Variable Dynamic Mode Decomposition for Estimating Time Eigenvalues in Nuclear Systems

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Abstract — We present a new approach to calculating time eigenvalues of the neutron transport operator (also known as $\alpha$ eigenvalues) by extending the dynamic mode decomposition (DMD) to allow for nonuniform time steps. The new method, called variable dynamic mode decomposition (VDMD), is shown to be accurate when computing eigenvalues for systems that were infeasible with DMD due to a large separation in timescales (such as those that occur in delayed supercritical systems). The $\alpha$ eigenvalues of an infinite medium neutron transport problem with delayed neutrons, and consequently having multiple, very different relevant timescales, are computed. Furthermore, VDMD is shown to be of similar accuracy to the original DMD approach when computing eigenvalues in other systems where the previously studied DMD approach can be used.

Keywords — Time eigenvalues, data-driven algorithms, time-dependent neutronics.

Note — Some figures may be in color only in the electronic version.

I. INTRODUCTION

The time behavior of neutron transport problems can be understood through the spectrum of the transport operator given by time eigenvalues,$^1$ also known as $\alpha$ eigenvalues. The corresponding eigenfunctions for the time eigenvalues are angular fluxes, and therefore are more challenging to compute than the more well-known $k$ eigenvalue problem where the eigenfunctions are scalar fluxes.

The conventional approach to computing $\alpha$ eigenvalues is via the $k$-$\alpha$ iteration procedure.$^2,3$ This method is ill suited for many subcritical problems because the iteration procedure can introduce total cross sections that are effectively negative. Moreover, $k$-$\alpha$ iterations can only calculate the eigenvalue farthest to the right in the complex plane. In a given scenario, especially at short times, other eigenvalues may be more important to the dynamics. We also note that the time eigenvalues of the transport operator do not describe the complete dynamics of a system. The spectrum of the transport operator has discrete eigenvalues as well as a continuum of eigenvalues.$^4$ These continuum eigenvalues will be important at short timescales to deal with the neutrons that have not undergone several collisions.

Dynamic mode decomposition (DMD) has been used in the neutron transport community for the purpose of estimating time eigenvalues in calculations$^5$ and experiments,$^6,7$ as well as to create reduced-order models,$^8$ improve the convergence of power iteration in $k$-eigenvalue problems,$^9,10$ and accelerate source iteration.$^{11,12}$ Originally introduced for fluid dynamics problems,$^{13,14}$ DMD takes the solution to a time-dependent transport problem and uses the solution at several time steps to estimate an approximate transport operator based solely on the available solutions. This approximate operator has eigenvalue-eigenvector pairs that are also eigenvalues and eigenvectors of the full transport operator. DMD is a fully data-driven method; this means that it will find the eigenmodes that are important in the system’s evolution. Additionally, the approximate operator that DMD estimates can be used as a reduced-order model to evolve the system forward in time.

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The DMD procedure requires that data snapshots be spaced at regular intervals (i.e., have the same time step between the snapshots). This is a significant drawback for transport problems with delayed neutrons or problems very near critical, as we will demonstrate. One would prefer to use variable time steps to resolve important transients without losing efficiency. This was the motivation for developing a variable dynamic mode decomposition (VDMD) algorithm that allows for irregularly spaced steps. In this paper, we develop this method and show how it can be used for a variety of time integration techniques. The underlying idea is the same as in Ref. 5: use solutions to a time-dependent transport problem to estimate the α eigenvalues of a system.

We demonstrate on a variety of problems that our method can accurately estimate the eigenvalues of the system without the requirement of equal-sized time steps. One restriction of our approach is that it does require knowledge of the type of time discretization used in producing the solution. In practice, this restriction may be relaxed. Concurrent with the submission of this work, a recent paper showed that for computational fluid dynamics data, a similar approach to ours can be used on data that were generated using a different (or perhaps unknown) time integrator in order to allow a modal analysis of the data. We discuss this further in the our conclusions in Sec. V.

