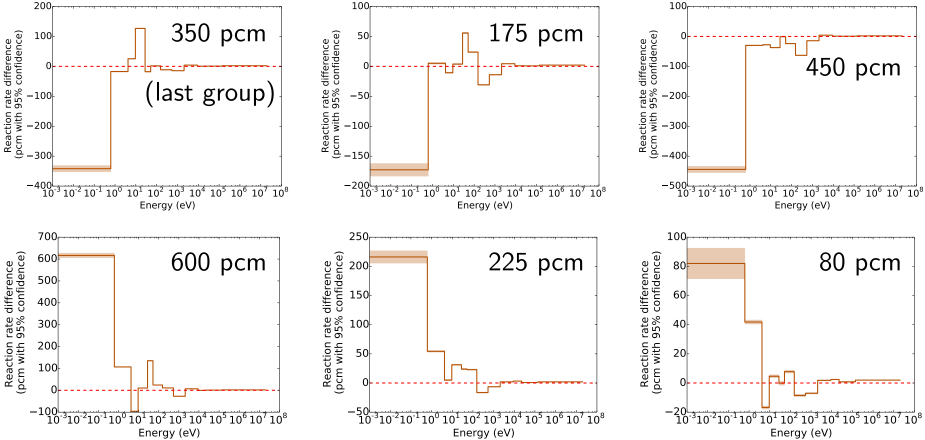
30 elements in the RRR | 108 elements in the RRR | 225 elements in the RRR



# Slab vs MCNP results — U-235 fission rate errors

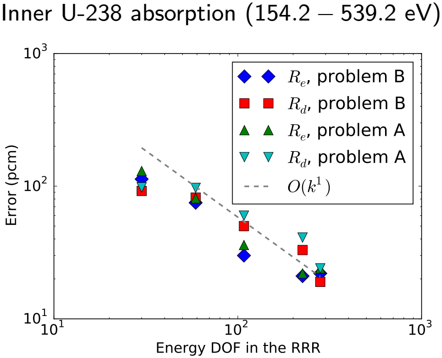
Top row: MG (SHEM boundaries)
Bottom row: FEDS

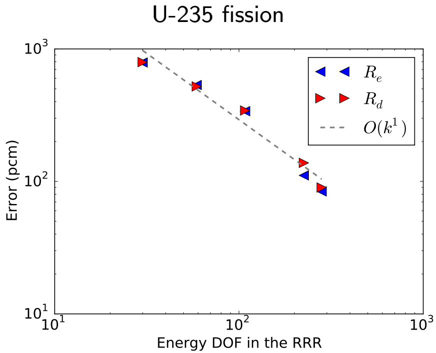
30 elements in the RRR | 108 elements in the RRR | 225 elements in the RRR



# Slab vs MCNP results — Convergence rates

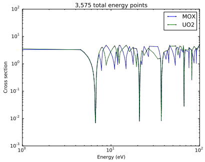
## FEDS Errors



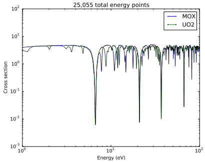



# Problem: No method is perfect

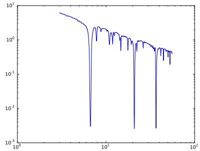
Unesolved spectra




Resolved spectra




Unnormalized spectra



## Solution: How to break FEDS

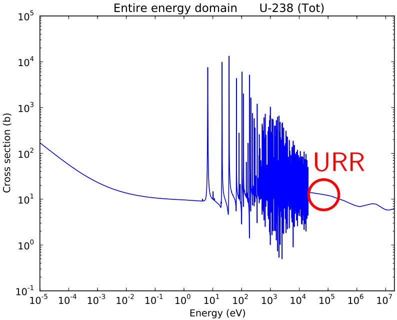
1. Use microscopic cross sections instead of spectra as inputs to the minimization problem
2. Do not resolve the resonances in the spectra (left, top)
3. Fail to renormalize the spectra (left, bottom)
4. Use an expensive clustering algorithm
5. Fail to use coarse groups (rely on energy penalties alone for dividing in energy space)
6. Use too many elements at high energies, which yields too many subelements for NJOY
7. Use the wrong escape cross section for the basis function
8. Use a MG solver that cannot handle upscattering
9. Fail to increase spatial / angular resolution when going from MG to FEDS

