

# Gappy POD and GNAT

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# Outline

- Nonlinear partial differential equations
- An issue with the model reduction of nonlinear equations
- The gappy proper orthogonal decomposition
- The discrete empirical interpolation method (DEIM)
- The Gauss-Newton with approximated tensors method (GNAT)
- Two applications

# Nonlinear PDE

- Parametrized partial differential equation (PDE)

$$\mathcal{L}(\mathcal{W}, \mathbf{x}, t; \boldsymbol{\mu}) = 0$$

- Associated boundary conditions

$$\mathcal{B}(\mathcal{W}, \mathbf{x}_{\text{BC}}, t; \boldsymbol{\mu}) = 0$$

- Initial condition

$$\mathcal{W}_0(\mathbf{x}) = \mathcal{W}_{\text{IC}}(\mathbf{x}, \boldsymbol{\mu})$$

- $\mathcal{W} = \mathcal{W}(\mathbf{x}, t) \in \mathbb{R}^q$ : state variable
- $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ ,  $d \leq 3$ : space variable
- $t \geq 0$ : time variable
- $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^p$ : parameter vector

# Discretization of nonlinear PDE

- The PDE is then discretized in space by one of the following methods
  - Finite Differences approximation
  - Finite Element method
  - Finite Volumes method
  - Discontinuous Galerkin method
  - Spectral method....
- This leads to a system of  $N_{\mathbf{w}} = q \times N_{\text{space}}$  ordinary differential equations (ODEs)

$$\frac{d\mathbf{w}}{dt} = \mathbf{f}(\mathbf{w}, t; \boldsymbol{\mu})$$

in terms of the discretized state variable

$$\mathbf{w} = \mathbf{w}(t; \boldsymbol{\mu}) \in \mathbb{R}^{N_{\mathbf{w}}}$$

with initial condition  $\mathbf{w}(0; \boldsymbol{\mu}) = \mathbf{w}(\boldsymbol{\mu})$

- This is the high-dimensional model (HDM)

# Model reduction of nonlinear equations

- High-dimensional model (HDM)

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

- Reduced-order modeling assumption using a reduced basis  $\mathbf{V}$

$$\mathbf{w}(t) \approx \mathbf{V}\mathbf{q}(t)$$

- $\mathbf{q}(t)$ : reduced (generalized) coordinates
- Inserting in the HDM equation

$$\mathbf{V} \frac{d\mathbf{q}}{dt}(t) \approx \mathbf{f}(\mathbf{V}\mathbf{q}(t), t)$$

- $N_{\mathbf{w}}$  equations in terms of  $k$  unknowns  $\mathbf{q}$
- Galerkin projection

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

# Issue with the model reduction of nonlinear equations

- Galerkin projection

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

- $k$  equations in terms of  $k$  unknowns
- To evaluate  $\mathbf{f}_k(\mathbf{V}\mathbf{q}(t), t)$ :
  - 1 Compute  $\mathbf{w}(t) = \mathbf{V}\mathbf{q}(t)$
  - 2 Evaluate  $\mathbf{f}(\mathbf{V}\mathbf{q}(t), t)$
  - 3 Left-multiply by  $\mathbf{V}^T$ :  $\mathbf{V}^T \mathbf{f}(\mathbf{V}\mathbf{q}(t), t)$
- The computational cost associated with these three steps scales linearly with the dimension  $N_{\mathbf{w}}$  of the HDM
- Hence no significant speedup can be expected when solving the projection-based ROM

# The Gappy POD

- First applied to face recognition (Emerson and Sirovich, "Karhunen-Loeve Procedure for Gappy Data" 1996)
- Procedure
  - 1 Build a database of  $m$  faces (snapshots)
  - 2 Construct a POD basis  $\mathbf{V}$  for the database
  - 3 For a new face  $\mathbf{f}$ , record a few pixels  $f_1, \dots, f_n$
  - 4 Using the POD basis  $\mathbf{V}$ , approximately reconstruct the new face  $\mathbf{f}$

# The Gappy POD

- First applied to face recognition (Emerson and Sirovich, "Karhunen-Loeve Procedure for Gappy Data" 1996)

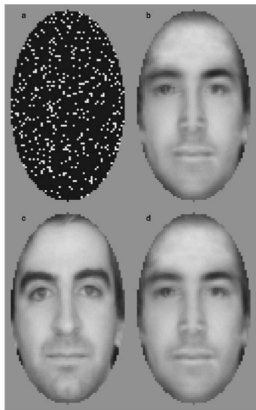


Fig. 1. Reconstruction of a face, not in the original ensemble, from a 10% mask. The reconstructed face, b, was determined with 50 empirical eigenfunctions and only the white pixels shown in a. The original face is shown in c, and a projection (with all the pixels) of the face onto 50 empirical eigenfunctions is shown in d.



