

Intrusive Reduced Order Modeling for Inverse Problems

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ABSTRACT Inverse problems are one of the challenging in engineering perspective, as estimating the unknown parameter from give sets of measurable data that characterizes the system often leading to optimization problem. With the advantage of being convex optimization, golden search optimization is gradient-free and robust for such problems. Four sets of equations were considered with increasing complexity that resembles the system of interest (Electrohydrodynamics- EHD) and to build confidence on inverse search, coupling equations, estimating non-linear term using POD-DEIM then extend to EHD. It was observed that inverse search with ROM offers an advantage on elapsed time while maintaining similar error as FOM. With gradient methods such as gradient descent optimization, one can further reduce the elapsed time to the point where ROM's are used for digital twin.

Keywords: Intrusive Reduced order models, Inverse search, Golden Search, Convex optimization

I. INTRODUCTION

Inverse problems are the class of engineering problems, often estimating the unknown parameter value(s) through set of given experimental/ observed data that characterizes the system. This is exactly opposite of forward problems, for example- given a set of temperature distribution profiles at certain time intervals and estimating the thermal diffusivity of that system is class of inverse problems. These problems arise in experimental field where based on some observable/ measurable quantities, unmeasurable quantities has to be estimated with precision. This problems are rather difficult as it involves engineering, optimization fields merging together. Thus the aim is to uncover the importance of Intrusive Reduced Order Models (ROM) over Full Order Models (FOM) for inverse search problems. To understand the significance and advantages of ROM, we have considered different cases with increasing complexity.

II. MATHEMATICAL FORMULATION

To understand the behaviour of Intrusive ROM over various Partial differential equations (PDE), four cases in the order of increasing complexity has been considered,

- 1) **Transient heat conduction:** One dimensional transient heat conduction with constant thermal diffusivity for intrusive ROM formulation including boundary lifting techniques to enhance the accuracy of ROM models and measure speedup of ROM in inverse problem estimation.

- 2) **Reaction- Diffusion:** One dimensional linear coupled PDE and validating the FOM, ROM through Methods of Manufactured Solution (MMS) for validation and to identify the speedup through uni-direction golden search approach.
- 3) **Transient Wave Propagation:** One dimensional nonlinear wave equation with discrete empirical interpolation method (DEIM) to enhance the ROM calculations for non-linear equation.
- 4) **Electrohydrodynamics:** One dimensional nonlinear third order equation and is the system of interest of inverse problem

A. TRANSIENT HEAT CONDUCTION

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

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

The intrusive ROM has to be formulated snapshot matrix, $\mathcal{T} = [T(t_1), T(t_2), \dots, T(t_n)]$ such that modes (\mathbf{U}_T) are extracted through Singular Valued Decomposition (SVD). Truncation rank, ρ_T is chosen for energy of atleast 99.9% ($\rho_T = 3$) and reduced order model (ROM) is formulated as,

$$\frac{\partial \hat{T}}{\partial x} = \mathbf{U}_T^\top \alpha \mathbf{U}_T \frac{\partial^2 \hat{T}}{\partial x^2} = \hat{\mathbf{A}} \hat{T} \quad (2)$$

where $\hat{\mathbf{A}} = \mathbf{U}_T^\top \alpha \mathbf{U}_T D_2$ and D_2 is second order differentiation matrix. Analytical solution employed for validation is written as sum of boundary solution ($\tilde{T}_s(x)$) and internal solution ($\theta(x, t)$),

$$T(x, t) = \tilde{T}(x) + \theta(x, t) \quad (3)$$

$$\tilde{T}(x) = T(x = 0, t) \frac{L - x}{L} + T(x = L, t) \frac{x}{L} \quad (4)$$

$$\theta(x, t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x/L) \exp(-\alpha(n\pi/L)^2 t) \quad (5)$$

$$\text{where, } B_n = \frac{2}{L} \int_0^L (T(x, t = 0) - \tilde{T}(x)) \sin(n\pi x/L) \quad (6)$$

Validation of FOM, ROM is in Fig. 1

- 1) **BOUNDARY LIFTING:** Boundary lifting is an mathematical formulation where the non-homogeneous are converted to homogeneous boundary conditions then ROM are formulated and at last converting back to non-homogeneous solutions [1]. The lifting function, $\tilde{T}(x)$ from Eq. (4) used for this case. Further SVD is performed on reduced temperature, $T_R(x, t)$ as $T_R(x, t) = T(x, t) - \tilde{T}(x)$, and temperature

