CSMA 2024
16ème Colloque National en Calcul des Structures
13-17 Mai 2024, Presqu'île de Giens (Var)

Non-intrusive reduced order approximation for multi-physics problems

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Résumé — This paper essentially depicts a methodology to address computational frugality of multi-physics problem using COMSOL Multiphysics. The first step is to decouple the involved physics using MATLAB Livelink with COMSOL. After the decoupling is established, a non-intrusive reduced order approximation is used through response surface method to replace the full order simulation of the most expensive physics. This essentially provides reduction in computational cost with acceptable accuracy as is depicted by an academic example.

Mots clés — multi-physics, Reduced Order Model, thermo-fluid.

1 Introduction

The ultimate objective of this research is to address the computational aspects of multi-physics problem of metal transfer process which has extensive application in the automobile industry especially in cases of laser welding and additive manufacturing processes. The main set of physical equations to model such processes at the melt pool scale involves the heat transfer equation, the Navier-Stokes equation involving Newtonian fluid under laminar flow, and finally a level set transport equation to represent the phase transformation [1]. A more complex model can also be employed that includes electromagnetism as an extra physics [2]. Nevertheless, the complexity of such problems renders the computational time of simulations extremely high and therefore necessitates inculcation of a strategy that facilitates numerical frugality. One of such strategy involves usage of different meshes for different physics [1] to reduce computation time. However, in this case the idea is to use a more comprehensive reduced-order approximation strategy like the Proper Orthogonal Decomposition (POD) for the reduction of computational cost [3]. Also, it has to be mentioned that the intend herein is to be as non-intrusive as possible therefore a response surface method namely Radial Basis Functions (RBF) is to be used in conjunction with POD [4].

In this proceeding, to depict the efficacy of the methodology, an academic problem involving only two physics (heat transfer and fluid flow) is chosen . Also it has to be mentioned that the finite element (FE) resolutions (wherever needed) have to be performed through COMSOL Multiphysics (commercial FE software) and the POD-RBF to be implemented through MATLAB.

2 Reference problem

As mentioned before, the physics considered here are fluid flow and heat transfer. Consider the two dimensional domain to be studied with applied boundary conditions as shown in Figure 1. For the fluid

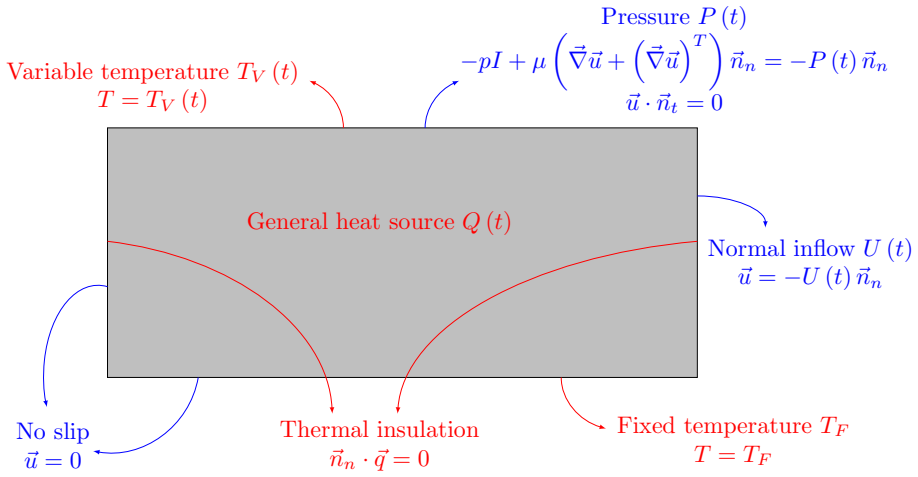

FIGURE 1 – Two dimensional domain to be studied

flow the equations considered are

$$\rho\left(\frac{\partial\vec{u}}{\partial t}+\left(\vec{u}\cdot\vec{\nabla}\right)\vec{u}\right)=\vec{\nabla}\cdot\left(-pI+\mu\left(\vec{\nabla}\vec{u}+\left(\vec{\nabla}\vec{u}\right)^{T}\right)\right)+\vec{F}, \tag{1}$$

$$\rho\vec{\nabla}\cdot\vec{u}=0, \tag{2}$$

and for the heat transfer problem the equation considered is

$$d\rho C_p\frac{\partial T}{\partial t}+d\rho C_p\vec{u}\cdot\vec{\nabla}T+\vec{\nabla}\cdot\left(-dk\vec{\nabla}T\right)=dQ+q_0+dQ_p+dQ_{vd}. \tag{3}$$

