# <span id="page-0-0"></span>AA216/CME345: PROJECTION-BASED MODEL ORDER REDUCTION

Parameterized Partial Differential Equations (PDEs)

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## Outline

- [Initial Boundary Value Problems](#page-2-0)
- [Typical Parameters of Interest](#page-6-0)
- [Untypical Parameters of Interest](#page-7-0)
- [Semi-discretization Processes and Dynamical Systems](#page-8-0)
- [The Case for Model Order Reduction](#page-11-0)
- [Subspace Approximation](#page-27-0)

<span id="page-2-0"></span> $\overline{\phantom{a}}$ [Initial Boundary Value Problems](#page-2-0)

■ Linear or Nonlinear Partial Differential Equation (PDE)

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

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

 $\overline{\phantom{a}}$ [Initial Boundary Value Problems](#page-2-0)

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- **Boundary Conditions (BCs)**

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

- Dirichlet BCs
- **Neumann BCs**

 $\mathbf{A} \equiv \mathbf{A} + \mathbf{A} + \mathbf{B} + \mathbf{A} + \math$ 

 $\overline{\phantom{a}}$ [Initial Boundary Value Problems](#page-2-0)

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- **Boundary Conditions (BCs)**

$$
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$$

Dirichlet BCs

**Neumann BCs** 

**n** Initial Condition (IC)

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

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<span id="page-5-0"></span> $\overline{\phantom{a}}$ [Initial Boundary Value Problems](#page-2-0)

[Parameterized PDE](#page-5-0)

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

**parameter vector (also referred to as parameter "point"):**  $\boldsymbol{\mu} = [\mu_1 \ \cdots \ \mu_p]^{\mathcal{T}} \in \mathcal{D} \subset \mathbb{R}^p$ 

where the superscript  $T$  designates the transpose operation

**Parameterized PDE** 

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

**Boundary conditions** 

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

**Initial condition** 

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

 $\mathbf{E} = \mathbf{A} \mathbf{E} \mathbf{b} + \mathbf{A} \mathbf{E} \mathbf{b} + \mathbf{A} \mathbf{B} \mathbf{b} + \mathbf{A} \mathbf{b}$ 

### <span id="page-6-0"></span>[Typical Parameters of Interest](#page-6-0)

#### **Physical parameters**

- shape parameters
- **n** material (properties) parameters
- operation parameters (for example, flight conditions, cruise conditions,  $\cdots$ )
- **boundary conditions**
- $\blacksquare$  initial condition



#### <span id="page-7-0"></span> $\overline{\phantom{a}}$  [Untypical Parameters of Interest](#page-7-0)

#### ■ Other types of parameters

- **n** modeling parameters
- abstract parameters



Input to the UCP: 9 components of the deformation gradient  $F_k$ Output of the UCP: 3 components of the symmetric plane stress tensor

<span id="page-8-0"></span> $\mathsf{\mathsf{L}}$  [Semi-discretization Processes and Dynamical Systems](#page-8-0)

 $\mathsf{\mathsf{L}}$  [Semi-discretized problem](#page-8-0)

- 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 ...

 $\mathsf{\mathsf{L}}$  [Semi-discretization Processes and Dynamical Systems](#page-8-0)

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	- a finite difference method
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	- a spectral method ...
- **This leads to a system of**  $N = \ell \times N_{\text{space}}$  **Ordinary Differential** Equations (ODEs) that can be written as

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

where

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

with the initial condition  $w(0; \mu) = w_0(\mu)$ 

 $\mathbf{E} = \mathbf{A} \oplus \mathbf{A} + \mathbf{A} \oplus \mathbf{A} + \mathbf{A} \oplus \mathbf{A} + \mathbf{A} \oplus \mathbf{A}$ 

 $\mathsf{\mathsf{L}}$  [Semi-discretization Processes and Dynamical Systems](#page-8-0)

 $\mathsf{\mathsf{L}}$  [Semi-discretized problem](#page-8-0)

