Assignment for the Postgraduate Course: Numerical Methods for Ordinary and Partial Differential Equations.

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Abstract

Reduced Order Models (ROM) provide a lower dimensional framework for the computation of a system of differential equations, resulting in faster computational results. In this assignment we are dealing with the stationary Navier-Stokes equation. We solve the equation by using the Finite Element Method in conjunction with Newton's Iteration Method for the nonlinearity. Then to produce a Reduced Order Model, the Proper Orthogonal Decomposition (POD) is introduced using a Singular Value Decomposition (SVD) of the FEM sample solutions. In the last chapter we compare the compression and prediction error of the POD method and provide some graphical results.

Contents

1 The Navier-Stokes equation **1**

2 Error Estimates for the Navies-Stokes equation **2**

3 Proper Orthogonal Decomposition **3**

4 Numerical Results **5**

1 The Navier-Stokes equation

In this assignment we are dealing with the stationary (or steady-state) Navier-Stokes equation (standard 2D cavity flow) whose governing equation is:

$$\mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = 0 \tag{1}$$
$$\nabla \cdot u = 0 \tag{2}$$

where $\mathbf{u}$ is the velocity, p is the pressure, $\nu = \frac{1}{Re}$ is the viscocity of the fluid and Re is the Reynolds number. We derive the weak form of the stationary Navier-Stokes equation by multiplying (1) by a test vector $\mathbf{v}$ and integrate. We obtain

$$\int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} + \mathbf{u} \cdot \nabla \mathbf{u} \cdot \mathbf{v} + p \nabla \cdot \mathbf{u} \, d\Omega = 0 \quad \forall \mathbf{v} \in H_0^1(\Omega) \tag{3}$$
$$\int_\Omega q \nabla \cdot \mathbf{u} \, d\Omega = 0 \quad \forall q \in L_0^2(\Omega) \tag{4}$$

Here L_0^2 is the space of square-integrable functions having inner product $(p, q) = \int_\Omega pq \, d\Omega$ and norm $\|q\|_0 = (q, q)^{\frac{1}{2}}$. To handle the term $\nabla\mathbf{u} : \nabla\mathbf{v}$ we define the bilinear form

$$a(\mathbf{u}, \mathbf{v}) = \nu \int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v} \, d\Omega = \nu \int_\Omega \sum_{j=1}^{n} \sum_{i=1}^{N} \frac{\partial \mathbf{u}_i}{\partial x_j} \frac{\partial \mathbf{v}_i}{\partial v_j} \, d\Omega \quad \forall \mathbf{u}, \mathbf{v} \in H^1(\Omega) \tag{5}$$

where $N = 2$ for the two-dimensional problem. To handle the incompressibility term, we define the bilinear form

$$b(\mathbf{v}, q) = \int_\Omega q \nabla \cdot \mathbf{v} \, d\Omega = \int_\Omega q \sum_{i=1}^{N} \frac{\partial \mathbf{v}}{\partial x_i} \, d\Omega \quad \forall \mathbf{v} \in H^1(\Omega) \quad q \in L_0^2(\Omega) \tag{6}$$

$N = 2$ for the two-dimensional problem. To handle the nonlinear term $\mathbf{u} \cdot \nabla\mathbf{u} \cdot \mathbf{v}$, we define the trilinear form

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) = \int_\Omega \mathbf{w} \cdot \nabla\mathbf{u} \cdot \mathbf{v} \, d\Omega = \int_\Omega \sum_{i=1}^{N} \sum_{j=1}^{N} \mathbf{w}_j \frac{\partial \mathbf{u}_i}{\partial x_j} \mathbf{v}_i \, d\Omega \quad \forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in H^1(\Omega) \tag{7}$$

