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Time-Eigenvalue Estimation using the Dynamic Mode Decomposition

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Dynamic Mode Decomposition (DMD)

Consider an evolution equation over time that can we written in the generic form

$$\frac{\partial y}{\partial t} = A(r)y(r,t), \tag{1}$$

where $y(r,t)$ is a function of a set of variables denoted by r, which could be space, angle, energy, etc., and time t. Consider the solution to the equation at a sequence of equally spaced times, $y(r,t_0), y(r,t_1), \dots, y(r,t_{N-1}), y(r,t_N)$, separated by a time Δt. These solutions are formally determined by the relationship:

$$[y(r,t_N), y(r,t_{N-1}), \dots, y(r,t_1)] = e^{\mathbf{A}\Delta t}[y(r,t_{N-1}), y(r,t_{N-2}), \dots, y(r,t_0)]. \tag{2}$$

If we constrain ourselves to finite dimensional problems, the solution is now a vector and the operator is a matrix. In this case the original equation has the form

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{A}\mathbf{y}(t). \tag{3}$$

We will say that $\mathbf{y}_n$ is of length $M > N$ and $\mathbf{A}$ is an $M \times M$ matrix. In this case, the solutions are related through the matrix exponential:

$$[\mathbf{y}_N, \mathbf{y}_{N-1}, \dots, \mathbf{y}_1] = e^{\mathbf{A}\Delta t}[\mathbf{y}_{N-1}, \mathbf{y}_{J-2}, \dots, \mathbf{y}_0]. \tag{4}$$

In shorthand we can define the $N \times M$ matrix

$$\mathbf{Y}_+ = [\mathbf{y}_N, \mathbf{y}_{N-1}, \dots, \mathbf{y}_1], \qquad \mathbf{Y}_- = [\mathbf{y}_{N-1}, \mathbf{y}_{N-2}, \dots, \mathbf{y}_0],$$

as the matrices formed by appending the column vectors $\mathbf{y}_n$ and to get

$$\mathbf{Y}_+ = e^{\mathbf{A}\Delta t}\mathbf{Y}_-. \tag{5}$$

Equation (5) is exact; however the matrix $\mathbf{A}$ may be too large to compute the exponential, $e^{\mathbf{A}\Delta t}$. Therefore, we desire to use just the solution to estimate the eigenvalues of $e^{\mathbf{A}\Delta t}$.

To this end we will use the solution vectors collected in $\mathbf{Y}_+$ and $\mathbf{Y}_-$ to produce an approximation to $\mathbf{A}$. We compute the thin singular-value decomposition (SVD) of the matrix $\mathbf{Y}_-$:

$$\mathbf{Y}_- = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^*, \tag{6}$$

where $\mathbf{U}$ is an $M \times N$ unitary matrix, $\mathbf{V}$ is a $N \times N$ unitary matrix, and $\mathbf{\Sigma}$ is an $N \times N$ diagonal matrix with non-negative elements. The asterisk denotes the conjugate-transpose of a matrix. Typically, some of the diagonal elements of $\mathbf{\Sigma}$ are effectively zero. Therefore, we make $\mathbf{\Sigma}$ the $r \times r$ matrix that contains all r values greater than some small, positive ϵ.

Substituting Eq. (6) into Eq. (5) we get

$$\mathbf{Y}_+ = e^{\mathbf{A}\Delta t}\mathbf{U}\mathbf{\Sigma}\mathbf{V}^*.$$

Rearranging this equation gives

$$\mathbf{V}^*\mathbf{Y}_+\mathbf{V}\mathbf{\Sigma}^{-1} = \mathbf{U}^* e^{\mathbf{A}\Delta t}\mathbf{U} \equiv \tilde{\mathbf{S}}. \tag{7}$$

