LA-UR-13-27327
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Title: Calculating Alpha Eigenvalues and Eigenfunctions of One-Dimensional Media

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Intended for: 23rd International Conference on Transport Theory,
2013-09-15/2013-09-20 (Santa Fe, New Mexico, United States)

Issued: 2013-09-20

Calculating α Eigenvalues and Eigenfunctions of One-Dimensional Media

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19 September 2013

Motivation: α eigenvalues

- The time- or α-eigenvalue spectrum is necessary for calculating eigenfunction expansions for time-dependent problems
- When the spectrum (and its eigenfunctions) is known, the flux response within the system may be calculated for any source
- Some applications of this work are pulsed neutron experiments and accelerator-driven subcritical systems, where the flux varies spatially in time
- Even critical systems have higher α eigenvalues and shape eigenfunctions that may be excited by a change in neutron population
- Objective is to show the Transition Rate Matrix Method (TRMM) is able to calculate these eigenvalues and eigenfunctions during a Monte Carlo random walk

Methods: α eigenvalues

- **To formulate the eigenvalue problem, separate the temporal dimension from position, energy, and direction:**

$$\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}) \exp(\alpha t)$$
$$C_j(\mathbf{r}, t) = C_j(\mathbf{r}) \exp(\alpha t).$$

- **The largest real eigenvalue (the fundamental) has the trend**

$$\alpha_0 \begin{cases} > 0 & \text{if supercritical,} \\ = 0 & \text{if critical,} \\ < 0 & \text{if subcritical.} \end{cases}$$

and its corresponding eigenvector must be all one sign

- **All other eigenvalues and eigenvectors may be real or complex (complex eigenvalue must have a conjugate)**

Methods: α eigenvalues

- **Introducing this separation into the time-dependent neutron transport equation yields the eigenvalue problem:**

$$\begin{bmatrix} v & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -\mathbf{L}+\mathbf{F_p} & \chi_d \lambda_j \\ \mathbf{F_d} & -\lambda_j \end{bmatrix} \begin{bmatrix} \psi \\ C_j \end{bmatrix} = \alpha \begin{bmatrix} \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}) \\ C_j(\mathbf{r}) \end{bmatrix}$$

- **We desire the eigenvalues of the combination of the left hand matrices, but the elements of this matrix are unphysical (speed times a decay constant does not have real physical meaning and cannot be obtained during a Monte Carlo run)**
- **Using the same work to formulate the time-dependent neutron importance (adjoint) equation yields a matrix of more physical quantities**

Methods: α eigenvalues

- **The adjoint α-eigenvalue problem is**

$$\begin{bmatrix} v & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -\mathbf{L}^\dagger + \mathbf{F_p}^\dagger & \mathbf{F_d}^\dagger \\ (\chi_d \lambda_j)^\dagger & -\lambda_j \end{bmatrix} \begin{bmatrix} \psi^\dagger \\ C_j^\dagger \end{bmatrix} = \alpha^\dagger \begin{bmatrix} \psi^\dagger(\mathbf{r}, E, \hat{\mathbf{\Omega}}) \\ C_j^\dagger(\mathbf{r}) \end{bmatrix}$$

- **The matrix elements are now rates (decay rates or speeds multiplied by cross sections) and if we divide the state space (position, energy, and angle) we are left with a finite matrix composed of rates**
- **These rates describe transitions among the divided state space, for example: (1) a precursor at a position *decaying* into a neutron traveling with a given energy and direction or (2) a neutron at a given energy and direction *scattering* to another energy and direction**
- **The transition rate matrix is the left side of the adjoint problem**

Methods: Transition rate matrix

- **This matrix is similar to a continuous-time Markov process where we describe a transition rate matrix**

$$\mathbf{Q} = \begin{bmatrix} -q_{11} & q_{12} & \cdots \\ q_{21} & -q_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

- **The diagonal elements *q* are rates of transitions out of that state**
- **The off-diagonal elements are rates of transition between states**
- **Note: Fission matrix formulation is a discrete-time Markov process where fission generations represent “time”**

Methods: Eigenfunction expansion

- **The time-dependent flux solutions is described as a linear combination of the shape eigenfunctions multiplied by a time function**

$$\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \sum_{n=1}^{\infty} A_n(t)\psi_n(\mathbf{r}, E, \hat{\mathbf{\Omega}})$$

- **The time dependence of the initial source determines the function; for a pulsed neutron source, it is**

$$A_n(t) = A_n(0)e^{\alpha_n t}$$

- **The coefficients are calculated with the adjoint and forward shape eigenfunctions and the given initial source**

$$A_n(0) = \frac{\left\langle \psi_n^{\dagger}, S_0 \right\rangle}{\left\langle \psi_n^{\dagger}, v^{-1}\psi_n \right\rangle + \sum_m \left\langle C_{m,n}^{\dagger}, C_{m,n} \right\rangle}$$

Methods: Tallies and calculation

- The entire transition rate matrix is calculated from tallies; no known quantities are used
- Probabilities, times, and distances for given states are tallied during a *k*-eigenvalue Monte Carlo calculation
- At the completion of the run, the transition rates are calculated from this tallied information and the transition rate matrix is formed
- The velocity matrix is formed and forward matrix is obtained by swapping the speeds and transposing the matrix
- Eigenvalues and eigenfunctions of the matrix are solved using LAPACK (direct Schur factorization)