Here $\vec{u}$ is the velocity field, ρ is the density, t represents time coordinate, p is the pressure field, μ represents dynamic viscosity, $\vec{F}$ is the volumetric force and I represents the identity tensor. Also, d is the thickness of the domain, C_p is the specific heat at constant pressure, T is the temperature field, k is the thermal conductivity, Q is general heat source, q_0 a general inward heat flux, Q_p a work done by pressure change and Q_{vd} a viscous dissipation term. From Figure 1, $\vec{n}_n$ and $\vec{n}_t$ represent the unit normal and tangential vectors for the corresponding surfaces, and $U(t)$, $P(t)$, $Q(t)$, $T_V(t)$, T_F are user defined.

All these equations are pre-existent in COMSOL Multiphysics and these loading conditions can be easily applied. This non-isothermal laminar single phase problem is solved for a time range 0 s to 1 s, with time step size being 0.1 s. The simulation is conducted using 378 triangular element with 216 nodes, and the solution at the final time step is shown in Figure 2. It has to be mentioned that velocity, pressure and temperature are the main quantities of interest, and the spatial-temporal discretisations remain the same for the subsequent analyses.

3 Separation of physics

The next step is now to separate the physics and simulate each individually and the output of one physics is provided as input to the other. The main process is through a fixed-point iteration which

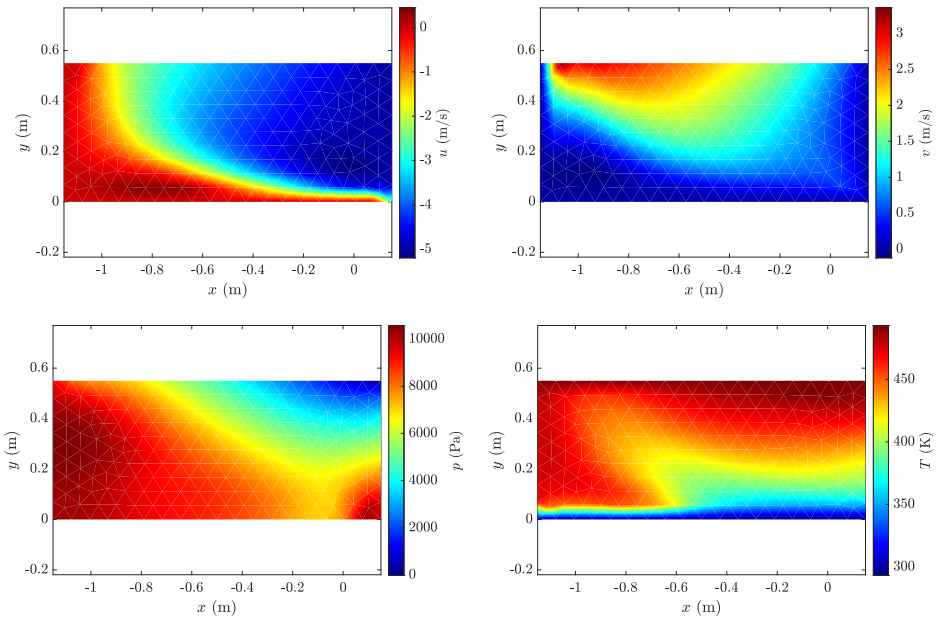

FIGURE 2 – Solution of the coupled problem at the final time step

is controlled by a main MATLAB programme and each physics is solved by COMSOL. The coupled COMSOL model is now decoupled into two separate model files, one for the heat transfer problem and the other for the fluid flow problem. Temperature field is provided as an input for the fluid flow problem and pressure, velocity are provided as inputs to the heat transfer problem. The fixed-point iteration can start with any physics and after its resolution the output is extracted in MATLAB from which a separate MATLAB function is created which is then called in COMSOL while solving the other physics (i.e. output from one physics is given as an input to the other physics). This iterative procedure will continue till a convergence is achieved, and the convergence criteria is measured through a relative error with respect to the previous iteration for each variable. This methodology is depicted in Figure 3. For the first