$N = 2$ for the two-dimensional problem. We may then rewrite (1) as

$$a(\mathbf{u}, \mathbf{v}) + c(\mathbf{u}, \mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) = 0 \tag{8}$$

$$b(\mathbf{u}, q) = 0 \tag{9}$$

The system is nonlinear and we will use Newton's Iteration Scheme for the nonlinearity. We will now seek a discretization of the weak form above. We seek $\mathbf{u}^h \in V_0^h \subset H_0^1(\Omega)$ and
$p^h \in S_0^h \subset L_0^2(\Omega)$, such that

$$a(\mathbf{u}^h, \mathbf{v}^h) + c(\mathbf{u}^h, \mathbf{u}^h, \mathbf{v}^h) + b(\mathbf{v}^h, p^h) = 0 \quad \forall \mathbf{v}^h \in V_0^h \tag{10}$$

$$b(\mathbf{u}^h, q^h) = 0 \quad \forall q^h \in S_0^h \tag{11}$$

The bases functions are $\{\mathbf{v}_k\}_{k=1}^K$ for V_0^h and $\{q_j\}_{j=1}^J$ for S_0^h. We have a nonlinear system of equations in (10) and (11) and substituting $\mathbf{v}$ and q our approximate solutions are

$$\mathbf{u}^h = \sum_{k=1}^{K} \beta_k \mathbf{v}_k(x), \quad p^h = \sum_{j=1}^{J} a_j q_j(x) \tag{12}$$

and from (2) yields $\sum_{k=1}^K b(\mathbf{v}_k, q_i)\beta_k = 0, \quad i = 1, ..., J$

2 Error Estimates for the Navies-Stokes equation

The discrete solutions of FEM satisfy the following error estimates (1)

$$\|u - u^h\|_1 \le C_1 \inf_{\mathbf{v}^h \in V_0^h} \|\mathbf{u} - \mathbf{v}^h\|_1 + C_2 \Theta \inf_{q \in S_0^h} \|p - q^h\|_0 \tag{13}$$

$$\|p - p^h\|_0 \le C_3 \inf_{\mathbf{v}^h \in V_0^h} \|\mathbf{u} - \mathbf{v}^h\|_1 + C_4 \inf_{q^h \in S_0^h} \|p - q^h\|_0 \tag{14}$$

where Θ is given by,

$$\Theta = \sup_{\mathbf{z}^h \in \mathbf{Z}^h,\ \|\mathbf{z}\|_1 = 1} \inf_{\mathbf{z} \in \mathbf{Z}} \|\mathbf{z} - \mathbf{z}^h\|_1, \quad \mathbf{z} \in \mathbf{Z},\ \mathbf{z}^h \in \mathbf{Z}^h$$

$$\mathbf{Z} = \left\{ \mathbf{v} \in H_0^1(\Omega) : b(\mathbf{v}, q) = 0 \quad \forall q \in L_0^2(\Omega) \right\}$$

$$\mathbf{Z}^h = \left\{ \mathbf{v}^h \in V_0^h : b(\mathbf{v}^h, q^h) = 0 \quad \forall q \in S_0^h \right\}$$

3 Proper Orthogonal Decomposition

In the context of solving PDEs using the finite element method, the ROM solution is a linear combination of basis vectors which are obtained from a collection of solutions to the PDE model, where each solution has a different set of values assigned to parameters of interest. We use POD to obtain reduced order model basis vectors from a collection of solutions with known parameters, using Singular Value Decomposition (SVD) (2). Using linear combinations of a small number of these basis vectors allows the dimensionality of the problem to be reduced with a small sacrifice of information, thus reducing the computational work. One requirement of this technique is that any combination of parameters in the model for which we wish to obtain a solution must be bracketed by the parameter values used in the collection of solutions to which SVD has been applied.

The typical process for producing a reduced order model of a PDE or system of PDEs solved using FEM involves the following steps.

1. Sampling of the parameter space.
2. The generation of the set of sample solutions, commonly referred to as "snapshots," with the sampled parameter sets.
3. The creation of the reduced order model basis vectors.
4. Obtaining the approximate solution as a linear combination of the ROM basis vectors that satisfy the given PDEs.

