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Analysis of the LRA Reactor Benchmark Using Dynamic Mode Decomposition

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LRA Benchmark

Write something about LRA and a slide or two about Detran

Reduced Order Modeling

ROM

$$\boldsymbol{f}(\boldsymbol{x}) \approx \boldsymbol{g}(\mathcal{M}(\boldsymbol{x})); \quad \boldsymbol{x} \subseteq \mathbb{R}^n, \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}^{r_x}; r_x << n$$

- This is usually done by projecting the problem high dimensional space onto a lower space that captures most of the data variance (i.e POD).
- In this work, Dynamic Mode Decomposition (DMD) was used to construct a data-driven surrogate model.

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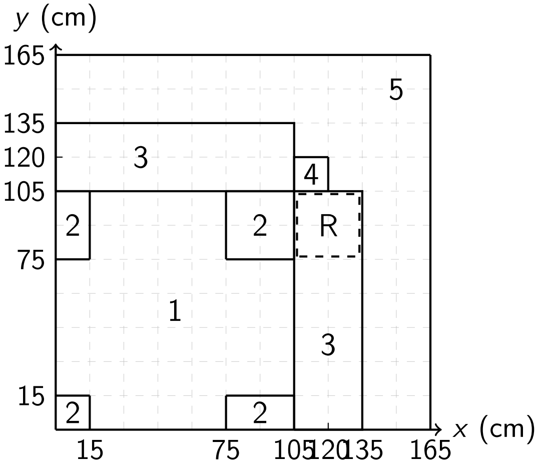
Physical Model



Model Description

- Super Prompt-critical Transient.
- 2D Diffusion.
- Adiabatic Heatup and Doppler Feedback in thermal reactor.

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Governing Equations

2D Diffusion with two Delayed Neutron Precursor groups.

$$
\begin{aligned}
&\nabla D_1(\boldsymbol{x},t)\nabla\phi_1(\boldsymbol{x},t) - [\Sigma_{a1}(\boldsymbol{x},t) + \Sigma_{1\to 2}(\boldsymbol{x},t)]\phi_1(\boldsymbol{x},t) \\
&+ \nu(1-\beta)[\Sigma_{f1}(\boldsymbol{x},t)\phi_1(\boldsymbol{x},t) + \Sigma_{f2}(\boldsymbol{x},t)\phi_2(\boldsymbol{x},t)] \\
&+ \Sigma_{i=1}^{2}\lambda_i c_i(\boldsymbol{x},t) = \frac{1}{v_1}\frac{\partial}{\partial t}\phi_1(\boldsymbol{x},t). \\
&\nabla D_2(\boldsymbol{x},t)\nabla\phi_2(\boldsymbol{x},t) - \Sigma_{a2}(\boldsymbol{x},t)\phi_2(\boldsymbol{x},t) + \Sigma_{1\to 2}(\boldsymbol{x},t)\phi_1(\boldsymbol{x},t) \\
&= \frac{1}{v_2}\frac{\partial}{\partial t}\phi_2(\boldsymbol{x},t). \\
&\nu\beta_i[\Sigma_{f1}(\boldsymbol{x},t)\phi_1(\boldsymbol{x},t) + \Sigma_{f2}(\boldsymbol{x},t)\phi_2(\boldsymbol{x},t)] - \lambda_i c_i(\boldsymbol{x},t) \\
&= \frac{\partial}{\partial t}c_i(\boldsymbol{x},t), \;\; i = 1,2.
\end{aligned}
$$

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Adiabatic Heatup

$$\alpha[\Sigma_{f1}(\boldsymbol{x},t)\phi_1(\boldsymbol{x},t)+\Sigma_{f2}(\boldsymbol{x},t)\phi_2(\boldsymbol{x},t)]=\frac{\partial}{\partial t}T(\boldsymbol{x},t).$$

Doppler Feedback

$$\Sigma_{a1}(\boldsymbol{x},t)=\Sigma_{a2}(\boldsymbol{x},t=0)[1+\gamma(\sqrt{(}T(\boldsymbol{x},t))-\sqrt{(}T_0))].$$

Power

$$P(\boldsymbol{x},t)=\varepsilon[\Sigma_{f1}(\boldsymbol{x},t)\phi_1(\boldsymbol{x},t)+\Sigma_{f2}(\boldsymbol{x},t)\phi_2(\boldsymbol{x},t)].$$

DMD Overview

- DMD was first used by Schmid in 2008, in fluid dynamics [?].
- It is used to explore the behavior of dynamical systems.
- It can be viewed as a PCA (spatial domain) + DFT (frequency domain).