An eigenvalue of $\tilde{\mathbf{S}}$ is also an eigenvalue of $e^{\mathbf{A}\Delta t}$. To see this, we consider an eigenvalue λ and eigenvector $\mathbf{v}$ of $\tilde{\mathbf{S}}$. By definition we have $\tilde{\mathbf{S}}\mathbf{v} = \lambda\mathbf{v}$, which is equivalent to $\mathbf{U}^* e^{\mathbf{A}\Delta t}\mathbf{U}\mathbf{v} = \lambda\mathbf{v}$. Left multiplying this equation by $\mathbf{U}$ we get

$$e^{\mathbf{A}\Delta t}\mathbf{U}\mathbf{v} = \lambda\mathbf{U}\mathbf{v},$$

which shows that λ is an eigenvalue of $e^{\mathbf{A}\Delta t}$. Additionally, $\hat{\mathbf{v}} = \mathbf{U}\mathbf{v}$ is the associated eigenvector of $e^{\mathbf{A}\Delta t}$ to eigenvalue λ.

The matrix $\tilde{\mathbf{S}}$ is much smaller than that for $e^{\mathbf{A}\Delta t}$ and we can form $\tilde{\mathbf{S}}$ *without knowing* $\mathbf{A}$. To create $\tilde{\mathbf{S}}$ we need to know the result of $e^{\mathbf{A}\Delta t}$ applied to an initial condition several times. Then we need to compute the SVD of the data matrix $\mathbf{U}_{J-1}$. A direct computation requires $O(M^2N)$ operations, though iterative methods for computing the SVD exist. As a comparison, the QR factorization of $e^{\mathbf{A}\Delta t}$, requires $O(M^3)$ operations.

α Eigenvalues for Neutron Transport

The discussion above suggests the following algorithm for estimating alpha eigenvalues of the discrete transport equation:

1. Compute N time dependent steps starting from ψ_0 using a numerical method of choice and fixed Δt.
2. Compute the SVD of the resulting data matrix $\mathbf{Y}_-$, and form $\tilde{\mathbf{S}}$.
3. Compute the eigenvalues/eigenvectors λ of $\tilde{\mathbf{S}}$, and calculate the α eigenvalues from $\lambda = e^{\alpha\Delta t}$.

This is an approximate method because the time steps typically will not be computed using the matrix exponential, rather a time integration technique such as the backward Euler method will be used. The backward Euler algorithm estimates the matrix exponential as

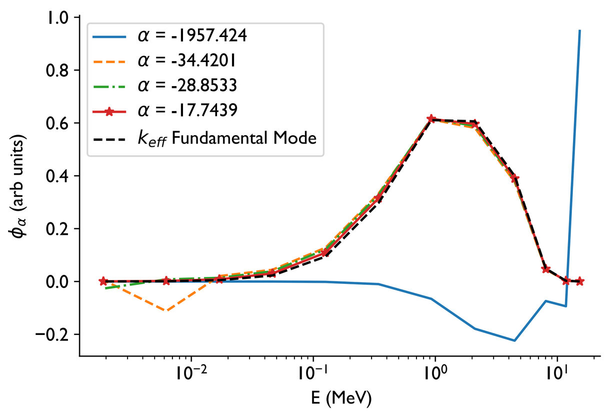
$$e^{\mathbf{A}\Delta t} \approx (\mathbf{I} - \Delta t\mathbf{A})^{-1}.$$

When we use the DMD method on a data matrix generated by the backward Euler method, we are computing eigenvalues of $(\mathbf{I} - \Delta t\mathbf{A})^{-1}$. To relate these eigenvalues to the α eigenvalues we use the relation

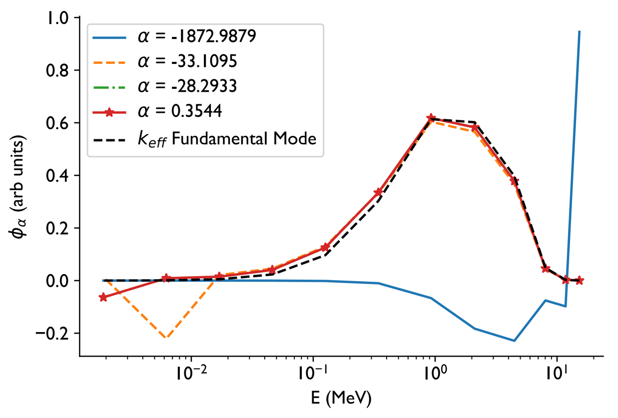
$$\alpha \approx \frac{1}{\Delta t}\left(1 - \frac{1}{\lambda}\right).$$

This approximation will improve at first order as $\Delta t \to 0$.

