Higher-Order DGFEM Transport Calculations on Polytope Meshes for Massively-Parallel Architectures

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Outline

We need a better treatment of the energy variable when simulating nuclear systems

The continuous-energy transport equation is averaged over energy to produce the multigroup transport equation

The continuous-energy transport equation

$$\mathbf{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \mathbf{\Omega}) + \Sigma_t(\mathbf{r}, E)\, \psi(\mathbf{r}, E, \mathbf{\Omega}) = Q(\mathbf{r}, E, \mathbf{\Omega})$$

where
$\mathbf{\Omega}$ is the direction of travel of the particle (solid angle in steradians or ster),
E is the energy of the particle (measured in MeV),
$\mathbf{r}$ is the spatial location of the particle (measured in cm),
ψ is the angular flux (particles/cm^2-s-ster-MeV),
Q is the source term (particles/cm^3-s-ster-MeV), and
$\Sigma_t(\mathbf{r}, E)$ is the continuous-energy macroscopic total cross section (1/cm)

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Averaging over a group

$$\int_{\Delta E_g} \mathrm{d}E \left[\boldsymbol{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \boldsymbol{\Omega}) + \Sigma_t(\mathbf{r}, E)\, \psi(\mathbf{r}, E, \boldsymbol{\Omega}) \right] = \int_{\Delta E_g} \mathrm{d}E\, Q(\mathbf{r}, E, \boldsymbol{\Omega})$$

Non-standard group definitions

$$\psi_g(\mathbf{r}, \boldsymbol{\Omega}) \equiv \int_{\Delta E_g} \mathrm{d}E\, \psi(\mathbf{r}, E, \boldsymbol{\Omega}) \qquad \Sigma_{t,g}(\mathbf{r}, \boldsymbol{\Omega}) = \frac{\int_{\Delta E_g} \mathrm{d}E\, \Sigma_t(\mathbf{r}, E)\, \psi(\mathbf{r}, E, \boldsymbol{\Omega})}{\int_{\Delta E_g} \mathrm{d}E\, \psi(\mathbf{r}, E, \boldsymbol{\Omega})}$$

Non-standard MG equation (exact)

$$\boldsymbol{\Omega} \cdot \psi_g(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_{t,g}(\mathbf{r}, \boldsymbol{\Omega})\, \psi_g(\mathbf{r}, \boldsymbol{\Omega}) = Q_g(\mathbf{r}, \boldsymbol{\Omega})$$

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The actual spectrum can vary significantly within a typical spectral region.

The standard MG formulation does not allow for spectrum variation with $\mathbf{r}$ and $\mathbf{\Omega}$ within a spectral region

The best MG can do is have $f_i(E)$ approximate $\psi(\mathbf{r}, E, \mathbf{\Omega})$ in some average sense

$$\Sigma_{t,g,i} = \frac{\int_{\Delta E_g} \mathrm{d}E\, \overline{\Sigma}_{t,i}(E)\, f_i(E)}{\int_{\Delta E_g} \mathrm{d}E\, f_i(E)} = \frac{\int_{\Delta E_g} \mathrm{d}E\, \overline{\Sigma}_{t,i}(E)\, \overline{\phi}_i(E)}{\int_{\Delta E_g} \mathrm{d}E\, \overline{\phi}_i(E)} \qquad \overline{\phi}_i(E) = \frac{1}{V_i} \int_{V_i} \mathrm{d}^3\mathbf{r} \int_{4\pi} \mathrm{d}\Omega\, \psi(\mathbf{r}, E, \mathbf{\Omega})$$

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Our method builds on the successes of previous multiband (MB) methods, though our method is **not** a MB method

Previous work:

- Opacity density function (ODF), probability tables (PT), and some implementations of subgroup (SG) and MB base unknowns on bands tied to the local cross sections
- MB methods often deal approximately with correlation of cross sections among nuclides because bands may be different for each nuclide
- We propose to use global (discontiguous) energy elements that are obtained by an optimization process that takes into account several characteristic or bounding infinite-medium spectra
- We will show we are choosing our energy unknowns to minimize the within-element spectral variance
- Unlike MB but like MG, our energy intervals apply to the entire problem: all nuclides, all spatial locations, all angular directions use the same energy mesh