II. THEORY OF A VARIABLE STEP DECOMPOSITION

We extend the DMD procedure to accept a variable time step for determining α eigenvalues by leveraging the fact that we know which time discretization method was used to create the data matrix. We begin with a generic, linear system of differential equations of the form

$$\frac{d}{dt} y(t) = A y(t),$$

with initial conditions $y(0) = y^0$. The vector $y$ is of length $M$, and the matrix $A$ is of size $M \times M$. In neutron transport applications, $A$ represents a discretized transport operator, but for most neutron transport calculations this matrix is never explicitly formed. The vector $y$ contains the spatial, angular, and energy degrees of freedom in the solution.

To develop our VDMD method, we consider common, implicit time integration procedures for Eq. (1). The backward Euler method applied to this equation is

$$\frac{y^{n+1} - y^n}{\Delta t} = Ay^{n+1}. \quad \text{Backward Euler,} \tag{2}$$

where the superscripts denote a time step number: $y^n \approx y(t^n)$ is the approximation of the solution at time $t^n$. The time step size is the difference between $t^{n+1}$ and $t^n$. Commonly, this equation would be factored to show how to produce $y^{n+1}$ from $y^n$. However, the form in Eq. (2) will be most useful to us in developing a DMD-like procedure for approximating the operator $A$.

The Crank-Nicolson and BDF-2 ([Ref. 17], Chap. V.1) methods applied to Eq. (1) yield the following equations:

$$\frac{y^{n+1} - y^n}{\Delta t} = \frac{1}{2} A (y^{n+1} + y^n) \quad \text{Crank-Nicolson} \tag{3}$$

and

$$\frac{y^{n+1} - \frac{4}{3} y^n + \frac{1}{3} y^{n-1}}{\Delta t} = Ay^{n+1} \quad \text{BDF-2}. \tag{4}$$

For each of these methods we can write the update as

$$u^{n+1} = Av^n, \tag{5}$$

where

$$u^{n+1} = \frac{1}{\Delta t} \begin{cases} y^{n+1} - y^n & \text{Backward Euler} \\
\frac{\Delta t}{2} (y^{n+1} - \frac{4}{3} y^n) & \text{Crank-Nicolson} \\
\frac{\Delta t}{3} (y^{n+1} + \frac{1}{2} y^n - \frac{1}{3} y^{n-1}) & \text{BDF-2} \end{cases} \tag{6}$$

and

$$v^n = \left( \frac{1}{2} (y^{n+1} + y^n) \right) \quad \text{Backward Euler or BDF-2} \tag{7}$$

Crank-Nicolson.

If we consider the repeated application of the time integration method from time $t^0 = 0$ over $N$ time steps,
we could collect via concatenation the vectors \( \mathbf{u}^n \) and \( \mathbf{u}^{n+1} \) into matrices of size \( M \times N \), \( \mathbf{U}^+ \), and \( \mathbf{V}^- \) defined as
\[
\mathbf{U}^+ = [\mathbf{u}^N \mathbf{u}^{N-1} \ldots \mathbf{u}^1]
\]
and
\[
\mathbf{V}^- = [\mathbf{v}^{N-1} \mathbf{v}^{N-2} \ldots \mathbf{v}^0].
\]
Using these definitions, we can write
\[
\mathbf{U}^+ = \mathbf{A} \mathbf{V}^-.
\]

We note that BDF-2 is not self-starting because it needs the two previous solutions. Either backward Euler or Crank-Nicolson can be used to compute \( \mathbf{u}^1 \) from the initial condition and still fit the form we have here. In our formulation, the operator \( \mathbf{A} \) does not depend on time so that the time step size does not affect it; all of the information regarding the time step size is contained in vectors \( \mathbf{u} \) and \( \mathbf{v} \).