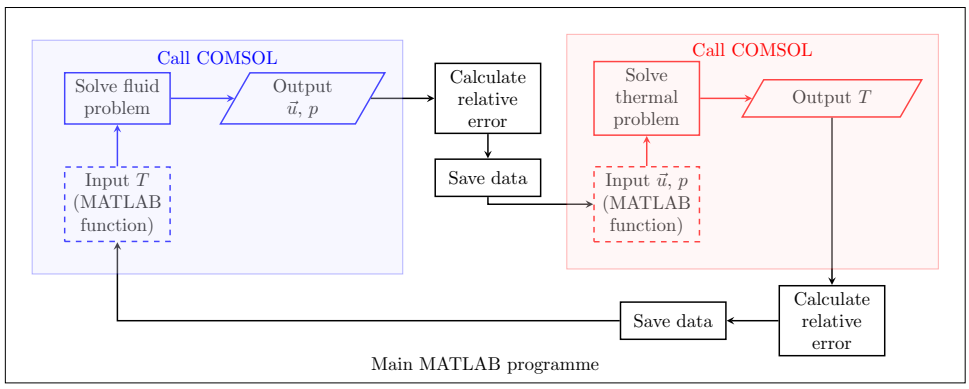

FIGURE 3 – Flow diagram of the fixed point iteration between the two physics

separation attempt, the total decoupled solutions are calculated at each iteration for all the time steps in COMSOL. The errors measured in terms of L2 norms with respect to the coupled reference solutions for every time steps are shown in Figure 4.

Now, the next step is to find the solutions time step by time step, i.e. instead of computing for all time steps through COMSOL with the fixed point iteration acting as an external loop, COMSOL is used to compute the solutions (in a decoupled manner) for each time step and fixed point iterations are performed at each time step till convergence. Also the final solutions of the previous time step is provided as initial condition of the current time step through MATLAB functions. The idea is depicted in Figure 5, where the green boxes essentially represent the fixed point of Figure 3 but for single time steps. The error with