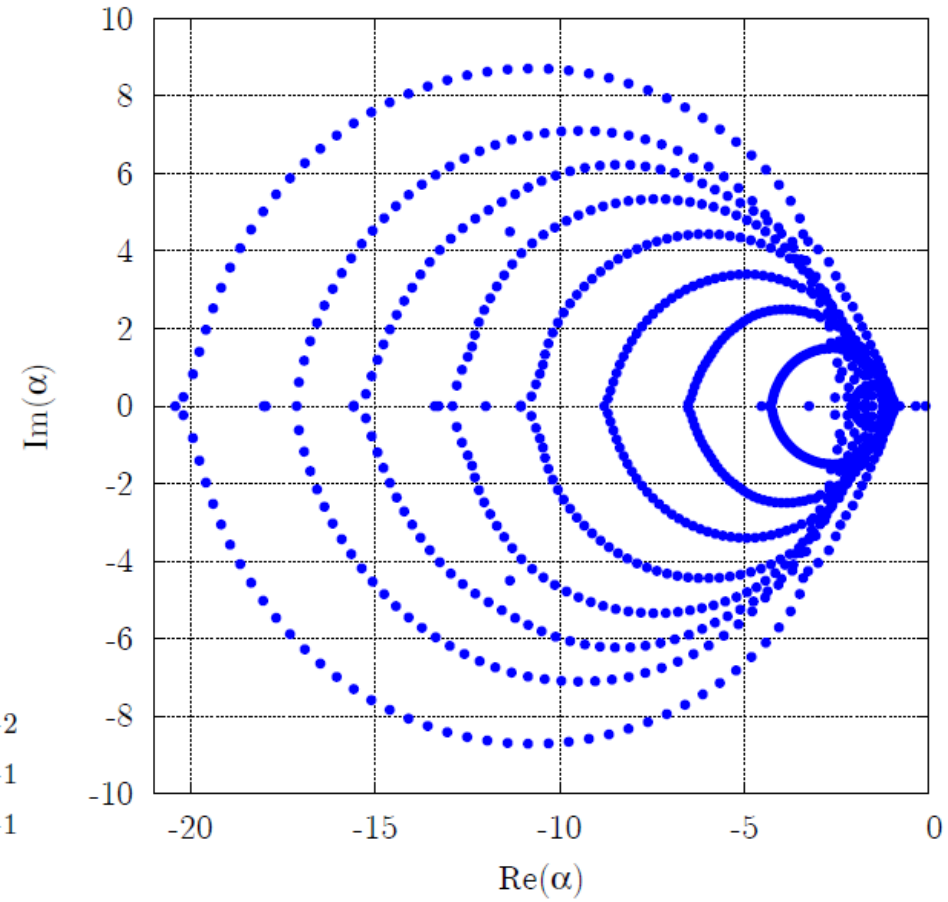
Results: One-Speed Slabs

- One-speed slabs problems are selected to reflect the simplified problems whose eigenvalues and eigenfunctions are obtained via the Green's Function Method (GFM)
- All dimensions are in mean free paths and the speed and total cross sections are set to unity
- These problems have a few real eigenvalues that exist before the start of the continuum spectrum; because the TRMM calculates a finite number of eigenvalues, many fall within the continuum portion of the spectrum as a set of points dependent on the definition of the spatial and angular states
- The simplest homogeneous scattering and multiplying slabs show good agreement to GFM calculations for calculated eigenvalues

Results: Spectrum

- This homogeneous slab with a thickness of five mfp has three real eigenvalues before the continuum portion of the spectrum (less than -1)
- This calculation uses 50 equal position states and 18 equal angle states
- Eigenvalues form along rings in the continuum
-

TRMM	GFM
-8.10462×10^{-2}	-8.10933×10^{-2}
-3.42167×10^{-1}	-3.41216×10^{-1}
-8.46262×10^{-1}	-8.34837×10^{-1}

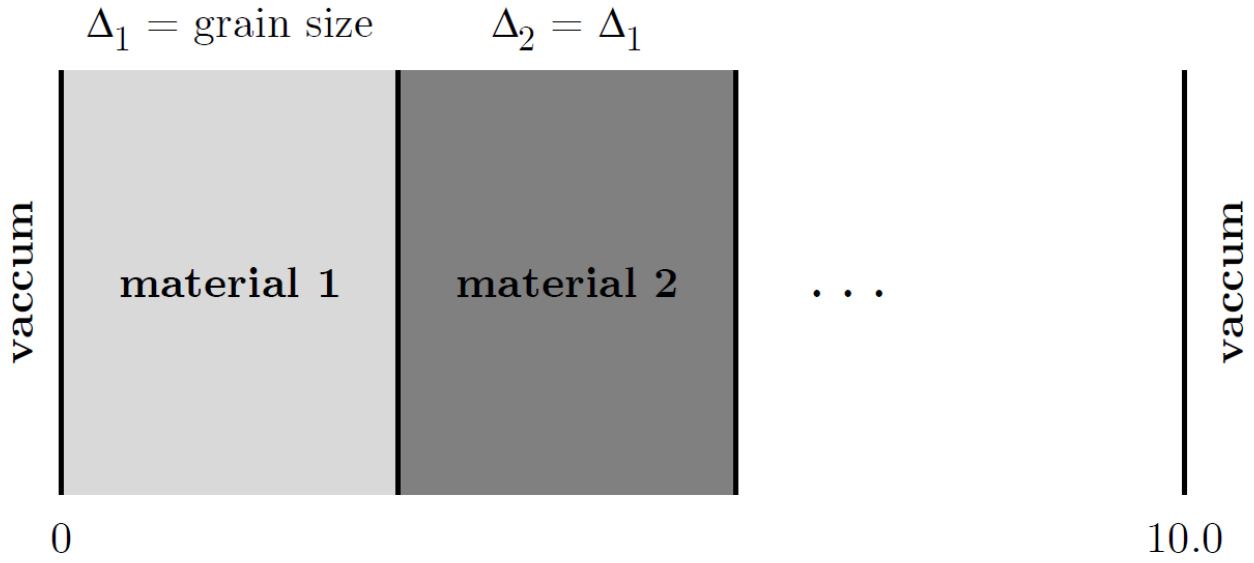


Results: Spectrum

- The number of rings of eigenvalues in the continuum is half that of the number of angular states used in the TRMM formulations
- The diameter of the “rings” increases with the number of position states; this is attributed to the position states being smaller, and thus, events (leakages from the position state) occurring faster
- Some eigenvalues that are part of the continuum leak into the real portion of the spectrum (greater than -1), but this occurrence decreases as the number of angles and positions is increased
- These behaviors with the point spectrum in the continuum is seen in previous work using an S_n-method for numerically solving for the eigenvalue spectrum