We now proceed as is standard for DMD. We first take the thin singular value decomposition (SVD) of \( \mathbf{V}^- \) and write this as
\[
\mathbf{V}^- = \mathbf{LSR}^T,
\]
where \( \mathbf{L} \) is of size \( M \times r \), \( \mathbf{S} \) is a diagonal matrix of size \( r \times r \) with positive entries called singular values, and \( \mathbf{R} \) is of size \( N \times r \) where \( r \) is number of nonzero singular values (or singular values with a magnitude larger than some threshold). The matrices \( \mathbf{L} \) and \( \mathbf{R} \) have the property that
\[
\mathbf{L}^T \mathbf{L} = \mathbf{I}_M
\]
and
\[
\mathbf{R}^T \mathbf{R} = \mathbf{I}_N,
\]
where \( \mathbf{I}_K \) is an identity matrix of size \( K \times K \). Using this property, we right multiply Eq. (9) by \( \mathbf{RS}^{-1} \) and then left multiply by \( \mathbf{L}^T \) to get
\[
\mathbf{L}^T \mathbf{U}^+ \mathbf{RS}^{-1} = \mathbf{L}^T \mathbf{A} \mathbf{L} = \mathbf{\tilde{A}}.
\]

The matrix \( \mathbf{\tilde{A}} \) is an \( r \times r \) approximation to the operator \( \mathbf{A} \). Moreover, we can compute this approximation using only the known data matrices \( \mathbf{U}^+ \) and \( \mathbf{V}^- \) as indicated by the left-hand side of Eq. (12).

As shown in previous work, the eigenvalues of \( \mathbf{L}^T \mathbf{AL} \) are also eigenvalues of \( \mathbf{A} \), and if \( \mathbf{w} \) is an eigenvector of \( \mathbf{L}^T \mathbf{AL} \), then \( \mathbf{L} \mathbf{w} \) is an eigenvector of \( \mathbf{A} \). These properties allow us to estimate the eigenvalues/eigenvectors of \( \mathbf{A} \) without any knowledge of the operator itself, other than the results of calculating solutions using one of the time discretization schemes described previously.

Equation (12) has the same form as the standard DMD approximation, except we have arrived at it using different data matrices. We call this approach the VDMD. One key difference between VDMD and the standard DMD method is that we require knowledge of how the solution is updated because the time integration method and the time step sizes influence the matrices \( \mathbf{U}^+ \) and \( \mathbf{V}^- \). This means that we cannot apply this method directly to experimental measurements without having an approximation of the time derivative of the measurement. Further investigation of the application of this approach to measured data should be the subject of future research.

II.A. Demonstration on a Simple Problem

Consider the system
\[
\frac{\partial}{\partial t} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\alpha^2 & -\lambda \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \mathbf{A} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix},
\]
with initial conditions \( y_1(0) = 1 \) and \( y_2(0) = 0 \). This system is the first-order system corresponding to the second-order ordinary differential equation (ODE)
\[
y''_1 + \lambda y'_1 + \omega^2 y_1 = 0,
\]
with solution
\[
y_1(t) = \left( \cos(\omega t) + \frac{\sin(\omega t)}{\omega t} \right) e^{-t/\tau},
\]
where
\[
\tau = \frac{2}{\lambda}.
\]
and

$$w^2 = \omega^2 - \frac{\lambda^2}{4}. \quad (16)$$

For this problem, the matrix $A$ has eigenvalues given by $(-\lambda \pm \sqrt{\lambda^2 - 4\omega^2})/2$.

We will solve system (13) using the various time integrators mentioned previously. Setting $\lambda = 1/10$ and $\omega = 13\sqrt{29}/20 \approx 3.500357$, we can analytically determine the eigenvalues of $A$ to be $-0.05 \pm 3.5i$. To demonstrate the VDMD method, we solve this problem with 20 logarithmically spaced time steps starting from $10^{-3}$ and increasing to a final step size of $3.0$ (i.e., the step size increases by a factor of about 1.524 each step).