# The Gappy POD

- Other applications
  - Flow sensing and estimation (Willcox, 2004)
  - Flow reconstruction
  - Nonlinear model reduction

# Nonlinear function approximation by gappy POD

- Approximation of the nonlinear function  $\mathbf{f}$  in

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

- The evaluation of all the entries in the vector  $\mathbf{f}(\cdot, t)$  is expensive (scales with  $N_w$ )
- Only a small subset of these entries will be evaluated (gappy approach)
- The other entries will be reconstructed either by interpolation or a least-squares strategy using a pre-computed specific reduced-order basis  $\mathbf{V}_f$
- The solution space is still reduced by any preferred model reduction method (by POD for instance)

# Nonlinear function approximation by gappy POD

A complete model reduction method should then provide algorithms for

- Selecting the evaluation indices  $\mathcal{I} = \{i_1, \dots, i_{N_i}\}$
- Selecting a reduced-order bases  $\mathbf{V}_f$  for the nonlinear function
- Reconstructing the complete approximated nonlinear function vector  $\hat{\mathbf{f}}(\cdot, t)$

# Construction of a POD basis for $\mathbf{f}$

- Construction of a POD basis  $\mathbf{V}_f$  of dimension  $k_f$ 
  - 1 Collection of snapshots for the nonlinear function from a transient simulation

$$\mathbf{F} = [\mathbf{f}(\mathbf{w}(t_1), t_1), \dots, \mathbf{f}(\mathbf{w}(t_{m_f}), t_{m_f})] \in \mathbb{R}^{N_{\mathbf{w}} \times m_f}$$

- 2 Singular value decomposition

$$\mathbf{F} = \mathbf{U}_f \mathbf{\Sigma}_f \mathbf{Z}_f^T$$

- 3 Basis truncation ( $k_f \ll m_f$ )

$$\mathbf{V}_f = [\mathbf{u}_{f,1}, \dots, \mathbf{u}_{f,k_f}]$$

# Reconstruction of an approximated nonlinear function

- Assume  $k_i$  indices have been chosen

$$\mathcal{I} = \{i_1, \dots, i_{k_i}\}$$

- The choice of indices will be specified later
- Consider the  $N_{\mathbf{w}}$ -by- $k_i$  matrix

$$\mathbf{P} = \begin{bmatrix} \mathbf{e}_{i_1}, \dots, \mathbf{e}_{i_{k_i}} \end{bmatrix}$$

- At each time  $t$ , for a given value of the state  $\mathbf{w}(t) = \mathbf{V}\mathbf{q}(t)$ , only the entries in the function  $\mathbf{f}$  corresponding to those indices will be evaluated

$$\mathbf{P}^T \mathbf{f}(\mathbf{w}(t), t) = \begin{bmatrix} f_{i_1}(\mathbf{w}(t), t) \\ \vdots \\ f_{i_{k_i}}(\mathbf{w}(t), t) \end{bmatrix}$$

- This is cheap if  $k_i \ll N_{\mathbf{w}}$
- Usually only a subset of the entries in  $\mathbf{w}(t)$  will be required to construct that vector (case of sparse Jacobian)

# Discrete Empirical Interpolation Method

- Case where  $k_i = k_f$ : interpolation

- Idea:  $\hat{f}_{i_j}(\mathbf{w}, t) = f_{i_j}(\mathbf{w}, t)$ ,  $\forall \mathbf{w} \in \mathbb{R}^{N_w}$ ,  $\forall j = 1, \dots, k_i$
- This means that

$$\mathbf{P}^T \hat{\mathbf{f}}(\mathbf{w}(t), t) = \mathbf{P}^T \mathbf{f}(\mathbf{w}(t), t)$$

- Remember that  $\hat{\mathbf{f}}(\cdot, t)$  belongs to the span of the vectors in  $\mathbf{V}_f$ , that is

$$\hat{\mathbf{f}}(\mathbf{V}\mathbf{q}(t), t) = \mathbf{V}_f \mathbf{f}_r(\mathbf{q}(t), t)$$

- Then

$$\mathbf{P}^T \mathbf{V}_f \mathbf{f}_r(\mathbf{q}(t), t) = \mathbf{P}^T \mathbf{f}(\mathbf{V}\mathbf{q}(t), t)$$

