REDUCED ORDER MODELLING CONVECTION DIFFUSION

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Nomenclature

ϵ	Diffusion Coefficient
Re	Reynolds number
f	force vector
$\vec{w}$	Convection Velocity Vector
ψ	Basis Function
Ω	Domain
M	Mass Matrix
S	Stiffness Matrix
C	Convection Matrix

I. Introduction

This study presents a comprehensive Reduced Order Modeling (ROM) approach for solving the convection-diffusion equation. The proposed ROM technique leverages Proper Orthogonal Decomposition (POD) coupled with Galerkin Projection to construct a low-dimensional model that accurately captures the dynamics of convection-diffusion process. IFISS (Incompressible Flow &Iterative Solver) Finite element-based solver is used to generate snapshot data for POD, creating a reduced space. The reduced model of convection-diffusion is created by applying Galerkin projection to the governing equation onto the reduced space. The discussion is restricted to the two-dimensional (2D) context and introduces Reduced Order Modeling (ROM) within Computational Fluid Dynamics (CFD).

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II. Theory

A. Background

The convection-diffusion equation plays a fundamental role in mathematically modeling physical systems in which particles, energy, or other quantities are transferred due to convection and diffusion. It accurately represents the behavior of various phenomena, such as heat movement in fluids and gases, and the spread of pollutants in both the atmosphere and water bodies. As a result, this equation is crucial for studies in engineering and environmental science.

B. So what are convection diffusion problems?

In convection diffusion problem, elliptic operator feature a parameter ϵ, which can approach zero. These second-order derivatives are associated with diffusion, whereas the first-order derivatives are linked to convection or transport mechanisms. In standard boundary value problems where ϵ is not near zero, diffusion predominates in the model, and the convective first-order derivatives are less influential in the analysis. However, when ϵ is close to zero, and the differential operator includes convective terms, it's referred to as a convection-diffusion operator. In this scenario, the convection term significantly impacts the solution to the boundary value problem. Under these conditions, the convection component substantially affects the solution of the boundary value problem. Despite being termed "lower-order terms," the convective elements are crucial in both the theoretical and numerical analysis of these problems and cannot be overlooked..[4]

$$\frac{\partial u}{\partial t} - \epsilon\nabla^2 u + \vec{w} \cdot \nabla u = f \tag{1}$$

In the numerical treatment of convection-diffusion problems, the choice of discretization strategy, particularly regarding mesh refinement, is of critical importance. Convection-diffusion equations, which are used to model phenomena where transport by convection is balanced by diffusion, often exhibit sharp gradients and thin boundary layers, particularly in high Péclet number scenarios. These features pose significant challenges in numerical simulations, necessitating a careful consideration of mesh width. Studies have demonstrated that parameter estimates dependent on mesh width can be rigorously established, enabling enhanced accuracy in numerical simulations [2]. The refinement of the mesh leads to an increased resolution of the spatial domain, which is particularly beneficial for accurately capturing the steep gradients and layers typical of convection-diffusion problems.

1. *Finite Element Model of Convection-Diffusion*

Finite Elements and Fast Iterative Solvers with Applications in Incompressible Fluid Dynamics(IFISS) [3] was used for modelling the unsteady convection diffusion problem. The 2dimensional unsteady convection diffusion problem was setup with the zero source term, variable vertical wind, and characteristic boundary-layers [1]

In this problem, the wind is vertical,$\vec{w} = (0, 1 + (x + 1)^2/4)$, but increases in strength from left to right. Dirichlet boundary values apply on the inflow and characteristic boundary segments; u is set to unity on the inflow boundary, and decreases to zero quadratically on the