As can be seen from Fig. 1, the various numerical solutions to this problem do not agree with the analytic solution with these large time step sizes. Nevertheless, applying the VDMD method to these numerical solutions produces eigenvalues that agree with the exact values to within machine precision (i.e., relative errors on the order of $10^{-14}$). Other numerical experiments indicate that with as few as three time steps we can approximate the eigenvalues to machine precision. This is an important result because it indicates that VDMD, because it has knowledge of the numerical method used to approximate the solution, is able to estimate properties of $A$ even when the numerical solutions in the snapshot matrices have large amounts of time discretization error.

### III. VDMD AND TIME EIGENVALUES FOR NEUTRONICS

Now that we have presented the VDMD method in general, we turn to the neutron transport problem. We begin with the time-dependent transport equation including delayed neutrons:

$$\frac{\partial \psi}{\partial t} = A\psi + \sum_{i=1}^{I} \frac{\chi_{di}(E)}{4\pi} \lambda_i C_i(x, t) \quad (17)$$

and

$$\frac{\partial C_i}{\partial t} = \int_0^\infty dE\beta_i \nu \Sigma_f(E) \phi(x, E, t) - \lambda_i C_i(x, t), \quad i = 1, \ldots, I, \quad (18)$$

where $\psi(x, \Omega, E, t)$ is the angular flux at position $x \in \mathbb{R}^3$ in direction $\Omega \in S_2$ at energy $E$ and time $t$, and $C_i(x, t)$ is the delayed precursor density of flavor $i$. The transport operator $A$ is given by

$$A = \nu(E)(-\Omega \cdot V - \Sigma_t + S + \mathcal{F}),$$

with $S$ and $\mathcal{F}$ the scattering and fission operators

$$S\psi = \int_0^\infty d\Omega' \int_0^\infty dE' \Sigma_s(\Omega' \rightarrow \Omega, E' \rightarrow E) \psi(x, \Omega', E', t) \quad (19)$$

and

$$\mathcal{F}\psi = \frac{\chi_p(E)}{4\pi} \int_0^\infty dE' (1 - \beta) \nu \Sigma_f(E') \phi(x, E', t), \quad (20)$$

where $\Sigma_s(\Omega' \rightarrow \Omega, E' \rightarrow E)$ is the double-differential scattering cross section from direction $\Omega'$ and energy $E'$ to direction $\Omega$ and energy $E$, $\nu \Sigma_f(E')$ is the fission cross section times the expected number of fission neutrons at energy $E'$, $\chi_p(E)$ is the probability of a fission neutron being emitted with energy $E$, $\chi_{di}(E)$ is the probability of a delayed neutron of flavor $i$ being emitted with energy $E$, $\beta_i$ is the fraction of fission neutrons that come from delayed flavor $i$, $\sum_i \beta_i$ is the $\beta_i$, and $\lambda_i$ is the decay constant for precursor flavor $i$.

The scalar flux $\phi(x, E, t)$ is defined as the integral of the angular flux over the unit sphere,

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**Fig. 1.** Data used to estimate the eigenvalues of the damped oscillator problem using VDMD. The solutions shown here used 20 logarithmically spaced time steps where the first step was of size 0.001 and the final step was of size 3. Despite the numerical error, VDMD is able to estimate the eigenvalues of the underlying operator to machine precision.
\[ \phi(x, E, t) = \int_{4\pi} d\Omega \psi(x, \Omega, E, t). \]  

(21)

We study the use of VDMD on the transport equation with discretizations of the multigroup method in energy, discrete ordinates in angle, and various spatial discretizations. To connect with Eq. (1), the time-dependent transport equation can be written as a system of differential equations

\[ \frac{\partial \Psi}{\partial t} = \Lambda \Psi(t), \]

(22)

where \( \Psi(t) \) is a time-dependent vector of the discrete values of the angular flux \( \psi \) at each space, energy, and angle degree of freedom and the delayed neutron precursor densities at each spatial degree of freedom. The discrete transport/delayed neutron operator matrix is written as \( \Lambda \). Notice that the time-eigenvalue problem that supposes a form for \( \Psi(t) \) of \( e^{i\alpha t} \psi \) leads to the eigenvalue problem

\[ \alpha \psi = \Lambda \psi. \]

(23)

From this form we can directly apply the VDMD method as detailed previously:

1. Take \( N \) backward Euler (or Crank-Nicolson or BDF-2) steps of the discrete transport problem and form the matrices \( U^+ \) and \( V^- \) [Eq. (8)].
2. Compute the SVD of \( V^- \) and form \( \tilde{\Lambda} \) [Eq. (12)].
3. Compute the eigenvalues of \( \tilde{\Lambda} \) and the associated eigenvectors.

