Data-Driven Model Reduction to Support Decision Making in Complex Systems

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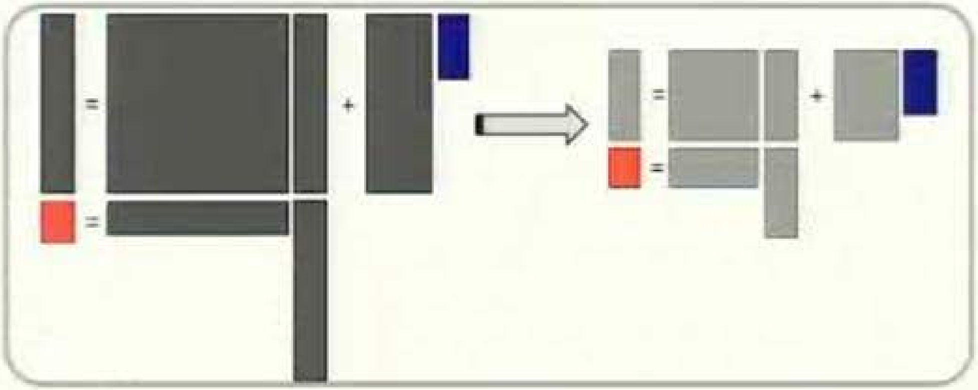
SIAM CSE15

Salt Lake City, UT
March 14, 2015



PROJECTION-BASED REDUCED MODELS

Data-driven reduced models

Reduced models are typically built and used in a static way:

- *offline phase*: sample a high-fidelity model, build a low-dimensional basis, project to build the reduced model
- *online phase*: use the reduced model

A single and/or static model is insufficient in many situations

- Complex physical system
- Other information sources, besides models
- Decision goal changes dynamically
- Physical system changes dynamically

→ A need for (online) adaptation of models

Data-driven reduced models

Adaptation is data-driven, where data could be:

- Sensor data collected online (e.g., structural sensors on board an aircraft)
- Simulation data collected online (e.g., over the path to an optimal solution)

Achieve adaptation in a variety of ways:

- Adapt the basis
- Adapt the way in which nonlinear terms are approximated
- Adapt the reduced model itself
- Construct localized reduced models; adapt through model choice

Start with a physics-based model

Arising, for example, from systems of ODEs or spatial discretization of PDEs describing the system of interest

- which in turn arise from governing physical principles (conservation laws, etc.)

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A}(\mathbf{p})\mathbf{x} + \mathbf{B}(\mathbf{p})\mathbf{u} \\ \mathbf{y} &= \mathbf{C}(\mathbf{p})\mathbf{x} \end{aligned}$$

$$\begin{aligned} \dot{\mathbf{x}} &= f(\mathbf{x}, \mathbf{p}, \mathbf{u}) \\ \mathbf{y} &= g(\mathbf{x}, \mathbf{p}, \mathbf{u}) \end{aligned}$$

$\mathbf{x} \in \mathbf{R}^N$: state vector

$\mathbf{u} \in \mathbf{R}^{N_i}$: input vector

$\mathbf{p} \in \mathbf{R}^{N_p}$: parameter vector

$\mathbf{y} \in \mathbf{R}^{N_o}$: output vector

Projection-based model reduction

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A}(\mathbf{p})\mathbf{x} + \mathbf{B}(\mathbf{p})\mathbf{u} \\ \mathbf{y} &= \mathbf{C}(\mathbf{p})\mathbf{x} \end{aligned}$$

$\mathbf{x} \approx \mathbf{V}\mathbf{x}_r$

$$\begin{aligned} \mathbf{r} &= \mathbf{V}\dot{\mathbf{x}}_r - \mathbf{A}\mathbf{V}\mathbf{x}_r - \mathbf{B}\mathbf{u} \\ \mathbf{y}_r &= \mathbf{C}\mathbf{V}\mathbf{x}_r \end{aligned}$$

$\mathbf{W}^T\mathbf{r} = 0$

$$\begin{aligned} \dot{\mathbf{x}}_r &= \mathbf{A}_r(\mathbf{p})\mathbf{x}_r + \mathbf{B}_r(\mathbf{p})\mathbf{u} \\ \mathbf{y}_r &= \mathbf{C}_r(\mathbf{p})\mathbf{x}_r \end{aligned}$$

$$\begin{aligned} \mathbf{A}_r(\mathbf{p}) &= \mathbf{W}^T\mathbf{A}(\mathbf{p})\mathbf{V} \\ \mathbf{B}_r(\mathbf{p}) &= \mathbf{W}^T\mathbf{B}(\mathbf{p}) \\ \mathbf{C}_r(\mathbf{p}) &= \mathbf{C}(\mathbf{p})\mathbf{V} \end{aligned}$$

