

AA216/CME345: PROJECTION-BASED MODEL ORDER REDUCTION

Parameterized Partial Differential Equations (PDEs)

Charbel Farhat
Stanford University
cfarhat@stanford.edu

Outline

- 1 Initial Boundary Value Problems
- 2 Typical Parameters of Interest
- 3 Untypical Parameters of Interest
- 4 Semi-discretization Processes and Dynamical Systems
- 5 Case for Model Order Reduction
- 6 Subspace Approximation

- Linear or Nonlinear Partial Differential Equation (PDE)

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

- $\mathcal{W} = \mathcal{W}(\mathbf{x}, t) \in \mathbb{R}^\ell$: State variable
 - $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, $d \leq 3$: Space variable
 - $t \geq 0$: Time variable
- Examples
 - Navier-Stokes equations or linearized counterparts
 - elastodynamic equations of motion
 - wave equation

- Linear or Nonlinear Partial Differential Equation (PDE)

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

- $\mathcal{W} = \mathcal{W}(\mathbf{x}, t) \in \mathbb{R}^\ell$: State variable
- $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, $d \leq 3$: Space variable
- $t \geq 0$: Time variable

- Examples

- Navier-Stokes equations or linearized counterparts
- elastodynamic equations of motion
- wave equation

- Boundary Conditions (BCs)

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

- Dirichlet BCs
- Neumann BCs
- Robin (mixed) BCs

■ Linear or Nonlinear Partial Differential Equation (PDE)

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

- $\mathcal{W} = \mathcal{W}(\mathbf{x}, t) \in \mathbb{R}^\ell$: State variable
- $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, $d \leq 3$: Space variable
- $t \geq 0$: Time variable

■ Examples

- Navier-Stokes equations or linearized counterparts
- elastodynamic equations of motion
- wave equation

■ Boundary Conditions (BCs)

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

- Dirichlet BCs
- Neumann BCs
- Robin (mixed) BCs

■ Initial Condition (IC)

$$\mathcal{W}(\mathbf{x}, 0) = \mathcal{W}_0(\mathbf{x}) = \mathcal{W}_{\text{IC}}(\mathbf{x})$$

└ Initial Boundary Value Problems

└ Parameterized PDE

- Parameter domain: $\mathcal{D} \subset \mathbb{R}^p$

- parameter vector (also referred to as parameter “point”):

$$\boldsymbol{\mu} = [\mu_1 \cdots \mu_p]^T \in \mathcal{D} \subset \mathbb{R}^p$$

where the superscript T designates the transpose operation

- Parameterized PDE

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

- Boundary conditions

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

- Initial condition

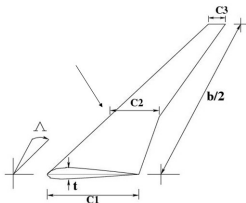
$$\mathcal{W}_0(\mathbf{x}) = \mathcal{W}_{\text{IC}}(\mathbf{x}; \boldsymbol{\mu})$$

└ Typical Parameters of Interest

■ Physical parameters

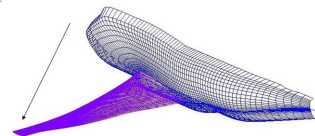
- shape parameters
- material (properties) parameters
- operation parameters (for example, flight conditions, cruise conditions, $\dots$)
- boundary conditions
- initial condition

6 planform variables
(sweep, span, t/c , 3 chords)



Simplified Planform Model

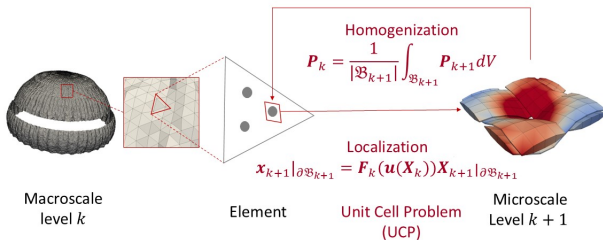
+ 4 224 mesh points on the wing
surface as design variables



CAD-Free Section Definition

■ Other types of parameters

- modeling parameters
- abstract parameters



Input to the UCP: 9 components of the deformation gradient $\mathbf{F}_k$

Output of the UCP: 3 components of the symmetric plane stress tensor

➡ Parameterization of the UCP: 9 components of $\mathbf{F}_k$

└ Semi-discretization Processes and Dynamical Systems

└ Semi-discretized problem

- The PDE is discretized in space using, for example
 - a finite difference method
 - a finite volume method
 - a finite element method
 - a discontinuous Galerkin method
 - a spectral method ...