Previously published versions of DMD for estimating time eigenvalues required a fixed-sized time step to generate the data matrices. VDMD does not have this constraint, though it does require knowledge of the time integration method used. The ability to handle variable-sized time steps is an important advance because, for problems where delayed neutrons are significant, computing the prompt and delayed modes of the system would require minuscule steps to capture the prompt scales and a large number of these steps to integrate to times when delayed neutrons are significant, as we demonstrate in the following.

The algorithm has flexibility in that the initial condition for the time-dependent calculation can be chosen based on the analysis being performed. For example, to model an experiment and extract the important eigenmodes, one would initialize the problem with the appropriate experimental initial condition. Alternatively, to compute the dominant eigenmodes in a system, one could use a random initial condition to assure that all of the modes are excited in the system.

IV. NUMERICAL RESULTS

IV.A. Infinite Medium Problem with Delayed Neutrons

To demonstrate the need for a variable time-step method, we consider the neutron flux solution of a 12-group problem with six delayed neutron precursor groups and a spherical buckling approximation for the leakage. This problem results in a transport operator that is an \( 18 \times 18 \) matrix for which we can use numerical linear algebra software to estimate the eigenvalues. A subcritical and delayed supercritical case are considered by modifying the radius of the sphere in the buckling. The numerical solution is computed using both backward Euler and Crank-Nicolson time integration, and logarithmically spaced timesteps are used.

The systems considered had a radius of 11.7335 cm for the subcritical case and a radius of 11.735 cm for the supercritical case. These unsteady problems were initialized with a single neutron per \( \text{cm}^3 \) in the highest energy group at time zero (to approximate probing the system with a fast-neutron source), and used a logarithmically spaced time grid to a final time of \( 10^3 \) s using 200 time steps; the first time step is of size \( \Delta t = 10^{-11} \) s. A challenge of using the traditional DMD algorithm to analyze these kinds of problems lies in the very different timescales over which the features of the system manifest. As an example, the prompt multiplication peak occurs around 10 ns into the problem, while the delayed multiplication continues until well into the hundreds of seconds. This is most evident in Fig. 3, where the supercritical behavior of the system is not evident until over 100 s into the evolution of the problem.

Figures 2 and 3 plot the neutron population in the sphere over time. Resolving the early and late time features of this delayed subcritical system would be extremely expensive using a uniform time step; the present example uses just 200 time points. In these figures, the black line corresponds to the exact solution based on the matrix exponential, the red dashed line is the backward Euler solution, and the green dash-dot line is the Crank-Nicolson solution. The vertical blue lines correspond to the magnitude of the periods of the exact eigenvalues \( |\alpha|^{-1} \), where blue and red colors, respectively, indicate negative and positive value. We also note that the Crank-
Nicolson solution is closer to the analytic solution obtained using a matrix exponential. The biggest errors in the numerical solutions occur during the rapid transition between 10^{-6} and 10^{-4} s.

The exact eigenvalues, along with the relative error in pcm (1 pcm = 10^{-3}) for the eigenvalues estimated with VDMD and either backward Euler or Crank-Nicolson, are tabulated for both the subcritical and supercritical cases in Table I. In the table, we can see that for all 18 eigenvalues, the VDMD estimates are within 1 pcm of the reference. We also observe that there does not appear to be a clear benefit to using Crank-Nicolson over backward Euler, despite the fact that Crank-Nicolson is a second-order accurate method. This speaks to part of the benefit of VDMD: VDMD is aware of the discretization so it can reasonably approximate the operator that generated the data.