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■ This is the High-Dimensional Model (HDM)

<span id="page-11-0"></span> $\overline{\phantom{a}}$  [The Case for Model Order Reduction](#page-11-0)



 $\overline{\phantom{a}}$  [The Case for Model Order Reduction](#page-11-0)

**Multi-query context** 



**n** routine analysis

[The Case for Model Order Reduction](#page-11-0)

**Multi-query context** 



**n** routine analysis

uncertainty quantification

**L** [The Case for Model Order Reduction](#page-11-0)



- **n** routine analysis
- uncertainty quantification
- design optimization

**L** [The Case for Model Order Reduction](#page-11-0)



- **routine analysis**
- uncertainty quantification
- design optimization
- $\blacksquare$  inverse problems

[The Case for Model Order Reduction](#page-11-0)



- **routine analysis**
- uncertainty quantification
- design optimization
- nverse problems
- optimal control

[The Case for Model Order Reduction](#page-11-0)

**Multi-query context** 



- **routine analysis**
- uncertainty quantification
- design optimization
- $\blacksquare$  inverse problems
- optimal control
- model predictive control

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 $\mathbf{E} = \mathbf{A} \oplus \mathbf{A} + \mathbf{A} \oplus \mathbf{A} + \mathbf{A} \oplus \mathbf{A} + \mathbf{A} \oplus \mathbf{A}$ 

<span id="page-18-0"></span>**L** [The Case for Model Order Reduction](#page-11-0)

[Multi-query Context](#page-18-0)

Routine analysis





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**L** [The Case for Model Order Reduction](#page-11-0)

[Multi-query Context](#page-18-0)

**Uncertainty quantification** 



- $\overline{\phantom{a}}$  [The Case for Model Order Reduction](#page-11-0)
	- [Multi-query Context](#page-18-0)
		- **Design optimization**



- [The Case for Model Order Reduction](#page-11-0)
	- [Multi-query Context](#page-18-0)
		- **Model predictive control**





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<span id="page-22-0"></span>**L** [The Case for Model Order Reduction](#page-11-0)

[Model Parameterized PDE](#page-22-0)

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

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

with appropriate boundary and initial conditions

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

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

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

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**L** [The Case for Model Order Reduction](#page-11-0)

[Model Parameterized PDE](#page-22-0)

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$$

$$
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$$

**Parameters of interest** 

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

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<span id="page-24-0"></span>[The Case for Model Order Reduction](#page-11-0)

[Parameterized Solutions](#page-24-0)

**T** Two-dimensional advection-diffusion equation

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

with boundary and initial conditions

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

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

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



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[The Case for Model Order Reduction](#page-11-0)

 $L$ [Parameterized Solutions](#page-24-0)

**Two-dimensional advection-diffusion equation** 

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

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

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

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

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

where  $\mu_D$  is a specified constant value of  $W_D(\mathbf{x}, t; \mu_D)$  $\textbf{w} \in \mathbb{R}^N$  with  $N=5\,402$ 

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<span id="page-26-0"></span>[The Case for Model Order Reduction](#page-11-0)

 $L$ [Parameterized Solutions](#page-24-0)

Solution snapshots at some time  $t_i$ , for six sampled parameter points  $\boldsymbol{\mu}^{(j)},\,j=1,\;\cdots,\;6$  (recall that  $\boldsymbol{\mu}=[\mathcal{U}_1\;\mathcal{U}_2\;\kappa\;\boldsymbol{\mu}_\mathrm{D}]^{\textstyle\mathcal{T}}\in\mathbb{R}^4)$ 



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<span id="page-27-0"></span> $\mathsf{\mathsf{L}}$ [Subspace Approximation](#page-27-0)

Question: Can we reuse the pre-computed snapshots to reconstruct a solution for a queried but unsampled parameter point  $\mu^{\star}$ ?