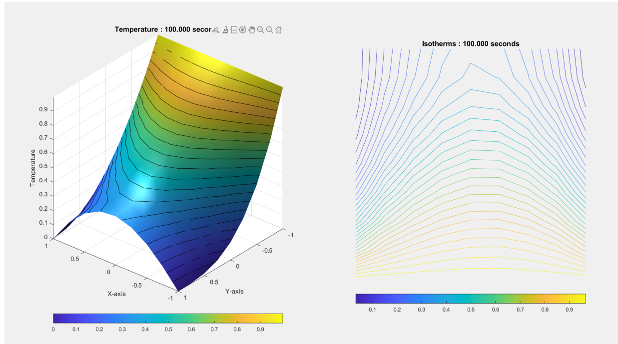

Figure 1. Contour plot Diffusion Dominant

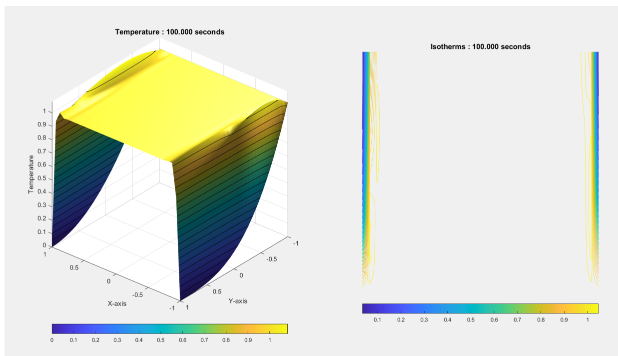

Figure 2. Contour plot Convection Dominant

right wall, and cubically on the left wall. A zero Neumann condition on the top boundary ensures that there is no exponential boundary layer in this case. The fact that the reduced solution $\hat{u} \equiv 1$ is incompatible with the specified values on the characteristic boundary, generates characteristic layers on each side. These layers are typical of so-called shear layers that commonly arise in fluid flow models [1].

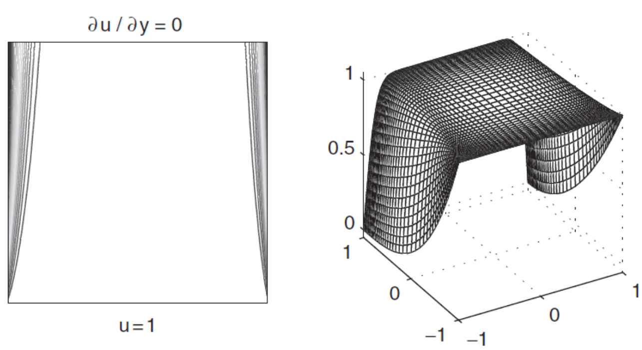

Figure 3. Contour plot Convection-Diffusion

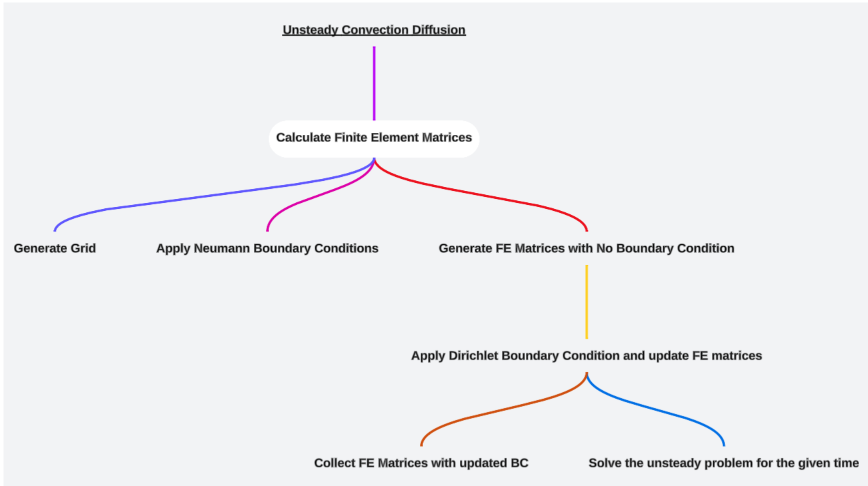

Figure 4. IFISS FE Matrices calculation

2. Reduce Order Modelling

Reduced Order Models (ROMs) are simplified versions of complex systems that preserve essential features and dynamics while significantly reducing the computational cost. Convection-diffusion equations, which typically require solving large-scale problems that can be computationally expensive, ROMs offer a promising alternative by reducing the dimensionality of the problem space.

In this study we are using Galerkin-ROMs a projection-based method where the high-dimensional solution space of a convection-diffusion problem is approximated by a lower-dimensional subspace constructed using basis functions. These basis functions are derived from the solutions of the full order model (e.g., solutions obtained via Finite Element Method) and capture the dominant modes of the system dynamics.

Construction of G-ROM for Convection-Diffusion Problem:

- Snapshot Collection: Generate a set of high-fidelity solutions (snapshots) at different time instances (or parameter values).
- Proper Orthogonal Decomposition (POD): Apply POD to the snapshot matrix to extract the most energetic modes, which serve as the basis for the reduced space.
- Projection: Project the full-order model onto the reduced basis to form the G-ROM, which now governs the dynamics in the reduced space.