IV.B. Modak and Gupta Problem

To demonstrate that VDMD is also applicable to numerical solutions to transport problems, and to compare it with the original DMD formulation, we consider a transport problem first published by Modak and Gupta\(^{18}\) with semi-analytic results published by Kornreich and Parsons.\(^{19}\) Unlike the infinite medium problem, the exact time evolution operator cannot be explicitly formed. The problem is defined as a 10 mean free path, nonmultiplying slab of two materials, with \(\Sigma_S = 10\) in one material and \(\Sigma_S = 9\) in the other. The other nuclear properties are defined as \(\Sigma_F = 10\), \(\nu\Sigma_F = 0\), and \(\chi = 0\). The grain size is varied for separate runs of this simulation; this parameter defines the fraction of the overall length that each slice of material is, compared to the whole. These material slices are arranged in alternating order. The zero-grain-size case indicates a homogeneous material with average properties. Given that we did not see a large benefit in using Crank-Nicolson in the previous problem, in this problem we exclusively use backward Euler time discretization.

Previous work has demonstrated that to accurately estimate eigenvalues on these problems, high resolution in space and angle is necessary. The Modak and Gupta problem was solved with VDMD using \(S_{96}\) discrete ordinates and a diamond difference approach with 1000 spatial grid points and 101 logarithmically spaced time steps, with the first time step ending at \(t = 10^{-5}\) and the last ending at \(t = 100\); results using the original, equi-spaced time-step formulation of DMD used 101 equally spaced time steps over a time range of 100 using the same spatial and angular discretizations. For this problem, the snapshots used in DMD are of size \(1000 \times 196 \approx 2 \times 10^4\), and the data matrices then have approximately \(2 \times 10^6\) entries for the 101 time steps. In applying DMD, we truncated the SVD once the relative contribution of the singular values reached \(10^{-13}\). That is, the rank of the SVD was chosen so that

\[
\frac{\sum_{i=1}^{R} s_i}{\sum_{i=1}^{R} s_i} \leq 10^{-13},
\]

where \(R\) is the total rank of the data matrix and \(s_i\) are the singular values.
### TABLE I