Bare Plutonium Sphere



Subcritical



Supercritical

Here we present results for a sphere of 99 atom-% ^{239}Pu and 1 atom-% natural carbon using 12 group cross-sections and a simple buckling model for leakage so that we can solve an infinite medium problem. We will consider sub- and super-critical systems by adjusting the radius of the sphere.

Subcritical Case

We consider a sphere of radius 4.77178 cm with an associated k_{eff} in our model of 0.95000. The fundamental mode for this reactor is shown in above along with several α eigenmodes. The α eigenvalues for this system have a fast decaying mode with a large number of neutrons in the fastest energy group, and the slowest decaying mode closely follows the fundamental mode.

To test the DMD estimation of α eigenvalues we run a time dependent problem where at time zero the system has 1000 neutrons in the energy group corresponding to 14.1 MeV. This is a crude approximation to an experiment where a pulse of DT fusion neutrons irradiates the sphere. The problem is run in time dependent mode out to various final times with uniform time steps, and the time steps are used in the DMD procedure to estimate α eigenvalues. The number of neutrons in the system as a function of time demonstrates that subcritical multiplication is happening in the first 0.002 μs of the problem. As we argue next, DMD finds the eigenvalues that are important in the time dependent solution over the time scales considered and that are resolved by the time step size.

From the table we can see that during the phase where subcritical multiplication is occurring (before $t = 0.002$ μs) DMD accurately computes to six digits the α eigenmode that corresponds to a large population of 14.1 MeV neutrons. This is the mode most excited by the initial condition. It also accurately computes the eigenvalues with magnitudes larger than 200 to several digits. However, we note that the "dominant" or slowest decaying eigenmode is not detected by the DMD algorithm, indicating that its contribution at this early time is insignificant or cannot be distinguished from other slowly decaying modes. This indicates an important phenomenon in time dependent transport: the slowest decaying eigenvalue may not be important in a given problem.

As we look at simulations run to later time, more eigenvalues are identified using DMD. Running the simulation to intermediate times, 0.02 and 0.2 μs, we see that DMD finds all of the eigenvalues in the problem to several digits of accuracy. In both of these solutions DMD does not find the eigenvalue near -28.85 μs^{-1}. This eigenmode has more neutrons in the slowest group, group 12, relative to the next slowest group, group 11. Given that this problem has very little thermalization due to the small amount of carbon, this mode is not important at these intermediate times relative to other modes.

At a much later time, 2 μs, DMD identifies all of the slowly decaying modes but cannot find the rapidly decaying modes. This is due to the fact that the larger time steps used make it so that the solution steps over the time scale where these modes are important. As a result DMD estimates a pair of complex eigenvalues with a real part that does not correspond to an actual eigenvalue.

Table 1: Alpha eigenvalues (μs^{-1}) for subcritical sphere computed using DMD using the solution obtained using different values of Δt and final times.