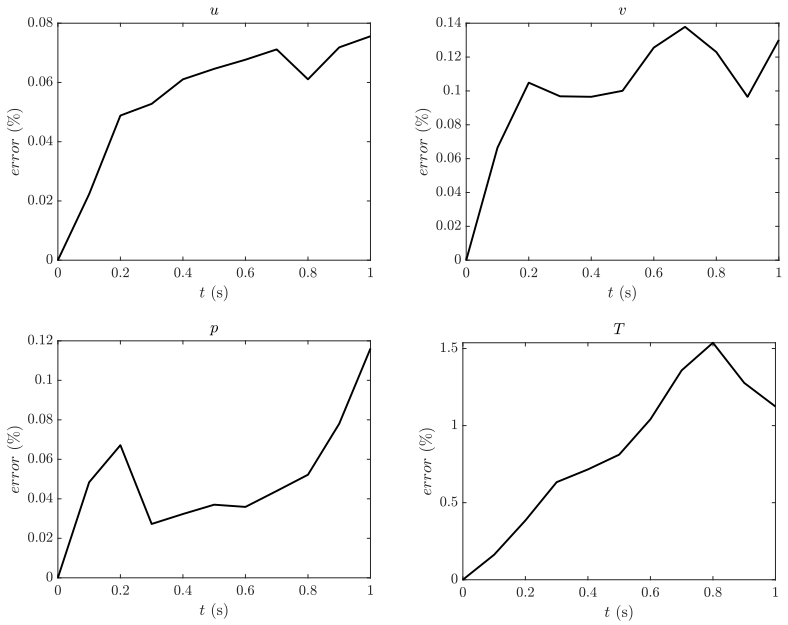

FIGURE 4 – Error of the decoupled solution with respect to coupled solutions

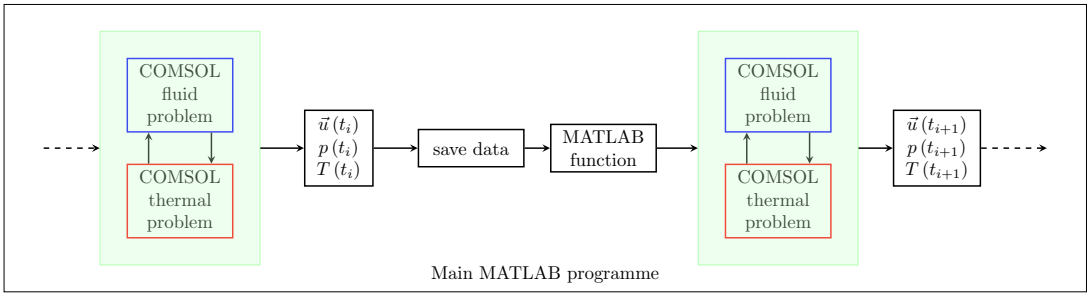

FIGURE 5 – Flow diagram of the time stepping scheme

respect to the coupled reference solution is shown in Figure 6.

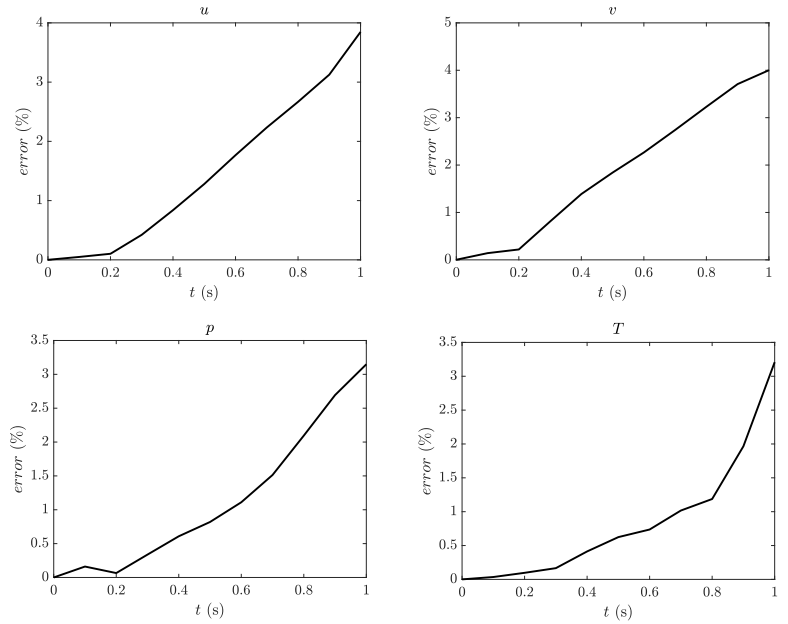

FIGURE 6 – Error of the decoupled solution using the time stepping scheme with respect to coupled solutions

4 Reduced-order modelling

Now the idea herein is to replace one of the full order computation of a physics by a surrogate model. As the fluid flow problem is generally computationally more expensive, herein this physics will be replaced by a reduced-order model.

Consider, for instance the time step $[t_i, t_{i+1}]$. For the first iteration of the fixed point method the full order solutions (through FE in COMSOL) are computed and will serve as the training stage. More precisely, these will serve as the snapshot matrices, and Singular Value Decompositions (SVDs) of the matrices are performed such that

$$\vartheta\left(t_0,\ldots,t_{i+1}\right) = \Phi_\vartheta \Sigma_\vartheta \Psi_\vartheta^T, \text{ with } \vartheta = \{\vec{u}, p, T\}. \tag{4}$$

where Φ_ϑ and Ψ_ϑ are the matrices of left and right singular vectors, and Σ_ϑ is the diagonal matrix containing singular values. From the singular values, it has to be determined how many modes are to be included for each variable. Consider for instance m_ϑ modes are chosen based on the first m_ϑ singular values. Then the matrix containing left singular vectors is truncated to the first m_ϑ columns as

$$\Phi_\vartheta = \Phi_\vartheta^{1,\ldots,m_\vartheta}. \tag{5}$$

These are the spatial modes or the basis vectors. Now the time functions are calculated as

$$\alpha_\vartheta = \Sigma_\vartheta \Psi_\vartheta^T, \tag{6}$$

which are again truncated using the first m_ϑ rows as

$$\alpha_\vartheta = \alpha_\vartheta^{(1,\ldots,m_\vartheta)^T}. \tag{7}$$

Thereby, eq (4) can be rewritten as

$$\vartheta\left(t_0,\ldots,t_{i+1}\right) \approx \Phi_\vartheta \alpha_\vartheta. \tag{8}$$

Now a radial basis function neural network (RBFNN) is created for each $\alpha_{\vec{u}}^j, \alpha_p^j$ using α_T as parameters evolving in the design space (where $j \in [1,\ldots,m_{\vec{u}}]$ or $j \in [1,\ldots,m_T]$). Each row of α_T will represent independent coordinate in the response surface, and each separate network $\text{RBFNN}_{\vec{u}}^j$ and RBFNN_p^j is created for each $\alpha_{\vec{u}}^j, \alpha_p^j$ using α_T as the parametric space of the response surface. It has to be mentioned that the same procedure was applied for the previous time step and therefore through the SVD a maximum of one mode is added in the current time step.