| VDMD Eigenvalue Errors for Subcritical and Delayed Supercritical Spheres Using Backward Euler and Crank-Nicolson* |
|----------------------------------------------------------------------------------------------------------------|
| **Subcritical** | **Supercritical** |
| Analytic (s⁻¹) | Backward Euler Error | Crank-Nicolson Error | Analytic (s⁻¹) | Backward Euler Error | Crank-Nicolson Error |
| −1.67621 × 10⁹ | 4.12074 × 10⁻⁷ | 9.15307 × 10⁻⁷ | −1.67597 × 10⁹ | 3.5385 × 10⁻⁷ | 3.48643 × 10⁻⁷ |
| −1.46266 × 10⁹ | 1.04743 × 10⁻⁶ | 2.41354 × 10⁻⁶ | −1.46245 × 10⁹ | 8.39863 × 10⁻⁷ | 8.98227 × 10⁻⁷ |
| −1.17322 × 10⁹ | 7.94049 × 10⁻⁷ | 2.67553 × 10⁻⁶ | −1.17306 × 10⁹ | 1.38875 | 9.82629 × 10⁻⁷ |
| −7.9423 × 10⁸  | 1.40458 × 10⁻⁷ | 1.97333 × 10⁻⁶ | −7.94119 × 10⁸  | 3.57139 × 10⁻⁷ | 7.95791 × 10⁻⁷ |
| −4.99878 × 10⁸ | 5.88453 × 10⁻⁷ | 1.61807 × 10⁻⁶ | −4.99804 × 10⁸ | 8.25479 × 10⁻⁷ | 5.93383 × 10⁻⁷ |
| −2.92659 × 10⁸ | 4.74705 × 10⁻⁷ | 1.42446 × 10⁻⁶ | −2.92606 × 10⁸ | 1.03237 × 10⁻⁷ | 7.47564 × 10⁻⁷ |
| −1.66397 × 10⁸ | 1.48477 × 10⁻⁸ | 1.43941 × 10⁻⁶ | −1.66365 × 10⁸ | 2.66235 × 10⁻⁷ | 5.597 × 10⁻⁷ |
| −9.36139 × 10⁷ | 9.43281 × 10⁻⁸ | 1.49989 × 10⁻⁶ | −9.35967 × 10⁷ | 5.99602 × 10⁻⁷ | 5.64083 × 10⁻⁷ |
| −5.28136 × 10⁷ | 2.51533 × 10⁻⁷ | 1.89254 × 10⁻⁶ | −5.28057 × 10⁷ | 3.02384 × 10⁻⁶ | 5.04243 × 10⁻⁷ |
| −3.3247 × 10⁷  | 1.57121 × 10⁻⁷ | 3.51607 × 10⁻⁶ | −3.32436 × 10⁷ | 5.85692 × 10⁻⁶ | 1.14324 × 10⁻⁶ |
| −2.64094 × 10⁷ | 3.76945 × 10⁻⁷ | 1.03666 × 10⁻⁵ | −2.64085 × 10⁷ | 0.000125423 | 9.61842 × 10⁻⁷ |
| −6.09650       | 2.07949 × 10⁻⁸ | 5.25697 × 10⁻⁸ | −5.40139 | 9.785 × 10⁻⁹  | 9.24618 × 10⁻⁸ |
| −2.6143        | 0.0002196     | 0.0015871 | −2.60143 | 0.000776098 | 0.00106403 |
| −0.743522      | 0.00158942    | 0.00683878 | −0.732142 | 0.00555557 | 0.00462957 |
| −0.196729      | 0.0077539     | 0.0202177  | −0.187957 | 0.0212489  | 0.0141573  |
| −0.0766105     | 0.0123597     | 0.0339459  | −0.0699507 | 0.0301533  | 0.0208952  |
| −0.0158092     | 0.0221887     | 0.0445097  | −0.0149391 | 0.0202711  | 0.018085   |
| −0.00467553    | 0.0408661     | 0.0300762  | 0.000441678 | 0.00430661 | 0.000104375 |

*VDMD eigenvalue errors in pcm.

### TABLE II

| Computed Eigenvalues for the Modak and Gupta Problem Using VDMD and DMD Compared with the Semi-analytic Results* |
|---------------------------------------------------------------------------------------------------------------|
| **Grain Size** | **Semi-analytic** | **VDMD** | **DMD** |
| 0.5             | −0.551429 | −0.550814 | −0.550814 |
|                 | −1.71149  | −1.70646  | −1.70645  |
|                 | −2.94399  | −2.94235  | −2.94235  |
|                 | −5.28234  | −5.19691  | −5.17338  |
| 0.25            | −0.703578 | −0.704010 | −0.704010 |
|                 | −1.45315  | −1.45044  | −1.45044  |
|                 | −3.07282  | −3.07073  | −3.07073  |
|                 | −5.26925  | −5.15114  | −5.15081  |
| 0.1             | −0.749672 | −0.749256 | −0.749255 |
|                 | −1.56062  | −1.55665  | −1.55665  |
|                 | −2.96323  | −2.96002  | −2.96002  |
|                 | −5.18772  | −5.09398  | −5.11195  |
| 0.05            | −0.758893 | −0.757022 | −0.757022 |
|                 | −1.56062  | −1.56447  | −1.56447  |
|                 | −2.97899  | −2.97842  | −2.97842  |
|                 | −5.21764  | −5.10019  | −5.10619  |
| 0               | −0.763507 | −0.763508 | −0.763508 |
|                 | −1.57201  | −1.57202  | −1.57202  |
|                 | −2.98348  | −2.98352  | −2.98352  |
|                 | −5.10866  | −5.13648  | −5.47278  |

