Intrusive Reduced Order Modeling for Inverse Problems

AS5401: Data-driven modeling of complex aerospace systems and fluid flows

S. Ananth Narayan

AM24D038

Department of Applied Mechanics and Biomedical Engineering

IIT Madras

November 8, 2025

Agenda

Aim and Motivation

Aim and Motivation

Aim

- Inverse Problems are the tasks of using observed data and estimating the values of unknown parameters that characterize the system.
- The aim of this project is to **formulate and demonstrate the inverse problem through Reduced order models (ROM)** for various partial equations.

Motivation

- How effectively one can leverage ROM's for such problems. **Example:** Calculation of thermal diffusivity from set(s) of temperature profile data.

- Transient Heat Conduction (1D **linear** PDE)- **Inverse problem**
- Reaction- Diffusion (1D **linear coupled** PDE)- **Coupling systems**
- Wave (1D **nonlinear** PDE)- **POD-DEIM**
- Electrohydrodynamics (1D **nonlinear coupled** PDE)- **Actual system of interest**

Transient Heat Conduction

Transient Heat Conduction

Intrusive ROM

- One-dimensional transient temperature variation (first order linear PDE) with thermal diffusivity (α),

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}, \qquad 0 < \alpha \leq 1, \quad 0 \leq x \leq 1$$

- For snapshot matrix, $\mathcal{T} = [T(t_1), T(t_2), \cdots, T(t_n)]$ modes ($\mathbf{U_T}$) are extracted through SVD. Truncation rank is chosen for energy of atleast 99.9% ($\rho_T = 3$) and reduced order model (ROM) is formulated as,

$$\frac{\partial \hat{T}}{\partial x} = \mathbf{U_T}^\top \alpha \mathbf{U_T} \frac{\partial^2 \hat{T}}{\partial x^2} = \hat{\mathbf{A}} \hat{T}$$

Transient Heat Conduction

Validation

- **Boundary lifting**, decomposing solution as sum of lifting function (satisfy BC's) and ROM expansion [1].
- **Golden search** technique has been implemented for convex optimization. The objective $\mathcal{J}$ is written as,

$$\mathcal{J}_\alpha = \frac{1}{2}\|T - \bar{T}\|^2$$

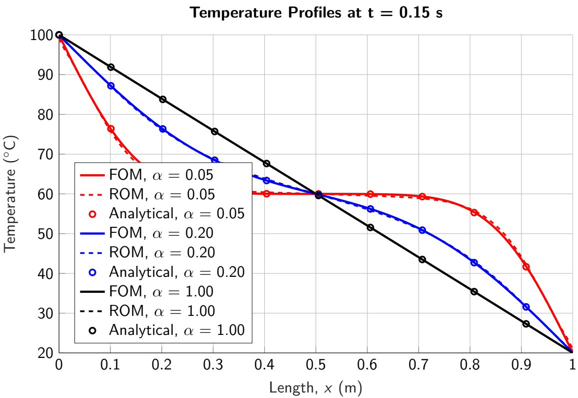


Figure: FOM and ROM validation

Transient Heat Conduction

Inverse Problem- Golden Search

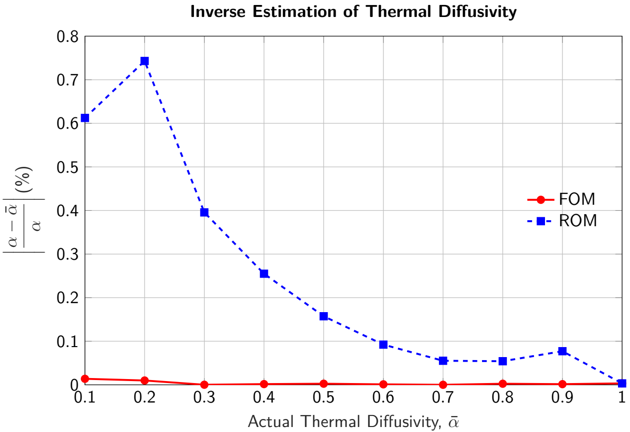
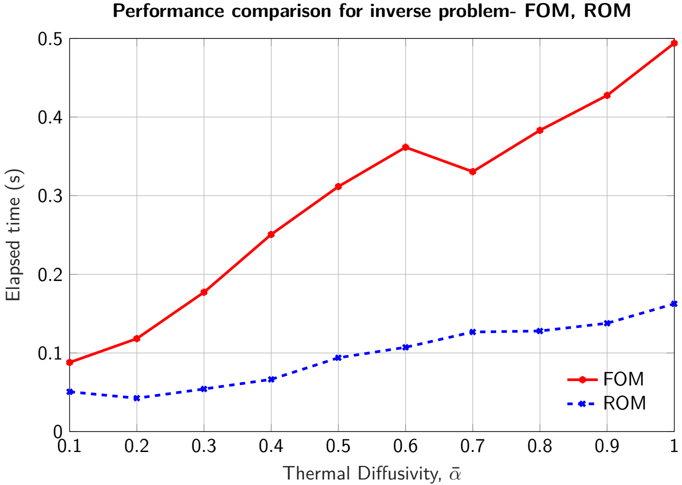