Now for the subsequent iteration of the fixed point method, the thermal problem is solved (full order FE using COMSOL) to get updated $T^{\text{up}}\left(t_{i+1}\right)$ thereby to eventually obtain updated $T^{\text{up}}\left(t_0,\ldots,t_{i+1}\right)$ which is then projected on the basis vectors to obtain the updated time function, i.e.

$$\alpha_T^{\text{up}} = \Phi_T^T T^{\text{up}}. \tag{9}$$

The superscript up indicates the update of the corresponding variables at each fixed point iteration. Using this updated time function α_T^{up}, the updated time functions $\alpha_{\vec{u}}^{\text{up}}$ and α_p^{up} are calculated using

$$\alpha_p^{j,\,\text{up}} = \text{RBFNN}_p^j\left(\alpha_T^{\text{up}}\right), \alpha_{\vec{u}}^{j,\,\text{up}} = \text{RBFNN}_{\vec{u}}^j\left(\alpha_T^{\text{up}}\right). \tag{10}$$

Using these time functions the updated variables are calculated as

$$p^{\text{up}}\left(t_{i+1}\right) = \Phi_p \alpha_p^{\text{up}}\left(t_{i+1}\right), \vec{u}^{\text{up}}\left(t_{i+1}\right) = \Phi_{\vec{u}} \alpha_{\vec{u}}^{\text{up}}\left(t_{i+1}\right), \tag{11}$$

and thereby $p^{\text{up}}\left(t_0,\ldots,t_{i+1}\right)$ and $\vec{u}^{\text{up}}\left(t_0,\ldots,t_{i+1}\right)$. Hence using RBF-POD the FE simulation of the fluid flow problem is avoided and this essentially modifies Figure 5 as shown in Figure 7. The errors with respect to the reference solution are shown in Figure 8.

A total of 11 modes are generated (one for each time step) for approximating each variable. The first three modes (both spatial and temporal) are depicted in Figure 9 and Figure 10 for the velocity field and Figure 11 for the pressure field.

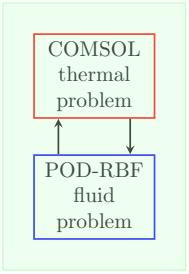

FIGURE 7 – Modification of time stepping scheme to include POD-RBF

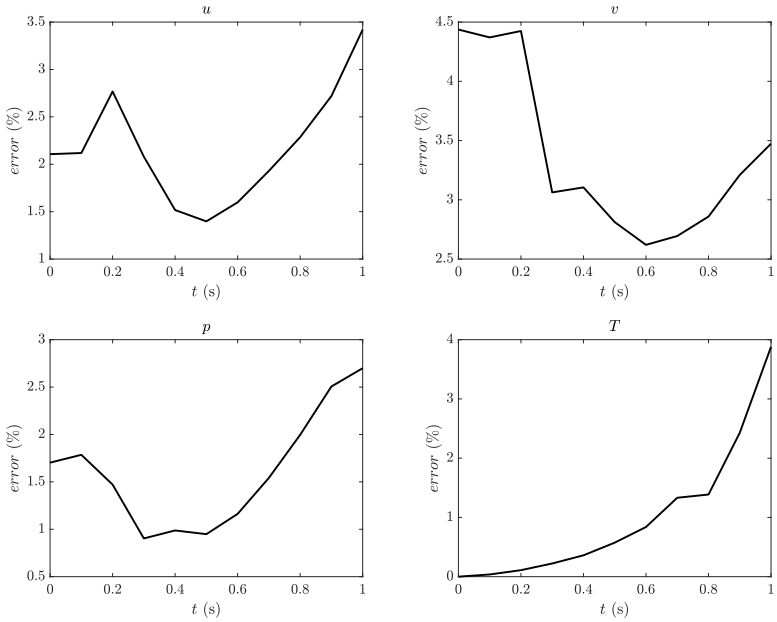

FIGURE 8 – Error of the decoupled solution using the RBF-POD with respect to coupled solutions