DMD Methodology

Consider a sequential dataset ($\mathbf{X} \subseteq \mathbb{R}^{n \times m}$) spaced by Δt.

$$
\begin{array}{cc}
 & \xrightarrow{\text{Time}} \\
\text{Space}\big\downarrow & \begin{bmatrix} | & | & & | \\ \boldsymbol{x}_1 & \boldsymbol{x}_2 & \cdots & \boldsymbol{x}_m \\ | & | & & | \end{bmatrix}
\end{array}
$$

$$
\underbrace{\begin{bmatrix} | & & | \\ \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_{m-1} \\ | & & | \end{bmatrix}}_{\mathbf{X}_1}
\qquad\qquad
\underbrace{\begin{bmatrix} | & & | \\ \boldsymbol{x}_2 & \cdots & \boldsymbol{x}_m \\ | & & | \end{bmatrix}}_{\mathbf{X}_2}
$$

Assumption: With sufficiently small Δt, there is a linear time marching operator **A** that approximates the system's dynamic, such that;

$$\mathbf{X_2} \approx \mathbf{A}\mathbf{X_1}$$

DMD Methodology

A is the operator that best fits the data in a least-squares sense;

$$\mathbf{A} = \underset{\mathbf{A}}{\operatorname{argmin}} \left\| \mathbf{X_2} - \mathbf{A}\mathbf{X_1} \right\|_F ,$$

$$\mathbf{A} \approx \mathbf{X_2}\mathbf{X_1}^\dagger$$

In practice, **A** is very large $\rightarrow$ DMD tries to approximate its eigenpairs.

The Singular Value Decomposition(**SVD**) is computed for $\mathbf{X_1}$;

$$\mathbf{X_1} = \mathbf{U}\mathbf{\Sigma}\mathbf{V^H}$$

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Singular Value Decomposition

The SVD is exploited to reveal the low dimensional structure in the data by keeping the first r singular values that recovers most of the data variance;

$$\mathbf{X_1} \approx \mathbf{U_r \Sigma_r V_r^H}$$

The columns of $\mathbf{U_r}$ are the **POD** modes onto which the data will be projected.

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DMD Surrogate

The Algorithm

- $\mathbf{U_r^H X_2} \approx \underbrace{\mathbf{U_r^H A U_r}}_{\tilde{\mathbf{A}}} \mathbf{\Sigma_r V_r^H}.$
- $\mathbf{A}$ and $\tilde{\mathbf{A}}$ are similar.

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DMD Surrogate

The Algorithm

- $\mathbf{U_r^H X_2} \approx \underbrace{\mathbf{U_r^H A U_r}}_{\tilde{\mathbf{A}}} \Sigma_\mathbf{r} \mathbf{V_r^H}.$
- $\tilde{\mathbf{A}} = \mathbf{U_r^H X_2 V_r} \Sigma_\mathbf{r}^{-1}.$
- $\mathbf{A}$ and $\tilde{\mathbf{A}}$ are similar.
- Compute $\tilde{\mathbf{A}}$.

DMD Surrogate

The Algorithm

- $\mathbf{U_r^H X_2} \approx \underbrace{\mathbf{U_r^H A U_r}}_{\tilde{\mathbf{A}}} \mathbf{\Sigma_r V_r^H}$.
- $\tilde{\mathbf{A}} = \mathbf{U_r^H X_2 V_r \Sigma_r^{-1}}$.
- $\tilde{\mathbf{A}}\tilde{\mathbf{W}} = \tilde{\mathbf{W}}\mathbf{\Lambda}$

- $\mathbf{A}$ and $\tilde{\mathbf{A}}$ are similar.
- Compute $\tilde{\mathbf{A}}$.
- Eigendecomposition of $\tilde{\mathbf{A}}$.