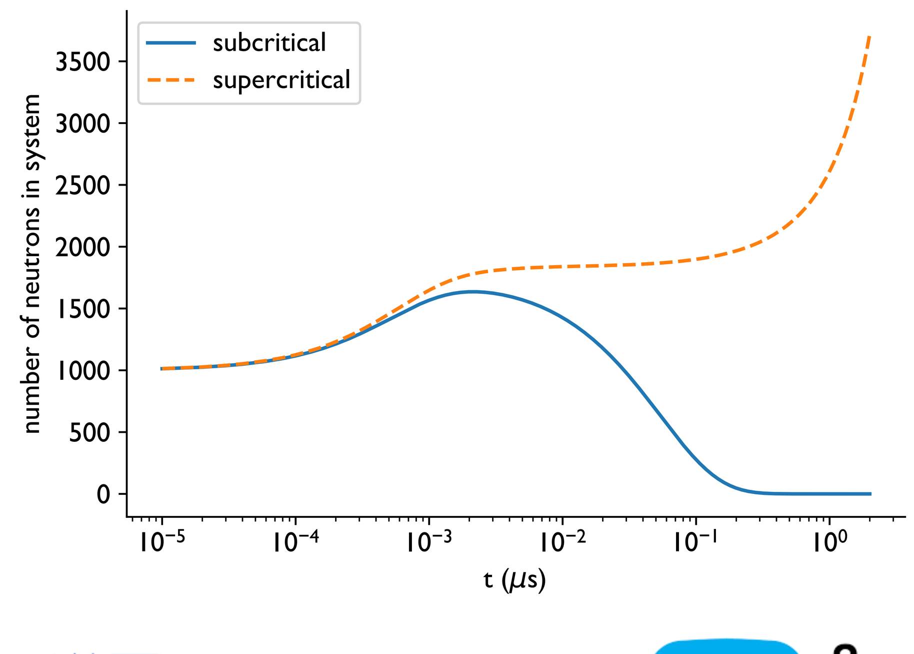
Exact	t_{final} (μs) = 0.002	0.02	0.2	2
-17.7439		-17.5504	-17.7588	-17.7437
-28.8533	-24.5669			-28.8628
-34.4201		-35.7281	-34.1948	-34.3999
-48.4269		-46.6817	-48.0231	-48.4613
-75.0701		-75.7798	-75.2787	-74.9998
-132.352		-132.183	-132.197	-132.587
-261.942	-262.78	-261.974	-262.127	-260.218
-547.732	-531.575	-547.719	-547.11	-585.536
-893.385	-893.314	-893.399	-895.262	-763.974
-1368.92	-1335.16	-1368.90	-1362.45	
-1732.99	-1721.75	-1733.01	-1725.84	$-1708 \pm 381i$
-1957.42	-1957.42	-1957.41	-1957.42	
	Δt (μs) = 0.0002	0.0002	0.001	0.01

Table 2: Alpha eigenvalues (μs^{-1}) for supercritical sphere computed using DMD using the solution obtained using different values of Δt and final times.

Exact	t_{final} (μs) = 0.002	0.02	0.2	2
0.354439	-4.02079	0.332366	0.354291	0.354439
-28.2933				-28.2932
-33.1095		-32.8048	-33.1151	
-46.0832		-45.3512	-45.817	-46.0703
-70.7945		-70.4805	-70.9448	-70.8261
-124.497		-124.568	-124.38	-124.381
-247.14	-247.914	-247.127	-247.281	-248.057
-521.689	-506.467	-521.693	-521.216	-507.684
-853.58	-853.733	-853.577	-855.008	
-1309.4	-1279.91	-1309.4	-1305.12	$-1050 + 23i$
-1659.02	-1649.68	-1659.02	-1655.16	
-1872.99	-1872.99	-1872.99	-1872.98	-2059.43
	Δt (μs) = 0.0002	0.0002	0.001	0.01

Supercritical Case

We consider a sphere of radius 5.029636 cm with an associated k_{eff} in our model of 1.000998. We perform the same calculations as performed before on the subcritical sphere. Table 2 compares the eigenvalues computed with DMD with the eigenvalues computed by solving the equivalent infinite medium problem. At an early time (0.002 μs), the DMD computation does not identify the exponentially increasing mode. We see that at this time the supercritical and subcritical systems have neutron populations that are very similar. The subcritical multiplication observed in the smaller sphere where modes associated with the fusion neutrons contributed to the growth of the neutron population, is also present in this supercritical system. However, there are very few neutrons emitted in the fusion energy range from fission ($\chi_1 \approx 1.37 \times 10^{-4}$), so these modes decay away.