The technique employed for ROM in this chapter is POD, using SVD. Computationally, the SVD is implemented as a built-in routine in Python packages, such as NumPy and SciPy. To generate a complete set of POD modes, a data set is compiled and represented as the matrix $\mathbf{X}$. Each row of the matrix consists of a sample solution taken at a specific value of time, and the number of rows in the matrix is the number of samples taken at evenly spaced values in time. Therefore if the data consists of m samples with n points per sample. The process of computing the SVD for a full rank matrix $\mathbf{X}$ can be summarized as solving two eigenvalue problems for the associated square and symmetric, positive-definite, covariance matrices constructed by taking the products $\mathbf{X}\mathbf{X}^T$ and $\mathbf{X}^T\mathbf{X}$. We seek the decomposition $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$, where $\mathbf{U} \in \mathbb{R}^{m\times m}$, $\mathbf{V} \in \mathbb{R}^{n\times n}$, and $\boldsymbol{\Sigma} \in \mathbb{R}^{m\times n}$ anticipating $\mathbf{U}$ and $\mathbf{V}$ will be orthogonal matrices, and Σ will be diagonal matrix. From $\mathbf{X}^T\mathbf{X} = \mathbf{V}\boldsymbol{\Sigma}^T\mathbf{U}^T\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$ and $\mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{V}\boldsymbol{\Sigma}^T\mathbf{U}^T$ we observe $\mathbf{X}^T\mathbf{X} = \mathbf{V}\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\mathbf{V}^T$ and $\mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\mathbf{U}^T$ if our speculation regarding the orthogoniality of $\mathbf{U}$ and $\mathbf{V}$ holds. Since we are anticipating $\mathbf{U}$ and $\mathbf{V}$ to be orthogonal, $\mathbf{U}$ and $\mathbf{V}$ are the (normalized) matrices of eigenvectors obtained from them. The matrix $\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}$ is, then, the diagonal matrix of squared eigenvalues which are the same for both matrices, $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}\mathbf{X}^T$. The singular values $\sigma_1 \ldots \sigma_n$ of the $m \times n$ matrix A are the square roots $\sigma_i = \sqrt{\lambda_i}$ of the eigenvalues, λ_i, of $\mathbf{X}^T\mathbf{X}$. The eigenvectors of $\mathbf{X}^T\mathbf{X}$ are the singular vectors of $\mathbf{X}$. The entries of matrix $\mathbf{\Sigma}$ are σ_i the singular values of $\mathbf{X}$ in descending order. In a matrix form the factorization above is expressed as

$$\mathbf{X} = \begin{bmatrix} \vec{u}_1 \\ \vdots \\ \vec{u}_i \\ \vdots \\ \vec{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_j & & \\ & & & \ddots & \\ & & & & \sigma_n \\ 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} \vec{\phi}_1 \\ \vdots \\ \vec{\phi}_j \\ \vdots \\ \vec{\phi}_n \end{bmatrix} \tag{15}$$

As a result the singular value decomposition of the k-th row of $\mathbf{X}$ into

$$\vec{\chi}_k = \sum_{j=1}^{n} \sigma_j u_{kj} \vec{\phi}_j \tag{16}$$

Hence, the SVD returns a complete orthonormal set of basis functions for the rows of the data matrix $\mathbf{X}$. The elements of this basis are the vectors $\vec{\phi}_j$ and are referred to as the POD modes. The key idea is embodied in the previous equation. Specifically, the POD method attempts to provide an accurae approximation of the $\sigma_j u_{kj}$ with a system of ordinary differential equations.

The relative importance of the j-th POD mode $\vec{\phi}_j$ in the approximation of the matrix $\mathbf{X}$ is determined by the relative energy E_j of that mode, defined as

$$E_j = \frac{\sigma_j^2}{\sum_{i=1}^{n} \sigma_i^2} \tag{17}$$

where the total energy is normalized such that $\sum_{j=1}^{n} E_j = 1$. If the sum of the energies of the retained modes is unity, then these modes can be used to completely reconstruct $\mathbf{X}$. By examining the slope of σ_i versus i, we determine at which i the σ_i no longer decrease significantly in magnitude, and designate p to equal the value of i. The first p columns of $\mathbf{U}$ are selected as the most significant POD basis vectors.