# Problem: I would like to graduate

Research: Common practice

## Solution: Future Work

- Applying FEDS to 2-D and 3-D pin-cell problems and comparing to MCNP with consistent continuous-energy cross sections (with Milan Hanuš)
- Applying FEDS to the fully resolved C5 problem (Carolyn McGraw)
- Applying FEDS to traveling-wave reactor problems (Pablo Vaquer)
- Passing the torch (Jijie Lou)




## Possible extensions of FEDS

- To the unresolved resonance region (URR, left)
- To thermal radiation problems (to preserve Planck and Rosseland opacity limits simultaneously with $S_n$ transport or IMC)
- As a basis for estimating discretization error in energy

# I look forward to your feedback and questions regarding my FEDS method

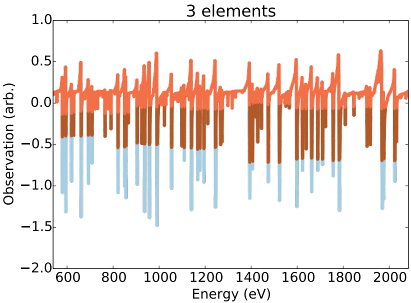
## And to possible future collaboration

Questions?

A special acknowledgment to the Department of Energy Computational Science Graduate Fellowship program (DOE CSGF - grant number DE-FG02-97ER25308), which provides strong support to its fellows and their professional development.

# Problem: How do we form accurate spectra for the minimization problem

Research: Integral form of the transport equation, equivalence theory, physics of downscattering




Snapshot are spectra that come from solving:

$\left(\Sigma_e + \Sigma_{t,g}\right)\phi_{g,p} = q_{\mathrm{scat},g,p} + q_{\mathrm{ext},g,p}$

Minimization problem:

$\mathbb{S}_e = \mathrm{argmin} \sum_p \sum_e \sum_{g \in \mathbb{S}_e} \left|\phi_{g,p} - \bar{\phi}_{e,p}\right|^2$

## Solution: Infinite-medium calculations

Parametrize particle advection with $s$:

$(\mathbf{r}, t) = (\mathbf{r}_{\mathrm{bdr}}, t_{\mathrm{bdr}}) + s\,(\mathbf{\Omega}, 1/v)$

$\Rightarrow (1/v)\partial_t + \mathbf{\Omega}\cdot\nabla \rightarrow \partial_s$

Transport equation becomes:

$\left[\partial_s + \Sigma_t(s,E)\right]\psi(s,E) = q_{(\mathrm{total})}(s,E)$

$\psi(s,E)$ is the convex sum of upstream $q(s,E)/\Sigma_t(s,E) \sim q_p(E)/\Sigma_{t,p}(E)$