└ Semi-discretization Processes and Dynamical Systems

└ Semi-discretized problem

- The PDE is discretized in space using, for example
 - a finite difference method
 - a finite volume method
 - a finite element method
 - a discontinuous Galerkin method
 - a spectral method ...
- This leads to a system of $N = \ell \times N_{\text{space}}$ Ordinary Differential Equations (ODEs) that can be written as

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

where

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

with the initial condition $\mathbf{w}(0; \mu) = \mathbf{w}_0(\mu)$

└ Semi-discretization Processes and Dynamical Systems

└ Semi-discretized problem

- The PDE is discretized in space using, for example
 - a finite difference method
 - a finite volume method
 - a finite element method
 - a discontinuous Galerkin method
 - a spectral method ...
- This leads to a system of $N = \ell \times N_{\text{space}}$ Ordinary Differential Equations (ODEs) that can be written as

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

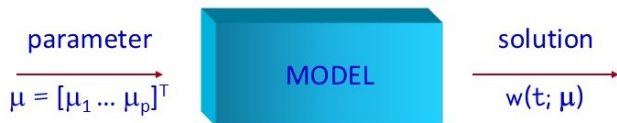
where

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

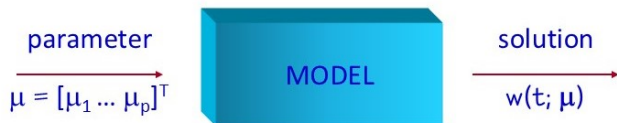
with the initial condition $\mathbf{w}(0; \mu) = \mathbf{w}_0(\mu)$

- This is the High-Dimensional Model (HDM)

■ Multi-query context

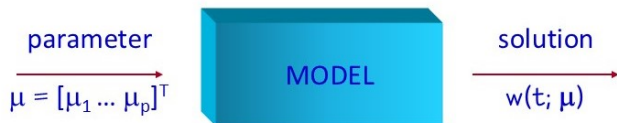


■ Multi-query context



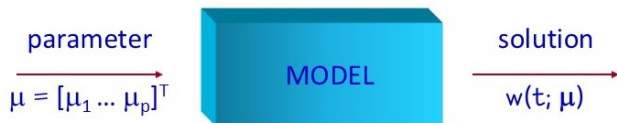
■ routine analysis

- Multi-query context



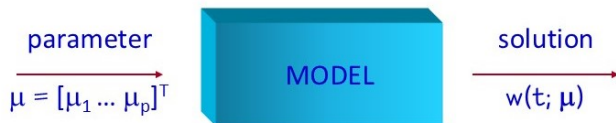
- routine analysis
- uncertainty quantification

■ Multi-query context



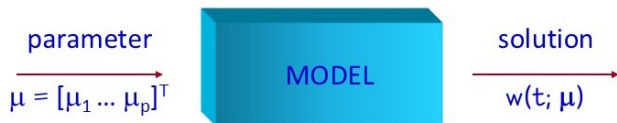
- routine analysis
- uncertainty quantification
- design optimization

■ Multi-query context



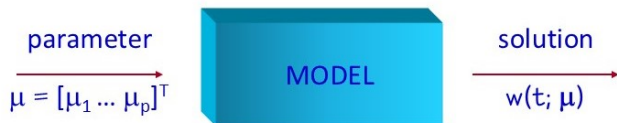
- routine analysis
- uncertainty quantification
- design optimization
- inverse problems

■ Multi-query context



- routine analysis
- uncertainty quantification
- design optimization
- inverse problems
- optimal control