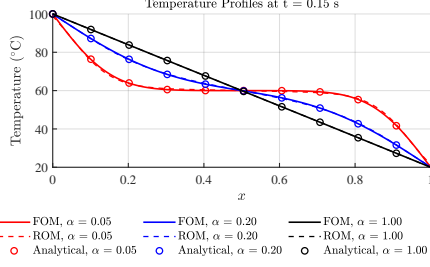


Figure 1: Validation of FOM and ROM with analytical

is reconstructed as $T(x, t) = T_R(x, t) + \tilde{T}(x)$. The effects of boundary lifting on accuracy is in Fig. 2 and can infer that at $x = 0$, there is an error for without lifting but with lifting ensures that boundary conditions are satisfied.

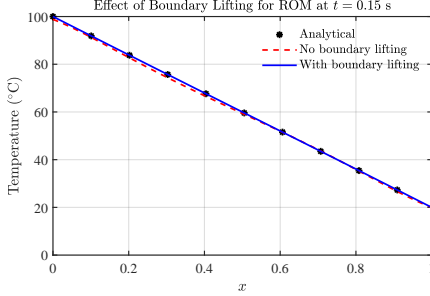


Figure 2: Effects with and without boundary lifting

B. COUPLED DIFFUSION-REACTION

One-dimensional coupled reaction- diffusion equation with system constants, a, b, α, β has no particular solution for validation of FOM and ROM.

$$\frac{\partial u}{\partial t} = a \frac{\partial^2 u}{\partial x^2} + \alpha(v - u) + F_u \quad (7)$$

$$\frac{\partial v}{\partial t} = b \frac{\partial^2 v}{\partial x^2} + \beta(u - v) + F_v \quad (8)$$

$$x \in [0, L = 1], \quad t > 0 \quad (9)$$

Thus to gain the confidence, the methods of manufactured solution (MMS) was implemented. The idea of MMS is that we find a equation that satisfies the governing equation for certain forcing function, F_u, F_v , then verify if this solution is similar to FOM and ROM.

1) METHODS OF MANUFACTURED SOLUTIONS:

Solution of u, v are assumed to have form as,

$$u = \tilde{u} + U \sin(\pi x) \cos(2\pi t) \quad (10)$$

$$\tilde{u} = u(x=0, t) \frac{1-x}{L} + u(x=L, t) \frac{x}{L} \quad (11)$$

$$v = \tilde{v} + V \sin(\pi x) \cos(2\pi t) \quad (12)$$

$$\tilde{v} = v(x=0, t) \frac{L-x}{L} + v(x=L, t) \frac{x}{L} \quad (13)$$

where U, V are some constant. Further, F_u, F_v are calculated as which satisfy the governing equation as,

$$F_u = \frac{\partial u}{\partial t} - a \frac{\partial^2 u}{\partial x^2} - \alpha(v - u) \quad (14)$$

$$F_v = \frac{\partial v}{\partial t} - b \frac{\partial^2 v}{\partial x^2} - \beta(u - v) \quad (15)$$

Further forcing functions, F_u, F_v is solved as,

$$\begin{aligned} F_u = & \alpha(u(x=L, t)x - v(x=L, t)x \\ & - u(x=0, t)(x-1) + v(x=0, t)(x-1) \\ & + U \cos(2\pi t) \sin(\pi x) - V \cos(2\pi t) \sin(\pi x) \\ & - 2\pi U \sin(2\pi t) \sin(\pi x) + U a \pi^2 \cos(2\pi t) \sin(\pi x) \end{aligned} \quad (16)$$

$$\begin{aligned} F_v = & -\beta(u(x=L, t)x - v(x=L, t)x \\ & - u(x=0, t)(x-1) + v(x=0, t)(x-1) \\ & + U \cos(2\pi t) \sin(\pi x) - V \cos(2\pi t) \sin(\pi x) \\ & - 2\pi V \sin(2\pi t) \sin(\pi x) + V b \pi^2 \cos(2\pi t) \sin(\pi x) \end{aligned} \quad (17)$$

which are then computed, and solved for u, v from Eqs. (7) and (8) through FOM and ROM to verify correctness of Eqs. (10) and (12) for any constant values of U, V, α, β . The validation result is in Fig. 3