Our spectra: $\phi_{g,p} = q_{\infty,p}(E_g)/\Sigma_{t,p}(E_g)$

Best case: $\phi_{g,p} = \phi(\mathbf{r}_p, E_g)$

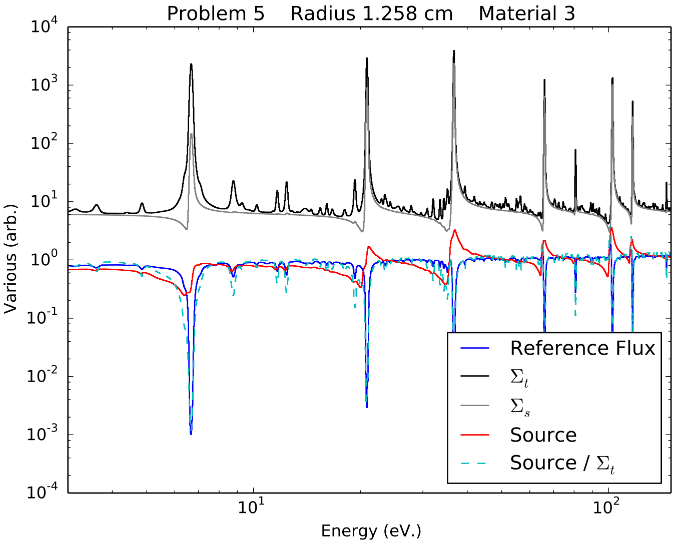
Worst case: $\phi_{g,p}$ are solution indicators

Desire:

$\phi_{g,p}$ spans behavior of $\psi(\mathbf{r}, E, \mathbf{\Omega}, t)$ by spanning behavior of $q_p(E)/\Sigma_{t,p}(E)$

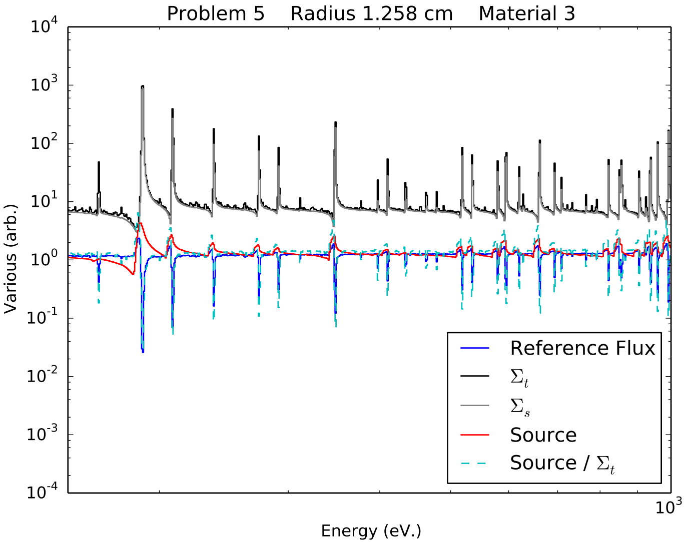
# Research: The scalar flux is often well approximated by $q(E)/\Sigma_t(E)$

Low-energy resolved RR



# Research: The scalar flux is often well approximated by $q(E)/\Sigma_t(E)$

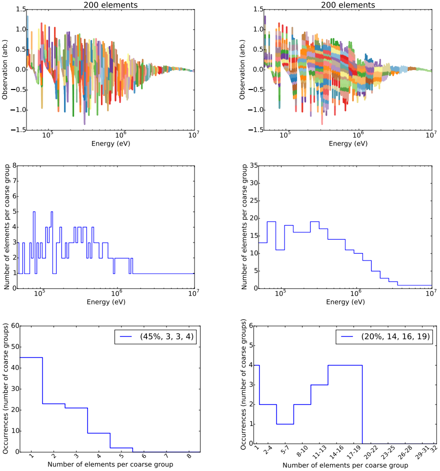
Medium-energy resolved RR



# Problem: How do we automatically apportion energy unknowns among the coarse groups?

Research: Applied mathematics, the minimization problem

100 coarse groups ($r = 2$) | 20 coarse groups ($r = 10$)




## Solution: Apportion based on relative standard deviation within a coarse group

- Reuse the spectra to calculate the standard deviation in each coarse group:
- $S_c = \sqrt{\frac{1}{N_g P} \sum_{g=g_{c-1/2}}^{g_{c+1/2}} \sum_{p=1}^{P} \left| O_{g,p} - \bar{O}_{c,p} \right|^2}$
- Give coarse group $c$ approximately $\frac{S_c}{S_{tot}} N_e$ elements
- Assigns more unknowns to groups with higher variance (left)