Results: Multi-Region Problem

- This multi-region problem has alternating materials of equal thickness
- Material 1 is purely scattering and material 2 has a small absorption cross section
- For this problem the speed is effectively 10 so and continuum portion of the spectrum starts at -10



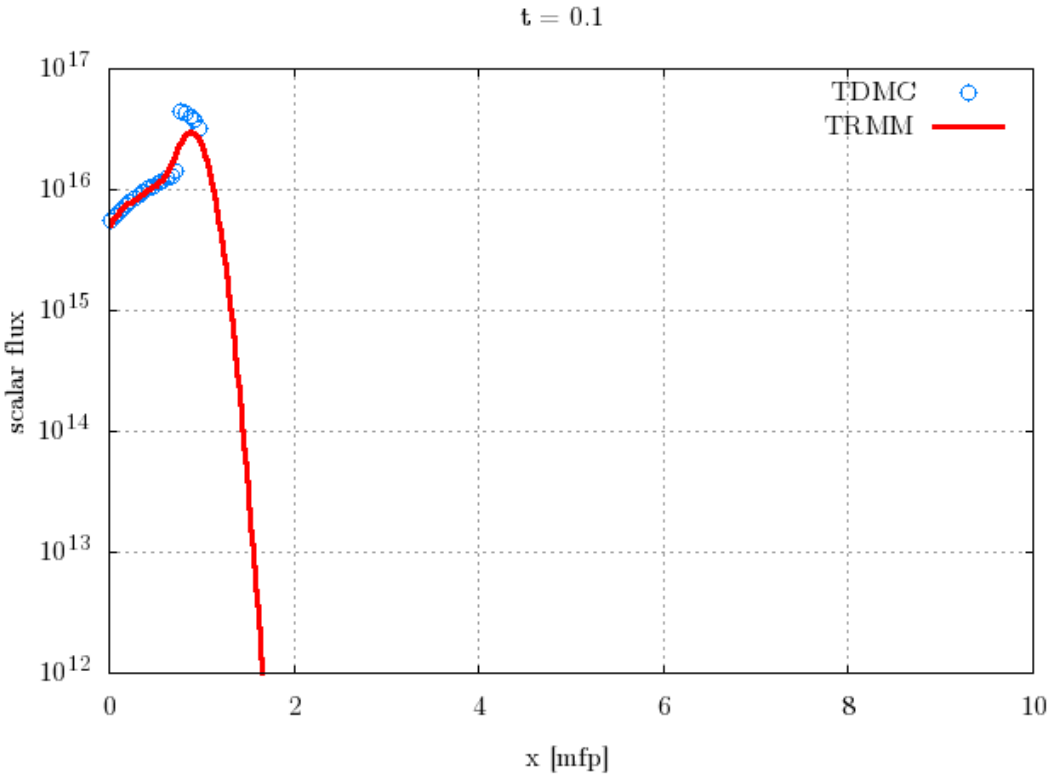
Results: Multi-Region Problem

- **All calculated eigenvalues match within 1% to GFM-calculated values**

Grain Size	TRMM	GFM	% relative error
5.0	−0.550522	−0.550812	0.0526
	−1.70897	−1.70645	0.148
	−2.94639	−2.94231	0.139
	−5.15743	−5.16275	0.103
2.5	−0.702916	−0.703133	0.526
	−1.44948	−1.44826	0.0842
	−3.07481	−3.07065	0.135
	−5.14246	−5.14979	0.142
1.0	−0.748572	−0.748792	0.0294
	−1.55628	−1.55474	0.0991
	−2.96333	−2.96021	0.105
	−5.06238	−5.06991	0.149
0.5	−0.756954	−0.757198	0.0322
	−1.56677	−1.56505	0.120
	−2.97862	−2.97523	0.114
	−5.09076	−5.09813	0.145
0.0	−0.763313	−0.763507	0.0254
	−1.57345	−1.57201	0.0916
	−2.98655	−2.98348	0.103
	−5.10018	−5.10866	0.166

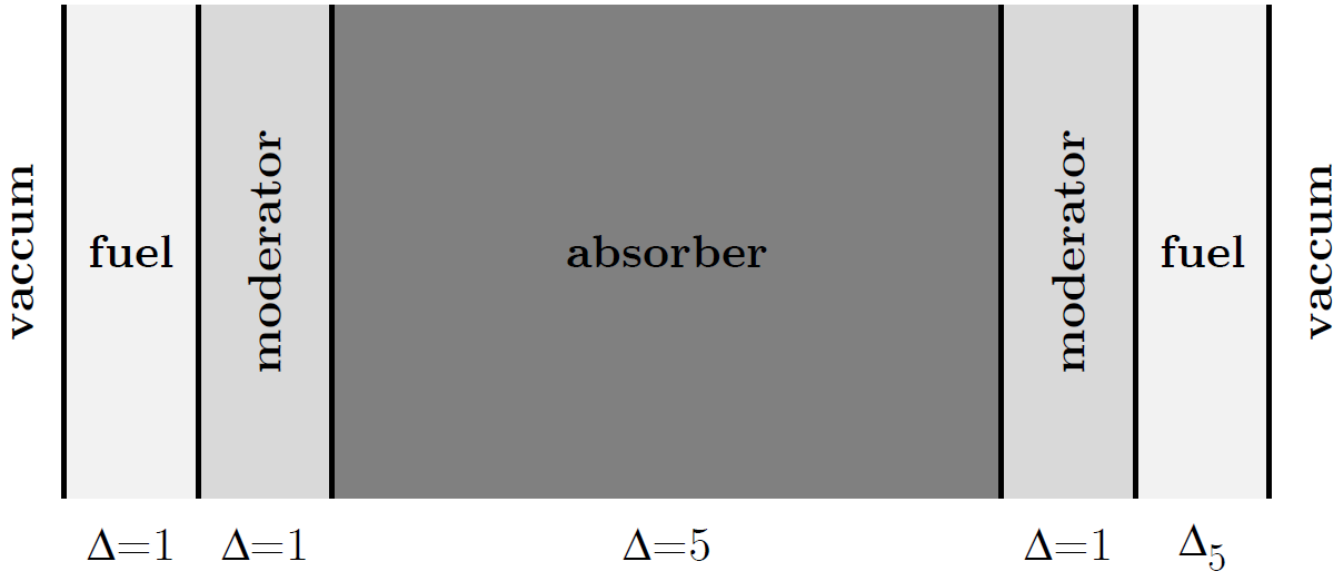
Results: Multi-Region Problem

- **The eigenfunction expansion solution matches that of the Time Dependent Monte Carlo (TDMC) for a rightward-directed incident pulse**