We call our method the finite-element-with-discontiguous-support multigroup (FEDS-MG) method

We discretize the problem using a finite element method in energy

- We split the energy domain into a mesh made up of energy elements, $\mathbb{E}_k$: $[E_{\text{min}}, E_{\text{max}}] = \mathbb{E}_1 \cup \mathbb{E}_2 \cup \ldots \cup \mathbb{E}_\Gamma, \quad \mathbb{E}_k \cap \mathbb{E}_n = 0 \text{ if } k \neq n$
- We represent the flux in a basis function expansion (our *only* approximation): $\psi(\mathbf{r}, E, \mathbf{\Omega}) \simeq \varphi(\mathbf{r}, E, \mathbf{\Omega}) \equiv \sum_k \Psi_k(\mathbf{r}, \mathbf{\Omega}) b_k(E)$
- Each unknown, $\Psi_k(\mathbf{r}, \mathbf{\Omega})$, corresponds to a single energy element, $\mathbb{E}_k$; the corresponding basis function, $b_k(E)$, has support only on that element: $b_k(E) = 0 \text{ if } E \notin \mathbb{E}_k$
- MG uses energy elements/basis functions that have contiguous support: $\mathbb{E}_k = \{E \mid E \in [E_{k-1/2}, E_{k+1/2}]\}$
- FEDS-MG uses energy elements that have discontiguous support: $\mathbb{E}_k = \{E \mid E \in [E_{k,1}, E_{k,2}] \cup [E_{k,3}, E_{k,4}] \cup [E_{k,5}, E_{k,6}] \cup \ldots\}$
  - Multiple contiguous subelements are combined into one discontiguous element
  - $\Psi_k(\mathbf{r}, \Omega)$ is still physically the integral of the flux over the energies in $\mathbb{E}_k$
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FEDS-MG is a finite element discretization of the energy variable where elements have discontiguous support

Groups are contiguous

Elements are discontiguous
(if they were contiguous,
we would have standard MG)

Our method consists of two parts

Part I: Determine the energy mesh

- The energy mesh is a discontiguous partitioning of the energy domain
- It is determined by solving a minimization problem
- Each element of the mesh has minimal within-element spectral variance

Part II: Condense cross sections and solve a transport equation

- We define a finite element space that lives on this energy mesh, where basis functions have support on one and only one energy element
- Using only the approximation that the angular flux can be represented by this finite element in energy, we can rigorously define an energy-discretized transport equation
- This equation uses basis-function-weighted cross sections, where the averaging is done over energy elements, which are discontiguous
- This equation with its cross sections is solvable with existing MG transport codes
- (Provided these codes can efficiently handle the added effective block-upscattering to the scattering matrix produced by the method)

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Part II: Condense cross sections and solve a transport equation

- We define a finite element space that lives on this energy mesh, where basis functions have support on one and only one energy element
- Using only the approximation that the angular flux can be represented by this finite element in energy, we can rigorously define an energy-discretized transport equation
- This equation uses basis-function-weighted cross sections, where the averaging is done over energy elements, which are discontiguous
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1. 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. Choose several characteristic or bounding material compositions and denote by index p
   3. Solve an infinite-medium, fixed-source, slowing-down equation to determine spectra on this hyperfine group structure for each material: $\phi_{g,p}$
   4. Choose a final number of energy elements, E, with $e = 1, \ldots, E$
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Our minimization problem has several useful properties

We choose $\mathbb{S}_e$ to minimize $F = \sum_p \sum_e \sum_{g \in \mathbb{S}_e} \Delta E_g |\phi_{g,p} - \bar{\phi}_{e,p}|$

- F is a variance / projection error that indicates how well the energy elements capture the fine-scale behavior of the spectra
- Choosing energy elements that minimize F results in an energy mesh that maximally captures the resonance-scale behavior of the spectra with a fixed final number of elements, E
- Because the spectra, $\phi_{g,p}$, do not use any geometric information and may use approximate material compositions applicable to several types of problems, the resultant energy mesh may be applicable to several types of problems (*e.g.*, to all BOL LEU PWRs)
- We can generalize the minimization problem to use more general averages, norms, and weights (cf. PhD Proposal)
- There exists a class of algorithms called clustering algorithms that can solve these minimization problems efficiently
- Clustering algorithms often solve the minimization problem iteratively and do not explicitly search the entire combinatoric space of $\mathbb{S}_e$