# Problem: How do we compare against an optimal MG method?

## Research: The minimization problem

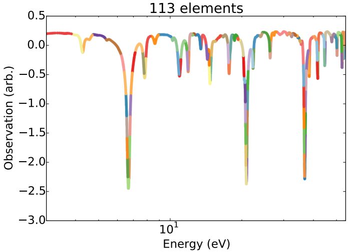
**Solution: Solve the minimization problem with contiguous clustering**

- Goal: minimize solution variance within a group
- Spectra indicate which energies have large solution variance
- Define group boundaries s.t. **each fine group has the same squared error**:
- $S_c = \sum_{g'=g_{c-1/2}}^{g_{c+1/2}} \max_p \left| O_{g',p} - O_{g'-1,p} \right|^2$
- Able to group hierarchically (coarse groups / fine groups per coarse group)

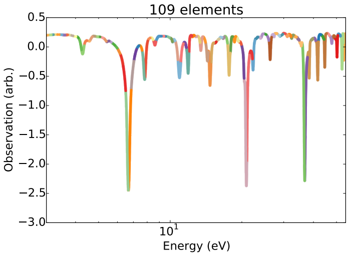
Low-energy RRR

(DOF count sufficient to resolve resonances)

Adaptive MG:




Standard MG:



# Problem: How can we predict convergence order?

Research: First mean value theorem for integration, Taylor series

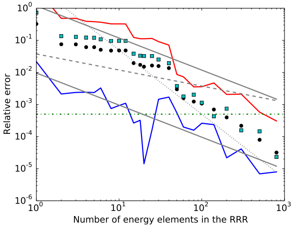
## Solution: We should expect first-order convergence for most cross section definitions

- Define $\sigma_{t,g} = \frac{\int\limits_{\Delta E_g} \mathrm{d}E\, f(E)\sigma_t(E)}{\int\limits_{\Delta E_g} \mathrm{d}E\, f(E)}$, with $\sigma_t(E)$ continuous and $f(E) > 0$, bounded
- First mean value theorem for integration: $\exists\ E_*$ st. $\sigma_t(E_*) = \sigma_{t,g}$, with $E_{g-1/2} \leq E_* \leq E_{g+1/2}$
- Collocate the transport equation at $E_*$: $[(1/v(E_*))\,\partial_t + \mathbf{\Omega}\cdot\nabla + \sigma_t(E_*)]\,\psi(E_*) = q(E_*)$
- Make $\psi_g = \Delta E_g\,\psi(E_*)$ by choosing $q_g = \Delta E_g\, q(E_*)$, $v_g = v(E_*)$, etc.
- Assume smoothness and Taylor-expand $\psi(E)$: $\psi(E) = \psi(E_*) + (E - E_*)\,\partial_E\psi(E_*) + \frac{1}{2}(E - E_*)^2\,\partial_E^2\psi(E_*) + \ldots$
- Integrate over a group and collect terms
$$\int\limits_{\Delta E_g} \mathrm{d}E\,\psi(E) = \psi_g + (E_g - E_*)\,[\Delta E_g\partial_E\psi(E_*)] + \frac{1}{2}(E_g - E_*)^2\left[\Delta E_g\partial_E^2\psi(E_*)\right] + \frac{1}{24}\left(\Delta E_g\right)^2\left[\Delta E_g\partial_E^2\psi(E_*)\right] + \ldots$$
- $|E_g - E_*| \leq \frac{1}{2}\Delta E_g$
- Unless $E_* = E_g = \frac{1}{2}(E_{g-1/2} + E_{g+1/2})$, method is first-order
- MB has mapping to $\sigma_t$ space and integrals of $\int_{\sigma_{b-1/2}}^{\sigma_{b+1/2}} \mathrm{d}\sigma\, J(\sigma)(\cdot)$; $J = \mathrm{d}E/\mathrm{d}\sigma$