Figure: Prediction of thermal diffusivity

Transient Heat Conduction

Inverse Problem- Golden Search



Coupled Reaction- Diffusion

Coupled Reaction- Diffusion

Intrusive ROM

- One-dimensional coupled reaction- diffusion equation with system constants, a, b, α, β

$$
\begin{aligned}
\frac{\partial u}{\partial t} =& a\frac{\partial^2 u}{\partial x^2} + \alpha(v-u) + F_u, \quad u(0,t) = u_L, u(1,t) = u_R \\
\frac{\partial v}{\partial t} =& b\frac{\partial^2 v}{\partial x^2} + \beta(u-v) + F_v, \quad v(0,t) = v_L, u(1,t) = v_R \\
& x \in [0,1], \quad t > 0
\end{aligned}
$$

- The **methods of manufactured solution** was implemented for validation of FOM.

Coupled Reaction- Diffusion

Intrusive ROM

- For snapshot matrix, $\mathcal{U}, \mathcal{V}$, modes $(\mathbf{U_u}, \mathbf{U_v})$ for u, v truncated to 99.9% $(\rho_u = \rho_v = 1)$ of energy and ROM can be formulated as,

$$
\begin{aligned}
\frac{\partial \hat{u}}{\partial t} &= \mathbf{U_u}^\top a \mathbf{U_u} \frac{\partial^2 \hat{u}}{\partial x^2} + \mathbf{U_u}^\top \alpha(\mathbf{U_v}\hat{v} - \mathbf{U_u}\hat{u}) + \mathbf{U_u}^\top F_u + \alpha \mathbf{U_u}^\top(\tilde{v} - \tilde{u}) \\
\frac{\partial \hat{v}}{\partial t} &= \mathbf{U_v}^\top b \mathbf{U_v} \frac{\partial^2 \hat{v}}{\partial x^2} + \mathbf{U_v}^\top \beta(\mathbf{U_u}\hat{u} - \mathbf{U_v}\hat{v}) + \mathbf{U_v}^\top F_v + \beta \mathbf{U_v}^\top(\tilde{u} - \tilde{v})
\end{aligned}
$$

$$
\tilde{u} = u_L \frac{1-x}{L} + u_R \frac{x}{L}, \quad \tilde{v} = v_L \frac{1-x}{L} + v_R \frac{x}{L}
$$

- Coupling of ROM through **transformation of subspace from $\tilde{u} \leftrightarrow \tilde{v}$** is due to boundary lifting.

Coupled Reaction- Diffusion

Validation

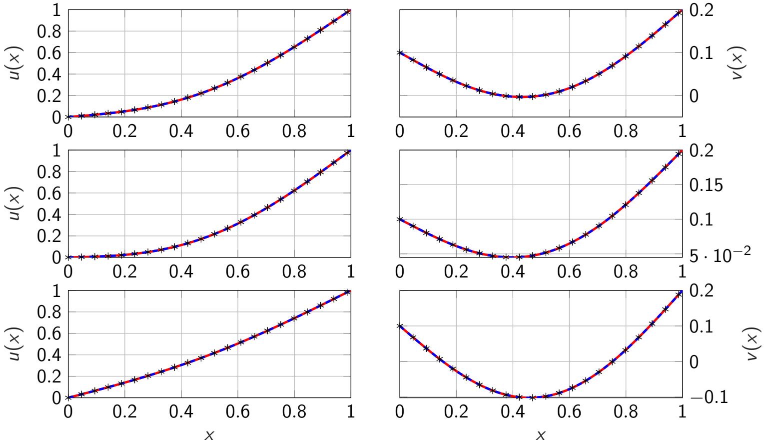


Figure: Validation for three U, V values. (FOM,ROM, $*$ Analytical)