3. Weak Formulation

$$\frac{\delta u}{\delta t} - \epsilon \nabla^2 u + \vec{w} \cdot \nabla u = f \tag{2}$$

choosing vr as a test function

$$(\frac{\delta u}{\delta t}, v_r) - (\epsilon \nabla^2 u, v_r) + (\vec{w} \cdot \nabla u, v_r) = (f, v_r) \tag{3}$$

In integral form:

$$\int_{\Omega} \frac{\delta u}{\delta t}\, v_r\; d\Omega - \int_{\omega} \epsilon\, \nabla^2 u\; v_r\; d\Omega + \int_{\omega} \vec{w}\cdot\nabla u\; v_r\; d\Omega = \int_{\omega} f\; v_r\; d\Omega \tag{4}$$

Using Integration by parts, weak form can be written as:

$$\int_{\Omega} \frac{\delta u}{\delta t}\, v_r\; d\Omega + \int_{\omega} \epsilon\, \nabla u\; \nabla v_r\; d\Omega + \int_{\omega} \vec{w}\cdot\nabla u\; v_r\; d\Omega = \int_{\omega} f\; v_r\; d\Omega \tag{5}$$

$$(\frac{\delta u}{\delta t},\; v_r)\; + (\epsilon\; \nabla u\;, \nabla v_r)\; + (\vec{w}\cdot\nabla u,\; v_r)\; = (f\;, v_r) \tag{6}$$

4. ROM Formulation

ROM solution can be approximated using:

$$(U^r(x))^n = \sum_{j=1}^{r} (U_j^r)^n * \psi_j^r(x) \tag{7}$$

where r are the number of dominant energy modes and ψ^r are the basis function in the ROM space.

$$(\frac{(u)^{n+1} - (u)^n}{\Delta t},\; v_r) + (\epsilon\; \nabla(u)^n\;, \nabla v_r)\; + (\vec{w}\cdot\nabla(u)^n,\; v_r)\; = (f\;, v_r) \tag{8}$$

$$\int_{\Omega} (u^{n+1} - u^n)\; \psi_i^r\; d\Omega + \Delta t \int_{\Omega} \epsilon\; \nabla u^n\; \nabla \psi_i^r\; d\Omega + \Delta t \int_{\Omega} \vec{w}\cdot\nabla u^n\; \psi_i^r\; d\Omega = \Delta t \int_{\Omega} f\; \psi_i^r\; d\Omega \tag{9}$$

$$\int_{\Omega} ((u^r)^{n+1} - (u^r)^n)\psi_i^r\; d\Omega + \Delta t \int_{\Omega} \epsilon\; \nabla(u^r)^n\; \nabla\psi_i^r\; d\Omega + \Delta t \int_{\Omega} \vec{w}\cdot\nabla(u^r)^n\; \psi_i^r\; d\Omega = \Delta t \int_{\Omega} f\; \psi_i^r\; d\Omega \tag{10}$$

$$\int_{\Omega} (u^r)^{n+1}\psi_i^r\; d\Omega = \int_{\Omega} (u^r)^n \psi_i^r\; d\Omega - \Delta t \int_{\Omega} \epsilon\; \nabla(u^r)^n\; \nabla\psi_i^r\; d\Omega - \Delta t \int_{\Omega} \vec{w}\cdot\nabla(u^r)^n\; \psi_i^r\; d\Omega + \Delta t \int_{\Omega} f\; \psi_i^r\; d\Omega \tag{11}$$

$$\begin{aligned} \sum_{j=1}^{r} (u_j^r)^{n+1} \int_{\Omega} \psi_j^r\; \psi_i^r\; d\Omega = \sum_{j=1}^{r} (u_j^r)^n \int_{\Omega} \psi_j^r\; \psi_i^r\; d\Omega - \Delta t\; \sum_{j=1}^{r} (u_j^r)^n \int_{\Omega} \epsilon\; \nabla\psi_j^r\; \nabla\psi_i^r\; d\Omega \\ -\Delta t\; \sum_{j=1}^{r} (u_j^r)^n \int_{\Omega} \vec{w}\cdot\nabla\psi_j^r\; \psi_i^r d\Omega + \Delta t \int_{\Omega} f\; \psi_i^r d\Omega \end{aligned} \tag{12}$$

This can be written as:

$$M_r u_r^{n+1} = M^r u_r^n - \Delta t S_r u_r^n - \Delta t C r u_r^n + \Delta t f_r^n \tag{13}$$

