# Data-Driven Algorithms for Transport 

Ryan G. McClarren<br>University of Notre Dame<br>Dept. of Aerospace and Mechanical Engineering

June 28, 2018

UNIVERSITY of
NOTRE DAME
College of Engineering

## 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.


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

- Consider a sequence of vectors $\left\{y_{0}, y_{1}, \ldots, y_{K}\right\}$ where $y_{k} \in \mathbb{R}^{N}$.
- The vectors are related by a potentially unknown linear operator of size $N \times N, A$, as

$$
y_{k+1}=A y_{k}
$$

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

$$
Y_{+}=\left(\begin{array}{cccc}
\mid & \mid & & \mid \\
y_{1} & y_{2} & \ldots & y_{K} \\
\mid & \mid & & \mid
\end{array}\right) \quad Y_{-}=\left(\begin{array}{cccc}
\mid & \mid & & \mid \\
y_{0} & y_{1} & \ldots & y_{K-1} \\
\mid & \mid & & \mid
\end{array}\right)
$$

we can write

$$
Y_{+}=A Y_{-}
$$

- At this point we only need to know the data vectors $y_{k}$, they could come from a calculation, measurement, etc.
- As $K \rightarrow \infty$ 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

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

where $U$ is a $N \times K$ orthogonal matrix, $\Sigma$ 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 $O\left(N K^{2}\right)$ 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.
- The matrix $U$ has columns that forms an orthonormal basis for the row space of $Y_{-} \subset \mathbb{R}^{N}$.
- Using the SVD we get

$$
Y_{+}=A U \Sigma V^{T}
$$

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

$$
Y_{+}=A U \Sigma V^{T} \quad \rightarrow \quad U^{T} A U=U^{T} Y_{+} \sqrt{ } \Sigma^{-1}
$$

- Define $\tilde{A}=U^{T} A U=U^{T} Y_{+} \sqrt{\Sigma^{-1}}$. This is a rank $K$ approximation to $A$.
- Using the approximate operator $\tilde{A}$, 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 $A$ :

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

- The dynamic mode decomposition (DMD) of the data matrix $Y_{+}$is then the decomposition of into vectors $\varphi$. The mode with the largest norm of $\lambda$ 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 $n_{k} \sim \mathcal{N}\left(0,10^{2}\right)$.

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


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: $U_{\varphi_{2}}$


Fourth DMD mode: $U \varphi_{4}$

## 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

## 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 $\mathrm{Ce}^{\alpha t}$.
- 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,

$$
\frac{\partial y}{\partial t}=A y(t)
$$

and are separated by a time, $\Delta t$, 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 $Y_{-}=U S V^{*}$, and approximate the matrix exponential:

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

- One can show the following:
- The eigenvalues of $U^{T} e^{A \Delta t} U$ are also eigenvalues of $e^{A \Delta t}$.
- If $\alpha$ 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

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

where the discretized transport operator $A$ is given by

$$
A=v(E)\left(-\Omega \cdot \nabla+-\sigma_{\mathrm{t}}+\mathcal{S}+\mathcal{F}\right)
$$

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 $\alpha$ is an eigenvalue of the transport operator.
- $\alpha>0$ implies that the system is supercritical and will have a divergent number of neutrons as $t \rightarrow \infty$.
- $\alpha=0$ 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 $t \rightarrow \infty$ 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 $\Delta t$ using a transport solver, we will have the relation

$$
\left(\begin{array}{cccc}
\mid & \mid & & \mid \\
\psi_{K} & \psi_{K-1} & \ldots & \psi_{1} \\
\mid & \mid & & \mid
\end{array}\right)=e^{A \Delta t}\left(\begin{array}{cccc}
\mid & \mid & & \mid \\
\psi_{K-1} & \psi_{K-2} & \ldots & \psi_{0} \\
\mid & \mid & & \mid
\end{array}\right)
$$

