Enforcing Boundary Conditions for Reduced-Order CFD Simulations

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Problem: High-fidelity CFD simulations are too computationally expensive for time sensitive applications.

Goal: Reduce computational complexity \textit{without} coarsening model or omitting relevant physics.
Consider a set of ODEs arising from the discretization in space of a space-time PDE:

\[
\frac{d\mathbf{w}(t)}{dt} = f(\mathbf{w}(t), t, \mu)
\]

\[
\mathbf{w}(0) = \mathbf{w}_0,
\]

where \( t \geq 0 \) denotes time, \( \mathbf{w}(t) \in \mathbb{R}^n \) denotes the fluid state vector, and \( \mu \in \mathbb{R}^d \) denotes a vector of parameters defining the operating point.
Using implicit time integration, the state $w^{(i)} \in \mathbb{R}^n$ at time $t^{(i)}$, $0 \leq i \leq N_t$ can be computed as the solution to a discrete nonlinear residual

$$r^{(i)}(w^{(i)}, \mu) = 0.$$
Using implicit time integration, the state \( \mathbf{w}^{(i)} \in \mathbb{R}^n \) at time \( t^{(i)}, 0 \leq i \leq N_t \) can be computed as the solution to a discrete nonlinear residual

\[
\mathbf{r}^{(i)}(\mathbf{w}^{(i)}, \mu) = 0.
\]

Introducing a reduced order basis (ROB), \( \mathbf{V} \in \mathbb{R}^{n \times k} \), leads to a system of \( n \) eq. for \( k \ll n \) variables

\[
\min_{\Delta \mathbf{w}^{(i)}_{k} \in \mathbb{R}^k} \left\| \mathbf{r}^{(i)}( \mathbf{w}^{(i-1)} + \mathbf{V} \Delta \mathbf{w}^{(i)}_{k}, \mu) \right\|_2^2
\]
Using implicit time integration, the state \( w^{(i)} \in \mathbb{R}^n \) at time \( t^{(i)} \), \( 0 \leq i \leq N_t \) can be computed as the solution to a discrete nonlinear residual

\[
r^{(i)}(w^{(i)}, \mu) = 0.
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Introducing a reduced order basis (ROB), \( V \in \mathbb{R}^{n \times k} \), leads to a system of \( n \) eq. for \( k \ll n \) variables

\[
\min_{\Delta w_k^{(i)} \in \mathbb{R}^k} \left\| r^{(i)}(w^{(i-1)} + V \Delta w_k^{(i)}, \mu) \right\|_2^2
\]

420x reduction in CPU with less than 1% error in outputs

GNAT method: Carlberg et al. 2011
Partitioning the residual into interior / boundary:

\[
\begin{bmatrix}
r^{(i)}_{\text{interior}}(w^{(i)}, \mu) \\
r^{(i)}_{\text{boundary}}(w^{(i)}, \mu)
\end{bmatrix} = 0
\]
Enforcing Boundary Conditions

Partitioning the residual into interior / boundary:

\[
\begin{bmatrix}
  r^{(i)}_{\text{interior}}(\mathbf{w}^{(i)}, \mu) \\
  r^{(i)}_{\text{boundary}}(\mathbf{w}^{(i)}, \mu)
\end{bmatrix} = 0
\]

If any basis vectors do not satisfy the boundary conditions, then the relative weighting of these terms becomes important in the minimization:

\[
\min_{\Delta \mathbf{w}_{k}^{(i)} \in \mathbb{R}^k} \left\| \begin{bmatrix}
  r^{(i)}_{\text{interior}}(\mathbf{w}^{(i-1)} + \mathbf{V}\Delta \mathbf{w}_{k}^{(i)}, \mu) \\
  \epsilon r^{(i)}_{\text{boundary}}(\mathbf{w}^{(i-1)} + \mathbf{V}\Delta \mathbf{w}_{k}^{(i)}, \mu)
\end{bmatrix} \right\|^2_2
\]
In practice, this weighted nonlinear least squares problem can be solved using the Gauss-Newton Algorithm, resulting in the following iterations:

$$
\min_{\Delta w^{(i)} \in \mathbb{R}^n} \left\| J^{(i,l-1)} V \Delta w^{(i,l)} + r^{(i,l-1)} \right\|^2_P
$$

$$
w^{(i,l+1)} = w^{(i,l)} + \gamma^{(i,l)} p^{(i,l)},
$$

where gamma is the step length, J is the Jacobian matrix and P is a weighting matrix,

$$
r^{(i,l-1)} \equiv r^{(i)}(w^{(i,l-1)}, \mu), \quad J^{(i,l-1)} \equiv \frac{\delta r^{(i)}}{\delta w}(w^{(i,l-1)}, \mu)
$$

$$
P = \begin{bmatrix}
I & 0 \\
0 & \epsilon^2 I
\end{bmatrix}.
$$
As a first (crude) attempt, I solved a regularized least squares problem instead of the true weighted least squares problem:

\[
\min_{\Delta w^{(i)} \in \mathbb{R}^n} \left( \left\| J^{(i,l-1)} V \Delta w^{(i,l)}_{k} + r^{(i,l-1)} \right\|^2 + \left\| (w^{(i,l-1)} + V \Delta w^{(i,l)}_{k}) - \tilde{w} \right\|_Q^2 \right)
\]

where \(\tilde{w}\) is an approximation to the true state (at least near the boundary) and the matrix \(Q\) defines a semi-norm.

\[
Q = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon^2 I \end{bmatrix}.
\]

(Note: \(Q\) masks all interior nodes, so the regularization term is only active for the boundary nodes)
Enforcing BCs for Nonlinear ROMs

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NACA 0015
$M_\infty = 0.75$
Re = 6 Million
SA Turbulence Model
Wall Model
Alpha = 0,1,2,3,4
40,922 Fluid Nodes
245,532 Degrees of Freedom
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Projection of (Predictive) HDM Solution onto ROB

Chord

\(-C_p\)

Projection of HDM solution onto ROB
Enforcing BCs for Nonlinear ROMs

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PG ROM, $\alpha=3.5$ (Predictive)

Unregularized Predictive Global ROM

Chord

$-C_p$

-1.5 -1 -0.5 0 0.5 1

HDM (DOF = 245532)

ROM (DOF = 594)
Predictive Operating Point (α=3.5)

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Predictive Operating Point ($\alpha=3.5$)

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Predictive Operating Point ($\alpha=3.5$)

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Contours of unweighted residual: \[ \left\| r^{(i)} \right\|_2^2 \]
Contours of raw (HDM) residual: \[ \| r^{(i)} \|_2^2 \]

Predictive Operating Point ($\alpha=3.5$)
Contour of regularized residual: \[ \left\| r(i) \right\|_2^2 + \left\| w(i) - \tilde{w} \right\|_Q^2 \]

Where \[ Q = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon^2 I \end{bmatrix} \].
Contours of regularized residual:

$$\|r^{(i)}\|_2^2 + \|w^{(i)} - \tilde{w}\|_Q^2$$

where

$$Q = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon^2 I \end{bmatrix}.$$
Contours of regularized residual:
\[ \| r^{(i)} \|_2^2 + \| w^{(i)} - \tilde{w} \|_Q^2 \]

where
\[ Q = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon^2 I \end{bmatrix} \]

\[ \epsilon = 10 \]
Contours of regularized residual: 
\[ \left\| r^{(i)} \right\|_2^2 + \left\| w^{(i)} - \tilde{w} \right\|_Q^2 \]

where 
\[ Q = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon^2 I \end{bmatrix} \]
Enforcing BCs for Nonlinear ROMs

Predictive Global ROM, Regularization Weight = $10^1$ ($\alpha = 3.5$)

- $\text{C}_p$ vs Chord

- HDM (DOF = 245532)
- ROM (DOF = 594)

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PG ROM, $\alpha=3.5$ (Predictive), $\varepsilon = 10^2$
Enforcing BCs for Nonlinear ROMs