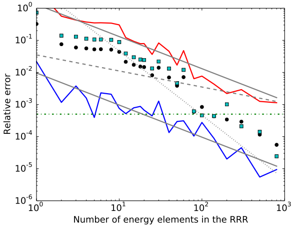
# Addendum: Selected results for cylindrical pin-cell problem

Problem 3 (multi-temperature, MOX), low-energy RRR (fewer resonances), case 1 ($1/E$ condensing spectrum), resolved MG reference solution

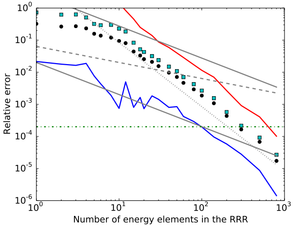
## Hierarchical agglomeration



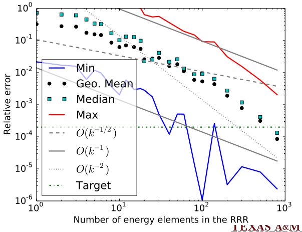

## K-means




## Adaptive MG



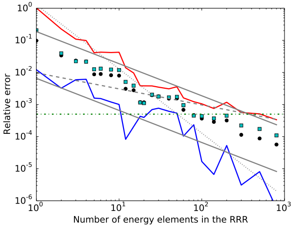

## Standard MG



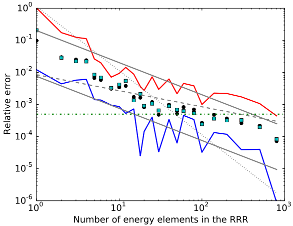
# Addendum: Selected results for cylindrical pin-cell problem

Problem 5 (MOX, moderator, $UO_2$), medium-energy RRR (more resonances), case 1 ($1/E$ condensing spectrum), resolved MG reference solution

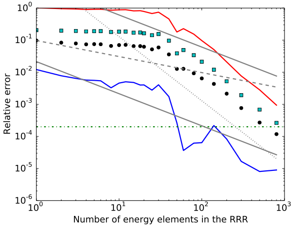
## Hierarchical agglomeration



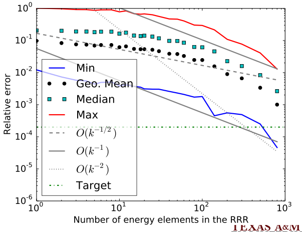

## K-means




## Adaptive MG



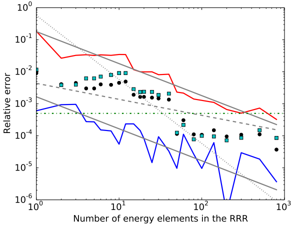

## Standard MG



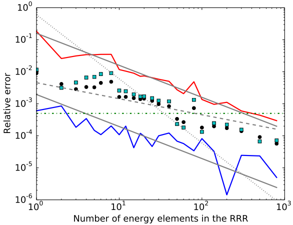
# Addendum: Selected results for cylindrical pin-cell problem

Problem 3 (multi-temperature, MOX), low-energy RRR (fewer resonances), case 2 (inf.-med.-equiv. condensing spectrum), resolved MG reference solution

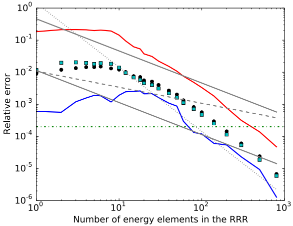
## Hierarchical agglomeration



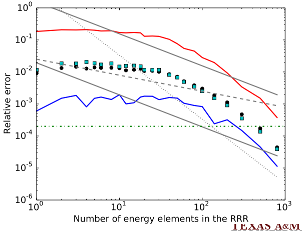

## K-means




## Adaptive MG



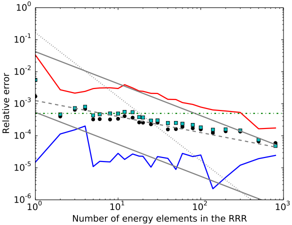

## Standard MG



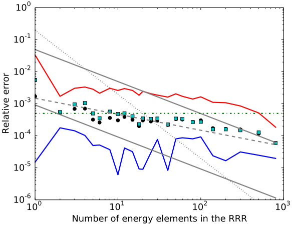
# Addendum: Selected results for cylindrical pin-cell problem