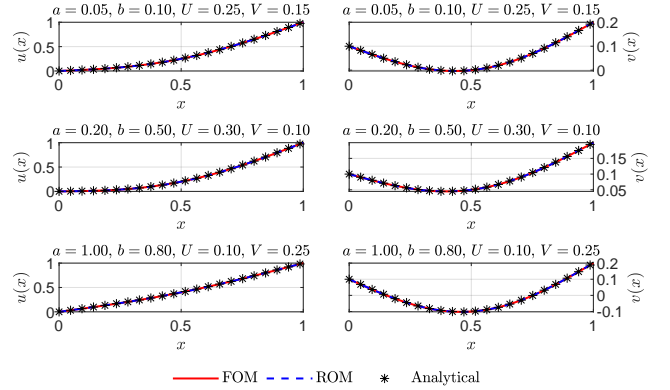


Figure 3: Validation of FOM, ROM through MMS

While computing $u - v$ and $v - u$ introduces the error (when boundary lifted) 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.

$$\frac{\partial u}{\partial t} = a \frac{\partial^2 u}{\partial x^2} + \alpha(v - u) + F_u + \alpha(\tilde{u} - \tilde{v}) \quad (18)$$

$$\frac{\partial v}{\partial t} = b \frac{\partial^2 v}{\partial x^2} + \beta(u - v) + F_v + \beta(\tilde{u} - \tilde{v}) \quad (19)$$

The intrusive ROM has been formulated such that snapshot matrix, $\mathcal{U} = [u(t_1), u(t_2), \dots, u(t_n)]^T$, $\mathcal{V} = [v(t_1), v(t_2), \dots, v(t_n)]^T$, modes $(\mathbf{U}_u, \mathbf{U}_v)$ are extracted through SVD for u, v truncated to 99.9% ($\rho_u = \rho_v = 1$)

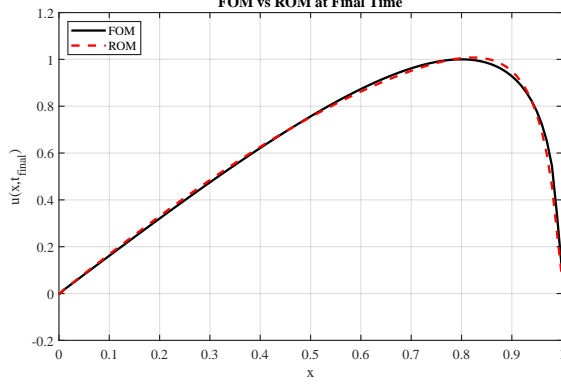


Figure 4: Comparison of FOM, ROM

of energy and ROM can be formulated as,

$$\frac{\partial \hat{u}}{\partial t} = \mathbf{U}_u^\top a \mathbf{U}_u \frac{\partial^2 \hat{u}}{\partial x^2} + \mathbf{U}_u^\top \alpha (\mathbf{U}_v \hat{v} - \mathbf{U}_u \hat{u}) + \mathbf{U}_u^\top F_u + \alpha \mathbf{U}_u^\top (\tilde{v} - \tilde{u}) \quad (20)$$

$$\frac{\partial \hat{v}}{\partial t} = \mathbf{U}_v^\top b \mathbf{U}_v \frac{\partial^2 \hat{v}}{\partial x^2} + \mathbf{U}_v^\top \beta (\mathbf{U}_u \hat{u} - \mathbf{U}_v \hat{v}) + \mathbf{U}_v^\top F_v + \beta \mathbf{U}_v^\top (\tilde{u} - \tilde{v}) \quad (21)$$

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

C. WAVE EQUATION

One-dimensional non-linear wave equation has been formulated in conservative form as,

$$\frac{\partial u}{\partial t} = -\frac{\partial(u^2/2)}{\partial x} = -\mathbf{N}, \quad (22)$$