Coupled Reaction- Diffusion

Inverse Problem- Golden Search

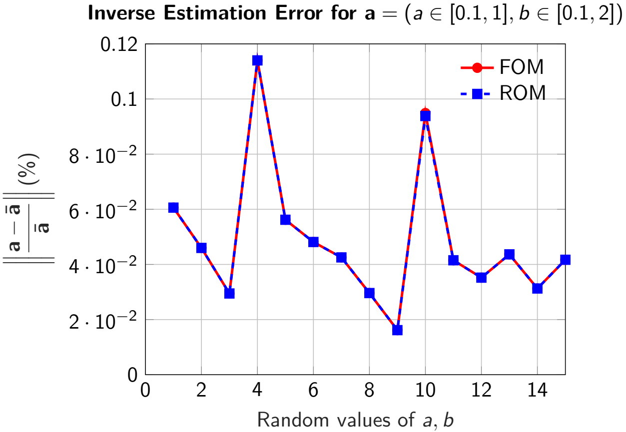


Figure: Inverse Error estimation

Coupled Reaction- Diffusion

Inverse Problem- Golden Search

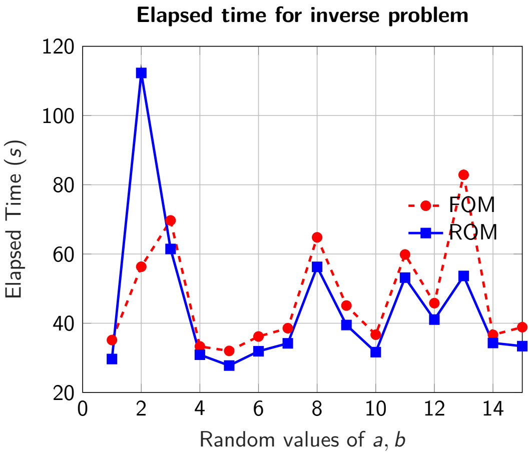


Figure: Elapsed time for inverse problem

Wave Equation

Wave Equation

Intrusive ROM

- Formulation of one-dimensional non-linear wave equation for FOM, ROM such that snapshot matrix, $\mathcal{U}$ has modes $(\mathbf{U_u})$ with 99.9% $(\rho_u = 3)$ energy are,

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} = -\frac{\partial (u^2/2)}{\partial x} = -N, \quad x \in [0,1], t \in (0, 0.3], \quad u(x,0) = \sin(\pi x/L)$$

$$\frac{\partial \hat{u}}{\partial t} = -\mathbf{U_u}^\top \left[\frac{\partial (\mathbf{U_u}\hat{u})^2/2}{\partial x}\right]$$

- Modes of non linear term, $\mathbf{N} = [N(t_1), N(t_2), \cdots, N(t_n)]$ is $\mathbf{U_N}$ with 99% $(\rho_N = 3)$ energy. Reduced non-linear model through DEIM [2] is,

$$\frac{\partial \hat{u}}{\partial t} = -\mathbf{U_u}^\top \hat{N}$$

$$\hat{N} = \mathbf{U_N}^\top (\mathbf{P}\,\mathbf{U_N})^\dagger \mathbf{P}^\top N, \quad \mathbf{P} \leftarrow \mathbf{DEIM}(\mathbf{U_N})$$