Problem 5 (MOX, moderator, $UO_2$), medium-energy RRR (more resonances), case 2 (inf.-med.-equiv. condensing spectrum), resolved MG reference solution

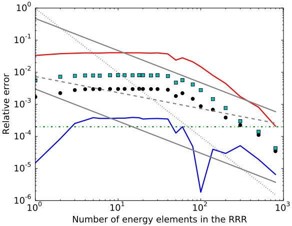
## Hierarchical agglomeration



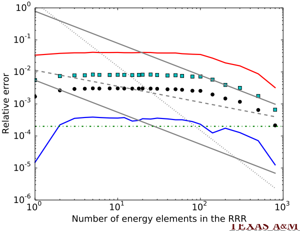

## K-means




## Adaptive MG

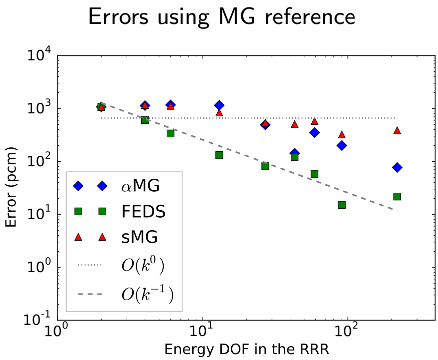


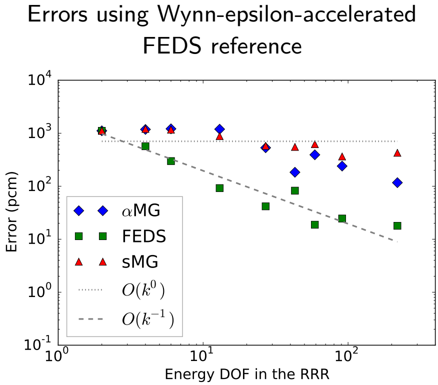

## Standard MG



# Addendum: Selected results for C5G$^\infty$ problem

## Errors in criticality eigenvalue

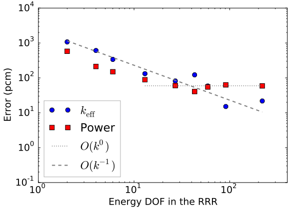


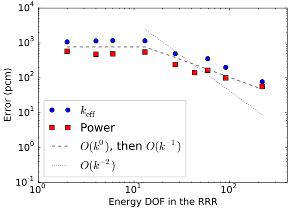
# Addendum: Selected results for C5G$^\infty$ problem

## Criticality eigenvalue error and average of pin-power-QOI errors

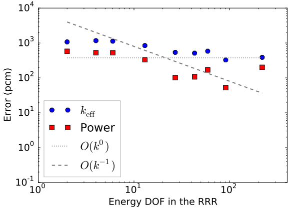
### FEDS with MG reference



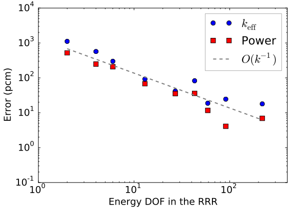

### $\alpha$MG with MG reference



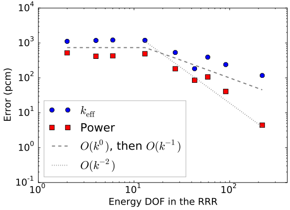

### sMG with MG reference




### FEDS with FEDS reference




### $\alpha$MG with FEDS reference




### sMG with FEDS reference