Data-Driven Algorithms for Transport

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Outline

Introduction

The Dynamic Mode Decomposition

Estimating Time Eigenvalues Time-dependent transport examples

DMD for Accelerating Source Iteration Slab geometry examples

Low-Rank Approximations to Dynamic Systems

Conclusions

We can use data to approximate operators and improve calculations.

- In scientific computing we are used to taking a known operator and making approximations to it.
- It is possible to use the action of an operator and use just the action of the operator to generate approximations to it.
 - This is the basis for many Krylov methods.
- In this talk I will detail how we can use the action of radiation transport operators to
 - Estimate time eigenvalues present in a subcritical system, and
 - Compute the slowly converging modes in source iteration to accelerate convergence without the need for diffusion-based preconditioning.
- I will also talk about how we can generate a low-rank approximation to the time-dependent transport system.

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We begin with a sequence of vectors related by an operator.

- Consider a sequence of vectors $\{y_0, y_1, \ldots, y_K\}$ where $y_k \in \mathbb{R}^N$.
- The vectors are related by a potentially unknown linear operator of size $N \times N$, A, as

$$y_{k+1} = Ay_k.$$

• If we construct the $N \times K$ data matrices Y_+ and Y_- ,

$$Y_{+} = \begin{pmatrix} | & | & | \\ y_{1} & y_{2} & \dots & y_{K} \\ | & | & | \end{pmatrix} \qquad Y_{-} = \begin{pmatrix} | & | & | \\ y_{0} & y_{1} & \dots & y_{K-1} \\ | & | & | \end{pmatrix}$$

we can write

$$Y_+ = AY_-.$$

- At this point we only need to know the data vectors y_k, they could come from a calculation, measurement, etc.
- As $K \to \infty$ we could hope to infer properties about A.

The SVD gives a representation of the data matrices.

• We take the thin singular value decomposition (SVD) of Y_{-} to write

$$Y_{-}=U\Sigma V^{\mathrm{T}},$$

where U is a $N \times K$ orthogonal matrix, Σ is a diagonal $K \times K$ matrix with non-negative entries on the diagonal, and V is a $K \times K$ orthogonal matrix.

- The SVD requires $O(NK^2)$ operations to compute.
- Later, we will want $K \ll N$, if, for example, N is the number of unknowns in a transport calculation.
- ► Also, if the column rank of Y₋ < K, then there is a further reduction in the SVD size.</p>
- The matrix U has columns that forms an orthonormal basis for the row space of Y₋ ⊂ ℝ^N.
- Using the SVD we get

$$Y_+ = AU\Sigma V^{\mathrm{T}}.$$

▶ If there are only r < K non-zero singular values in Σ , we use the compact SVD where U is $N \times r$, Σ is $r \times r$, and V is $K \times K$.

DMD gives a low rank approximation to the operator.

• We can rearrange the relationship between Y_+ and Y_- to be

$$Y_+ = AU\Sigma V^{\mathrm{T}} \qquad \rightarrow \qquad U^{\mathrm{T}}AU = U^{\mathrm{T}}Y_+V\Sigma^{-1}.$$

- Define $\tilde{A} = U^{T}AU = U^{T}Y_{+}V\Sigma^{-1}$. This is a rank K approximation to A.
- Using the approximate operator A, we can now find out information about A.
- The eigenvalues/vectors of \tilde{A} ,

$$\tilde{A}w = \lambda w$$

are used to define the dynamic modes of A:

$$\varphi = \frac{1}{\lambda} U^{\mathrm{T}} Y_{+} V \Sigma^{-1} w.$$

The dynamic mode decomposition (DMD) of the data matrix Y₊ is then the decomposition of into vectors φ. The mode with the largest norm of λ is said to be the dominant mode.

Example of operator approximation demonstrates the efficacy.

Consider the sequence

$$z_{k+1} = a z_k + n_k,$$

where a = 0.5, and $n_k \sim \mathcal{N}(0, 10^2)$.

• Using K = 500, we estimate a = 0.506552 from the data below.



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Evolution without an operator is possible: DMD infers the operator from the data.