Wave Equation

Intrusive ROM

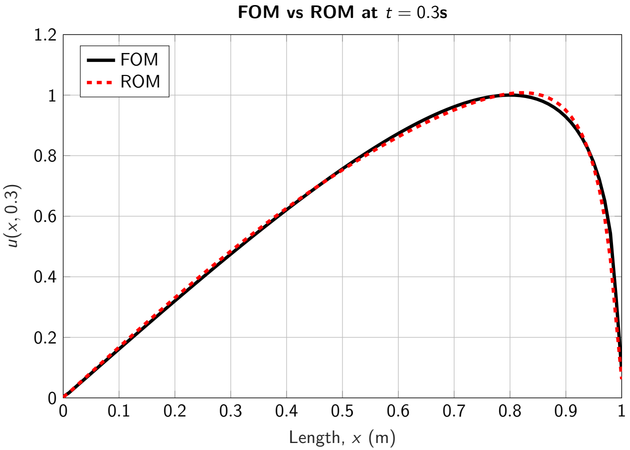


Figure: Velocity distribution at $t = 0.3$s

Wave Equation

Intrusive ROM

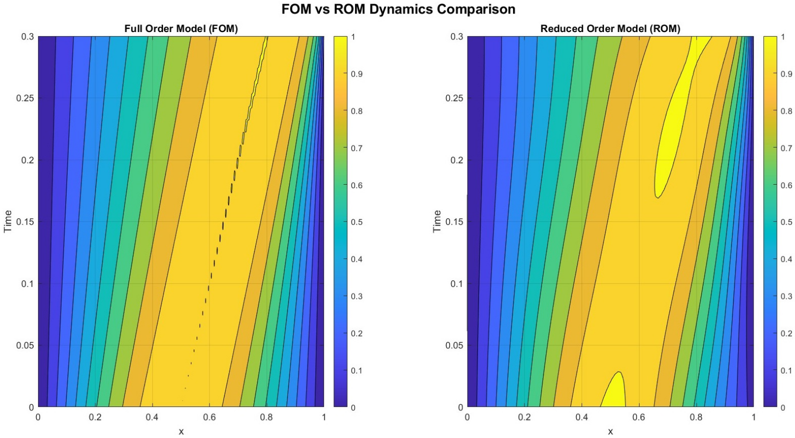


Figure: Transient Velocity distribution for FOM, ROM

Electrohydrodynamics

Electrohydrodynamics

Intrusive ROM

- EHD is one-dimensional coupled non-linear equation but expressed as,

$$\frac{1}{\mu_e}\frac{\partial}{\partial t}\left(\frac{\partial^2 \phi}{\partial x^2}\right) = \frac{\partial^3 \phi}{\partial x^3}\frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial x^2}\frac{\partial^2 \phi}{\partial x^2}$$

- Snapshot modes, $\mathbf{U}_\phi$ have 99.9% of energy,

$$\frac{\partial}{\partial t}\left(\frac{\partial^2 \hat{\phi}}{\partial x^2}\right) = \mu_e \mathbf{U}_\phi^\top \left(\mathbf{U}_\phi \frac{\partial^3 \hat{\phi}}{\partial x^3}\mathbf{U}_\phi \frac{\partial \hat{\phi}}{\partial x} + \mathbf{U}_\phi \frac{\partial^2 \hat{\phi}}{\partial x^2}\mathbf{U}_\phi \frac{\partial^2 \hat{\phi}}{\partial x^2}\right)$$

- Currently, ROM model is **numerically unstable and are under research**.

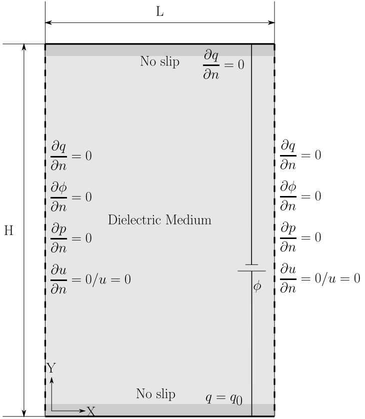


Figure: Schematic of the EHD [3]

Conclusions

Conclusions

- Inverse search problems are **faster** in execution than full order model
- Coupled diffusion-reaction ROM model is an **surrogate model** with minimal error and computing time
- Boundary lifting often **enhances ROM accuracy**
- Currently for EHD there is **numerical instability** and being researched upon.

Takeaway

- Gradient based solver with ROM lays a groundwork for **real time inverse prediction**
- One must **account human hours** into making ROM for digital twins.

References

[1] Fabian Key, Max von Danwitz, Francesco Ballarin, and Gianluigi Rozza. Model order reduction for deforming domain problems in a time-continuous space-time setting. *International Journal for Numerical Methods in Engineering*, 124(23): 5125–5150, August 2023. ISSN 1097-0207. doi: 10.1002/nme.7342.

[2] M. Rojas M.M. Baumann, M.B. Van Gijzen. Nonlinear model order reduction using pod/deim for optimal control of burgers' equation. mathesis, TU Delft, 2013. URL https://github.com/ManuelMBaumann/MasterThesis.

[3] P.A. Vázquez and A. Castellanos. Numerical simulation of ehd flows using discontinuous galerkin finite element methods. *Computers &; Fluids*, 84:270–278, September 2013. ISSN 0045-7930. doi: 10.1016/j.compfluid.2013.06.013.