- Assuming  $\mathbf{P}^T \mathbf{V}_f$  is nonsingular

$$\mathbf{f}_r(\mathbf{q}(t), t) = (\mathbf{P}^T \mathbf{V}_f)^{-1} \mathbf{P}^T \mathbf{f}(\mathbf{V}\mathbf{q}(t), t)$$

- In terms of  $\hat{\mathbf{f}}(\cdot, t)$ :

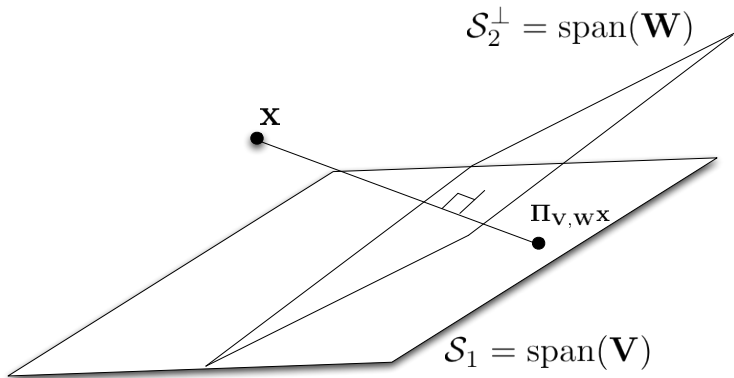
$$\hat{\mathbf{f}}(\cdot, t) = \mathbf{V}_f (\mathbf{P}^T \mathbf{V}_f)^{-1} \mathbf{P}^T \mathbf{f}(\cdot, t) = \mathbf{\Pi}_{\mathbf{V}_f, \mathbf{P}} \mathbf{f}(\cdot, t)$$

- This results in an oblique projection of the full nonlinear vector

# Oblique projection of the full nonlinear vector

$$\hat{\mathbf{f}}(\cdot, t) = \mathbf{V}_f(\mathbf{P}^T \mathbf{V}_f)^{-1} \mathbf{P}^T \mathbf{f}(\cdot, t) = \mathbf{\Pi}_{\mathbf{V}_f, \mathbf{P} \mathbf{f}}(\cdot, t)$$

- $\mathbf{\Pi}_{\mathbf{V}, \mathbf{W}} = \mathbf{V}(\mathbf{W}^T \mathbf{V})^{-1} \mathbf{W}^T$ : oblique projector onto  $\mathbf{V}$  orthogonally to  $\mathbf{W}$



# Reduced-order dynamical system

- Case where  $k_i > k_f$ : least-squares reconstruction
  - Idea:  $\hat{f}_{i_j}(\mathbf{w}, t) \approx f_{i_j}(\mathbf{w}, t)$ ,  $\forall \mathbf{w} \in \mathbb{R}^{N_w}$ ,  $\forall j = 1, \dots, N_i$  in the least squares sense
  - Idea: minimize

$$\mathbf{f}_r(\mathbf{q}(t)) = \underset{\mathbf{y}_r}{\operatorname{argmin}} \|\mathbf{P}^T \mathbf{V}_f \mathbf{y}_r - \mathbf{P}^T \mathbf{f}(\mathbf{V} \mathbf{q}(t), t)\|_2$$

- Note that  $\mathbf{M} = \mathbf{P}^T \mathbf{V}_f \in \mathbb{R}^{k_i \times k_f}$  is a skinny matrix
- One can compute its singular value decomposition

$$\mathbf{M} = \mathbf{U} \mathbf{\Sigma} \mathbf{Z}^T$$

- The left inverse of  $\mathbf{M}$  is then defined as

$$\mathbf{M}^\dagger = \mathbf{Z} \mathbf{\Sigma}^\dagger \mathbf{U}^T$$

where  $\mathbf{\Sigma}^\dagger = \operatorname{diag}(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_r}, 0, \dots, 0)$  if  $\mathbf{\Sigma} = \operatorname{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0)$  with  $\sigma_1 \geq \dots \sigma_r > 0$

- Then

$$\hat{\mathbf{f}}(\mathbf{q}(t)) = \mathbf{V}_f (\mathbf{P}^T \mathbf{V}_f)^\dagger \mathbf{P}^T \mathbf{f}(\mathbf{V} \mathbf{q}(t), t)$$