- Left: Data generated by moving a circle in a periodic motion with added noise. The data has two periods of motion.
- Right: Reconstruction generated by approximating \tilde{A} using one period of frames and starting from frame 1.

The DMD modes of the inferred operator are what we would expect.



Dominant DMD mode: $U\varphi_1$



Third DMD mode: $U\varphi_3$



Second DMD mode: $U\varphi_2$



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Current methods of estimating time-eigenvalues have issues for subcritical systems.

- In neutron transport for time-dependent problems alpha eigenvalues (also called time eigenvalues) are important quantities to understand system dynamics and safety.
 - These eigenvalues characterize the system evolution in terms of functions of the form Ce^{\alpha t}.
- ► The more well-known *k*-eigenvalue gives information about the long-term behavior of the system, but is less useful for diagnosing many experiments.
- Additionally, most alpha eigenvalue solvers have issues with subcritical problems due to "negative absorption".
- ► Furthermore, for subcritical systems it has been shown that the rightmost eigenvalue in the complex plane is not necessarily meaningful.
 - There can be an eigenvalue with negative real part that is arbitrarily close to 0 and decays arbitrarily slowly.

These eigenvalues correspond to the time scale of slow moving neutrons crossing the system. DMD can be used to estimate eigenvalues of the matrix exponential.

If we consider a sequence of vectors that are solutions to the system of differential equations,

$$\frac{\partial y}{\partial t} = Ay(t),$$

and are separated by a time, Δt , the relationship between vectors is

$$y^{n+1} = e^{A\Delta t} y^n.$$

• As before we can define Y_{-} and Y_{+} , compute the SVD of $Y_{-} = USV^{*}$, and approximate the matrix exponential:

$$U^{\mathrm{T}} e^{A\Delta t} U = U^{\mathrm{T}} Y_{+} V \Sigma^{-1}.$$

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One can show the following:

- The eigenvalues of $U^{T}e^{A\Delta t}U$ are also eigenvalues of $e^{A\Delta t}$.
- If α is an eigenvalue of A, then $e^{\alpha \Delta t}$ is an eigenvalue of $e^{A\Delta t}$.
- The eigenvectors of A are the same as those from $e^{A\Delta t}$.

We can cast the alpha eigenvalue problem into this framework.

Consider the time-dependent transport equation

$$\frac{\partial \psi}{\partial t} = A\psi_{z}$$

where the discretized transport operator A is given by

$$A = v(E)(-\Omega \cdot \nabla + -\sigma_{t} + S + F),$$

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

The alpha eigenvalues of the transport equation satisfy the following relationship

$$A\psi = \alpha\psi$$

that is, we are interested in the eigenvalues of the complete transport operator.

- ▶ The importance of the alpha eigenvalue can be found by noticing that if $\psi(t) = \psi_0 e^{\alpha t}$, then α is an eigenvalue of the transport operator.
 - ▶ $\alpha > 0$ implies that the system is supercritical and will have a divergent number of neutrons as $t \to \infty$.
 - $\alpha = 0$ means the system is critical and will reach a non-zero steady state when a neutron source is not present.
 - $\alpha < 0$ implies that the system is subcritical and as $t \to \infty$ the solution will go to zero without a source.
 - There is at most one non-negative eigenvalue.

The time evolution of the angular flux can be used to estimate alpha eigenvalues.

If we compute K + 1 time steps of size ∆t using a transport solver, we will have the relation

$$\begin{pmatrix} | & | & | \\ \psi_{K} & \psi_{K-1} & \dots & \psi_{1} \\ | & | & | \end{pmatrix} = e^{A\Delta t} \begin{pmatrix} | & | & | & | \\ \psi_{K-1} & \psi_{K-2} & \dots & \psi_{0} \\ | & | & | \end{pmatrix}$$

or $Y_+ = e^{A \Delta t} Y_-$ and we can take the SVD of Y_- as before.