Validation

Heat Equation

Analytical Solution

- For 1D transient heat conduction, analytical solution employed for validation is,

$$T(x,t) = T_s(x) + \theta(x,t)$$

$$T_s(x) = T_L \frac{1-x}{L} + T_R \frac{x}{L}$$

$$\theta(x,t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x/L) \exp(-\alpha(n\pi/L)^2 t)$$

$$B_n = \frac{2}{L} \int_0^L (T_0(x,t) - T_s(x)) \sin(n\pi x/L)$$

Reaction- Diffusion Equation

Methods of Manufactured Solutions

- Solution of u, v are assumed to have form, where U, V are unknown constants. Further, F_u, F_v are calculated as which satisfy the governing equation

$$u = \tilde{u} + U\sin(\pi x)\cos(2\pi t), \quad \tilde{u} = u_L\frac{1-x}{L} + u_R\frac{x}{L}$$
$$v = \tilde{v} + V\sin(\pi x)\cos(2\pi t), \quad \tilde{v} = v_L\frac{1-x}{L} + v_R\frac{x}{L}$$
$$F_u = \frac{\partial u}{\partial t} - a\frac{\partial^2 u}{\partial x^2} - \alpha(v-u)$$
$$F_v = \frac{\partial v}{\partial t} - b\frac{\partial^2 v}{\partial x^2} - \beta(u-v)$$

- The whole idea is to assume any constant values for $a, b, \alpha, \beta, U, V$ compute the F_u, F_v then solve the FOM for validation against analytical expression.

Reaction- Diffusion Equation

Coupling term- Boundary lifting

$$u - v = \tilde{u} - \tilde{v} + U\sin(\pi x)\cos(2\pi t) - V\sin(\pi x)\cos(2\pi t)$$
$$v - u = \tilde{v} - \tilde{u} + V\sin(\pi x)\cos(2\pi t) - U\sin(\pi x)\cos(2\pi t)$$

- $u - v$ and $v - u$ introduces the error of $\tilde{u} - \tilde{v}$ and $\tilde{v} - \tilde{u}$ and corrected with $\alpha(\tilde{u} - \tilde{v})$ and $\beta(\tilde{u} - \tilde{v})$. For the ROM, the subspace has to be transformed.

$$\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2} + \alpha(v - u) + F_u + \alpha(\tilde{u} - \tilde{v})$$
$$\frac{\partial v}{\partial t} = b\frac{\partial^2 v}{\partial x^2} + \beta(u - v) + F_v + \beta(\tilde{u} - \tilde{v})$$

Electrohydrodynamics

Numerical validation

- The coupled EHD system is formulated as,

$$\nabla \cdot (\epsilon \nabla \phi) = -q$$

$$\mathbf{E} = -\nabla \phi$$

$$\frac{\partial q}{\partial t} + \nabla \cdot (\mu_e q \mathbf{E}) = 0$$

- These set of equations are coupled as,

$$\frac{1}{\mu_e} \frac{\partial}{\partial t} \left(\frac{\partial^2 \phi}{\partial x^2} \right) = \frac{\partial^3 \phi}{\partial x^3} \frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial x^2} \frac{\partial^2 \phi}{\partial x^2}$$

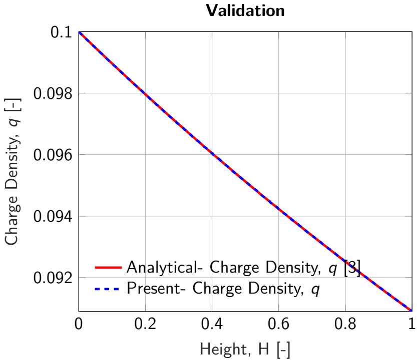


Figure: Validation of weak injection (C = 0.1)

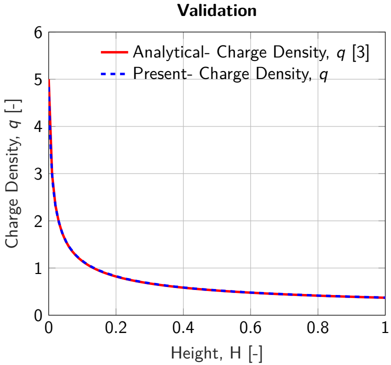


Figure: Validation of strong injection (C = 10)