$x \in [0, 1], \quad t \in (0, 0.3], \quad u(x, 0) = \sin(\pi x/L)$

The intrusive ROM has been formulated such that snapshot matrix, $\mathcal{U} = [u(t_1), u(t_2), \dots, u(t_n)]^\top$ has modes computed through SVD (\mathbf{U}_u) has been truncated to 99.9% ($\rho_u = 3$) energy,

$$\frac{\partial \hat{u}}{\partial t} = -\mathbf{U}_u^\top \left[\frac{\partial(\mathbf{U}_u \hat{u})^2/2}{\partial x} \right] \quad (23)$$

Modes of non linear term, $\mathcal{N} = [N(t_1), N(t_2), \dots, N(t_n)]^\top$ is \mathbf{U}_N with 99% ($\rho_N = 3$) energy. Reduced non-linear model through POD-DEIM [2] is,

$$\frac{\partial \hat{u}}{\partial t} = -\mathbf{U}_u^\top \hat{\mathbf{N}} \\ \hat{\mathbf{N}} = \mathbf{U}_N^\top (\mathbf{P} \mathbf{U}_N)^\dagger \mathbf{P}^\top \mathbf{N}, \quad \mathbf{P} \leftarrow \text{DEIM}(\mathbf{U}_N)$$

where \mathbf{P} is projection matrix to reduce the complexity of non-linear term but still maintaining accuracy. The comparison result is in Fig. 4

D. ELECTROHYDRODYNAMICS

The coupled EHD system with $\epsilon, q, \mathbf{E}, \phi, \mu_e$ being permittivity, charge density, electric field, potential difference, ion mobility is formulated as,

$$\nabla \cdot (\epsilon \nabla \phi) = -q \quad (24)$$

$$\mathbf{E} = -\nabla \phi \quad (25)$$

$$\frac{\partial q}{\partial t} + \nabla \cdot (\mu_e q \mathbf{E}) = 0 \quad (26)$$

This can be reformulated as one-dimensional non-linear equation as,

$$\frac{1}{\mu_e} \frac{\partial}{\partial t} \left(\frac{\partial^2 \phi}{\partial x^2} \right) = \frac{\partial^3 \phi}{\partial x^3} \frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial x^2} \frac{\partial^2 \phi}{\partial x^2} \quad (27)$$

1) **ANALYTICAL SOLUTION:** From Eq. (27), the steady state solution is calculated as,

$$\phi(x) = c_2(2x - c_1)^{1.5} + c_3 \quad (28)$$

with c_1, c_2, c_3 being integration constants being solved from boundary conditions,

$$\phi(x=0) = \phi_0 \quad (29)$$

$$\phi(x=L) = 0 \quad (30)$$

$$\frac{\partial^2 \phi}{\partial x^2}(x=0) = -q_0/\epsilon \quad (31)$$

Upon solving for c_1, c_2, c_3 ,

$$c_1 = -s_0^2 \quad (32)$$

$$c_2 = -\frac{q_0}{3\epsilon} s_0 \quad (33)$$

$$c_3 = -c_2 s_0^3 \quad (34)$$

$$\frac{q_0}{3\epsilon} s_0 ((2L + s_0^2)^{1.5} - s_0^3) - \phi_0 = 0, \quad s_0 > 0 \quad (35)$$

The intrusive ROM has been formulated such that snapshot matrix, $\Phi = [\phi(t_1), \phi(t_2), \dots, \phi(t_n)]^\top$, modes \mathbf{U}_ϕ are extracted through SVD for ϕ truncated to 99.9% ($\rho_\phi = 1$) of energy and formulated as,

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

For the schematic from Fig. 5 the numerical data from OpenFOAM and FDM models has been validated for steady state and is in Fig. 6

E. GOLDEN INVERSE SEARCH

The golden section search is a derivative-free optimization method used to locate the minimum (or maximum) of a uni-modal function on a closed interval.