Results: Five-Region Problem

- For this five-region problem, the right fuel region thickness is either 1 (symmetric) or 1.1 (asymmetric)
- The fuel is varied to make subcritical and near critical configurations
- All configurations have only two real eigenvalues



Results: Five-Region Problem

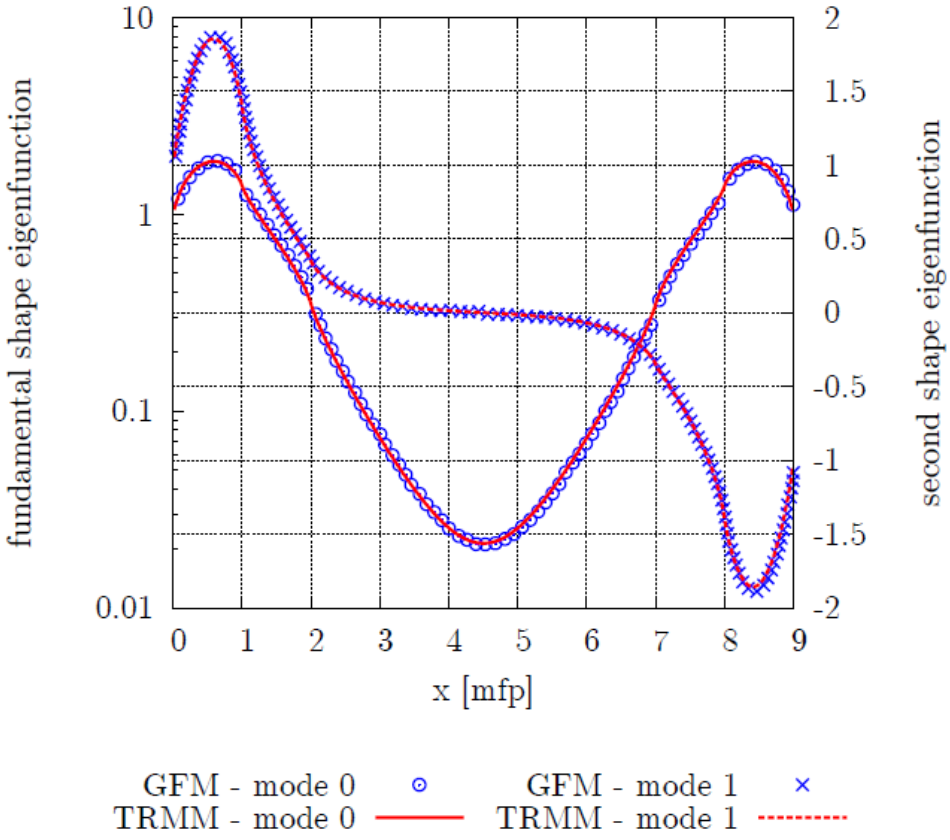
- **The calculated alpha eigenvalues from all configurations compare very well to those from the GFM**
- **The second alpha eigenvalue of the asymmetric supercritical case shows the most relative difference due to its small value**

n	$\nu\Sigma_f$	Δ_5	k_n		α_n	
			TRMM[a]	GFM	TRMM	GFM
0	0.3	1.0	0.4243228	0.4243163	−0.3196225	−0.3196537
1	0.3	1.0	-	0.4241317	−0.3229678	−0.3229855
0	0.3	1.1	0.4556890	0.4556758	−0.2930021	−0.2932468
1	0.3	1.1	-	0.4242237	−0.3211711	−0.3213939
0	0.7	1.0	0.9900525	0.9900716	−0.006153130	−0.006156369
1	0.7	1.0	-	0.9896407	−0.006442946	−0.006440766
0	0.7	1.1	1.063237	1.063244	0.03753544	0.03759991
1	0.7	1.1	-	0.9898554	−0.006969051	−0.006298843

[a] Uncertainties converged to less than a few pcm.

