Model Order Reduction for Multi-scale, Multi-physics Problems

Karthik Duraisamy

Computational AeroSciences Laboratory

caslab.engin.umich.edu & afcoe.engin.umich.edu

Projection

Consider a sub-space $\mathcal{S}_1 \subset \mathbb{R}^m$ spanned by the basis functions $\mathbf{U} = \{\mathbf{u}_1, \mathbf{u}_2, ...\mathbf{u}_n\}$, where $\mathbf{U} \in \mathbb{R}^{m \times n}$ and $\mathbf{u} \in \mathbb{R}^m$.

If $\mathbf{U}$ is an orthonormal matrix, then $\mathbf{U}^T\mathbf{U} = \mathbf{I}$.

A projection matrix $\mathbf{\Pi} \in \mathbb{R}^{m \times m}$ satisfies the following property : $\mathbf{\Pi}^2 = \mathbf{\Pi}$.

If $rank(\mathbf{\Pi}) = k$, then there exists a basis $\mathbf{X}$ such that

$$\mathbf{\Pi} = \mathbf{X} \begin{bmatrix} \mathbf{I}_k & . \\ . & \mathbf{0}_{m-k} \end{bmatrix} \mathbf{X}^{-1}.$$

We can separate the bases into two sets

$$\mathbf{X} = [\mathbf{X}_1 \;\; ; \;\; \mathbf{X}_2], \quad with \;\; \mathbf{X}_1 \in \mathbb{R}^{m \times k}, \quad \mathbf{X}_2 \in \mathbb{R}^{m \times (m-k)}.$$

For any vector $\mathbf{x} \in \mathbb{R}^m$, we have

- $\mathbf{\Pi x} \in \; range(\mathbf{X}_1) = \; range(\mathbf{\Pi}) = \mathcal{S}_1$
- $(\mathbf{I} - \mathbf{\Pi})\mathbf{x} \in \; range(\mathbf{X}_2) = range(\mathbf{I} - \mathbf{\Pi}) = \; kernel(\mathbf{\Pi}) = \mathcal{S}_2$.

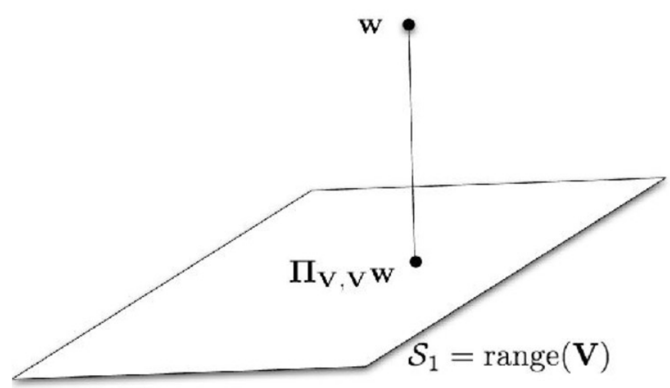
So $\mathbf{\Pi}$ defines the projection onto $\mathcal{S}_1$ parallel to $\mathcal{S}_2$.

Also, $\mathcal{S}_1 \oplus \mathcal{S}_2 = \mathbb{R}^m$.

Projection

An orthogonal projection is defined by $\mathbf{\Pi} = \mathbf{V}\mathbf{V}^{\mathrm{T}}$.
Where $\mathbf{V}$ is a basis set that spans $\mathcal{S}_1$.

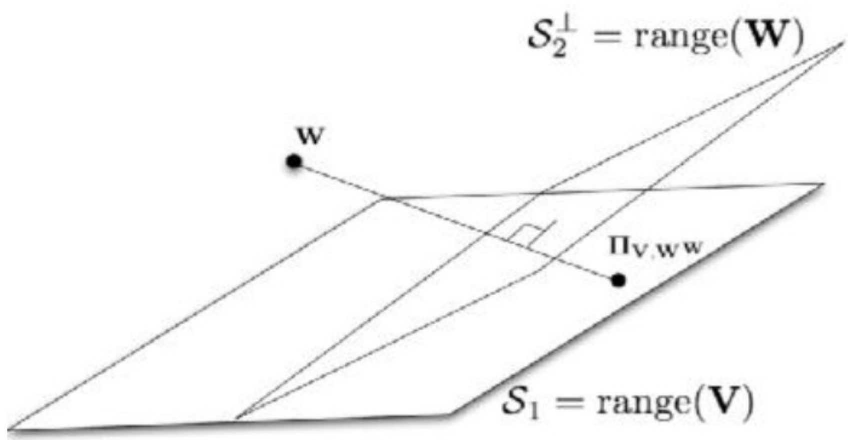
$$\mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\mathbf{w} = \mathbf{V}\mathbf{V}^T\mathbf{w}$$



Projection

An oblique projection is defined by $\mathbf{\Pi} = \mathbf{V}[\mathbf{W}^{\mathrm{T}}\mathbf{V}]^{-1}\mathbf{W}^{\mathrm{T}}$.