► Therefore, if we estimate the eigenvalues λ of the $K \times K$ matrix $U^{\mathrm{T}} e^{A\Delta t} U$, we can compute the alpha eigenvalues of the system as

$$\alpha = \frac{\log \lambda}{\Delta t}.$$

- We do not need to a special eigenvalue solver to do this.
- If the time discretization used in the time dependent transport solve is backward Euler (as is common), then a better approximation is

$$\alpha = \frac{\lambda - 1}{\Delta t \lambda},$$

because this method approximates

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

An example problem will allow us to investigate how these alpha eigenvalues behave.

- We consider a 12-group calculation of an infinite medium of Pu-239 with a buckling approximation to simulate a finite sphere.
- We set the radius in the buckling approximation to make $k_{\rm eff} = 0.95$.
- The eigenvalues we get from the full transport operator for this system are



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Pulsing the sphere with 14.1 MeV neutrons reveals that the DMD approximation computes the eigenmodes present in the system.

- Using an initial condition of only neutrons in the group containing 14.1 MeV, we run a time dependent problem to a specified final time.
- We then use the last 10 time steps to estimate the α eigenvalues.
- Early in time the modes corresponding to the spike at 14.1 MeV are present, late in time we relax to the fundamental, slowly decaying mode.
- ► The α = -0.291318 sh⁻¹ eigenmode is not present because it has a larger number of thermal neutrons than our system does.

	Exact	$t_{\sf final} = 0.01 \; {\sf sh}$	0.2 sh	2 sh	20 sh
	-0.179734			-0.182064	-0.179802
	-0.291318				
	-0.346882			-0.346326	-0.346946
	-0.48783				
	-0.756007			-0.73261	
	-1.33304	-1.40235		-1.5013	
	-2.64032			-2.59257	
	-5.52353		-5.31228		
	-9.00368	-7.65929	-7.60506		
	-13.7938				
	-17.4603				
	-19.7214	-19.7212	-19.7139		
►	$1 sh = 0.01 \mu s$			_	

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A heterogeneous, subcritical system will test this method on a nontrivial problem.

- We consider a slab-geometry problem where a plastic moderator is sandwiched between two slabs of plutonium with a small outer reflector.
- This system will have α eigenvalues associated with the time scale of slow neutrons crossing the moderator.
- The fundamental mode from a k-eigenvalue problem has many thermal neutrons in the middle of the problem.
- We consider the situation where DT neutrons enter the slab from both sides at time 0.
- Thermal: E < 5 eV, Fast: E > 0.5 MeV



 \ln 1 $\mu \rm s$ the spectrum does not approximate the fundamental k-eigenvalue mode.

Left: Neutron density (ϕ/ν) as a function of space and time. Right: Neutron spectrum at the center of the HDPE and the center of the fuel.

Using the DMD method at different times finds the predominant eigenmodes present in the system.





Scalar Flux for Right-most eigenvector

Using the DMD method at different times finds the predominant eigenmodes present in the system.



Extensions to the method could be made for more dynamic systems.

Because the method finds the eigenmodes that are present in the system it will not be susceptible to finding unimportant, slowly decaying modes.

- One can tailor initial conditions to look for certain eigenvalues.
- ► The DMD approximation can be used for nonlinear operators.
- If the system changed over time we could approximate effective eigenvalues of the changing transport operator:
 - Thermal expansion
 - Depletion/Breeding
- The theoretical interpretation of these eigenvalues is not obvious.

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The approximate operator can be used to find slowly converging modes in an iterative method.

- The discrete ordinates method for transport is typically solved using source iteration (Richardson iteration) and diffusion-based preconditioning/acceleration.
- Source iterations converge quickly for problems with a small amount of particle scattering.
- For strongly scattering media, the transport operator has a near nullspace that can be handled using a diffusion preconditioner.
- However, the question of efficiently preconditioning/accelerating transport calculation on high-order meshes with discontinuous fine elements is an open area of research.
- The approximate operator found from DMD can be used to remove this same near nullspace and improve iterative convergence without the need for a separate preconditioner or diffusion discretization/solve.

We consider source iteration for a simple transport problem.