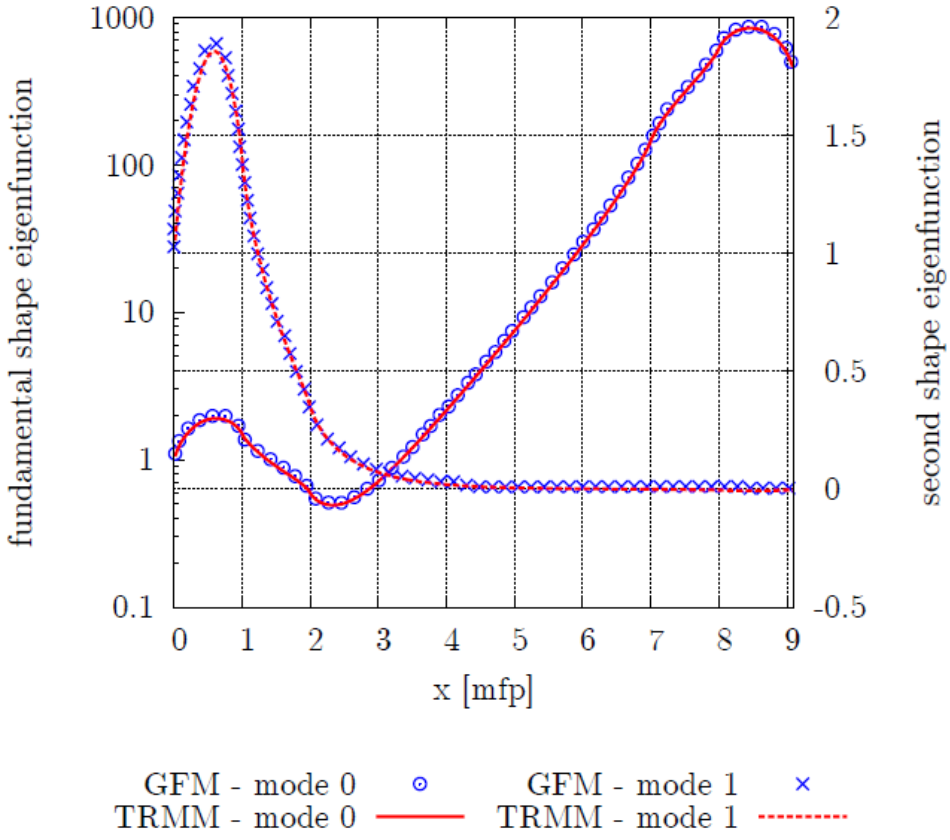
Results: Five-Region Problem

- The first two eigenfunctions for the symmetric, near critical case agree with the GFM results
- The second shape eigenfunction has rotational symmetry
- These eigenfunctions have the most difficulty converging due to the proximity of the first two alpha eigenvalues (-0.00615 and -0.00644)



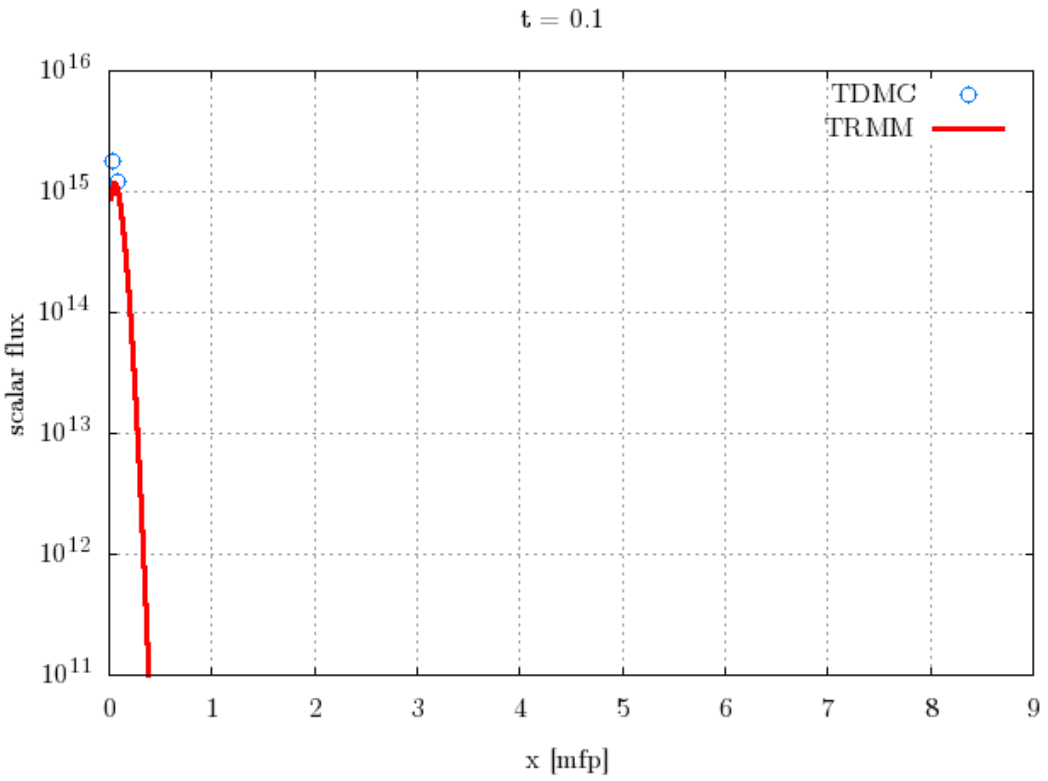
Results: Five-Region Problem

- The asymmetric fundamental shape eigefunction increases nearly three orders of magnitude towards the thicker fuel region, where the second shape eigenfunction is nearly flat
- These converge faster than the symmetric case because the first two eigenvalues differ greatly



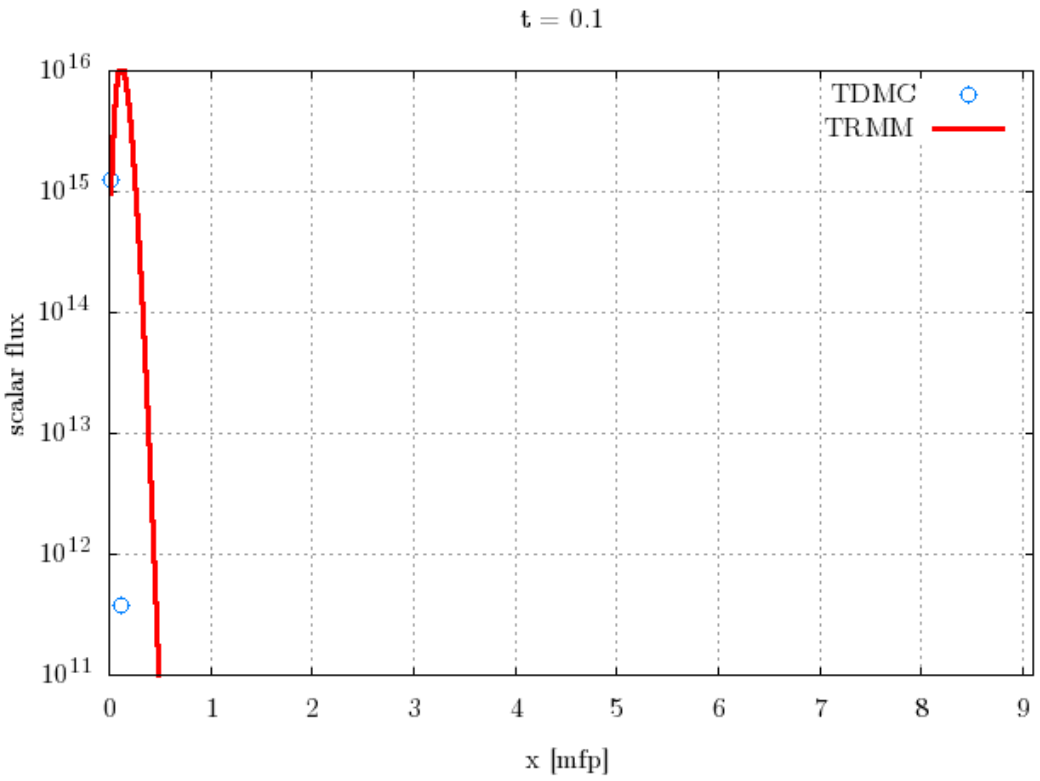
Results: Five-Region Problem

- **Eigenfunction expansion for the far subcritical symmetric configuration with a *constant* source incident on the left face**