For a uni-modal function $f(x)$ defined on the interval $[a, b]$. The method relies on the golden ratio, $\varphi = \frac{1+\sqrt{5}}{2} \approx 1.618$. Two interior points are chosen using the golden ratio, $x_1 = b - \frac{b-a}{\varphi}, x_2 = a + \frac{b-a}{\varphi}$

The function values $f(x_1)$ and $f(x_2)$ are compared. Since the function is assumed uni-modal, one of the sub-intervals contains the minimum:

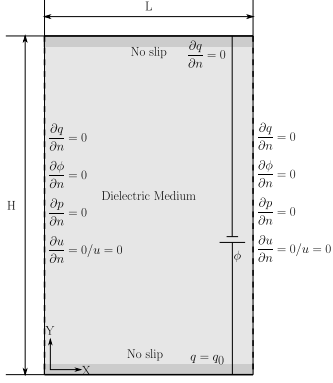


Figure 5: Schematic of EHD domain [3]

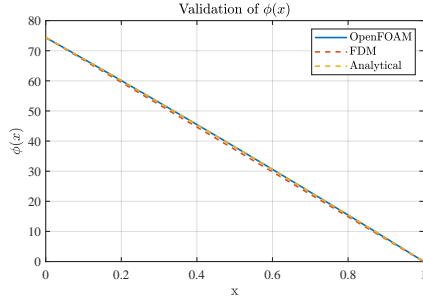


Figure 6: Validation of FOM and numerical with analytical

- If $f(x_1) > f(x_2)$, the minimum lies in $[x_1, b]$ and we set $a = x_1$.
- If $f(x_1) < f(x_2)$, the minimum lies in $[a, x_2]$ and we set $b = x_2$.

The process is repeated, shrinking the interval at each iteration. Because the ratio of interval reduction is constant, the algorithm is efficient and requires only one new function evaluation per iteration.

The algorithm stops when the interval length is below a prescribed tolerance, $|b - a| < \varepsilon$. The estimated minimizer is then taken as, $x^* = \frac{a+b}{2}$.

The uni-modal loss function is defined as $\mathcal{J}_p = \frac{1}{2} \|\mathbf{X} - \bar{\mathbf{X}}\|^2$, p being the parameter of optimization that characterizes the system based on experimental/ given data $\bar{\mathbf{X}}$, where \mathbf{X} is being solved for p such that $\mathcal{J}_p \rightarrow 0$ through golden optimization.

III. RESULTS AND DISCUSSION

To measure the performance of FOM, ROM the elapsed time for time-integration (Runge-Kutta 4th order) was measured apart from the inverse reconstruction error.

A. TRANSIENT HEAT CONDUCTION

From, Fig. 7 its evident that inverse error is less than 0.8% for range of α and Fig. 8 indicates that wall clock time for ROM is significantly lower than FOM. Further speedup of FOM, ROM was considered by varying the domain discretization count (while having other parameters

constant) and is in Fig. 9. The order of complexity was found to be $7.283 \times 10^{-8} N_x^{2.35}$, $1.764 \times 10^{-8} N_x^{2.45}$ respectively for FOM, ROM.

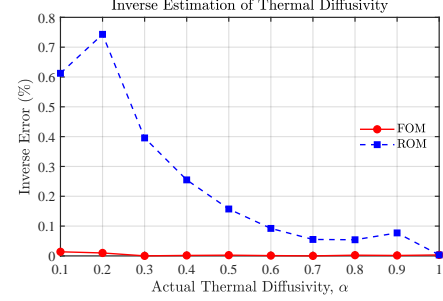


Figure 7: Inverse error estimation

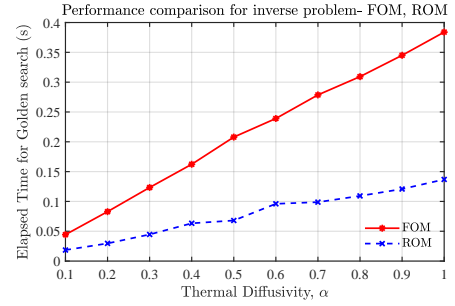


Figure 8: Elapsed time- transient heat conduction

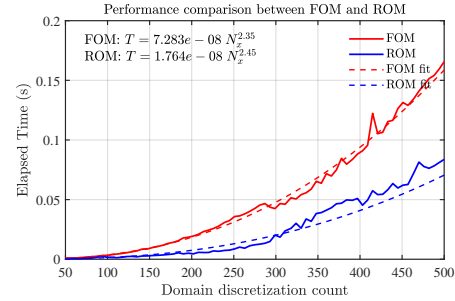


Figure 9: Scaling- transient heat conduction

B. COUPLED DIFFUSION-REACTION

From, Fig. 10 its evident that inverse error same as FOM for various cases of $a \in [0, 1]$, $b \in [0, 1]$ and Fig. 11 indicates that wall clock time for ROM is significantly lower than FOM. Further speedup of FOM, ROM was considered by varying the domain discretization count (while having other parameters constant) and is in Fig. 12.