■ Multi-query context

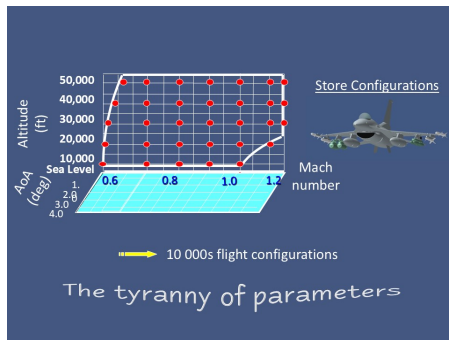
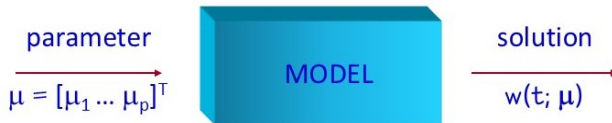


- routine analysis
- uncertainty quantification
- design optimization
- inverse problems
- optimal control
- model predictive control

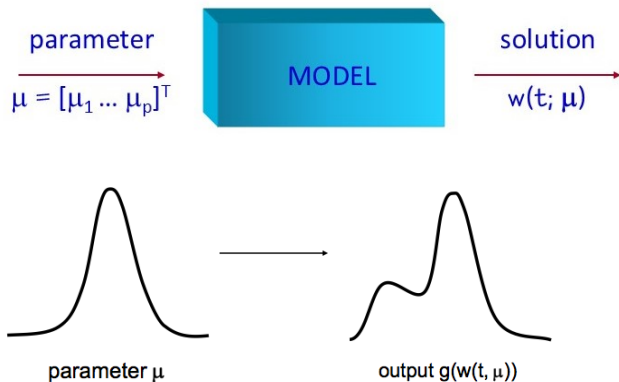
- Case for Model Order Reduction

- Multi-query Context

- Routine analysis



■ Uncertainty quantification

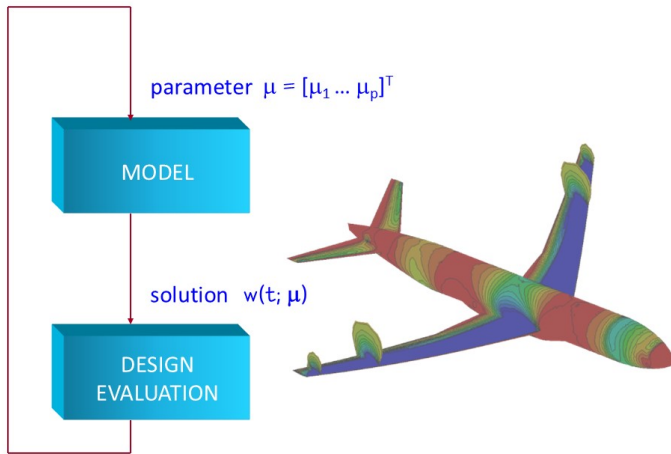


Monte-Carlo simulations ...

└ Case for Model Order Reduction

└ Multi-query Context

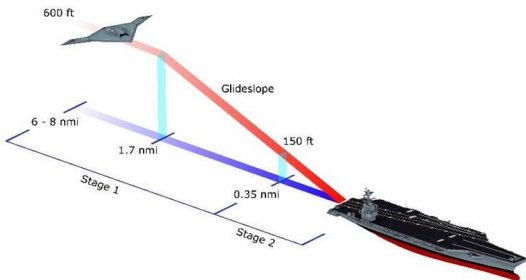
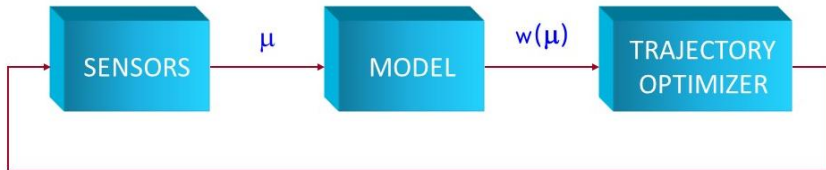
■ Design optimization



└ Case for Model Order Reduction

└ Multi-query Context

■ Model predictive control



└ Case for Model Order Reduction

└ Model Parameterized PDE

- Advection-diffusion-reaction equation: $\mathcal{W} = \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ solution of

$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \cdot \nabla \mathcal{W} - \kappa \Delta \mathcal{W} = f_{\text{R}}(\mathcal{W}, t; \boldsymbol{\mu}_{\text{R}}) \text{ for } \mathbf{x} \in \Omega$$

with appropriate boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_D) \text{ for } \mathbf{x} \in \Gamma_D$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_N$$