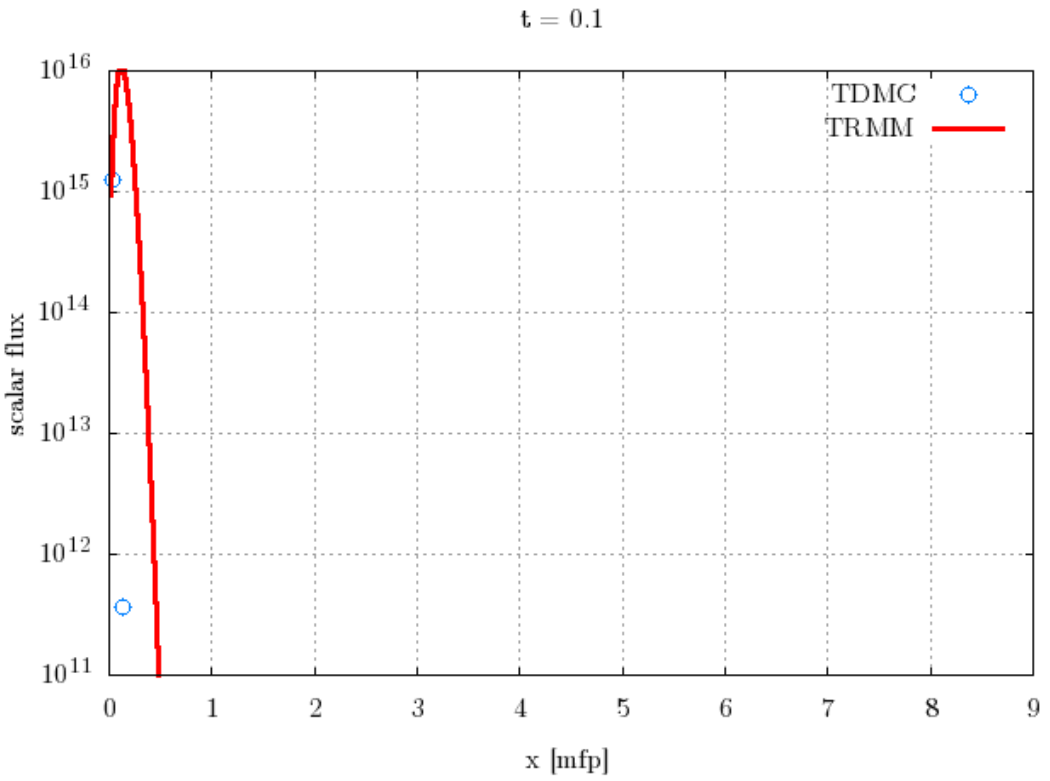
Results: Five-Region Problem

- **Eigenfunction expansion for the asymmetric supercritical configuration with a pulse incident on the left face**



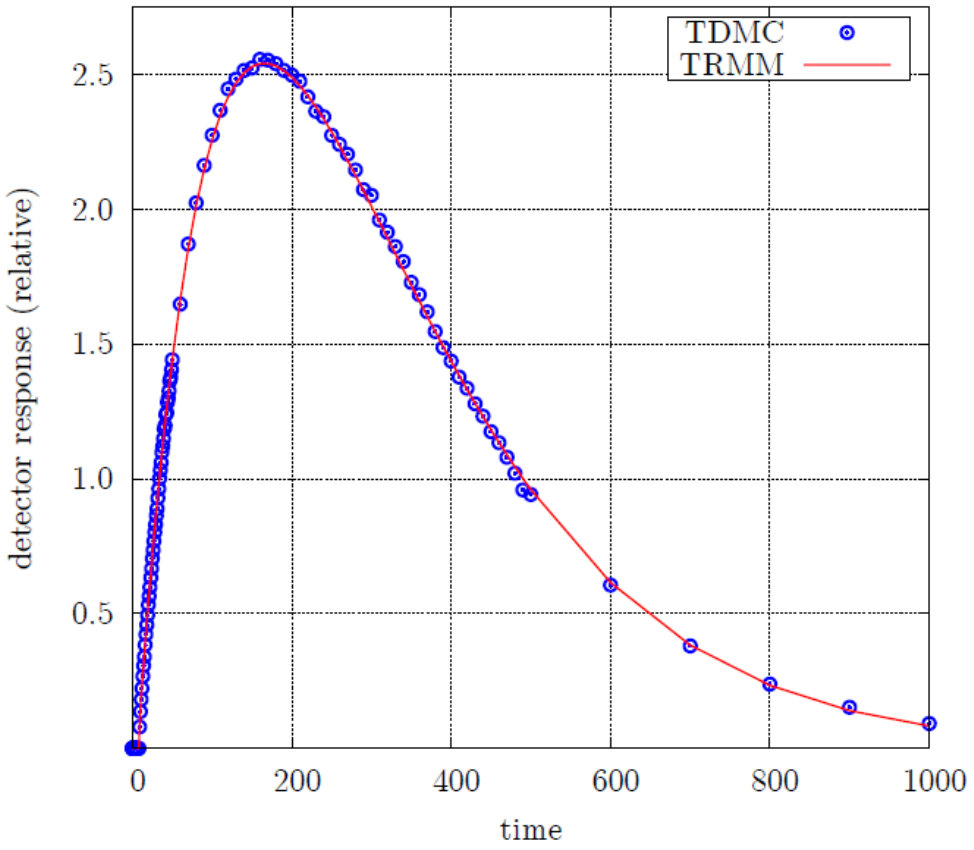
Results: Five-Region Problem

- **Eigenfunction expansion for the near critical symmetric configuration with a pulse incident on the left face**