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Our multiband-like method is a generalized multigroup method implemented using Petrov-Galerkin finite elements in energy

We consistently apply definitions

Our Finite-Element-with-Discontiguous-Support Multigroup (FEDS-MG) solution

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

Our weight functions

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

with $\{\mathbb{E}_k\}$ a global, **discontinuous** partitioning of the energy domain

Our basis functions

Product of normalized local weighting spectrum and global weight function:

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

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We derive a weak form of the equation

The transport equation

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

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

$$\int_0^\infty \mathrm{d}E\, w_n(E)\Big\{\mathbf{\Omega}\cdot\nabla\left[\sum_k b_k(\mathbf{r},E)\psi_k(\mathbf{r},\mathbf{\Omega})\right]+\Sigma_t(\mathbf{r},E)\sum_k b_k(\mathbf{r},E)\psi_k(\mathbf{r},\mathbf{\Omega})=\frac{1}{4\pi}\int_0^\infty \mathrm{d}E'\Sigma_s(\mathbf{r},E'\rightarrow E)\sum_{k'} b_{k'}(\mathbf{r},E')\phi_{k'}(\mathbf{r})+\frac{\chi(\mathbf{r},E)}{4\pi\,k_{\mathrm{eff}}}\int_0^\infty \mathrm{d}E'\nu\Sigma_f(\mathbf{r},E')\sum_{k'} b_{k'}(\mathbf{r},E')\phi_{k'}(\mathbf{r})\Big\}$$

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$$\frac{\chi(\mathbf{r},E)}{4\pi\, k_{\mathrm{eff}}}\int_0^\infty \mathrm{d}E'\nu\Sigma_f(\mathbf{r},E')\sum_{k'} b_{k'}(\mathbf{r},E')\phi_{k'}(\mathbf{r})\Bigg\}$$

After algebraic manipulation and application of definitions we get

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

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The FE definitions give us expressions for the cross sections

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

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

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

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

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

with $\{\mathbb{E}_k\}$ a global, discontinuous partitioning of the energy domain, and $b_k(\mathbf{r}, E)$ piecewise constant in space (for a given E), normalized st $\int_{\Delta E_k} \mathrm{d}E\, b_k(\mathbf{r}, E) \equiv 1 \quad \forall \mathbf{r}$.

I will test the proposed method on a variety of problems

These problems will increase in complexity and be applicable to reactor physics simulations

1. A series of one-dimensional cylindricized pin cells to test energy convergence on small reactor-themed problems
2. An energy-generalized version of the C5G7 benchmark called the C5G$^{\infty}$ benchmark to test energy convergence on a realistic reactor problem
3. A 2D model of the NSC TRIGA core with depletion to test viability of using a single generalized energy mesh for time-dependent problems

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I have investigated one-dimensional, cylindricized pin-cell problems

The test cases used

- A cylindricized version of a multi-material problem (below)
- One of two subsets of the full RRR:
  3 to 55.6 eV (right, above) and
  55.6 to 1060 eV (right, below)
- Different weighting spectra and basis functions (bottom)

Case	Spectra Used	Basis Functions Used
1	Infinite-medium	$1/E$
2	Infinite-medium	Infinite-medium with escape XS
3	Reference-solution partial currents	Reference-solution material-averaged fluxes

A class of convergent cases empirically show the viability of the proposed method

Top: Low-energies (3 eV – 55.6 eV); Bottom: Medium-energies (55.6 eV – 1060 eV)

Weighting spectra — Case 1: $1/E$; Case 2: ∞-medium + σ_0; Case 3: Reference

Fission production rate in outer U-235	Absorption rate in inner U-238	k-Eigenvalue

The minimization problem yields an energy mesh with minimized within-element spectral variance

∞-medium spectra — Top: In the inner MOX; Bottom: In the outer UO_2

Low Energies	Low Energies	Medium Energies
10 energy elements	50 energy elements	10 energy elements