Which describes the projection onto $\mathcal{S}_1$ (spanned by V) perpendicular to $\mathcal{S}_2^{\perp}$ (spanned by $\mathbf{W}$).



Projection-based Model Reduction

Consider the high-fidelity model (HFM),

$$\frac{d\mathbf{q}(t)}{dt} = \mathbf{f}(\mathbf{q}(t)) \quad ; \quad \mathbf{q}(0) = \mathbf{q}_0$$

From modal expansion of the solution $\mathbf{q}$ we have,

$$\tilde{\mathbf{q}} = \mathbf{V}\mathbf{q}_r$$

Substitute the modal expansion in the HFM,

$$\frac{d\mathbf{V}\mathbf{q}_r(t)}{dt} = \mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{V}\mathbf{q}_r(0) = \mathbf{q}_0$$

$\mathbf{q} \in \mathbb{R}^n$

$\mathbf{V} \in \mathbb{R}^{n\times k}$

$\mathbf{q}_r \in \mathbb{R}^k$

$\mathbf{W} \in \mathbb{R}^{n\times k}$

Projection-based Model Reduction

Let's define a test basis $\mathbf{W}$ and project the equation onto the test subspace,

$$\mathbf{W}^T\mathbf{V}\frac{d\mathbf{q}_r(t)}{dt} = \mathbf{W}^T\mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{W}^T\mathbf{V}\mathbf{q}_r(0) = \mathbf{W}^T\mathbf{q}_0$$

Special case: Galerkin projection

If the test subspace is the same as the trial subspace (i.e., $\mathbf{W} = \mathbf{V}$), then the ROM ODE is,

$$\frac{d\mathbf{q}_r(t)}{dt} = \mathbf{V}^T\mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{q}_r(0) = \mathbf{V}^T\mathbf{q}_0$$

Errors in ROMs

$$
\begin{aligned}
\boldsymbol{\epsilon}(t) &= \mathbf{q}(t) - \tilde{\mathbf{q}}(t) \\
&= \mathbf{q}(t) - \mathbf{V}\mathbf{q}_r(t) \\
&= \mathbf{q}(t) - \boldsymbol{\Pi}\mathbf{q}(t) + \boldsymbol{\Pi}\mathbf{q}(t) - \mathbf{V}\mathbf{q}_r(t) \\
&= [(\mathbf{I} - \boldsymbol{\Pi})\mathbf{q}(t)] + [\boldsymbol{\Pi}\mathbf{q}(t) - \mathbf{V}\mathbf{q}_r(t)] \\
&= \boldsymbol{\epsilon}_{\boldsymbol{\Pi}}(t) + \boldsymbol{\epsilon}_{\|}(t).
\end{aligned}
$$

$$
\begin{aligned}
\frac{d\boldsymbol{\epsilon}_{\|}}{dt} &= \frac{d}{dt}[\boldsymbol{\Pi}\mathbf{q}(t)] - \frac{d}{dt}[\mathbf{V}\mathbf{q}_r(t))] \\
&= \frac{d}{dt}[\boldsymbol{\Pi}\mathbf{q}(t)] - \frac{d}{dt}\tilde{\mathbf{q}}(t) \\
&= \frac{d}{dt}[\boldsymbol{\Pi}\mathbf{q}(t)] - \boldsymbol{\Pi}\mathbf{f}(\tilde{\mathbf{q}}(t), t)
\end{aligned}
$$

Errors in ROMs

$$\frac{d\boldsymbol{\epsilon}_{\|}}{dt} = \boldsymbol{\Pi}\left[\mathbf{f}(\mathbf{q}(t),t) - \mathbf{f}(\tilde{\mathbf{q}}(t),t)\right] \qquad \boldsymbol{\epsilon}_{\|}(0) = \mathbf{0}.$$

$$\frac{d\mathbf{q}(t)}{dt} = \mathbf{f}(\mathbf{q}(t),t) \tag{7.37}$$

$$\boldsymbol{\Pi}\frac{d\mathbf{q}(t)}{dt} + (\mathbf{I}-\boldsymbol{\Pi})\frac{d\mathbf{q}(t)}{dt} = \mathbf{f}(\boldsymbol{\Pi}\mathbf{q}(t),t) + [\mathbf{f}(\mathbf{q}(t),t) - \mathbf{f}(\boldsymbol{\Pi}\mathbf{q}(t),t)] \tag{7.38}$$

$$\frac{d\boldsymbol{\Pi}\mathbf{q}(t)}{dt} = \boldsymbol{\Pi}\mathbf{f}(\boldsymbol{\Pi}\mathbf{q}(t),t) + \boldsymbol{\Pi}[\mathbf{f}(\mathbf{q}(t),t) - \mathbf{f}(\boldsymbol{\Pi}\mathbf{q}(t),t)] \tag{7.39}$$