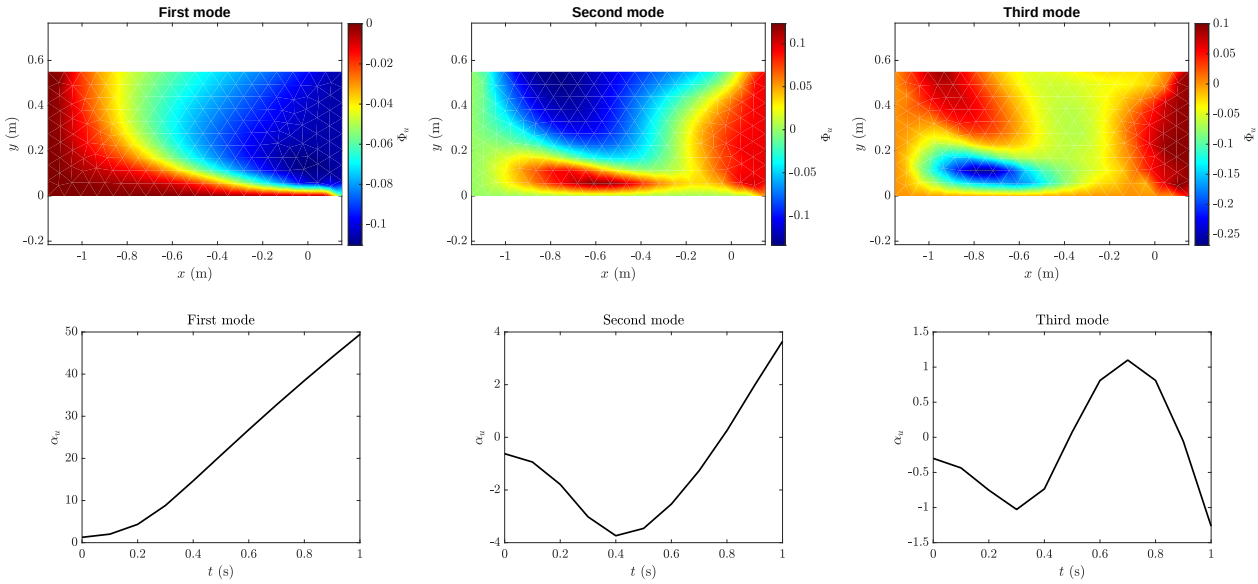

FIGURE 9 – First three space time modes for x-velocity

5 Discussion and conclusion

It is seen that the separation of physics is successful both using fixed point algorithm as an external loop (Figure 4) as well as as a nested loop (Figure 6). It has to be kept in mind that the ultimate goal is