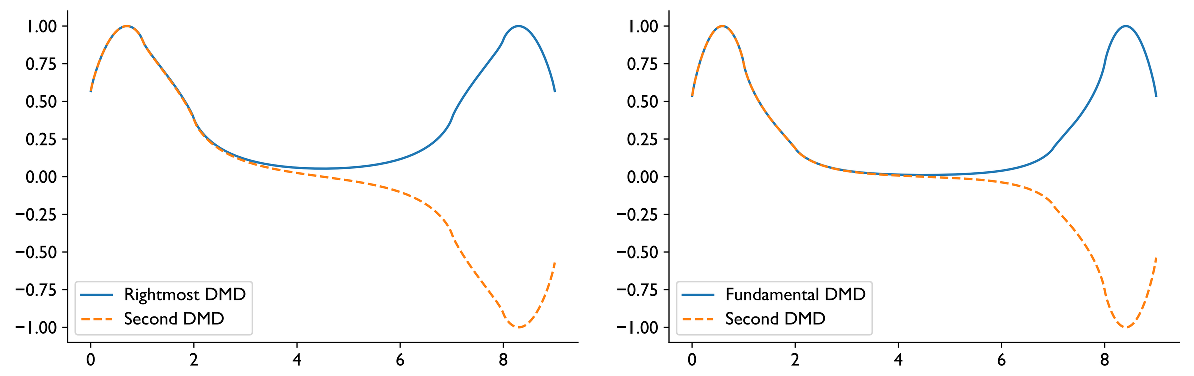


Hetergeneous, 1-Speed Benchmark

We solve the benchmark problems published by Kornreich and Parsons as solved by the Green's function method (GFM). Their work defines a slab problem for single-speed neutrons (i.e., one group) consisting of an absorber surrounded by a moderator and fuel. They define configurations of this problem that are symmetric and asymmetric, as well as subcritical and supercritical versions.

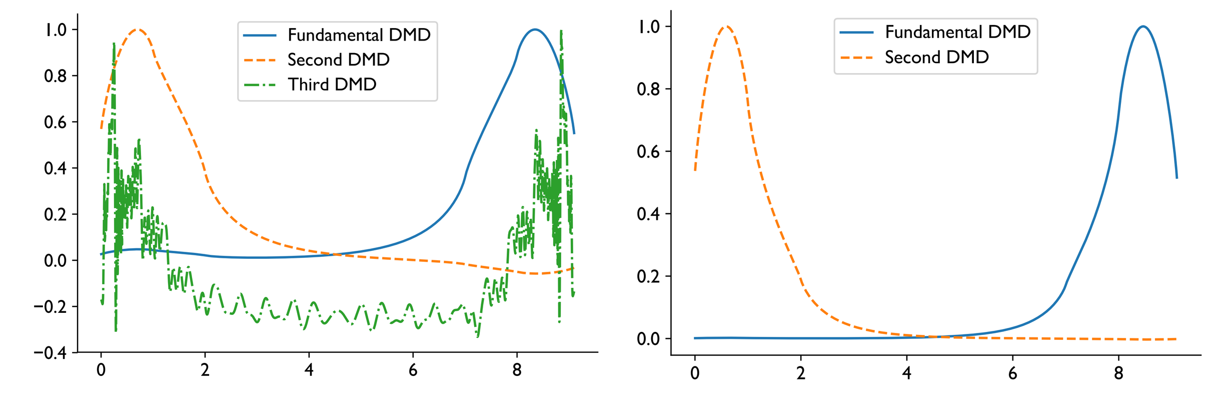
Table 3: Alpha eigenvalues for the one-group slab problem in different configurations as computed via the Green's function method (GFM) and the difference between the GFM eigenvalues and the DMD estimates in units of pcm (10^{-5}).