Thus if we have the exact $\tilde{\mathbf{q}}(t) = \boldsymbol{\Pi}\mathbf{q}(t)$,

$$\frac{d\tilde{\mathbf{q}}(t)}{dt} = \boldsymbol{\Pi}\mathbf{f}(\tilde{\mathbf{q}}(t),t) + \boldsymbol{\Pi}\left[\mathbf{f}(\mathbf{q}(t),t) - \mathbf{f}(\tilde{\mathbf{q}}(t),t)\right] \tag{7.40}$$

Thus, the term $\boldsymbol{\Pi}\left[\mathbf{f}(\mathbf{q}(t),t) - \mathbf{f}(\tilde{\mathbf{q}}(t),t)\right]$ represents the impact of the unresolved modes on the resolved modes, also known as the sub-scale terms. If not accounted for, this term contributes directly to the evolution of the parallel error.

Errors in ROMs

$$\frac{1}{2}\frac{d\boldsymbol{\epsilon}_{\parallel}^{T}\boldsymbol{\epsilon}_{\parallel}}{dt} = \frac{1}{2}\boldsymbol{\epsilon}_{\parallel}^{T}[\boldsymbol{\Pi}\mathbf{A} + [\boldsymbol{\Pi}\mathbf{A}]^{T}]\boldsymbol{\epsilon}_{\parallel} + \boldsymbol{\epsilon}_{\parallel}^{T}\boldsymbol{\Pi}\mathbf{A}\boldsymbol{\epsilon}_{\perp} \quad (7.44)$$

we get the necessary condition [2], that $\boldsymbol{\Pi}\mathbf{A} + [\boldsymbol{\Pi}\mathbf{A}]^{T}$ should be negative definite. Additionally, the interaction between the parallel and orthogonal errors may also affect stability in a profound manner.

In Galerkin ROMs, we do not have a great degree of control over $\boldsymbol{\Pi}$. Petrov Galerkin methods give us additional control knobs to improve both accuracy and stability.

Petrov-Galerkin Projection

Consider the fully-discrete equations (e.g. with Euler explicit time-stepping):

$$\frac{\mathbf{V}\mathbf{q}_r^n - \mathbf{V}\mathbf{q}_r^{n-1}}{\Delta t} = \mathbf{f}(\mathbf{V}\mathbf{q}_r^{n-1})$$

Let's define a residual,

$$\mathbf{r}(\mathbf{q}_r^n) = \frac{\mathbf{V}\mathbf{q}_r^n - \mathbf{V}\mathbf{q}_r^{n-1}}{\Delta t} - \mathbf{f}(\mathbf{V}\mathbf{q}_r^{n-1})$$

With Euler implicit we will have,

$$\mathbf{r}(\mathbf{q}_r^n) = \frac{\mathbf{V}\mathbf{q}_r^n - \mathbf{V}\mathbf{q}_r^{n-1}}{\Delta t} - \mathbf{f}(\mathbf{V}\mathbf{q}_r^n)$$

Petrov-Galerkin Projection

Then the update to the next time step is obtained by a residual minimization approach,

$$\mathbf{q}_r^n = arg \min_{\hat{\mathbf{q}}_r \in range(\mathbf{V})} \|\mathbf{r}(\hat{\mathbf{q}}_r)\|_2^2$$

Let's define the function to be minimized as,

$$m(\mathbf{q}_r) = [\mathbf{r}(\mathbf{q}_r^n)]^T [\mathbf{r}(\mathbf{q}_r^n)]$$

Petrov-Galerkin Projection

The update to the next time step is obtained by a residual minimization approach,

$$\mathbf{q}_r^n = arg \min_{\hat{\mathbf{q}}_r \in range(\mathbf{V})} \|\mathbf{r}(\hat{\mathbf{q}}_r)\|_2^2$$

This can be written in a more general form as,

$$\mathbf{q}_r^n = arg \min_{\hat{\mathbf{q}}_r \in range(\mathbf{V})} \|\mathbf{A}\mathbf{r}(\hat{\mathbf{q}}_r)\|_2^2$$