The steady, single group transport equation with isotropic scattering can be written as

$$L\psi=\frac{c}{4\pi}\phi+\frac{Q}{4\pi},$$

where c is the scattering ratio, Q is a prescribed source, and the streaming and removal operator is

$$L = (\Omega \cdot \nabla + 1).$$

• $\psi(\mathbf{x}, \Omega)$, $\Omega \in \mathbb{S}_2$,

$$\phi(\mathbf{x}) = \int_{4\pi} \psi \, d\Omega = \langle \psi \rangle.$$

Source iteration solves this problem using the iteration strategy

$$\phi^{\ell} = \left\langle L^{-1} \left(\frac{c}{4\pi} \phi^{\ell-1} + \frac{Q}{4\pi} \right) \right\rangle$$

where ℓ is an iteration index.

- One iteration is often called a "transport sweep".
- A benefit of source iteration is that the angular flux, ψ does not have to be stored.
- As $c \rightarrow 1$, the convergence of source iteration can be arbitrarily slow.

We can write source iteration as a sequence of vectors related by a linear operator.

 Rearranging the transport equation we see that source iteration is an iterative procedure for solving

$$\phi - \left\langle L^{-1} \frac{c}{4\pi} \phi \right\rangle = L^{-1} Q,$$

or

$$(I-A)\phi=b.$$

Therefore, the source iteration vectors are

$$\phi^{\ell+1} = A\phi^\ell + b,$$

or

$$\phi^{\ell+1} - \phi^{\ell} = A(\phi^{\ell} - \phi^{\ell-1})$$

▶ Therefore, we can cast the difference between iterates in a form that is amenable to the approximation of A using DMD, $Y_+ = AY_-$,

$$\begin{aligned} \mathbf{Y}_{+} &= \left[\phi^{2} - \phi^{1}, \phi^{3} - \phi^{2}, \dots, \phi^{K} - \phi^{K-1}\right], \\ \mathbf{Y}_{-} &= \left[\phi^{1} - \phi^{0}, \phi^{2} - \phi^{3}, \dots, \phi^{K-1} - \phi^{K-2}\right]. \end{aligned}$$

Source iteration can be accelerated by taking several iterates and approximating the solution as $\ell\to\infty$

► As before we define an approximate A as the K × K matrix:

$$\tilde{A} = U^{\mathrm{T}} A U = U^{\mathrm{T}} Y_{+} V \Sigma^{-1},$$

We can use à to construct the operator (*I*−Ã)⁻¹ and use this to approximate the solution:

$$(I - A)(\phi - \phi^{K-1}) = b - (I - A)\phi^{K-1}$$

= $b - \phi^{K-1} + (\phi^K - b)$
= $\phi^K - \phi^{K-1}$.

► The difference φ - φ^{K-1} is the difference between step K - 1 and the converged answer. We define a new vector Δy as the length K vector that satisfies

$$\phi - \phi^{K-1} = U \Delta y. \tag{1}$$

 \blacktriangleright We then substitute and multiply by ${\it U}^{\rm T}$ to get

$$(I - \tilde{A})\Delta y = U^{\mathrm{T}}(\phi^{K} - \phi^{K-1}).$$
⁽²⁾

This is a linear system of size K that we can solve to get Δy and then compute the update to ϕ^{K-1} as

$$\phi \approx \phi^{K-1} + U\Delta y. \tag{3}$$

DMD acceleration requires only source iteration and SVD: no diffusion solver.

- The algorithm is as follows
 - 1. Perform *R* source iterations: $\phi^{\ell} = A\phi^{\ell-1} + b$.
 - 2. Compute K source iterations to form Y_+ and Y_- . The last column of Y_- we call ϕ^{K-1} .
 - 3. Compute $\phi = \phi^{K-1} + U\Delta y$ as above.
- Each pass of the algorithm requires R + K source iterations.
- ▶ The *R* source iterations are used to correct any errors caused by the approximation of *A* using the SVD.
- It is easiest to assess convergence between the source iterations.
- This works regardless of the spatial discretization used.
- Other algorithms are possible:
 - Rather than extrapolate to an infinite number of iterations, we can use to approximate a finite number of source iterations.

 \blacktriangleright We could use a coarsened vector $\bar{\phi}$ in the DMD procedure to reduce the memory/computational cost.

DMD works perfectly on a homogenous slab, the ur-demonstration problem for acceleration schemes.