# Greedy function sampling

- This selection takes place after the vectors  $[\mathbf{v}_{f,1}, \dots, \mathbf{v}_{f,k_f}]$  have already been computed by POD
- Greedy algorithm (Chaturantabut et al. 2010):
  - 1:  $[s, i_1] = \max\{|\mathbf{v}_{f,1}|\}$
  - 2:  $\mathbf{V}_f = [\mathbf{v}_{f,1}], \mathbf{P} = [\mathbf{e}_{i_1}]$
  - 3: **for**  $l = 2 : k_f$  **do**
  - 4:   Solve  $\mathbf{P}^T \mathbf{V}_f \mathbf{c} = \mathbf{P}^T \mathbf{v}_{f,l}$  for  $\mathbf{c}$
  - 5:    $\mathbf{r} = \mathbf{v}_{f,l} - \mathbf{V}_f \mathbf{c}$
  - 6:    $[s, i_l] = \max\{|\mathbf{r}|\}$
  - 7:    $\mathbf{V}_f = [\mathbf{V}_f, \mathbf{v}_{f,l}], \mathbf{P} = [\mathbf{P}, \mathbf{e}_{i_l}]$
  - 8: **end for**

# Model reduction at the fully discrete level

- Semi-discrete level:  $\frac{d\mathbf{w}}{dt}(t) = \mathbf{f}(\mathbf{w}(t), t)$
- Subspace assumption  $\mathbf{w}(t) \approx \mathbf{V}\mathbf{q}(t)$

$$\mathbf{V} \frac{d\mathbf{q}}{dt}(t) \approx \mathbf{f}(\mathbf{V}\mathbf{q}(t), t)$$

- Fully discrete level (implicit, backward Euler scheme)

$$\mathbf{V} \frac{\mathbf{q}^{(n+1)} - \mathbf{q}^{(n)}}{\Delta t^{(n)}} \approx \mathbf{f}(\mathbf{V}\mathbf{q}^{(n+1)}, t^{(n+1)})$$

- Fully discrete residual

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

- Model reduction by least-squares (Petrov-Galerkin)

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{y}}{\operatorname{argmin}} \|\mathbf{r}_D^{(n+1)}(\mathbf{y})\|_2$$

- $\mathbf{r}_D(\mathbf{q}^{(n+1)})$  is nonlinear  $\Rightarrow$  use the gappy POD idea

# Gappy POD at the fully discrete level

- Gappy POD procedure for the fully discrete residual  $\mathbf{r}_D$
- Algorithm
  - 1 Build a reduced basis  $\mathbf{V}_r \in \mathbb{R}^{N_w \times k_r}$  for  $\mathbf{r}_D$
  - 2 Construct a sample mesh  $\mathcal{I}$  (indices  $i_1, \dots, i_{k_i}$ ) by a greedy procedure
  - 3 Consider the gappy approximation

$$\mathbf{r}_D^{(n+1)}(\mathbf{q}^{(n+1)}) \approx \mathbf{V}_r \mathbf{r}_{k_r}(\mathbf{q}^{(n+1)}) \approx \mathbf{V}_r \left( \mathbf{P}^T \mathbf{V}_r \right)^\dagger \mathbf{P}^T \mathbf{r}^{(n+1)}(\mathbf{V} \mathbf{q}^{(n+1)})$$

- 4 Solve

$$\begin{aligned} \mathbf{q}^{(n+1)} &= \underset{\mathbf{y}}{\operatorname{argmin}} \|\mathbf{V}_r \mathbf{r}_{k_r}(\mathbf{y})\|_2 \\ &= \underset{\mathbf{y}}{\operatorname{argmin}} \|\mathbf{r}_{k_r}(\mathbf{y})\|_2 \\ &= \underset{\mathbf{y}}{\operatorname{argmin}} \left\| \left( \mathbf{P}^T \mathbf{V}_r \right)^\dagger \mathbf{P}^T \mathbf{r}^{(n+1)}(\mathbf{V} \mathbf{y}) \right\|_2 \end{aligned} \tag{1}$$

# Gauss-Newton for nonlinear least squares problem

- Nonlinear least squares problem  $\min_{\mathbf{y}} \|\mathbf{r}(\mathbf{y})\|_2$
- Equivalent function to be minimized

$$f(\mathbf{y}) = 0.5\|\mathbf{r}(\mathbf{y})\|_2^2 = \mathbf{r}(\mathbf{y})^T \mathbf{r}(\mathbf{y})$$