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DMD Surrogate

The Algorithm

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- $\tilde{\mathbf{A}}\tilde{\mathbf{W}} = \tilde{\mathbf{W}}\mathbf{\Lambda}$
- $\omega_i = \log(\lambda_i)/\Delta t$.

- $\mathbf{A}$ and $\tilde{\mathbf{A}}$ are similar.
- Compute $\tilde{\mathbf{A}}$.
- Eigendecomposition of $\tilde{\mathbf{A}}$.
- Discrete to continuous.

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DMD Surrogate

The Algorithm

- $\mathbf{U_r^H X_2} \approx \underbrace{\mathbf{U_r^H A U_r}}_{\tilde{\mathbf{A}}} \mathbf{\Sigma_r V_r^H}$.
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- $\tilde{\mathbf{A}}\tilde{\mathbf{W}} = \tilde{\mathbf{W}}\mathbf{\Lambda}$
- $\omega_i = \log(\lambda_i)/\Delta t$.
- $\mathbf{\Phi}^{DMD} = \mathbf{X_2 V_r \Sigma_r^{-1}}\tilde{\mathbf{W}}$.

- $\mathbf{A}$ and $\tilde{\mathbf{A}}$ are similar.
- Compute $\tilde{\mathbf{A}}$.
- Eigendecomposition of $\tilde{\mathbf{A}}$.
- Discrete to continuous.
- The DMD modes.

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DMD Surrogate

The Algorithm

- $\mathbf{U_r^H X_2} \approx \underbrace{\mathbf{U_r^H A U_r}}_{\tilde{\mathbf{A}}} \mathbf{\Sigma_r V_r^H}$.
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- Discrete to continuous.
- The DMD modes.

The surrogate

$$\boldsymbol{x}^{DMD}(t) \approx \sum_{i=1}^{r} b_i \phi_i^{DMD} e^{\omega_i t} = \mathbf{\Phi}^{DMD}\mathbf{diag}(e^{\boldsymbol{\omega} t})\boldsymbol{b}$$

mode contribution (amplitudes)

- $\boldsymbol{b} = \Phi^{DMD\dagger}\boldsymbol{x_0}$.
- $\boldsymbol{b}_{opt} = \underset{\boldsymbol{b}}{\operatorname{argmin}} \|\mathbf{X_1} - \Phi^{DMD}\mathbf{D}_b\mathbf{V}_{and}\|_F$.
- $\boldsymbol{b}_{opt} = \underset{\boldsymbol{b}}{\operatorname{argmin}} \|\Sigma_{\boldsymbol{r}}\mathbf{V}^{\mathbf{H}} - \mathbf{W}\mathbf{D}_b\mathbf{V}_{and}\|_F$.
- $\boldsymbol{b}_{opt} = \Big((\mathbf{W}^{\mathbf{H}}\mathbf{W}) \circ (\overline{\mathbf{V}_{and}\mathbf{V}_{and}^{H}})\Big)^{-1}\overline{diag(\mathbf{V}_{and}\mathbf{V}\Sigma^{H}\mathbf{W})}$.

Partitioned DMD

- modes are **non-orthogonal**, increasing the rank does not necessarily enhance accuracy.
- In highly transient problems, what if there were modes that were important for while but disappeared after that?
- what if some interval required a certain rank where dynamics evolved slowly, but another required the full rank to capture the rapid evolution?
- can we use multiple sequential surrogates, with multiple ranks and maybe different amplitudes?
- This is the basic idea of Partitioned DMD.

Partitioned DMD

- The premise of Partitioned DMD is that it allows for scanning each time window for a sense of the time scale at which dynamics are evolving and hence select iteratively the number/location of partitions, proper rank, and mode contributions for each partition.