$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}; \boldsymbol{\mu}_{\text{IC}}) \text{ for } \mathbf{x} \in \Omega$$

└ Case for Model Order Reduction

└ Model Parameterized PDE

- Advection-diffusion-reaction equation: $\mathcal{W} = \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ solution of

$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \cdot \nabla \mathcal{W} - \kappa \Delta \mathcal{W} = f_R(\mathcal{W}, t; \boldsymbol{\mu}_R) \text{ for } \mathbf{x} \in \Omega$$

with appropriate boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_D) \text{ for } \mathbf{x} \in \Gamma_D$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_N$$

$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}; \boldsymbol{\mu}_{IC}) \text{ for } \mathbf{x} \in \Omega$$

- Parameters of interest

$$\boldsymbol{\mu} = [\mathcal{U}_1 \cdots \mathcal{U}_d \kappa \boldsymbol{\mu}_R \boldsymbol{\mu}_D \boldsymbol{\mu}_{IC}]^T$$

└ Case for Model Order Reduction

└ Parameterized Solutions

- Two-dimensional advection-diffusion equation

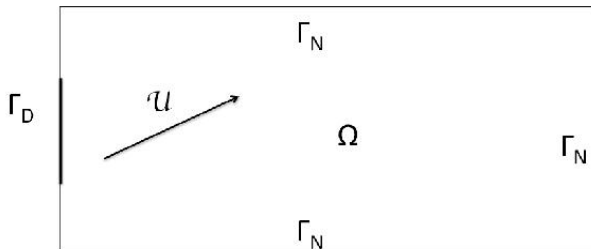
$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \cdot \nabla \mathcal{W} - \kappa \Delta \mathcal{W} = 0 \text{ for } \mathbf{x} \in \Omega$$

with boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_D) \text{ for } \mathbf{x} \in \Gamma_D$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_N$$

$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega$$



- Two-dimensional advection-diffusion equation

$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \cdot \nabla \mathcal{W} - \kappa \Delta \mathcal{W} = 0 \text{ for } \mathbf{x} \in \Omega$$

with boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_D) \text{ for } \mathbf{x} \in \Gamma_D$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_N$$

$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega$$

- 4 parameters of interest $\Rightarrow p = 4$

$$\boldsymbol{\mu} = [\mathcal{U}_1 \ \mathcal{U}_2 \ \kappa \ \boldsymbol{\mu}_D]^T \in \mathbb{R}^4$$

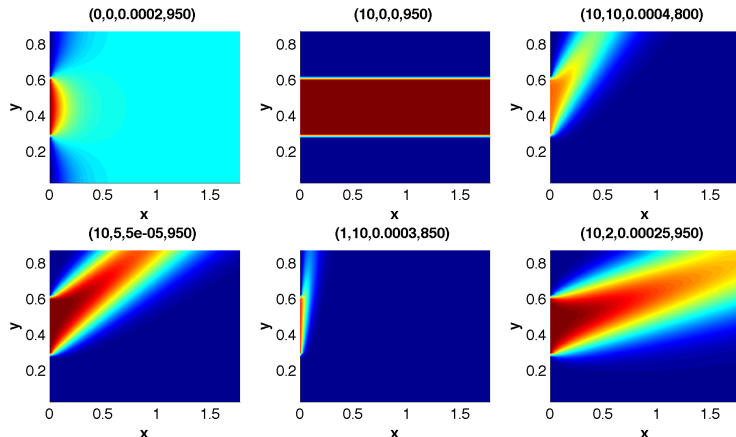
where $\boldsymbol{\mu}_D$ is a specified constant value of $\mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_D)$

- $\mathbf{w} \in \mathbb{R}^N$ with $N = 5402$

└ Case for Model Order Reduction

└ Parameterized Solutions

- Solution snapshots at some time t_i , for six sampled parameter points $\mu^{(j)}$, $j = 1, \dots, 6$ (recall that $\mu = [\mathcal{U}_1 \ \mathcal{U}_2 \ \kappa \ \mu_D]^T \in \mathbb{R}^4$)



- Question: Can we reuse the pre-computed snapshots to *reconstruct* a solution for a *queried but unsampled* parameter point μ^* ?