Petrov-Galerkin Projection

The minimization problem can be written in a more general form as,

$$\mathbf{q}_r^n = arg \min_{\hat{\mathbf{q}}_r \in range(\mathbf{V})} \|\mathbf{A}\mathbf{r}(\hat{\mathbf{q}}_r)\|_2^2$$

Which is equivalent to a Petrov-Galerkin projection,

$$\mathbf{W}(\mathbf{q}_r^n)^T[\mathbf{r}(\mathbf{q}_r^n)] = 0$$

Where,

$$\mathbf{W}(\mathbf{q}_r^n) = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}_r^n)}{\partial \mathbf{q}_r^n}\right] = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}^n)}{\partial \mathbf{q}^n}\right]\mathbf{V}$$

Petrov-Galerkin Projection

The test subspace in Petrov-Galerkin projection is,

$$\mathbf{W}(\mathbf{q}_r^n) = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}_r^n)}{\partial \mathbf{q}_r^n}\right] = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}^n)}{\partial \mathbf{q}^n}\right]\mathbf{V}$$

Which is the same as Galerkin if,

- $\Delta t \to 0$
- Scheme is explicit
- $\mathbf{A}^T\mathbf{A} = \left[\frac{\partial \mathbf{r}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}$

Petrov-Galerkin Projection

The test subspace in Petrov-Galerkin projection is,

$$\mathbf{W}(\mathbf{q}_r^n) = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}_r^n)}{\partial \mathbf{q}_r^n}\right] = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}^n)}{\partial \mathbf{q}^n}\right]\mathbf{V}$$

- For LSPG: $\mathbf{A} = \mathbf{I}$
- For balanced truncation: $\mathbf{W} = \mathcal{W}_c\mathcal{W}_o$

Linear Stability : 1/2

Continuous FOM

$$\frac{d\mathbf{q}}{dt} = \mathbf{J}\mathbf{q}, \quad \mathbf{q}(0) = \mathbf{q}_0,$$

Discrete FOM

$$(\mathbf{I} - \Delta t \mathbf{J})\mathbf{q}^n = \mathbf{q}^{n-1}, \quad \mathbf{q}^0 = \mathbf{q}_0$$

Decomposition

$$\tilde{\mathbf{q}}(t) \triangleq \mathbf{V}\mathbf{q}_r(t), \text{ where } \mathbf{V} \in \mathbb{R}^{N \times k} \text{ and } \mathbf{q}_r \in \mathbb{R}^k$$

Theorem 1 : *If the Discrete FOM above is asymptotically stable in the sense of* $\left\|(\mathbf{I} - \Delta t \mathbf{J})^{-1}\right\|_2 \leq 1$ *, then the Backward Euler Galerkin ROM is also asymptotically stable if* $\lambda_n\left(\mathbf{I} - 0.5\Delta t(\mathbf{J} + \mathbf{J}^T)\right) \geq 1$

Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation C Huang, C Wentland, K Duraisamy, C Merkle, JCP 2021.

Linear Stability : 2/2

Continuous FOM

$$\frac{d\mathbf{q}}{dt} = \mathbf{J}\mathbf{q}, \quad \mathbf{q}(0) = \mathbf{q}_0,$$

Discrete FOM

$$(\mathbf{I} - \Delta t \mathbf{J})\mathbf{q}^n = \mathbf{q}^{n-1}, \quad \mathbf{q}^0 = \mathbf{q}_0$$

Decomposition

$$\tilde{\mathbf{q}}(t) \triangleq \mathbf{V}\mathbf{q}_r(t), \text{ where } \mathbf{V} \in \mathbb{R}^{N \times k} \text{ and } \mathbf{q}_r \in \mathbb{R}^k$$

Theorem 2 : *If the Discrete FOM above is asymptotically stable in the sense of* $\left\|(\mathbf{I} - \Delta t \mathbf{J})^{-1}\right\|_2 \leq 1$ *, then the associated LSPG ROM is also asymptotically stable with no further assumptions required.*

Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation *C Huang, C Wentland, K Duraisamy, C Merkle, JCP 2021.*

Off-line/On-line costs in ROMs

Consider a linear system

$$\frac{d\mathbf{q}(t)}{dt} = \mathbf{A}\mathbf{q}(t) + \mathbf{B}\mathbf{u}(t) \quad ; \quad \mathbf{q}(0) = \mathbf{q}_0,$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{B} \in \mathbb{R}^{n \times p}$ and $\mathbf{u} \in \mathbb{R}^p$.