Case Study

- Building a surrogate for the responses of interest: i.e., Power, flux, and/or temperature.
- 300 snapshots.
- 22×22 spatial cells.
- 3 seconds simulation time.
- control rod:

$$\frac{\Sigma_{a2}(t)}{\Sigma_{a2}(0)} = \begin{cases} 1 - 0.0606184\ t & t \leq 0.2 \quad sec \\ 0.878763 & t > 0.2 \quad sec \end{cases}$$

Case Study

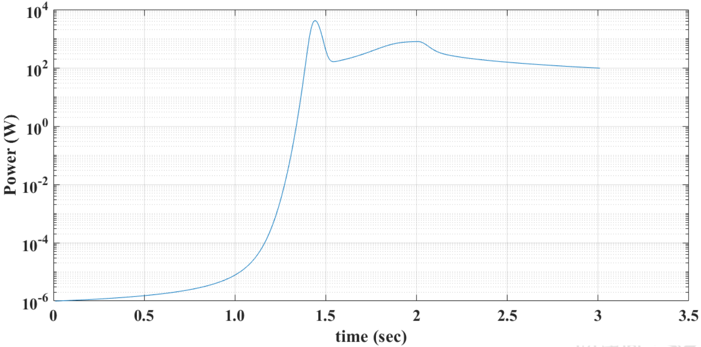

Figure: Power from Detran

Case Study

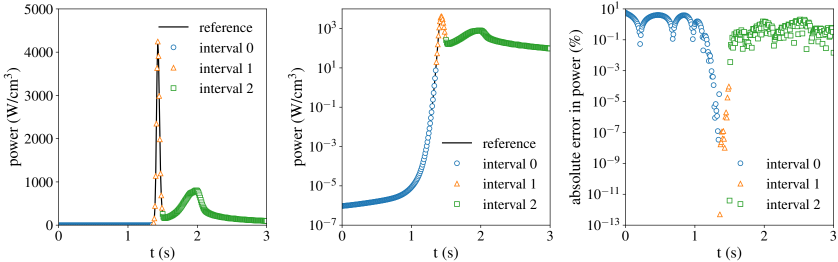

Figure: Partitioned DMD surrogates

Case Study

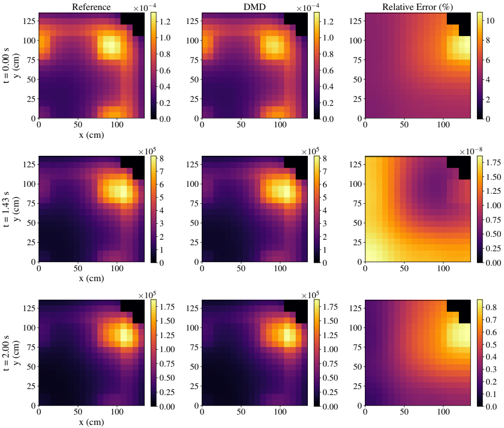

Figure: Partitioned DMD surrogates

Conclusion

- Partitioned DMD surrogate was able to represent the spatio-temporal dynamics of the LRA benchmark.
- The benchmark exhibits a rapid severe change in dynamics within a very short time scale.
- The surrogate offered a precision of $10^{-8}\%$ in the maximum power region, and a maximum error of 10% at the very beginning of the simulation. The surrogate was shown to be sensitive to the time partitioning.
- Work is ongoing to mitigate this sensitivity and to provide an automated way to select the number of partitions and their boundaries.

References I

Backup Slides

POD	DMD
Optimality and Orthogonality	Non-orthogonal

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Equations can be injected	Solely Data-driven

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as rank ↑ error ↓	Optimal rank is a challenge
Modes ordered (energy/variance)	numerous variants/criteria

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DMD UQ

Sandwich Rule

$$\mathbf{x}^{DMD}(t) = \underbrace{\Phi^{DMD}\mathbf{diag}(e^{\omega t})\Phi^{DMD\dagger}}_{\mathbf{S}}\mathbf{x_0}$$

$$\mathbf{C}_x^{DMD} = \mathbf{S}\mathbf{C}_0\mathbf{S}^T,$$

$$\mathbf{C}_0 = \frac{1}{N-1}\mathbf{X_0}\mathbf{X_0}^T$$