- ► We consider a slab with vacuum boundaries and a scattering ratio of c = 0.99 and 1.0 and 400 spatial zones, S₈ angular discretization, and the diamond difference spatial discretization.
- Solid lines are c = 0.99 results and dashed lines are c = 1.0



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A comparison of the number of iterations as a function of K and c indicates that the convergence is nearly independent of c.

On the same problem set up, the number of iterations to converge is shown below.

K/c	0.1	0.5	0.9	0.99	0.999	0.9999	0.99999	0.999999
3	8	15	39	70	70	70	70	70
5	10	11	28	90	90	90	90	90
10	15	15	29	60	140	140	140	140
20	25	25	25	49	74	76	76	76
50	55	55	55	56	57	57	57	57
SI	6	17	89	637	2439	3681	3889	3911

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Performance does degrade on an insanely heterogeneous problem.

• We consider a problem with vacuum boundaries, 1000 cells, unit domain length, with c = 0.9999 and

$$\sigma_{\rm t} = \begin{cases} 2^{p} & \mbox{cell number odd} \\ 2^{-p} & \mbox{cell number even} \end{cases}$$

Below we see convergence for p = 5 (dashed) and p = 8 (solid), a factor of about 1000 and 6.5 × 10⁴ between thick and thin cells, respectively.



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A version of the crooked pipe problem is a more realistic test.

- We solve a linear, xy-geometry version of the crooked pipe problem where all materials have a scattering ratio of 0.988 (to simulate a realistic sized time step).
- The density ratio between the tick and thin material is 1000.
- Problem solved using fully lumped, bilinear discontinous Galerkin in space and S₈ product quadrature.



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The number of iterations required increases slowly with mesh refinement.

► The number of iterations for source iteration and DMD-accelerated calculations with K = 10 and R = 3.

$(N_x \times N_y)$	DMD	SI
25 imes 15	53	811
50 imes25	52	873
100 imes 60	78	974
150 imes90	91	∞_{RML}
200 imes 120	104	∞_{RML}

 ∞_{RML} = functionally infinite on my laptop.

The increase seems to be the resolution to the 1/2 power (square root of the number of cells per dimension).

There are opportunities to this approach beyond the acceleration strategy outlined above.

- We could use DMD acceleration to compute a low-order transport acceleration (the so-called TSA method). In this case the we would use low-order in angle transport sweeps to estimate the slowly converging modes.
- ► Additionally, it is possible to estimate *Ã* using independently generated vectors. This would enable the Y_± matrices to be generated using sweeps computed in parallel.
- ► The big win could be from applying this to other iterative components:
 - Energy group iterations
 - Temperature iterations in radiative transfer.
- The performance of DMD on meshes with cycles is also a possible impact area.

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Is there a way to find an efficient, optimal approximation to time-dependent transport problems?

- This work is a collaboration with Cory Hauck (ORNL) and Martin Frank's group at Karlsruhe Institute of Technology.
- Consider the equation for the evolution of the $m \times n$ matrix A(t):

$$\dot{A}\equiv rac{d}{dt}A=f(A).$$

• We seek to find a rank r approximation to A(t),

$$Y(t) = U(t)S(t)V(t)^{\mathrm{T}},$$

where U(t) is $m \times r$, V(t) is $n \times r$ with orthonormal columns and S(t) is $r \times r$ and invertible.

- This looks like an SVD but it is more general because S(t) is not diagonal
- We want to find a dynamic system \dot{Y} such that
 - \dot{Y} lives in the tangent space of rank *r* matrices,
 - $\blacksquare \|\dot{Y} \dot{A}\| \text{ is minimized.}$

Is there a way to find an efficient, optimal approximation to time-dependent transport problems?