Geometry	$\nu\sigma_f^{\text{fuel}}$	Fundamental α (GFM)	$\alpha_{\text{GFM}} - \alpha_{\text{DMD}}$ (pcm)	Second α (GFM)	$\alpha_{\text{GFM}} - \alpha_{\text{DMD}}$(pcm)
Symmetric	0.3	-0.3196537	0.639	-0.3229855	0.694
	0.7	-0.006156369	0.7711	-0.006440766	0.7724
Asymmetric	0.3	-0.2932468	0.535	-0.3213939	0.666
	0.7	0.03759991	0.64	-0.006298843	0.7717



(a) Symmetric slab with $\nu\sigma_f = 0.3$ (b) Symmetric slab with $\nu\sigma_f = 0.7$

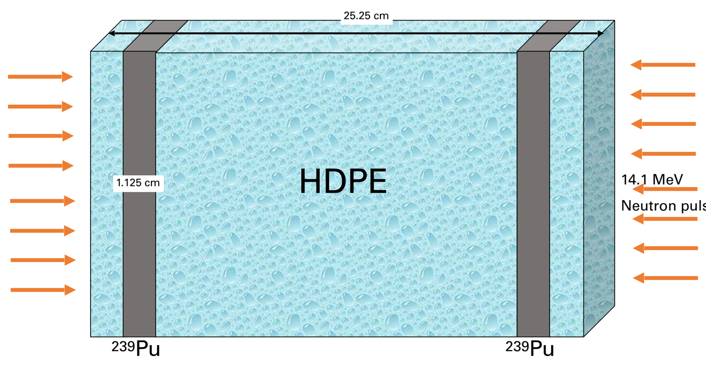
Fundamental and second eigenmodes for the one group slab problem in the symmetric configurations.

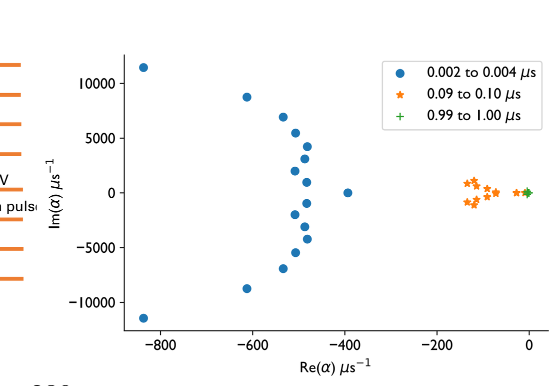


(a) Asymmetric slab with $\nu\sigma_f = 0.3$ (b) Asymmetric slab with $\nu\sigma_f = 0.7$

Fundamental and second eigenmodes for the one group slab problem in the asymmetric configurations. There is a third, real eigenvalue in the $\nu\sigma_f = 0.3$ case with $\alpha = -1.02158875$.