Results: Five-Region Problem

- The estimated detector response for the previous problem for a detector located in the right fuel region shows the ability of the TRMM to accurately predict the response in a given region of the problem
- The higher modes are still present throughout a large portion of the response, due to the proximity of the first two eigenvalues

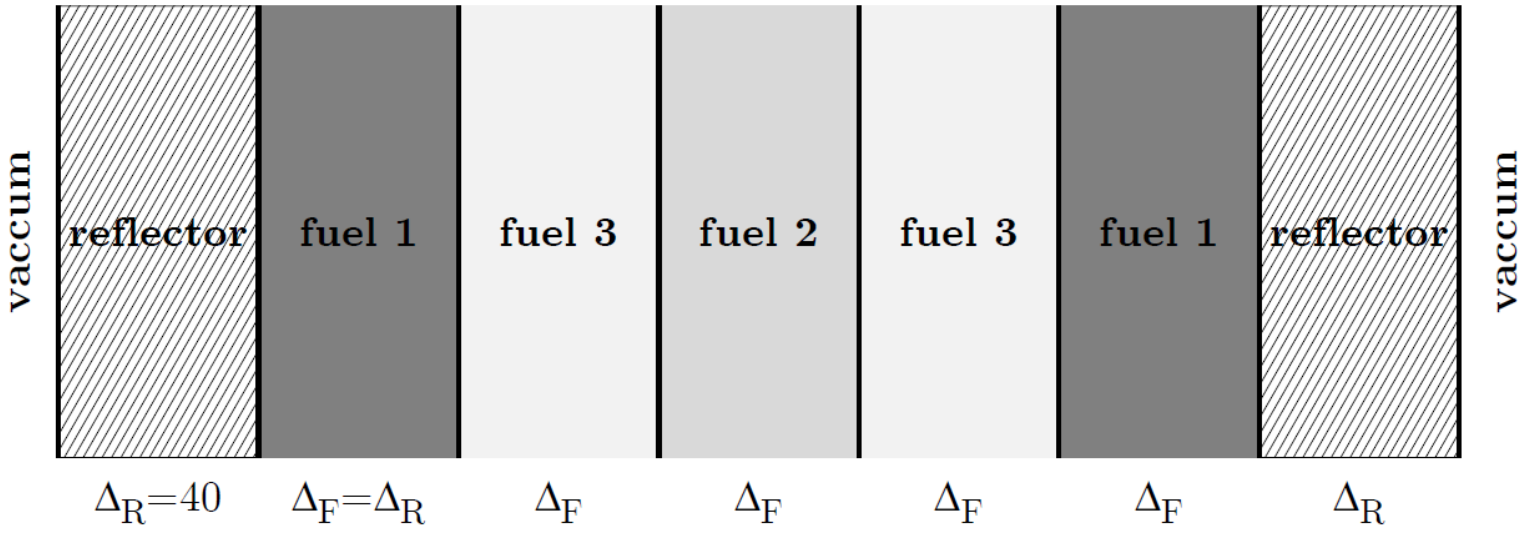


Results: Five-Region Problem

- The TRMM eigenfunction expansion solutions compare well to TDMC
- The eigenfunction expansions shown use all modes in the expansion, even those belonging to the eigenvalues calculated that fall within the continuum; these modes are necessary to model the earliest times where the flux is zero in much of the problem
- The smoothness of the expanded solution is not able to accurately describe sharp variations in the flux shape
- Differences at the front of the pulse shapes at early times are due to the differences in the angular dependence of the initial source and the source described to the eigenfunction expansion

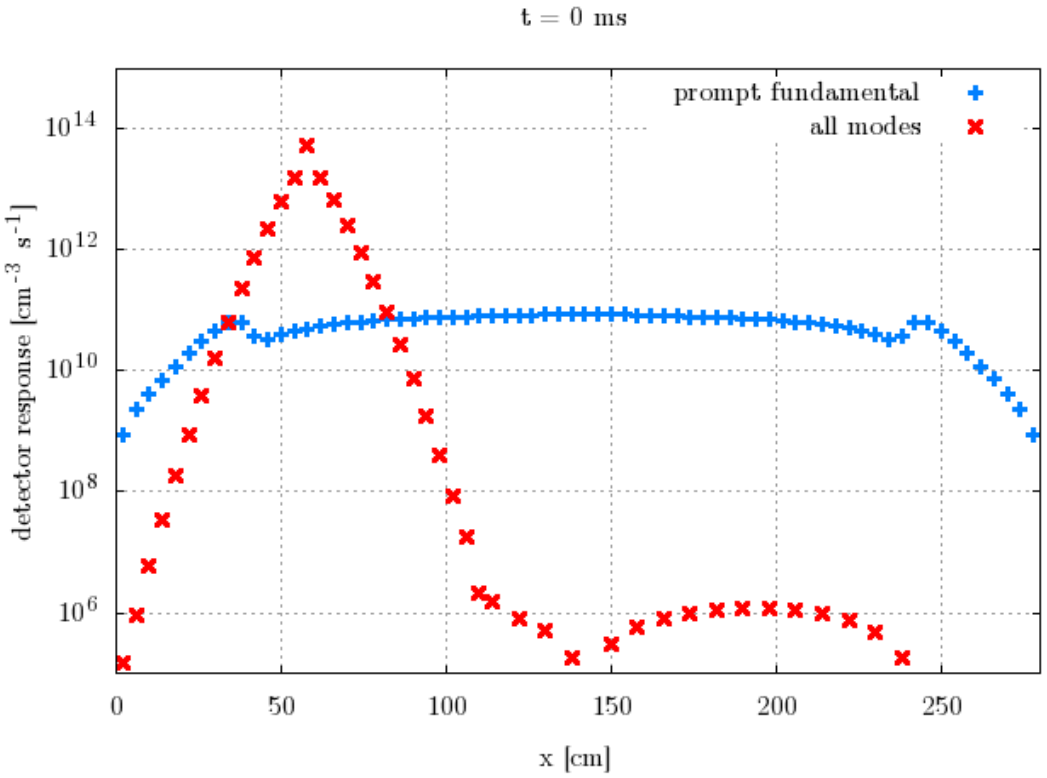
Results: Continuous Energy Problem

- This continuous energy problem is a subcritical hydrogenous medium set up with five homogenized fuel regions with an outer reflector
- The total problem size is 280 centimeters
- The detector response is a linear combination of the flux in each of the energy groups (mostly thermal)