*Bold numbers indicate an agreement for the number in that decimal place with the published results.¹⁹*
We compare the results of the new VDMD algorithm and the existing DMD algorithm. The problem is initialized with a random initial condition for the angular flux in all angles and all positions sampled uniformly between zero and one to ensure that all eigenmodes are excited. The four largest real eigenvalues from these numerical experiments are tabulated in Table II. Bold numbers indicate an agreement for the number in that decimal place with the published results.19 From the table, we notice that VDMD and DMD have nearly identical performance in the number of digits matched with the semi-analytic results. This demonstrates that we have not sacrificed accuracy in formulating a variable step version of DMD.

IV.C. Sood Two-Group Transport Problem

In this final problem, we consider a two-group, two-region critical slab system consisting of a fuel region and a reflector region from problem 59 in Ref. 20. The original problem, being a $k$-eigenvalue benchmark, does not specify neutron speeds. We set the neutron speeds in the two groups to be 1 and 10 cm/μs. The system is designed to be critical, and the rightmost eigenvalue is expected to be nonzero, but small as a consequence of the numerical solution. The ability of a data-driven method to capture this extremely small, negative eigenvalue necessarily requires computing the solution out to a very long time. Instead of requiring a corresponding very large number of time steps, allowing a variable time step greatly reduces the computational and storage costs associated with these kinds of problems.

This problem was simulated using $S_N$ approximations with varying angles, 100 spatial cells, and 300 time steps logarithmically spaced, having an initial time step of $\approx 0.001$ s and ending with a time step of $\approx 0.1$ s. The largest real eigenvalues recovered by VDMD are tabulated against the $\alpha$ eigenvalue estimated by the standard $k$-$\alpha$ iteration.21 We note that VDMD estimates other eigenvalues, while $k$-$\alpha$ iterations are limited to computing the rightmost eigenvalue in the complex plane. We are able to use $k$-$\alpha$ iterations for this problem because it is close to critical. If we reduced the slab size, the system would become far from critical and make the $k$-$\alpha$ iteration procedure unworkable.19,22

While the exact, dominant eigenvalue for this problem is zero, because we have numerical error in the numerical solution (due to spatial, time, and angular discretizations), the eigenvalues for a given numerical instantiation of the problem are expected to be “close” to zero. This is indeed what we observe in Table III. All of the eigenvalues estimated are subcritical and near zero. Note that as the number of angles in the discrete ordinate calculation increase, the eigenvalues get closer to zero. The results from the $k$-$\alpha$ iteration and from VDMD agree to four or more digits in all calculations.

V. CONCLUSIONS

The VDMD is an extension to the DMD method that is capable of determining time eigenvalues of the neutron transport operator as effectively as DMD but without the requirement of uniformly spaced time steps. We believe that this method will be useful to analyze systems where time-dependent phenomena are important and a range of timescales is also present, as is common in neutronics problems due to the separation of scales of prompt and delayed neutrons.

There are several directions for future exploration into VDMD. The VDMD approach is naturally suited to adaptive time-stepping methods. One could use the approximate operator estimated by VDMD to predict the solution after the next time step and use this result in a time-step controller. Additionally, because VDMD, and also DMD, can be applied to multiphysics problems (particularly those with thermal-hydraulic negative feedback), applications of it to estimate properties of the multiphysics system should be explored. Finally, how to apply VDMD to measurement data is an open question. Because measurement data are not generated by a time integration algorithm, VDMD is not directly applicable to these problems. It may be possible, however, to formulate the problem using time averages to use a similar approach. Applying DMD or VDMD to these problems may not be able to generate $\alpha$ eigenvalues, but looking at the modes generated from an experiment and comparing them to DMD applied to simulated diagnostics could indicate if the overall behavior of the simulation is consistent with the experiment. Recent work in computational fluid dynamics suggests that a VDMD approach is possible even if the data were not generated using
a numerical algorithm. How this applies to neutronics applications is an open question and should be the subject of future work.

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