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

- Therefore, if we estimate the eigenvalues $\lambda$ of the $K \times K$ matrix $U^{T} e^{A \Delta t} U$, 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 $k_{\text {eff }}=0.95$.
- The eigenvalues we get from the full transport operator for this system are

| $\alpha\left(\mathrm{sh}^{-1}\right)$ |
| ---: |
| -0.179734 |
| -0.291318 |
| -0.346882 |
| -0.48783 |
| -0.756007 |
| -1.33304 |
| -2.64032 |
| -5.52353 |
| -9.00368 |
| -13.7938 |
| -17.4603 |
| -19.7214 |



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 $\alpha$ 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 $\alpha=-0.291318 \mathrm{sh}^{-1}$ eigenmode is not present because it has a larger number of thermal neutrons than our system does.

| Exact | $t_{\text {final }}=0.01 \mathrm{sh}$ | 0.2 sh | 2 sh | 20 sh |
| ---: | ---: | ---: | ---: | ---: |
| -0.179734 |  |  | -0.182064 | -0.179802 |
| -0.291318 |  |  | -0.346326 | -0.346946 |
| -0.346882 |  |  | -0.73261 |  |
| -0.48783 |  | -1.5013 |  |  |
| -0.756007 |  |  | -2.59257 |  |
| -1.33304 | -1.40235 |  |  |  |
| -2.64032 |  | -5.31228 |  |  |
| -5.52353 |  | -7.60506 |  |  |
| -9.00368 | -7.65929 |  |  |  |
| -13.7938 |  |  |  |  |
| -17.4603 | -19.7212 | -19.7139 |  |  |
| -19.7214 |  |  |  |  |

- $1 \mathrm{sh}=0.01 \mu \mathrm{~s}$

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 $\alpha$ 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: $E<5 \mathrm{eV}$, Fast: $E>0.5 \mathrm{MeV}$



In $1 \mu$ s the spectrum does not approximate the fundamental $k$-eigenvalue mode.
$\mathrm{t}=0.0001 \mu \mathrm{~s}$


K

Left: Neutron density $(\phi / v)$ 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.
$\alpha\left(\mathrm{sh}^{-1}\right)$ eigenvalues
$\alpha$ computed over $\mathrm{t}=0.0005$ to $0.0025 \mu \mathrm{~s}$

$\alpha$ computed over $\mathrm{t}=0.01$ to $0.012 \mu \mathrm{~s}$


Scalar Flux for Right-most eigenvector



Using the DMD method at different times finds the predominant eigenmodes present in the system.
$\alpha\left(\mathrm{sh}^{-1}\right)$ eigenvalues


Scalar Flux for Right-most eigenvector

$\alpha$ computed over $\mathrm{t}=9.998$ to $10 \mu \mathrm{~s}$


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.


## 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

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 $\ell$ is an iteration index.

- One iteration is often called a "transport sweep".
- A benefit of source iteration is that the angular flux, $\psi$ 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

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

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

$$
\begin{gathered}
Y_{+}=\left[\phi^{2}-\phi^{1}, \phi^{3}-\phi^{2}, \ldots, \phi^{K}-\phi^{K-1}\right] \\
Y_{-}=\left[\phi^{1}-\phi^{0}, \phi^{2}-\phi^{3}, \ldots, \phi^{K-1}-\phi^{K-2}\right]
\end{gathered}
$$

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

- As before we define an approximate $A$ as the $K \times K$ matrix:

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

- We can use $\tilde{A}$ to construct the operator $(I-\tilde{A})^{-1}$ and use this to approximate the solution:

$$
\begin{aligned}
(I-A)\left(\phi-\phi^{K-1}\right) & =b-(I-A) \phi^{K-1} \\
& =b-\phi^{K-1}+\left(\phi^{K}-b\right) \\
& =\phi^{K}-\phi^{K-1}
\end{aligned}
$$

- The difference $\phi-\phi^{K-1}$ is the difference between step $K-1$ and the converged answer. We define a new vector $\Delta y$ as the length $K$ vector that satisfies

$$
\begin{equation*}
\phi-\phi^{K-1}=U \Delta y . \tag{1}
\end{equation*}
$$

- We then substitute and multiply by $U^{T}$ to get

$$
\begin{equation*}
(I-\tilde{A}) \Delta y=U^{\mathrm{T}}\left(\phi^{K}-\phi^{K-1}\right) \tag{2}
\end{equation*}
$$