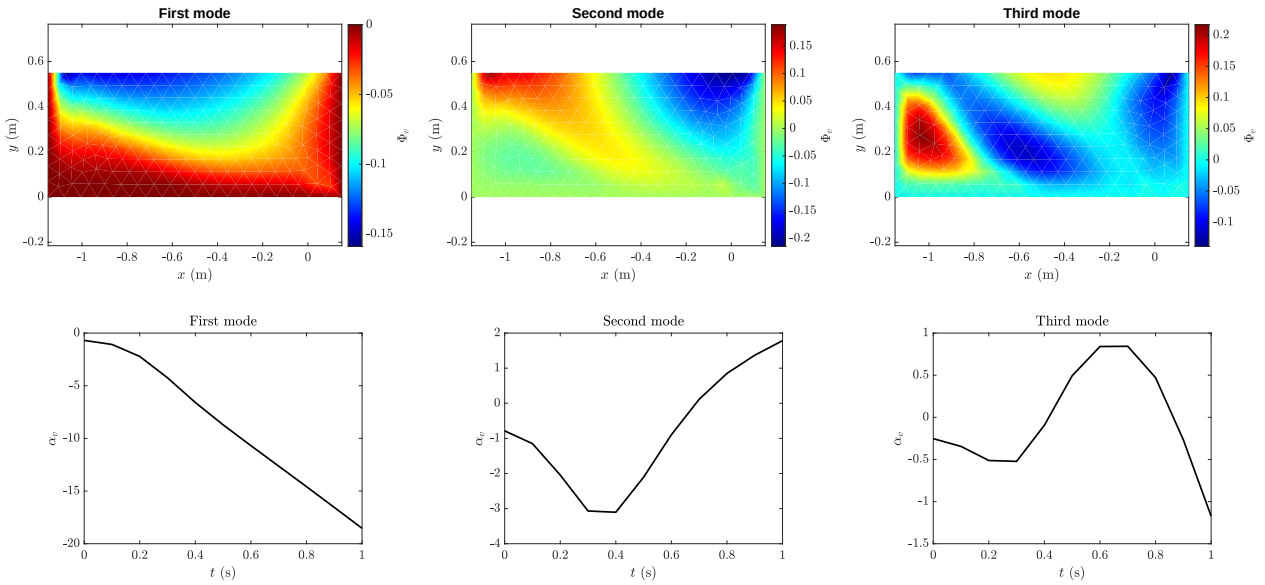

FIGURE 10 – First three space time modes for y-velocity

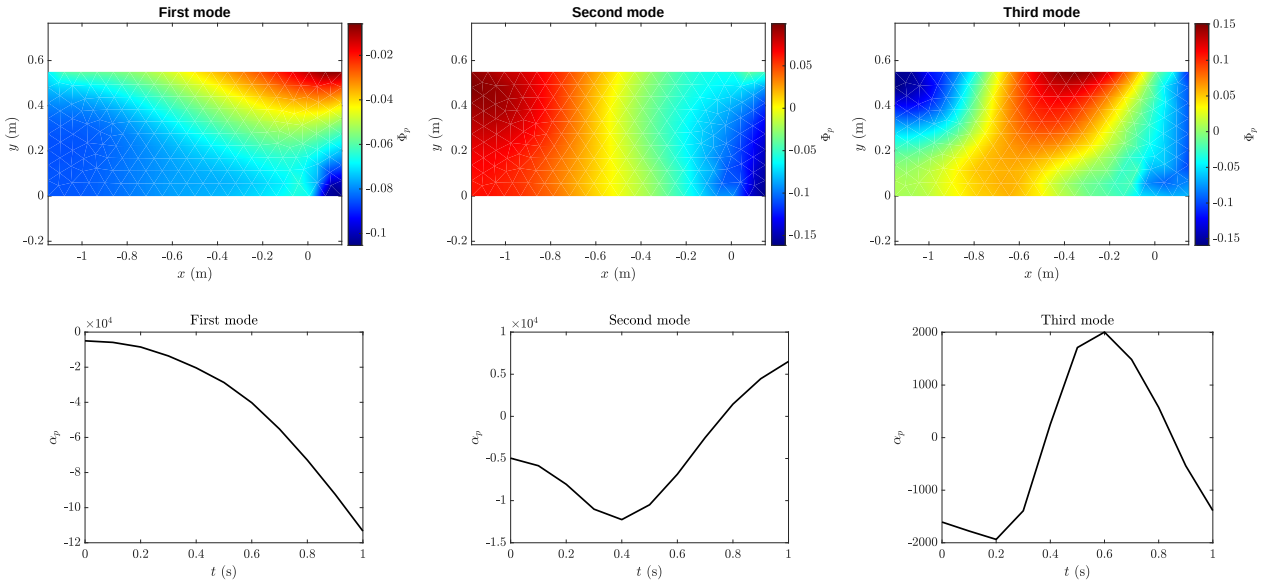

FIGURE 11 – First three space time modes for pressure

to address industrial problems and hence the time stepping decoupling scheme is chosen for inculcating reduced order approximations. The reason behind this is that for a large scale industrial problem a training stage for all the time steps (for the first fixed point iteration) may not be practically feasible, however for individual time steps it might not be a problem. Also creation of the RBFNN is much more accurate and precise when training stages are performed at individual time steps. Using the POD-RBF method, for a given fixed point iteration, the computational time is 47 % of the computation time without the reduced order approximation.

The next steps would be to incorporate phase change in the existing model through level set transport equation. Thereafter, when the methodology is well established, the idea is to apply this theory for large scale industrial problems dedicated to metal transfer processes.

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