The evolution equation in the tangent space can be found by differentiating Y(t):

$$\dot{Y} = \dot{U}(t)S(t)V(t)^{\mathrm{T}} + U(t)\dot{S}(t)V(t)^{\mathrm{T}} + U(t)S(t)\dot{V}(t)^{\mathrm{T}}.$$

- We impose the gauge conditions $U^{\mathrm{T}}\dot{U} = 0$, and $V^{\mathrm{T}}\dot{V} = 0$.
- We can operate on \dot{Y} by U^{T} and V to get the following three equations

$$\begin{split} U(t)^{\mathrm{T}} \dot{Y} &= \dot{S}(t) V(t)^{\mathrm{T}} + S(t) \dot{V}(t)^{\mathrm{T}}, \\ U(t)^{\mathrm{T}} \dot{Y} V(t) &= \dot{S}(t), \\ \dot{Y} V(t) &= \dot{U}(t) S(t) + U(t) \dot{S}(t). \end{split}$$

These can be rearranged to get

$$\dot{U} = (I - UU^{\mathrm{T}})\dot{Y}VS^{-1}$$
$$\dot{V} = (I - VV^{\mathrm{T}})\dot{Y}^{\mathrm{T}}U(S^{-1})^{\mathrm{T}}$$
$$\dot{S} = U(t)^{\mathrm{T}}\dot{Y}V(t).$$

• The best approximation to \dot{A} can be shown to be

$$\dot{Y} = (I - UU^{\mathrm{T}})\dot{A}VS^{-1} + U(t)^{\mathrm{T}}\dot{A}V(t) + (I - VV^{\mathrm{T}})\dot{A}^{\mathrm{T}}U(S^{-1})^{\mathrm{T}}.$$

There is a splitting of this equation keeps each step in the low rank space.

• Solve the $m \times r$ system over a time step from initial data $Y_0 = U_0 S_0 V_0^T$

$$K_1 = U_0S_0 + (A(t+\Delta t) - A(t))V_0,$$

- Compute $U_1 \tilde{S} = K_1$ using QR factorization.
- Solve the $r \times r$ system

$$S^* = ilde{S} - U_1^{ ext{T}}(A(t+\Delta t) - A(t))V_0,$$

Solve

$$L_1 = V_0(S^*)^{\mathrm{T}} + (A(t + \Delta t) - A(t))^{\mathrm{T}} U_1.$$

- Compute $V_1 S_1^{\mathrm{T}} = L_1$ using QR factorization.
- The value at the end of the step is $Y_1 = U_1 S_1 V_1^{T}$.
- Each step can be shown to keep the solution in the rank *r* space.
- This is a first-order algorithm, but higher order algorithms exist.
- ► To be a truly low rank update, we must be able to estimate $(A(t + \Delta t) A(t)) = \Delta t \int f(A) dt$ without evaluating the full operator.

A proof of principle calculation indicates there is merit to this algorithm.

- We consider the S_{10} solution to Brunner's lattice problem and use the full transport operator to estimate $(A(t + \Delta t) A(t))$.
- ▶ The data has 280 × 280 degrees of freedom in space and 100 degrees of freedom in angle.
- Figure below has pure scatter in orange, pure absorber in black, and a source in white. A solution with a logarithmic color scale is on the right.





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The low-rank comparisons give promising results on this problem.



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The low-rank comparisons give promising results on this problem.



The low-rank approximations are better at early time.



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The error decreases at second-order in the rank beyond rank 10.



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We need to derive the low-rank approximations to the update.

- As mentioned before, if we use the full system to approximate $(A(t + \Delta t) A(t))$ there is no savings.
- We need to express the projections U^T₁(A(t + ∆t) − A(t))V₀, U^T₁(A(t + ∆t) − A(t))V₀, and (A(t + ∆t) − A(t))^TU₁ in terms of the discretizations in space and angle.
- Then the update will only require the smaller memory footprint of the low rank operators during the update.

We have derived the equations for 1-D slab geometry, but do not have solutions yet.

Outline

Introduction

The Dynamic Mode Decomposition

Estimating Time Eigenvalues Time-dependent transport examples

DMD for Accelerating Source Iteration Slab geometry examples

Low-Rank Approximations to Dynamic Systems

Conclusions

Data-Driven algorithms are widely applicable in transport problems.

- Using a DMD approach to compute approximate operators gives one the ability to
 - Estimate eigenvalues for the system, and
 - Accelerate calculations.
- Furthermore, we can use similar techniques to derive a low-rank approximation to the dynamics of transport.
- There is much further research to be done, but progress is exciting.

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