Then the ROM that solves of $\mathbf{q}_r \in \mathbb{R}^k$ is

$$\frac{d\mathbf{q}_r(t)}{dt} = \mathbf{A}_r\mathbf{q}_r(t) + \mathbf{B}_r\mathbf{u}(t) \quad ; \quad \mathbf{q}_r(0) = \mathbf{V}\mathbf{q}_0,$$

where

$$\begin{aligned} \mathbf{A}_r &= [\mathbf{W}^T\mathbf{V}]^{-1}\mathbf{W}^T\mathbf{A}\mathbf{V} \in \mathbb{R}^{k \times k} \\ \mathbf{B}_r &= [\mathbf{W}^T\mathbf{V}]^{-1}\mathbf{W}^T\mathbf{B} \in \mathbb{R}^{k \times p} \end{aligned}$$

Off-line/On-line costs in ROMs

$$\frac{d\mathbf{q}(t)}{dt} = \mathbf{A}\mathbf{q}(t) + \mathbf{B}\mathbf{u}(t)$$

$$\frac{d\mathbf{q}_r(t)}{dt} = \mathbf{A}_r\mathbf{q}_r(t) + \mathbf{B}_r\mathbf{u}(t)$$

$\mathbf{A} \in \mathbb{R}^{n\times n}$ and $\mathbf{B} \in \mathbb{R}^{n\times p}$ and $\mathbf{u} \in \mathbb{R}^{p}$.

$$\frac{d\mathbf{q}(t)}{dt} = \mathbf{f}(\mathbf{q}(t))$$

$$\frac{d\mathbf{q}_r(t)}{dt} = [\mathbf{W}^T\mathbf{V}]^{-1}\mathbf{W}^T\mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t)$$

Off-line/On-line costs in ROMs

$$\frac{d\mathbf{q}_r(t)}{dt} = [\mathbf{W}^T\mathbf{V}]^{-1}\mathbf{W}^T\mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t)$$

To do this, we can represent snapshots of the non-linear function $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^n$ in terms of some basis $\mathbf{\Psi} \in \mathbb{R}^{n\times s}$

$$\mathbf{f} = \Psi\mathbf{a},$$

where $\mathbf{a} \in \mathbb{R}^s$ are the basis coefficients. These basis functions, can, for instance be constructed using POD on a collection of snapshots

$$\mathbf{F} \in \mathbb{R}^{n\times m} = [\mathbf{f}(\mathbf{x}(t_1)) \;\; \mathbf{f}(\mathbf{x}(t_2)) \;\; \mathbf{f}(\mathbf{x}(t_3))...\mathbf{f}(\mathbf{x}(t_m)).$$

Then, we can sub-sample $\mathbf{f}$ by multiplying it by a sample selection matrix $\mathbf{P} \in \mathbb{R}^{s\times n}$. Then we have a few measurements $\mathbf{Pf} = \mathbf{f}_s \in \mathbb{R}^s$, for which

$$\mathbf{Pf} = \mathbf{P}\Psi\mathbf{a}.$$

Now, based on the few samples, we can estimate $\hat{\mathbf{a}}$ using

$$\hat{\mathbf{a}} = [\mathbf{P}\Psi]^+\mathbf{f}_s.$$

and we can reconstruct the entire $\mathbf{f}$ as

$$\hat{\mathbf{f}} = \Psi[\mathbf{P}\Psi]^+\mathbf{f}_s.$$

Off-line/On-line costs in ROMs

$$\frac{d\mathbf{q}_r(t)}{dt} = [\mathbf{W}^T\mathbf{V}]^{-1}\mathbf{W}^T\mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t)$$

$$\frac{d\mathbf{q}_r(t)}{dt} \quad = \quad [\mathbf{W}^T\mathbf{V}]^{-1}\mathbf{W}^T\Psi[\mathbf{P}\Psi]^{+}\mathbf{f}_s(t)$$

Petrov-Galerkin Projection

The test subspace in Petrov-Galerkin projection is,

$$\mathbf{W}(\mathbf{q}_r^n) = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}_r^n)}{\partial \mathbf{q}_r^n}\right] = \left[\mathbf{A}^T\mathbf{A}\frac{\partial \mathbf{r}(\mathbf{q}^n)}{\partial \mathbf{q}^n}\right]\mathbf{V}$$

$$\left[\mathbf{W}^{p-1}\right]^T \mathbf{W}^{p-1}(\mathbf{q}_r^p - \mathbf{q}_r^{p-1}) = -\left[\mathbf{W}^{p-1}\right]^T \mathbf{r}(\mathbf{q}_r^{p-1}).$$