- M_r (Mass Matrix) $= \int_{\Omega} \psi_j^r\; \psi_i^r\; d\Omega$
- S_r (Stiffness Matrix) $= \int_{\Omega} \epsilon\; \nabla\psi_j^r\; \nabla\psi_i^r\; d\Omega$
- C_r (Convection Matrix) $= \int_{\Omega} \vec{w}\cdot\nabla\psi_j^r\; \psi_i^r d\Omega$
- f_r (Force Vector) $= \int_{\Omega} f\; \psi_i^r d\Omega$

5. Connecting ROM to FOM

The FOM matrices can be projected into the ROM space using the reduced basis matrix generated from the snapshot matrix. In this paper, Singular Value Decomposition(SVD) was used to determine the dominant energy modes and determine the reduce basis matrix. In SVD, the snapshot matrix is decomposed into three matrices: U_{svd}, S, and V^T. The matrix U_{svd} contains the left singular vectors, S is the diagonal matrix with singular values, and V^T contains the right singular vectors. The left singular vectors represents the POD modes. These modes are orthogonal and are ordered by the amount of variance (or energy) they capture from the snapshot matrix. The singular values in S give a measure of the energy captured by the corresponding modes.

Based on the dominant modes , a reduce basis matrix "C_r" was determined. And the ROM operators can be assembled from FOM operators as:

- M_r (Mass Matrix) = $C_r^T\ M^h\ C_r$
- S_r (Stiffness Matrix) = $C_r^T\ S^h\ C_r$
- C_r (Convection Matrix) = $C_r^T\ C^h\ C_r$
- f_r (Force Vector) = $C_r^T\ F^h$

III. FEM + ROM Model

A. Finite Element Model

A 2D Finite element model of the convection-diffusion problem, with $\epsilon = \frac{1}{1000}$, which is a convection dominated region is simulated for 1.5 second time interval. The finite element matrices and temperature snapshots are collected for this model. The snapshot matrix is usually very tall and thin, with spatial data along the rows and the snapshot of the solution at each time step along the columns.

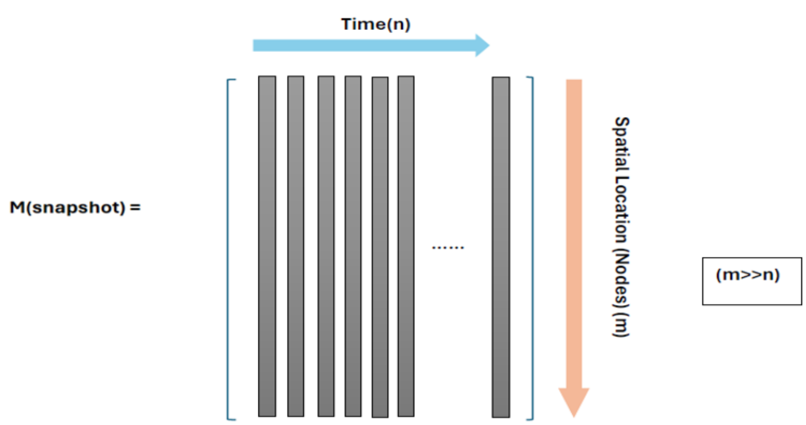

Figure 5. Snapshot Matrix

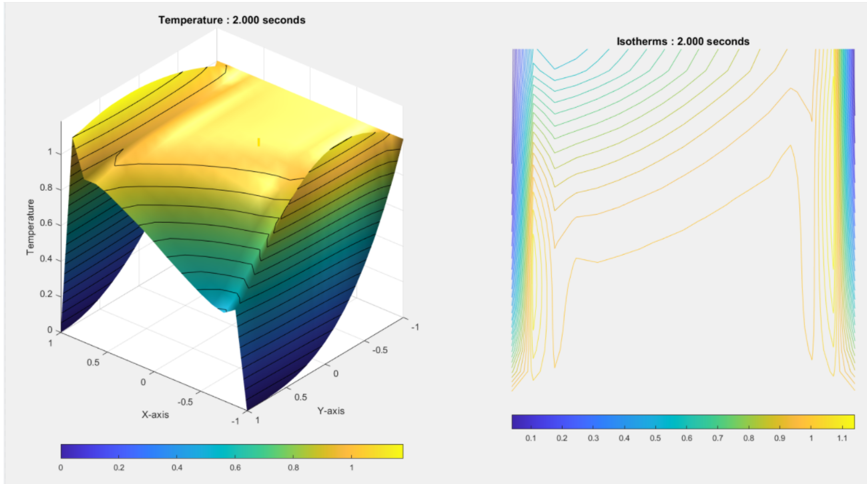

Figure 6. Finite Element Full Order Model (33x33 nodes)