This is a linear system of size $K$ that we can solve to get $\Delta y$ and then compute the update to $\phi^{K-1}$ as

$$
\begin{equation*}
\phi \approx \phi^{K-1}+U \Delta y \tag{3}
\end{equation*}
$$

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 $\phi^{K-1}$.
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 $\tilde{A}$ to approximate a finite number of source iterations.
- 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, $S_{8}$ angular discretization, and the diamond difference spatial discretization.
- Solid lines are $c=0.99$ results and dashed lines are $c=1.0$


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 |

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

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

- Below we see convergence for $p=5$ (dashed) and $p=8$ (solid), a factor of about 1000 and $6.5 \times 10^{4}$ between thick and thin cells, respectively.



## 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 $S_{8}$ product quadrature.


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 $R=3$.

| $\left(N_{x} \times N_{y}\right)$ | DMD | SI |
| ---: | ---: | ---: |
| $25 \times 15$ | 53 | 811 |
| $50 \times 25$ | 52 | 873 |
| $100 \times 60$ | 78 | 974 |
| $150 \times 90$ | 91 | $\infty_{\mathrm{RML}}$ |
| $200 \times 120$ | 104 | $\infty_{\mathrm{RML}}$ |

$\infty_{\mathrm{RML}}=$ 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 $\tilde{A}$ using independently generated vectors. This would enable the $Y_{ \pm}$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.


## 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


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 $A(t)$ :

$$
\dot{A} \equiv \frac{d}{d t} A=f(A)
$$

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

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

- These can be rearranged to get

$$
\begin{gathered}
\dot{U}=\left(I-U U^{\mathrm{T}}\right) \dot{Y} V S^{-1} \\
\dot{V}=\left(I-V V^{\mathrm{T}}\right) \dot{Y}^{\mathrm{T}} U\left(S^{-1}\right)^{\mathrm{T}} \\
\dot{S}=U(t)^{\mathrm{T}} \dot{Y} V(t) .
\end{gathered}
$$

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

$$
\dot{Y}=\left(I-U U^{\mathrm{T}}\right) \dot{A} V S^{-1}+U(t)^{\mathrm{T}} \dot{A} V(t)+\left(I-V V^{\mathrm{T}}\right) \dot{A}^{\mathrm{T}} U\left(S^{-1}\right)^{\mathrm{T}}
$$

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 $Y_{0}=U_{0} S_{0} V_{0}^{T}$

$$
K_{1}=U_{0} S_{0}+(A(t+\Delta t)-A(t)) V_{0}
$$

- Compute $U_{1} \tilde{S}=K_{1}$ using QR factorization.
- Solve the $r \times r$ system

$$
S^{*}=\tilde{S}-U_{1}^{\mathrm{T}}(A(t+\Delta t)-A(t)) V_{0},
$$

- Solve

$$
L_{1}=V_{0}\left(S^{*}\right)^{\mathrm{T}}+(A(t+\Delta t)-A(t))^{\mathrm{T}} U_{1} .
$$

- Compute $V_{1} S_{1}^{T}=L_{1}$ 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 $(A(t+\Delta t)-A(t))=\Delta t \int f(A) d t$ 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 $280 \times 280$ 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.



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


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


The low-rank approximations are better at early time.


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

Relative L2 error against full rank simulation (S10) over ranks


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 $U_{1}^{T}(A(t+\Delta t)-A(t)) V_{0}$, $U_{1}^{\mathrm{T}}(A(t+\Delta t)-A(t)) V_{0}$, and $(A(t+\Delta t)-A(t))^{\mathrm{T}} U_{1}$ 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

4ロ・4司｣

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.


## Acknowledgments

- Thanks to Terry Haut for valuable discussions regarding this work.
- The DMD acceleration work was sponsored by Lawrence Livermore National Laboratory project titled "Dynamic Mode Decomposition (DMD) Acceleration Methods for Thermal Radiative Transfer" contract B627130.