$\mathbf{x} \in \mathbf{R}^N$: state vector

$\mathbf{p} \in \mathbf{R}^{N_p}$: parameter vector

$\mathbf{u} \in \mathbf{R}^{N_i}$: input vector

$\mathbf{y} \in \mathbf{R}^{N_o}$: output vector

$\mathbf{x}_r \in \mathbf{R}^n$: reduced state vector

$\mathbf{V} \in \mathbf{R}^{N \times n}$: reduced basis

Projection-based model reduction of nonlinear systems

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x},\mathbf{u}) \\ \mathbf{y} &= \mathbf{g}(\mathbf{x})\end{aligned} \quad \xrightarrow{\mathbf{x}=\mathbf{V}\mathbf{x}_r} \quad \begin{aligned}\dot{\mathbf{x}}_r &= \mathbf{V}^T\mathbf{f}(\mathbf{V}\mathbf{x}_r,\mathbf{u}) \\ \mathbf{y}_r &= \mathbf{g}(\mathbf{V}\mathbf{x}_r)\end{aligned}$$

- Nonlinear systems: standard projection approach leads to a model that is low order but still expensive to solve

- The cost of evaluating the nonlinear term

$$\mathbf{f}_r(\mathbf{x}_r,\mathbf{u}) = \mathbf{V}^T\mathbf{f}(\mathbf{V}\mathbf{x}_r,\mathbf{u})$$

still depends on *N*, the dimension of the large-scale system

- Can achieve efficient nonlinear reduced models via interpolation, e.g., Missing Point Estimation [Astrid et al., 2008], (Discrete) Empirical Interpolation Method [Barrault et al., 2004; Chaturantabut & Sorensen, 2010]

$$\dot{\mathbf{x}}_r = \mathbf{A}_r\mathbf{x}_r + \mathbf{E}_r\,\mathbf{f}_r(\mathbf{D}_r\mathbf{x}_r,\mathbf{u})$$

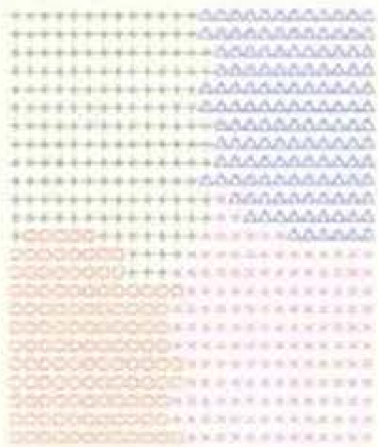
Computing the Basis: Proper Orthogonal Decomposition (POD)

(aka Karhunen-Loève expansions, Principal Components Analysis, Empirical Orthogonal Eigenfunctions, ...)

- Consider *K* **snapshots** $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_K \in \mathcal{R}^N$ [Sirovich, 1991] (solutions at selected times or parameter values)
- Form the snapshot matrix $X = [\mathbf{x}_1 \ \mathbf{x}_2 \ \ldots \ \mathbf{x}_K]$
- Choose the *n* basis vectors $\mathbf{V} = [\mathbf{V}_1 \ \mathbf{V}_2 \cdots \mathbf{V}_n]$ to be left singular vectors of the snapshot matrix, with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq \sigma_{n+1} \geq \cdots \geq \sigma_K$
- This is the optimal projection in a least squares sense:

$$\boxed{\min_{\mathbf{V}} \sum_{i=1}^{K} ||\mathbf{x}_i - \mathbf{V}\mathbf{V}^T\mathbf{x}_i||_2^2 = \sum_{i=n+1}^{K} \sigma_i^2}$$

- Similar idea to construct a basis for the nonlinear term using snapshots of $\mathbf{f}(\mathbf{x}, \mathbf{u})$ in DEIM approximation