When using POD, a measure of the fraction of total information contained in the snapshot set by the p basis vectors can be made. It is important to note that the following measure addresses the fidelity of the POD basis vectors to the snapshot set, not the fidelity of the approximate solution to the actual solution of the PDE. The ratio of the singular values of the rank-one elements which are preserved in the approximation, to the total sum of the singular values of the matrix. That is for a matrix M, of rank N, with singular values $\sigma_i,\ i = 1, ..., N$ if we choose to use p rank-one elements to approximate the matrix M_p, we describe information content e_{ROM} according to

$$e_{\mathrm{ROM}} = \frac{\sum_{i=1}^{p} \sigma_i^2}{\sum_{i=1}^{N} \sigma_i^2} \tag{18}$$

Let us consider the following PDE System:

$$\mathbf{u}_t = N(\mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, ..., x, t) \tag{19}$$

where $\mathbf{u}$ is a vector of physically relevant quantities and the subscripts t and x denote partial differentiation. The function $N(\cdot)$ captures the space-time dynamics that is specific to the system being considered. Along with this PDE are some prescribed boundary conditions and initial conditions. Here we deal with the stationary flow, where the velocity and the pressure do not change in time. Hence, $\mathbf{u}_t = 0$ and these flows are modelled by the so-called stationary or steady-state Navier–Stokes equations governed by

$$-\nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = f \text{ in } \Omega \tag{20}$$

$$\nabla\cdot\mathbf{u} = 0 \text{ in } \Omega \tag{21}$$

The discrete form of the FEM solutions are

$$p^h = \sum_{j=1}^{J} \eta_j q_j \quad \mathbf{u}^h = \sum_{k=1}^{K} \mu_k \mathbf{v}_k \tag{22}$$

Substituting into the discrete weak form, we obtain

$$\sum_{k=1}^{K} a(\mathbf{v}_k, \mathbf{v}_l)\mu_k + \sum_{k=1,\ \mu=1}^{K} c(\mathbf{v}_m, \mathbf{v}_k, \mathbf{v}_l)\mu_k\mu_m + \sum_{j=1}^{J} b(\mathbf{v}_l, q_j)\eta_j = 0, \quad l = 1, \dots, K \tag{23}$$

$$\sum_{k=1}^{K} b(\mathbf{v}_k, q_i)\mu_k = 0, \quad i = 1, \dots, J \tag{24}$$

Then with the basis set $(\phi_i, \psi_i)_{i=1}^{N}$ we built with the POD method, our weak form reads

$$\sum_{k=1}^{N} a(\phi_k, \phi_l)\mu_k + \sum_{k=1,\ m=1}^{N} c(\phi_m, \phi_k, \phi_l)\mu_k\mu_m + \sum_{j=1}^{N} b(\phi_l, \psi_j)\eta_j = 0 \quad l = 1, \dots, N \tag{25}$$

$$\sum_{k=1}^{N} b(\phi_k, \psi_i)\mu_k = 0 \quad i = 1, \dots, N \tag{26}$$

Since the basis $(\phi_i, \psi_i)_{i=1}^{N}$ has a much lower dimensionality than the (local) basis used during the offine phase (snapshot solutions), the solution of this new problem is expected to be much faster the standard FEM method.

4 Numerical Results

The following figure shows the POD basis that was produced by 61 sample FEM solutions inside the the parameter range $(1, 151)$ of the Reynolds number *Re* (3).