B. Reduced Order Model-Offline stage

In the offline stage data for ROM is collected and ROM model is developed. Proper orthogonal decomposition of the snapshot matrix was done to determine the significant modes in the snapshot matrix to create a reduced space. This reduced space was used for creating the Reduced order model. Singular Value Decomposition (SVD) was used to perform POD. The snapshot matrix was decomposed into a set of orthogonal modes (the left singular matrix), singular value matrix(energy of the mode) and the time coefficient matrix(the right singular vectors). The SVD results shows that the the dominant energy mode lies inside the region r=50. Therefore, the system can be approximated using first 50 modes.

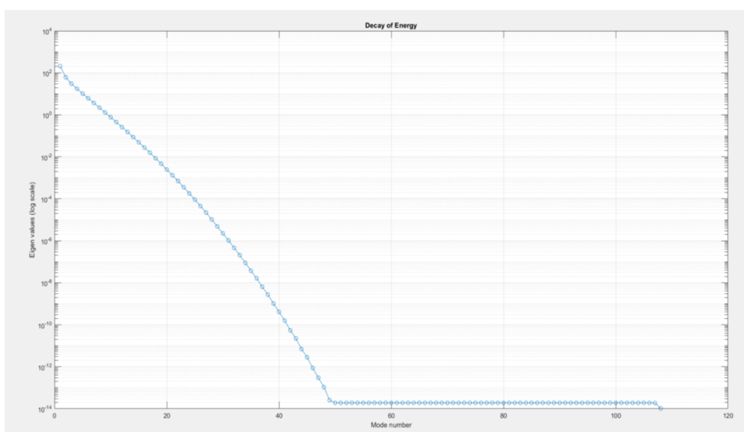

Figure 7. Decay of Energy

In the offline stage the Full order model of convection diffusion equation was simulated for t=1.5sec on a fine mesh setting (33x33 nodes). The viscosity parameter $\epsilon = \frac{1}{1000}$, therefore a convection dominant problem. The snapshot matrix was created using this setting and used for creating a reduced order model. At t=1.5 sec, flow is still developing and convection is setting in and overpowering diffusion, suggesting that the flow has developed where the convective transport is becoming more pronounced compared to the diffusive.

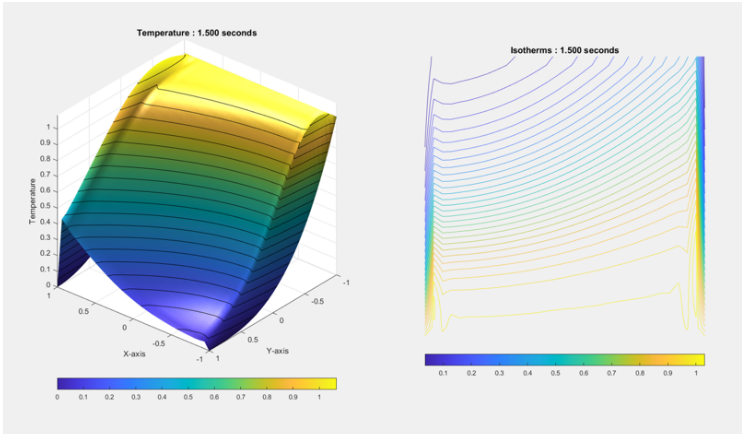

Figure 8. Reduced Order Model

L2-norm of ROM error in the offline stage, shows that the error increases initially but starts dropping after t=0.8 sec. The max L2 norm of the error is 0.013. The initial rise can be explained due to the sharp gradients at boundary that can be difficult to resolve accurately, which stabilizes as the solution marches in time.