I have developed a C5G$^{\infty}$ problem

1. I took the 2D C5G7 benchmark and kept the material / geometry definitions, but recomputed my own cross sections from scratch via ENDF cross sections and material compositions
2. I resolved 2/3 of the full RRR (from 3.0 eV to 1.06 keV). The SCALE 44-group boundaries were used outside this region
3. I solved infinite-medium, fixed-source, slowing-down problems to compute spectra in the highest-enriched MOX and UOX pins that were later used in the minimization problem to determine the energy element definitions
4. I used NJOY's default flux with $IWT = 5$ for the within-subelement spectra
5. I used infinite-medium, fixed-source, slowing-down problems with analytic escape cross sections from fuel-pin chord lengths as the weighting spectrum used to collapse energy subelements to elements
6. I chose a space/angle resolution and ran a reference solution using a 1024-group structure that maximally resolved the above spectra
7. I tested with the same space/angle resolutions and FEDS-MG XS with varying numbers of energy elements
8. I compared the following QOI: k-eigenvalue, min/max pin powers, and assembly-averaged pin powers

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I have computed pin-power rates for the C5G$^{\infty}$

C5 layout
(NEA/NSC/DOC(2001)4)

Pin-powers
(39 energy elements)

I have run the C5G$^{\infty}$ problem, varying the number of energy elements in the resolved resonance region (RRR)

QOI

Elements	Max Pin	Min Pin	Inner UO_2	MOX	Outer UO_2	k_{eff}
2	2.40189	0.20088	479.428	217.117	142.339	1.159180
4	2.41016	0.19826	480.770	216.683	141.864	1.177549
6	2.41215	0.19835	481.074	216.523	141.880	1.176155
13	2.42502	0.19892	482.926	215.588	141.898	1.174187
27	2.41386	0.19887	481.260	216.413	141.915	1.173490
43	2.41969	0.19927	482.055	215.999	141.946	1.171000
59	2.42113	0.19923	482.250	215.915	141.920	1.171352
91	2.42234	0.19923	482.409	215.842	141.906	1.171582
Reference	2.42321	0.19900	482.538	215.802	141.859	1.171695

Error in QOI

Elements	Max Pin (%)	Min Pin (%)	Inner UO_2 (%)	MOX (%)	Outer UO_2 (%)	k_{eff} (pcm)
2	0.8798	0.9447	0.6445	0.6094	0.3384	1068
4	0.5385	0.3719	0.3664	0.4082	0.0035	500
6	0.4564	0.3266	0.3034	0.3341	0.0148	381
13	0.0747	0.0402	0.0804	0.0992	0.0275	213
27	0.3859	0.0653	0.2648	0.2831	0.0395	153
43	0.1453	0.1357	0.1001	0.0913	0.0613	59
59	0.0858	0.1156	0.0597	0.0524	0.0430	29
91	0.0359	0.1156	0.0267	0.0185	0.0331	10

TEXAS A&M ENGINEERING

I have visualized the C5G$^{\infty}$ scalar flux in various energy elements

Fast element
URR element
RRR background element
RRR resonance element
Epithermal element
Thermal element

I have developed an NSC model with help from J. Vermaak, C. McGraw, and D. Bruss

2D slice of Jan's 3D MCNP model (zoom)

My 2D PDT model (full)

I have done preliminary calculations of the NSC core with 7-group cross sections

NSC mesh (zoom)

Fast flux (zoom)

I have done preliminary calculations of the NSC core with 7-group cross sections (cont.)

NSC materials (zoom)

Thermal flux (zoom)

I am making maximal use of Evaluated Nuclear Data Files (ENDF/B) whenever possible

Sed in primis **ad fontes** *ipsos properandum!*[1]

- Cross section files (MF 1–7)
- Energy per fission (MF 1)
- Decay modes, half-lives, and branching ratios (MF 8)
- Fission product yields (MF 8)
- Isomeric branching ratios for reactions (MF 8–10)

Fission of ^{235}U

Thermal fission of ^{235}U

$^{243}\mathrm{Am}(n, 2n)$ to ^{242}Am or ^{242m1}Am

[1] "Above all, one must hasten **to the sources** themselves," Erasmus of Rotterdam

I have developed tools for quantifying nuclide production and loss through fission, reaction, and decay

I use a directed graph, where nuclides are nodes and production/loss mechanisms are edges