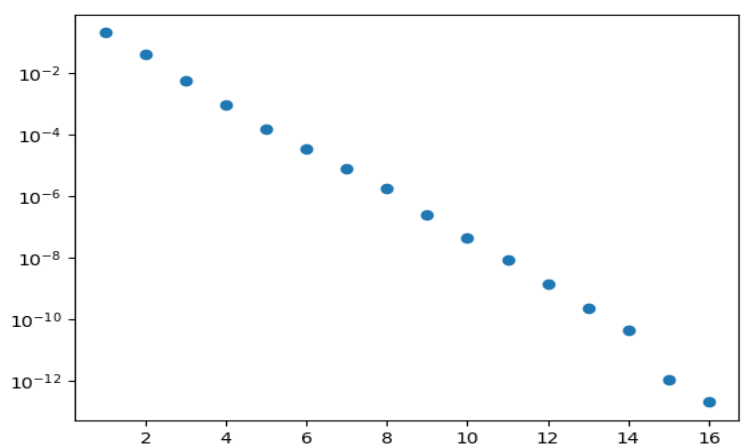
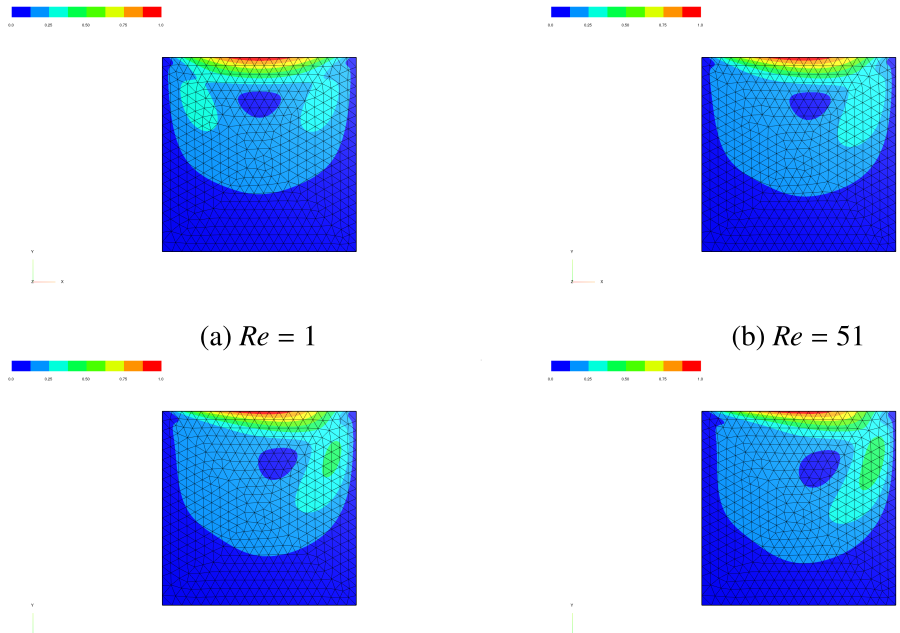


Figure 1: POD basis.

The figures below show 4 FEM solutions for 4 different Reynolds numbers.



(a) $Re = 1$

(b) $Re = 51$

(c) $Re = 101$

(d) $Re = 151$

Figure 2: FEM solutions for $Re = 1,\ 51,\ 101$ and 151.

The following table describes the compression (the convergence of the POD basis) and approximation error (the convergence of the computed ROM approximation) of the POD method for the target Reynolds number $Re = 101$ and P3/P2 elements of the stationary Navier-Stokes equation that was described at the beginning.

Table 1: ROM Approximation.

Dim.	% Energy	Comp.Error	Pred.Error
1	95.779	2.32494E-2	7.34205E-2
2	99.914	3.22230E-3	7.73318E-2
4	100.00	8.98000E-5	7.90192E-2
8	100.00	1.00000E-7	7.81678E-2
16	100.00	0.00000E-7	7.78539E-2

Below we provide the computational time of the snapshot generation function and the ROM method.

Table 2: Snapshot Generation Time.

No. of Snaps	10	20	30	40	50	60
Snap.Time	9.98	22.23	43.05	70.66	96.43	123.70

In the end we present the time for computing the POD basis and ROM solutions for different POD modes.

Table 3: Times of the POD algorithm.

no. of modes	POD basis	ROM recon.	ROM sol.
2	14.45	0.0067	0.10
4	14.84	0.0144	0.13
8	14.60	0.0085	0.22
16	19.04	0.0116	0.44

References

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[3] A. Gruber, M. Gunzburger, L. Ju, and Z. Wang, “A comparison of neural network architectures for data-driven reduced-order modeling,” *Computer Methods in Applied Mechanics and Engineering*, vol. 393, p. 114764, 2022.