- Gradient

$$\nabla f(\mathbf{y}) = \mathbf{J}(\mathbf{y})^T \mathbf{r}(\mathbf{y})$$

where  $\mathbf{J}(\mathbf{y}) = \frac{\partial \mathbf{r}}{\partial \mathbf{y}}(\mathbf{y})$

- Iterative solution using Newton's method  $\mathbf{y}^{(k+1)} = \mathbf{y}^{(k)} + \Delta \mathbf{y}^{(k+1)}$  with

$$\nabla^2 f(\mathbf{y}^{(k)}) \Delta \mathbf{y}^{(k+1)} = -\nabla f(\mathbf{y}^{(k)})$$

- What is  $\nabla^2 f(\mathbf{y})$ ?

$$\nabla^2 f(\mathbf{y}) = \mathbf{J}(\mathbf{y})^T \mathbf{J}(\mathbf{y}) + \sum_{i=1}^N \frac{\partial^2 r_i}{\partial \mathbf{y}^2}(\mathbf{y}) r_i(\mathbf{y})$$

- Gauss-Newton method

$$\nabla^2 f(\mathbf{y}) \approx \mathbf{J}(\mathbf{y})^T \mathbf{J}(\mathbf{y})$$

# Gauss-Newton for nonlinear least squares problem

- Gauss-Newton method  $\mathbf{y}^{(k+1)} = \mathbf{y}^{(k)} + \Delta\mathbf{y}^{(k+1)}$  with

$$\mathbf{J}(\mathbf{y}^{(k)})^T \mathbf{J}(\mathbf{y}^{(k)}) \Delta\mathbf{y}^{(k+1)} = -\mathbf{J}(\mathbf{y}^{(k)})^T \mathbf{r}(\mathbf{y}^{(k)})$$

- This is the normal equation for

$$\Delta\mathbf{y}^{(k+1)} = \underset{\mathbf{z}}{\operatorname{argmin}} \left\| \mathbf{J}(\mathbf{y}^{(k)})\mathbf{z} + \mathbf{r}(\mathbf{y}^{(k)}) \right\|_2$$

- QR decomposition of the Jacobian

$$\mathbf{J}(\mathbf{y}^{(k)}) = \mathbf{Q}^{(k)} \mathbf{R}^{(k)}$$

- Equivalent solution using the QR decomposition (assume  $\mathbf{R}^{(k)}$  is full rank)

$$\Delta\mathbf{y}^{(k+1)} = -\mathbf{J}(\mathbf{y}^{(k)})^\dagger \mathbf{r}(\mathbf{y}^{(k)}) = -\left(\mathbf{R}^{(k)}\right)^{-1} \left(\mathbf{Q}^{(k)}\right)^T \mathbf{r}(\mathbf{y}^{(k)})$$

# Gauss-Newton with Approximated Tensors

- GNAT = Gauss-Newton + Gappy POD
- Minimization problem

$$\min_{\mathbf{y}} \left\| (\mathbf{P}^T \mathbf{V}_r)^\dagger \mathbf{P}^T \mathbf{r}^{(n+1)}(\mathbf{V}\mathbf{y}) \right\|_2$$

- Jacobian

$$\mathbf{J}_D(\mathbf{y}) = (\mathbf{P}^T \mathbf{V}_r)^\dagger \mathbf{P}^T \mathbf{J}^{(n+1)}(\mathbf{V}\mathbf{y})$$

- Define a small dimensional operator (constructed offline)

$$\mathbf{A} = (\mathbf{P}^T \mathbf{V}_r)^\dagger$$

- Least-squares problem at iteration  $k$

$$\Delta \mathbf{y}^{(k)} = \underset{\mathbf{z}}{\operatorname{argmin}} \left\| \mathbf{A} \mathbf{P}^T \mathbf{J}^{(n+1)}(\mathbf{V}\mathbf{y}^{(k)}) \mathbf{V} \mathbf{z} + \mathbf{A} \mathbf{P}^T \mathbf{r}^{(n+1)}(\mathbf{V}\mathbf{y}^{(k)}) \right\|_2$$

- GNAT solution using QR decomposition  $\mathbf{Q}^{(k)} \mathbf{R}^{(k)} = \mathbf{A} \mathbf{P}^T \mathbf{J}^{(n+1)}(\mathbf{V}\mathbf{y}^{(k)}) \mathbf{V}$