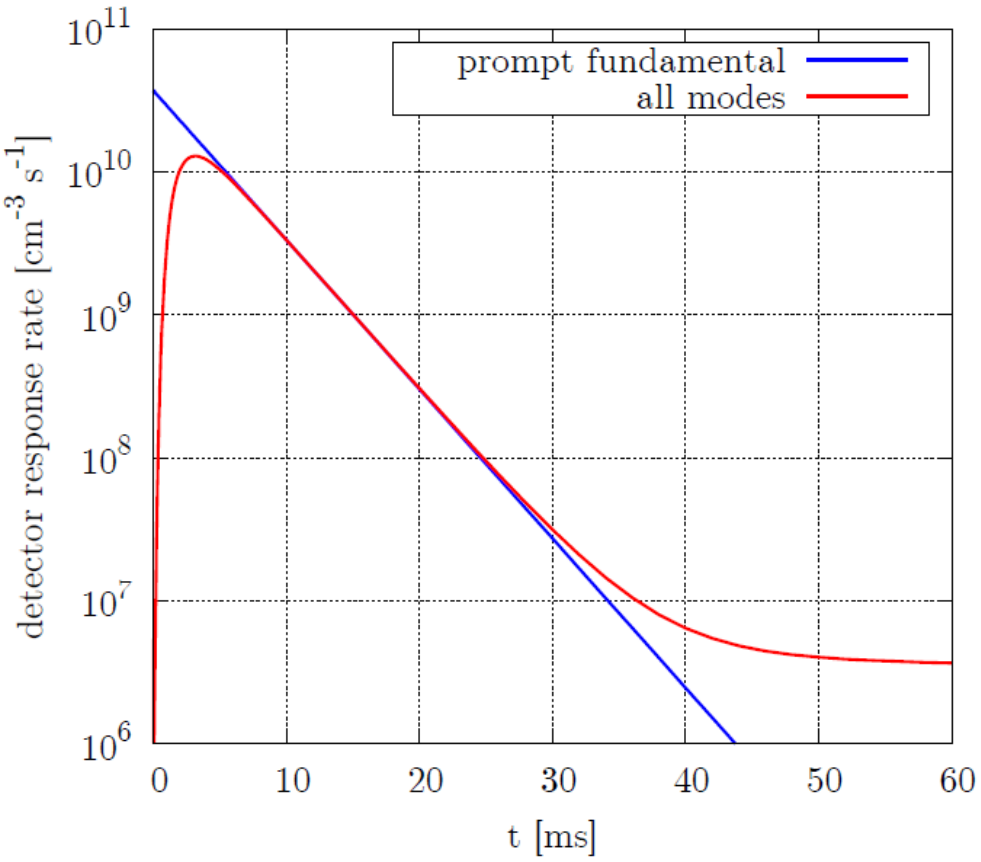
Results: Continuous Energy Problem

- **The eigenfunction expansion for a pulse in the left side of the problem (no TDMC ran for this problem)**



Results: Continuous Energy Problem

- The estimated response for a detector located in the right fuel region for the pulse incident from the left side of the reactor
- The prompt fundamental mode is plotted alongside the expected detector response
- After 40ms, the delayed neutron modes begin to dominate the response shape



Summary and Future Work

- **Formulated the Transiton Rate Matrix Method**
- **Tallied the continuous-time Markov process transition rate matrix with Monte Carlo**
- **Verified one-speed results with Green's Function Method**
- **Investigated the spectrum behavior**
- **Compared TRMM eigenfunction expansions to TDMC**

- **Sparse matrix storage and eigenvalue routines**
- **Continuous energy TDMC comparisions**
- **Calculate three-dimensional alpha modes**
- **Benchmark to experimental data**

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Methods: α eigenvalues

- **α-eigenvalue problem with precursors**

$$\frac{\alpha}{v}\psi + \hat{\mathbf{\Omega}}\cdot\nabla\psi + \Sigma\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}) = \iint \Sigma_s(E' \to E, \hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\psi' dE' d\mathbf{\Omega}'$$
$$+ \iint \frac{\chi_p}{4\pi}(1-\beta)\bar{\nu}\Sigma_f\psi' dE' d\mathbf{\Omega}' + \sum_j \frac{\chi_j}{4\pi}\lambda_j C_j,$$

$$\alpha C_j + \lambda_j C_j(\mathbf{r}) = \iint \beta_j \bar{\nu}\Sigma_f\psi' dE' d\mathbf{\Omega}'.$$

Methods: Eigenfunction expansion

- **Flux expansion in the time-dependent transport and precursor equations**

$$\sum_{i=0}^{\infty} \frac{dA_i(t)}{dt} \begin{bmatrix} v^{-1} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \psi_i(\mathbf{r}, E, \hat{\mathbf{\Omega}}) \\ C_{j,i}(\mathbf{r}) \end{bmatrix} =$$

$$\sum_{i=0}^{\infty} A_i(t) \begin{bmatrix} -\mathbf{L} + \mathbf{F}_p & \chi_d \lambda_j \\ \mathbf{F}_d & -\lambda_j \end{bmatrix} \begin{bmatrix} \psi_i(\mathbf{r}, E, \hat{\mathbf{\Omega}}) \\ C_{j,i}(\mathbf{r}) \end{bmatrix} + Q(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$$

- **Resulting differential equation**

$$\frac{dA_i(t)}{dt} = \alpha_i A_i(t) + \frac{\left\langle \psi_i^{\dagger}, Q \right\rangle_{\mathbf{r},E,\hat{\mathbf{\Omega}}}}{\gamma_i}$$