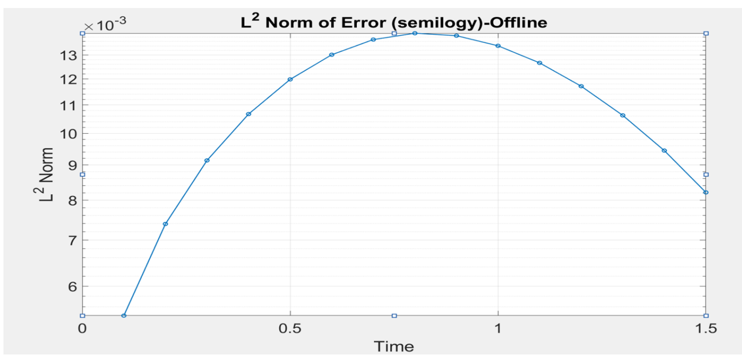

Figure 9. L2 error norm 1.5 sec-offline stage

C. Reduced Order Model-Online stage

In the online stage the ROM model is used for performing faster analysis and predictions. The Reduced Order Model developed in the previous section is now used to forecast solutions beyond the time frame utilized for the ROM development, and its predictive capability are evaluated. The ROM model is used to simulate the solution up-to t=5sec.

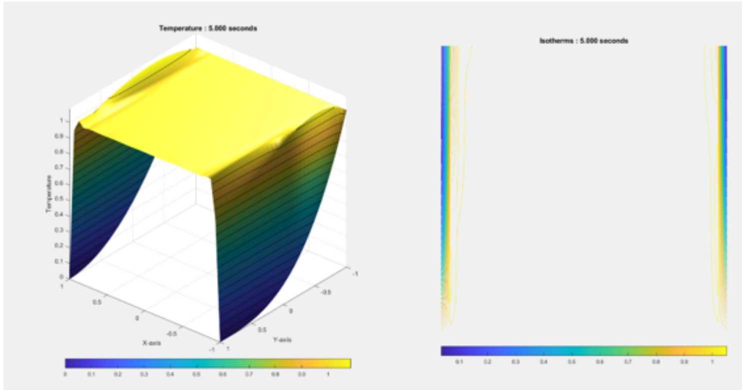

Figure 10. Reduced Order Model at 5 sec

The L2 error norm shows that as the error drops as the convection develops and reaches minimum as the solution approaches the steady state.

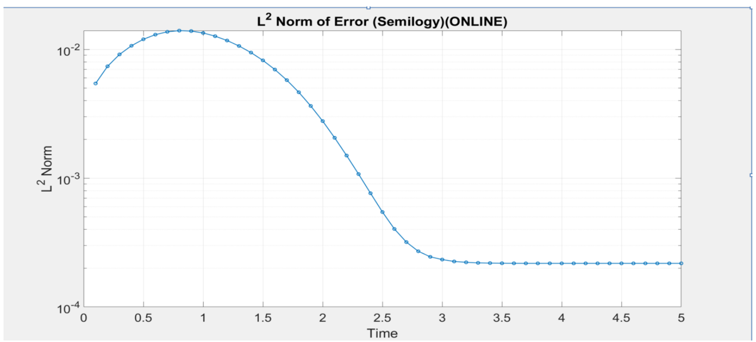

Figure 11. L2 Error t=0 to 5 sec

IV. Conclusion

This study introduced the concept of Reduced Order Models as a simplified approach to simulate unsteady convection-diffusion systems, which are commonly encountered in various fields of physics and engineering. Throughout the process, we focused on how ROMs can capture the essential dynamics of a system while significantly reducing computational cost compared to full-scale simulations. The ROM developed here was for specific time window, within which its performance was validated. This model demonstrated an ability to accurately approximate the behavior of the system for the time range. However, it is important to recognize that ROMs have limitations. The accuracy of the ROM is very much dependent on the initial FOM data. In the unsteady convection diffusion problem as time progresses, the transient effects dissipate, and the system approaches a steady state where the solution changes are very small, as the dynamics simply therefore the ROM predictions are accurate near the steady state. It was also noticed as the mesh size was reduced the ROM solution had oscillations, this can be stabilized using SUPG stabilization. This stabilization of ROM will be further explored.

References

[1] Howard C Elman, David J Silvester, and Andrew J Wathen. *Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics.* Oxford university press, 2014.

[2] Swetlana Giere et al. "SUPG reduced order models for convection-dominated convection–diffusion–reaction equations". In: *Computer Methods in Applied Mechanics and Engineering* 289 (2015), pp. 454–474.

[3] D Silvester, H Elman, and Alison Ramage. "Incompressible Flow and Iterative Solver Software (IFISS) version 3.2, May 2012". In: *URL http://www. manchester. ac. uk/ifiss* ().

[4] Martin Stynes and David Stynes. *Convection-diffusion problems.* Vol. 196. American Mathematical Soc., 2018.