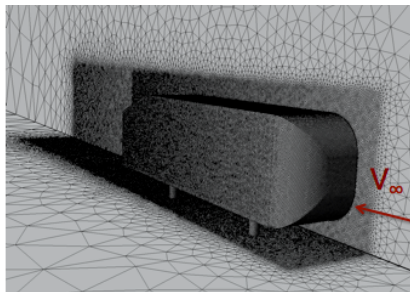
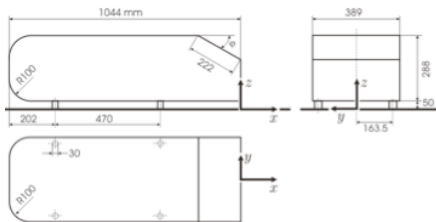
$$\Delta \mathbf{y}^{(k)} = - \left( \mathbf{R}^{(k)} \right)^{-1} \left( \mathbf{Q}^{(k)} \right)^T \mathbf{A} \mathbf{P}^T \mathbf{r}^{(n+1)}(\mathbf{V}\mathbf{y}^{(k)})$$

# Gauss-Newton with Approximated Tensors

- Further developments
  - Concept of reduced mesh
  - Concept of output mesh
  - Error bounds
  - GNAT using Local reduced bases
- More details in Carlberg et al., JCP 2013

# Application 1: compressible Navier-Stokes equations

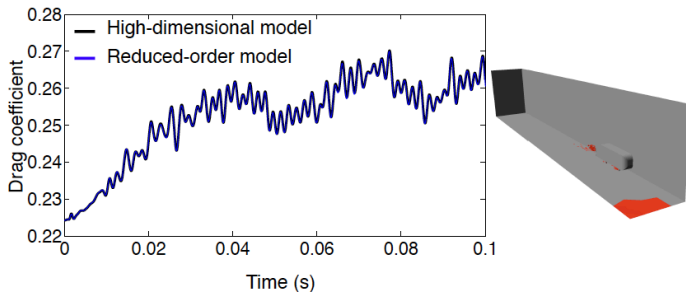
- Flow past the Ahmed body (automotive industry benchmark)
- 3D compressible Navier-Stokes equations
- $N_w = 1.73 \times 10^7$
- $Re = 4.48 \times 10^6$ ,  $M_\infty = 0.175$  (216km/h)
- More details in Carlberg et al., JCP 2013





# Application 1: compressible Navier-Stokes equations

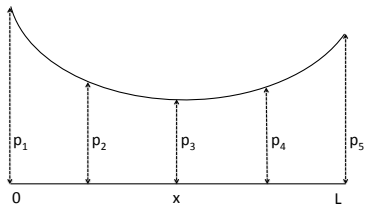
- Model reduction (POD+GNAT):  $k = 283$ ,  $k_f = 1,514$ ,  $k_i = 2,268$



Method	CPU Time	Number of CPUs	Relative Error
Full-Order Model	13.28 h	512	—
ROM (GNAT)	3.88 h	4	0.68%

## Application 2: design-optimization of a nozzle

- Full model:  $N_{\mathbf{w}} = 2,048$ ,  $p = 5$  shape parameters
- Model reduction (POD+DEIM):  $k = 8$ ,  $k_f = 20$ ,  $k_i = 20$

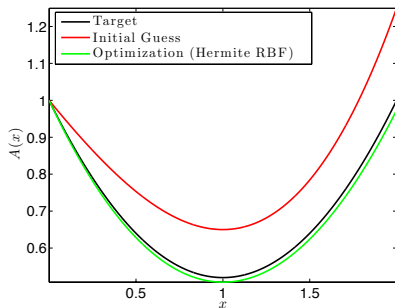
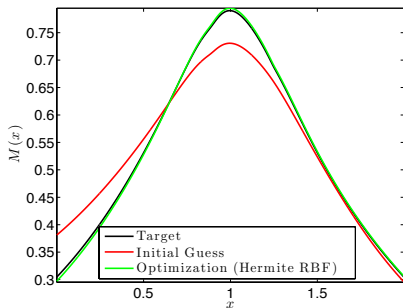


$$\min_{\boldsymbol{\mu} \in \mathbb{R}^5} \|M(\mathbf{w}(\boldsymbol{\mu})) - M_{\text{target}}\|_2$$

$$\text{s.t. } \mathbf{f}(\mathbf{w}(\boldsymbol{\mu}), \boldsymbol{\mu}) = \mathbf{0}$$

## Application 2: design-optimization of a nozzle

Method	Offline CPU Time	Online CPU Time	Total CPU Time
Full-Order Model	—	78.8 s	78.8 s
ROM (GNAT)	5.08 s	4.87 s	9.96 s



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