- Question: Can we reuse the pre-computed snapshots to *reconstruct* a solution for a *queried but unsampled* parameter point μ^* ?
- Idea: Use a linear combination of these snapshots such as, for example

$$\mathbf{w}(t; \mu^*) \approx \sum_{i=1}^{N_s^{(1)}} q_i^{(1)}(t; \mu^*) \mathbf{w}(t_i; \mu^{(1)}) + \cdots + \sum_{i=1}^{N_s^{(k)}} q_i^{(k)}(t; \mu^*) \mathbf{w}(t_i; \mu^{(k)})$$

where

- $N_s^{(j)}$, $j = 1, \dots, k$ denotes the number of pre-computed solution snapshots using the sampled parameter point $\mu^{(j)}$ and k denotes the total number of parameter points sampled in the parameter space $\mathcal{D}$
- $\mathbf{w}(t_i; \mu^{(j)}) \in \mathbb{R}^N$ denotes the pre-computed solution snapshots at time t_i using the sampled parameter point $\mu^{(j)}$
- $q_i^{(j)}(t; \mu) \in \mathbb{R}$ denotes the expansion coefficient associated with $\mathbf{w}(t_i; \mu^{(j)})$

- The linear expansion

$$\mathbf{w}(t; \mu) \approx \sum_{i=1}^{N_s^{(1)}} q_i^{(1)}(t; \mu) \mathbf{w}(t_i; \mu^{(1)}) + \cdots + \sum_{i=1}^{N_s^{(k)}} q_i^{(k)}(t; \mu) \mathbf{w}(t_i; \mu^{(k)})$$

can be written as

$$\mathbf{w}(t; \mu) \approx \mathbf{W} \mathbf{q}(t; \mu)$$

where

$$\mathbf{W} = \left[\mathbf{w}(t_1; \mu^{(1)}) \cdots \mathbf{w}(t_{N_s^{(1)}}; \mu^{(1)}) \cdots \mathbf{w}(t_1; \mu^{(k)}) \cdots \mathbf{w}(t_{N_s^{(k)}}; \mu^{(k)}) \right]$$

and

$$\mathbf{q}(t; \mu) = \left[q_1^{(1)}(t; \mu) \cdots q_{N_s^{(1)}}^{(1)}(t; \mu) \cdots q_1^{(k)}(t; \mu) \cdots q_{N_s^{(k)}}^{(k)}(t; \mu) \right]^T$$

- The parameterized approximation

$$\mathbf{w}(t; \boldsymbol{\mu}) \approx \mathbf{W}\mathbf{q}(t; \boldsymbol{\mu})$$

is a *subspace approximation* of $\mathbf{w}(t; \boldsymbol{\mu})$, where the subspace is

$$\mathcal{S} = \text{span} \left\{ \mathbf{w} \left(t_1; \boldsymbol{\mu}^{(1)} \right), \dots, \dots, \mathbf{w} \left(t_{N_s^{(k)}}; \boldsymbol{\mu}^{(k)} \right) \right\}$$

and its dimension is

$$\dim(\mathcal{S}) = \text{rank} \left[\mathbf{w} \left(t_1; \boldsymbol{\mu}^{(1)} \right) \cdots \cdots \mathbf{w} \left(t_{N_s^{(k)}}; \boldsymbol{\mu}^{(k)} \right) \right] \leq \sum_{j=1}^k N_s^{(j)}$$

- The parameterized approximation

$$\mathbf{w}(t; \boldsymbol{\mu}) \approx \mathbf{W}\mathbf{q}(t; \boldsymbol{\mu})$$

is a *subspace approximation* of $\mathbf{w}(t; \boldsymbol{\mu})$, where the subspace is

$$\mathcal{S} = \text{span} \left\{ \mathbf{w} \left(t_1; \boldsymbol{\mu}^{(1)} \right), \dots, \dots, \mathbf{w} \left(t_{N_s^{(k)}}; \boldsymbol{\mu}^{(k)} \right) \right\}$$

and its dimension is

$$\dim(\mathcal{S}) = \text{rank} \left[\mathbf{w} \left(t_1; \boldsymbol{\mu}^{(1)} \right) \cdots \cdots \mathbf{w} \left(t_{N_s^{(k)}}; \boldsymbol{\mu}^{(k)} \right) \right] \leq \sum_{j=1}^k N_s^{(j)}$$

- This approximation constitutes one of the pillars of projection-based model order reduction (PMOR): It raises the following questions
 - how to sample the parameter space $\mathcal{D}$?
 - how to reduce the dimensionality of $\mathbf{W}$ and therefore that of the approximation subspace $\mathcal{S}$ below $\sum_{j=1}^k N_s^{(j)}$?
 - how to compute the vector of generalized coordinates $\mathbf{q}(t; \boldsymbol{\mu})$?