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PG ROM, $\alpha=3.5$ (Predictive), $\varepsilon = 10^3$
Enforcing BCs for Nonlinear ROMs

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Enforcing BCs for Nonlinear ROMs

Washabaugh, FRG
Predictive Global ROM, Regularization Weight = $10^6$ ($\alpha = 3.5$)
Enforcing BCs for Nonlinear ROMs

Predictive Global ROM, Regularization Weight = $10^7$ ($\alpha = 3.5$)

HDM (DOF = 245532)
ROM (DOF = 594)
Predictive Global ROM, Regularization Weight = $10^8$ ($\alpha = 3.5$)

HDM (DOF = 245532)
ROM (DOF = 594)
Enforcing BCs for Nonlinear ROMs

Predictive Global ROM, Regularization Weight = $10^9$ ($\alpha = 3.5$)
Enforcing BCs for Nonlinear ROMs

Predictive Global ROM, Regularization Weight = $10^{10}$ ($\alpha = 3.5$)

- $-C_p$ vs Chord

HDM (DOF = 245532)
ROM (DOF = 594)
Enforcing BCs for Nonlinear ROMs

Predictive Global ROM, Regularization Weight = $10^{11}$ ($\alpha = 3.5$)

- $\alpha = 3.5$
- $\varepsilon = 10^{11}$
Enforcing BCs for Nonlinear ROMs

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\[ f_1 = \|r(w)\|^2_2 \]
\[ f_2 = \|w - w_\infty\|^2_A \]

- \( \varepsilon = 10 \)
- \( \varepsilon = 10^2 \)
- \( \varepsilon = 10^3 \)
- \( \varepsilon = 10^4 \)
- \( \varepsilon = 10^5 \)
- \( \varepsilon = 10^6 \)
- \( \varepsilon = 10^7 \)
- \( \varepsilon = 10^8 \)
- \( \varepsilon = 10^9 \)
- \( \varepsilon = 10^{11} \)
- \( \varepsilon = 10^{12} \)
\[ f_1 = \| \mathbf{r}(\mathbf{w}) \|_2^2 \]
\[ f_2 = \| \mathbf{w} - \mathbf{w}_\infty \|_A^2 \]

\[ \hat{A} \quad \text{ROM Error} \]
• The corner of this plot seems to correspond to low errors in the ROM results.

• In the next few weeks I’ll implement a method to find this corner automatically and efficiently.

• I’m also planning to implement the weighted least squares formulation of the problem rather than the regularized least squares formulation. It will be interesting to see whether the weighted least squares formulation exhibits the same behavior as the regularized formulation as the weighting on the boundary is increased.
Supporting Slides
Standard least-squares:

\[
\min_{x \in \mathbb{R}^n} \|Ax - b\|_P^2
\]

\[
x^* = (A^T PA)^{-1} (A^T Pb)
\]

Least-squares with Tikhonov regularization (generalized form):

\[
\min_{x \in \mathbb{R}^n} \left( \|Ax - b\|_P^2 + \|x - \tilde{x}\|_Q^2 \right), \text{ where } \tilde{x} \equiv E(x^*).
\]

\[
x^* = (A^T PA + Q)^{-1} (A^T Pb + Q\tilde{x})
\]
Residual minimization in the least squares sense

\[ w_r(t) = \arg\min_z \| r(w_0 + V_w z, t) \|_2 \]

\[ J(w) : \text{Jacobian of } r(., t) \text{ at } w \]

Solution by Newton’s method (Gauss-Newton iterations)

\[ (J(w^{(m)})V_w)^T(J(w^{(m)})V_w) z^{(m)} = -(J(w^{(m)})V_w)^T r(w^{(m)}, t) \]
I. **Full-order model** $\rightarrow$ Data collection $\rightarrow$ Compression

   **Approximation 1: Projection**

II. **Reduced-order model** $\rightarrow$ Data collection $\rightarrow$ Compression

   **Approximation 2: System approximation**

III. **Reduced-order model + system approximation**