### $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

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

$$
\mathbf{w}(t; \boldsymbol{\mu}^{\star}) \approx \sum_{i=1}^{N_{\rm s}^{(1)}} q_i^{(1)}(t; \boldsymbol{\mu}^{\star}) \mathbf{w}(t_i; \boldsymbol{\mu}^{(1)}) + \cdots + \sum_{i=1}^{N_{\rm s}^{(k)}} q_i^{(k)}(t; \boldsymbol{\mu}^{\star}) \mathbf{w}(t_i; \boldsymbol{\mu}^{(k)})
$$

where

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

### <span id="page-29-0"></span>[Subspace Approximation](#page-27-0)

**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

$$
\mathsf{w}(t;\mu) \approx \mathsf{Wq}(t;\mu)
$$

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

$$
\mathbf{q}(t; \boldsymbol{\mu}) = \left[q_{1}^{(1)}(t; \boldsymbol{\mu})\ \cdots\ q_{N_{\mathrm{S}}^{(1)}}^{(1)}(t; \boldsymbol{\mu})\ \ \cdots\ q_{1}^{(k)}(t; \boldsymbol{\mu})\ \cdots\ q_{N_{\mathrm{S}}^{(k)}}^{(k)}(t; \boldsymbol{\mu})\right]^{T}
$$

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### <span id="page-30-0"></span> $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

■ The parameterized approximation

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

is a subspace approximation of  $w(t; \mu)$ , where the subspace is

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

and its dimension is

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

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<span id="page-31-0"></span> $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

■ The parameterized approximation

 $w(t; \mu) \approx Wq(t; \mu)$ 

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

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

- This approximation constitutes one of the pillars of projection-based model order reduction (PMOR): It raises the following questions
	- $\blacksquare$  how to sample the parameter space  $\mathcal{D}$ ?
	- $\blacksquare$  how to reduce the dimensionality of W and therefore that of the approximation subspace  $\mathcal S$  below  $\sum\limits_{j=1}^k N_s^{(j)}?$

• how to compute the vector of generalized coordinates  $q(t; \mu)$ ?

 $\mathbf{E} = \mathbf{A} \mathbf{E} \mathbf{b} + \mathbf{A} \mathbf{E} \mathbf{b} + \mathbf{A} \mathbf{B} \mathbf{b} + \mathbf{A} \mathbf{b}$ 

<span id="page-32-0"></span> $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

■ The parameterized approximation

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• how to compute the vector of generalized coordinates  $q(t; \mu)$ ? These are some of the questions that this c[our](#page-31-0)[se](#page-33-0) [a](#page-29-0)[d](#page-32-0)d[re](#page-33-0)[s](#page-27-0)s[es](#page-38-0)  $x \equiv x$ 

<span id="page-33-0"></span>[Subspace Approximation](#page-27-0)

**Curse of dimensionality** 

 $\mathsf{\mathsf{L}}$ [Subspace Approximation](#page-27-0)

### **Curse of dimensionality**

high-dimensional parameter spaces (application-dependent)

 $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

### ■ Curse of dimensionality

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

 $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

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- $\Rightarrow$  at minimum,  $2^p$  parameter points must be sampled in  $\mathcal D$

 $\mathsf{\mathsf{L}}$  [Subspace Approximation](#page-27-0)

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- $\Rightarrow$  at minimum,  $2^p$  parameter points must be sampled in  $\mathcal D$
- $\blacksquare \Rightarrow$  for  $p = 20$ , at least  $N_p = 1048576$  parameter points must be sampled in  $D \Rightarrow$  at least 1048 576 high-dimensional solution snapshots must be computed!

### <span id="page-38-0"></span>[Subspace Approximation](#page-27-0)

### ■ Curse of dimensionality

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### 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

 $\mathbf{E} = \mathbf{A} \mathbf{E} \mathbf{b} + \mathbf{A} \mathbf{E} \mathbf{b} + \mathbf{A} \mathbf{B} \mathbf{b} + \mathbf{A} \mathbf{b}$