C. WAVE EQUATION

In order to verify the ROM formulation using POD-DEIM, non-linear wave equation has been considered and found that reconstruction for ROM is as accurate, represented in Fig. 13, thus giving confidence on POD-DEIM implementation for non-linear terms.

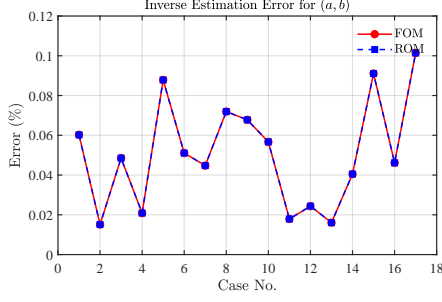


Figure 10: Inverse error estimation of coupled reaction-diffusion equations

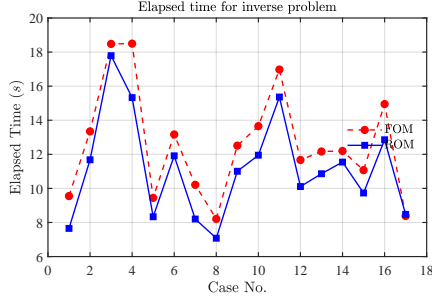


Figure 11: Elapsed time for coupled reaction-diffusion

D. ELECTROHYDRODYNAMICS

Currently analytical, FOM has been verified and ROM formulation seems to have fail due to non-homogeneous boundary conditions and non-linear third order governing equation, which amplify even small error in ROM thus leading to numerical instability. However this is under current research as the confidence on Intrusive ROM's for inverse problems have been demonstrated.

IV. CONCLUSIONS

Based on the studies performed, inverse search for intrusive ROM's takes less time than FOM. Gradient free optimization techniques are quite stable under noisy experimental data but are relatively slower than gradient methods. As these problems belong to class of convex optimization, gradient descent method is much powerful technique for predicting the solution to inverse problems. Gradient based solver with ROM lays a groundwork for real time inverse prediction. However one must account human hours and conclude on the feasibility of FOM or ROM into making ROM as digital twin. EHD being higher order non-linear system, small error could amplify the numerical instability, which is the actual scenario and upon being reviewed as future work. These process of estimating the elapsed time for FOM, ROM should give confidence on implementing the ROM's in digital twin.

ACKNOWLEDGMENT

First author would like to acknowledge the support taken from Wolfram alpha (analytical solution for EHD), LLM models (for speeding post-processing).

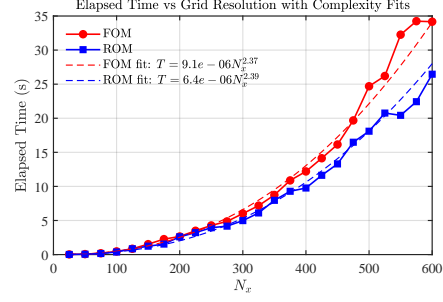


Figure 12: Scaling performance-coupled diffusion reaction

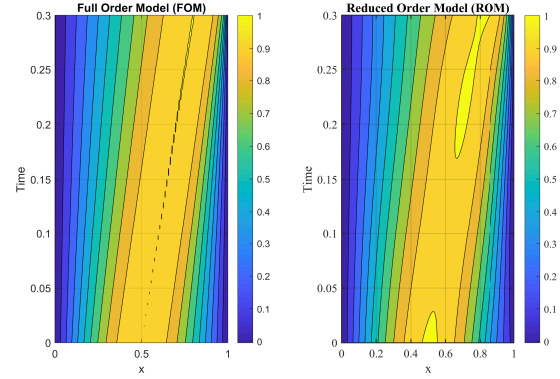


Figure 13: Contour plot of reconstruction of ROM

DATA AVAILABILITY

All the MATLAB codes used for this study can be located at <https://github.com/Ananth-Narayan-IITM/IntrusiveROM-InverseSearch.git>

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