Low-Z nuclide chains

Mid-Z nuclide chains

I will run the C5G$^{\infty}$ problem at higher space/angle resolutions

Current spatial resolution

$(2, 1, 1)$:

2 rings in the fuel meat, 1 ring in the fuel boundary, 1 ring in the moderator

Current angular resolution

$(2, 5)$:

Product Gauss-Legendre-Chebyshev with S_4 in polar and 5 equally-spaced azimuthal angles per quadrant

Desired spatial resolution

(extrapolating from McGraw's PHYSOR paper)

$(3, 2, 2)$:

Increase by a factor of 3.1

Desired angular resolution

(extrapolating from McGraw's PHYSOR paper)

$(8, 64)$:

Increase by a factor of 51.2

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We must increase our space/angle DOF by a factor of around 156.8

There are still unanswered questions regarding running depletion problems

Open questions

1. Which QOI to use? Possibilities include:
   k-eigenvalue, pin powers, per-pin nuclide densities, or per-pin/per-nuclide fission/absorption/production/loss rates
2. How to approximate the final material compositions when computing infinite-medium spectra for the minimization problem? Ideas include:
   1. Use material densities from the pin with the lowest U-235 concentrations from Jan's calculations and zero for nuclides not considered (which will contribute negligibly to absorption by his own metric)
   2. Do a single fuel pin calculation with all desired nuclides (would need a power peaking factor to know how much power to use; all locations burn approximately the same, just at different rates)
   3. Do predictor-corrector scheme, with predictor performing the entire burnup calculation with beginning-of-life spectra only when determining the energy mesh (using no depleted spectra)
3. How to handle nuclides lacking metastable-specific production data?
   - Absorption reactions: $(n, 2n)$, (n, γ)
   - Inelastic scattering reactions: What do MT 2 / MT 51 mean for a metastable state? If MT 50 is not allowed, where is this information put?
4. How to handle data sparsity for fission product yields?
   Interpolation by A may introduce errors when nuclides have different thermal/fast fission cross section ratios (fission product yields depend on incident neutron energy)

Questions?

A special acknowledgment to the Department of Energy Rickover Fellowship Program in Nuclear Engineering, which provides strong support to its fellows and their professional development.

TEXAS A&M ENGINEERING

A stretch goal is to compare my method to Monte Carlo

I claim the following is the best way to show our method has practical importance, because continuous-energy Monte Carlo codes do exact particle tracking / kinematics and use very accurate cross sections. Such codes may attain higher fidelity in all respects than DRAGON.

Start with a 0-D problem to isolate energy discretization effects

1. Come up with a reactor-themed problem
2. Solve the same problem in PDT and MCNP or OpenMC
3. Choose QOI, such as k-eigenvalue, radial power profile, absorption/fission rates per nuclide, etc.
4. Quantify how errors in PDT's QOI change as energy resolution is increased

Build up problem complexity slowly: cylindricized pin cell with white boundary conditions, infinite lattice of pin cells, heterogeneous lattice of pin cells, etc.

1. Quantify how errors in PDT's QOI change as spatial / angular / scattering moment resolution is increased
2. Quantify how errors in PDT's QOI change as energy resolution is increased
3. ...
4. Profit

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TEXAS A&M ENGINEERING

We wish to compute a reference solution that resolves all desired resonances

- Desirable properties are that the reference solution have sufficient:
  cross section fidelity (ENDF library, NJOY pointwise reconstruction tolerance, thermal / $S(\alpha, \beta)$ treatment, unresolved resonance range treatment), spatial resolution, angular resolution, temporal resolution, scattering moment expansion order, and energy (group) resolution outside the energy range of interest
- I claim it is both sufficient and necessary to choose a *reasonable* resolution in the above and a *high* energy resolution within the energy range of interest for the reference solution
- The only difference between the reference and method solutions will be the energy resolution within the energy range of interest, which is a subset of the entire resolved resonance range (RRR)
- This is the only fair way to make comparisons
- The reference solution is well-posed: given a space/angle resolution and material densities, cells' optical thicknesses are bounded as energy is resolved
- If the method solutions converge to the reference solution as energy resolution is increased, I claim that this shows our method is convergent in energy in the sense that we accurately treat the RRR, the source of all our troubles

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