70-group Problem

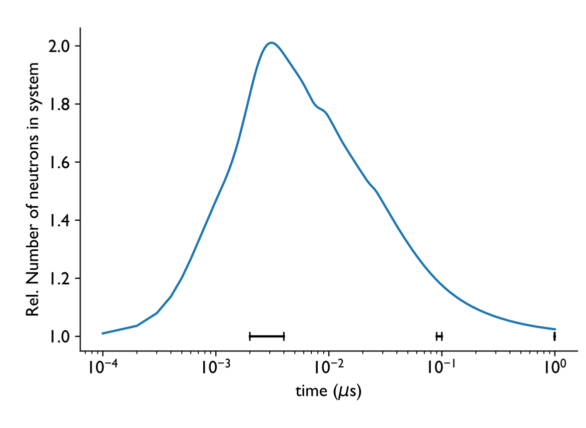




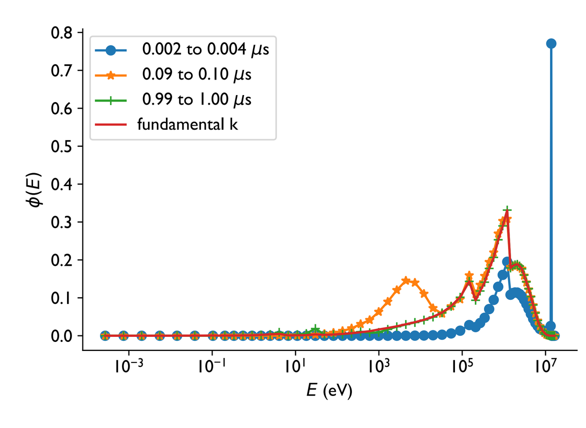
We solve a problem consisting of two slabs of ^{239}Pu with high-density polyethylene (HDPE) between them and a reflector of HDPE on the outside. The initial condition has a pulse of DT fusion neutrons striking the outer surface of the reflector. The system is subcritical when the fuel regions are each 1.125 cm thick with a resulting $k_{\text{eff}} \approx 0.97$ and isotropic scattering is assumed.

The behavior of the neutron population in time, as well as the three time intervals over which the eigenvalues were estimated is shown above. The time interval from 0.002 to 0.004 μs is during the subcritical multiplication phase of the simulation. It makes sense that during this phase the slowly decaying modes are not important in the solution.

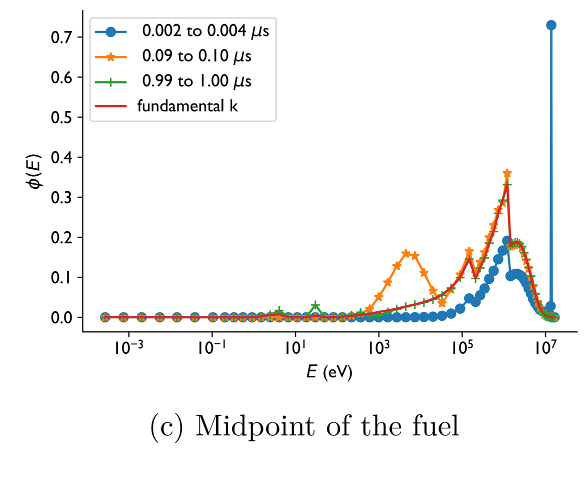
Early in the time the solution is dominated by the presence of 14.1 MeV neutrons, though fission neutrons are present in the fuel and outer reflector. At late times, near 1μs, the spectrum in the fuel and the reflector is close to the fundamental eigenmode of the k-eigenvalue problem. Nevertheless, the central moderator in the problem has not reached the fundamental k eigenmode, as there has not been enough time to fully thermalize the neutrons. Moreover, these results indicate that if this system were involved in an experiment, the neutrons produced in the first microsecond would give little information about the spectrum of the k eigenvalue problem.



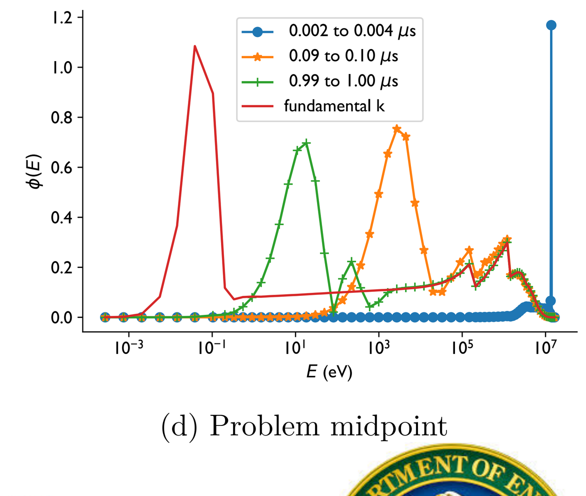
(a) Neutron population over time



(b) Midpoint in the outer reflector



(c) Midpoint of the fuel



(d) Problem midpoint

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