- The parameterized approximation

$$\mathbf{w}(t; \boldsymbol{\mu}) \approx \mathbf{W}\mathbf{q}(t; \boldsymbol{\mu})$$

is a *subspace approximation* of $\mathbf{w}(t; \boldsymbol{\mu})$, where the subspace is

$$\mathcal{S} = \text{span} \left\{ \mathbf{w} \left(t_1; \boldsymbol{\mu}^{(1)} \right), \dots, \dots, \mathbf{w} \left(t_{N_s^{(k)}}; \boldsymbol{\mu}^{(k)} \right) \right\}$$

and its dimension is

$$\dim(\mathcal{S}) = \text{rank} \left[\mathbf{w} \left(t_1; \boldsymbol{\mu}^{(1)} \right) \cdots \cdots \mathbf{w} \left(t_{N_s^{(k)}}; \boldsymbol{\mu}^{(k)} \right) \right] \leq \sum_{j=1}^k N_s^{(j)}$$

- This approximation constitutes one of the pillars of projection-based model order reduction (PMOR): It raises the following questions
 - how to sample the parameter space $\mathcal{D}$?
 - how to reduce the dimensionality of $\mathbf{W}$ and therefore that of the approximation subspace $\mathcal{S}$ below $\sum_{j=1}^k N_s^{(j)}$?
 - how to compute the vector of generalized coordinates $\mathbf{q}(t; \boldsymbol{\mu})$?
- These are *some* of the questions that this course addresses

- Curse of dimensionality

- Curse of dimensionality
 - high-dimensional parameter spaces (application-dependent)

- Curse of dimensionality
 - high-dimensional parameter spaces (application-dependent)
 - assume that at minimum, the dependence of $\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ is linear in each component μ_i of $\boldsymbol{\mu} \Rightarrow$ at minimum, 2 parameter points must be sampled in each direction of the parameter space $\mathcal{D}$

- Curse of dimensionality
 - high-dimensional parameter spaces (application-dependent)
 - assume that at minimum, the dependence of $\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ is linear in each component μ_i of $\boldsymbol{\mu} \Rightarrow$ at minimum, 2 parameter points must be sampled in each direction of the parameter space $\mathcal{D}$
 - $\Rightarrow$ at minimum, 2^p parameter points must be sampled in $\mathcal{D}$

- Curse of dimensionality
 - high-dimensional parameter spaces (application-dependent)
 - assume that at minimum, the dependence of $\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ is linear in each component μ_i of $\boldsymbol{\mu} \Rightarrow$ at minimum, 2 parameter points must be sampled in each direction of the parameter space $\mathcal{D}$
 - $\Rightarrow$ at minimum, 2^p parameter points must be sampled in $\mathcal{D}$
 - $\Rightarrow$ for $p = 20$, at least $N_p = 1\,048\,576$ parameter points must be sampled in $\mathcal{D} \Rightarrow$ at least 1 048 576 high-dimensional solution snapshots must be computed!

- Curse of dimensionality
 - high-dimensional parameter spaces (application-dependent)
 - assume that at minimum, the dependence of $\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ is linear in each component μ_i of $\boldsymbol{\mu} \Rightarrow$ at minimum, 2 parameter points must be sampled in each direction of the parameter space $\mathcal{D}$
 - $\Rightarrow$ at minimum, 2^p parameter points must be sampled in $\mathcal{D}$
 - $\Rightarrow$ for $p = 20$, at least $N_p = 1\,048\,576$ parameter points must be sampled in $\mathcal{D} \Rightarrow$ at least 1 048 576 high-dimensional solution snapshots must be computed!
- Exponential growth of N_p with p and linear growth of the training cost with $N_p \Rightarrow$ *adaptive* sampling and additional strategies for mitigating the curse of dimensionality