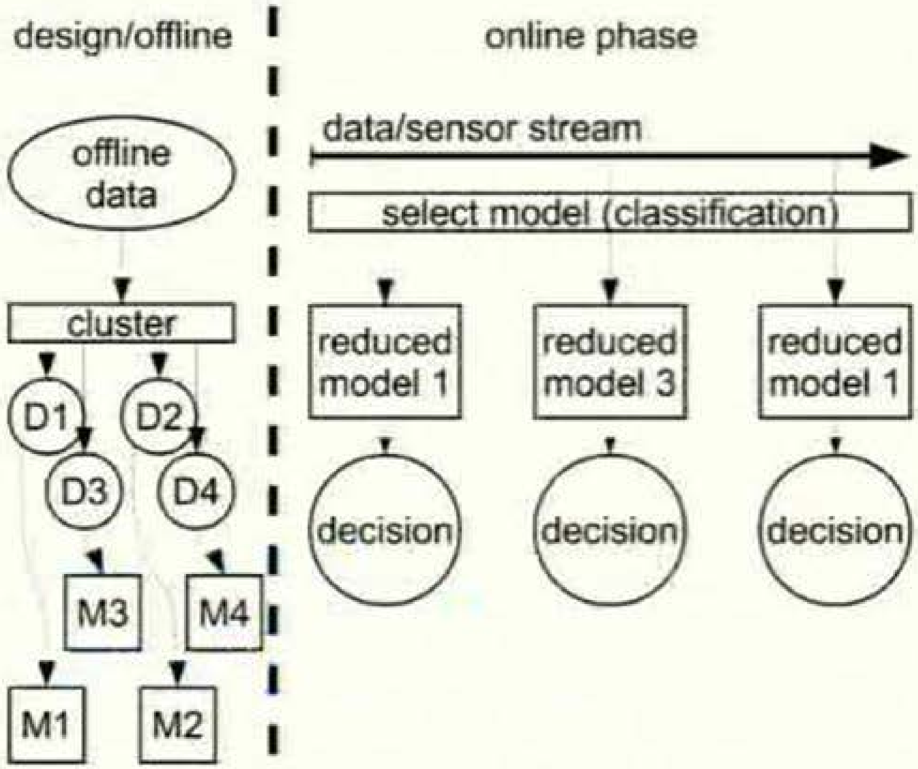


LOCALIZED REDUCED MODELS

Localized and adaptive reduced models

[Peherstorfer, Butnaru; W., Bungartz; SISC 2014]

- Automatic model management based on machine learning
  - Cluster set of snapshots $\mathcal{S} = \{x_1, \dots, x_M\} \subset \mathbb{R}^N$ into $\mathcal{S} = \mathcal{S}_1 \uplus \cdots \uplus \mathcal{S}_k$ (using e.g. k-means)
  - Create a separate local (reduced) model for each cluster
  - Derive a basis $Q \in \mathbb{R}^{N \times m}, m \ll N$ to obtain low-dimensional indicator $z_i = Q^T x_i$ that describes state x_i
  - Learn a classifier $g: Z \to \{1, \dots, k\}$ to map from low-dimensional indicator z to model index (using e.g. nearest neighbors)
  - Classify current state/indicator online and select model



→ Reduced models are tailored to local system behavior

Localized and adaptive reduced model

[Peherstorfer, Butnaru, W., Bungartz; SISC 2014]

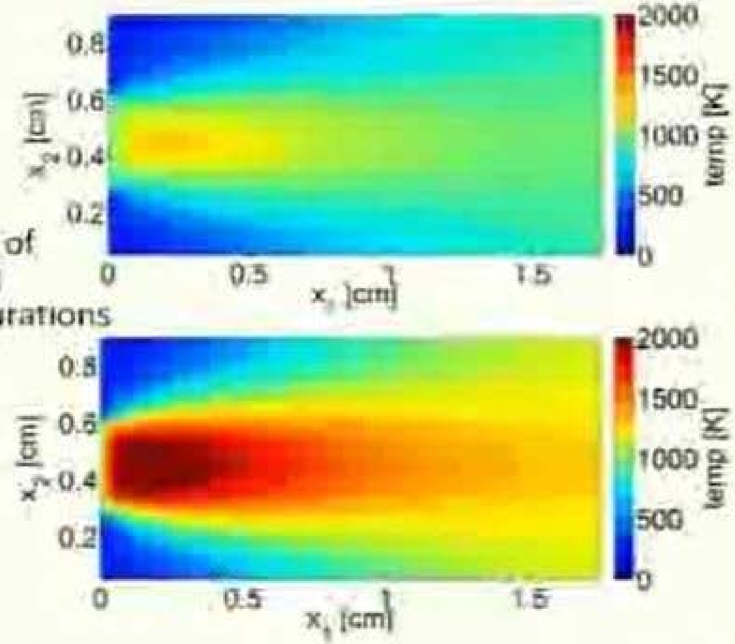
- Example: Reacting flow with one-step reaction

$$2H_2 + O_2 \rightarrow 2H_2O$$

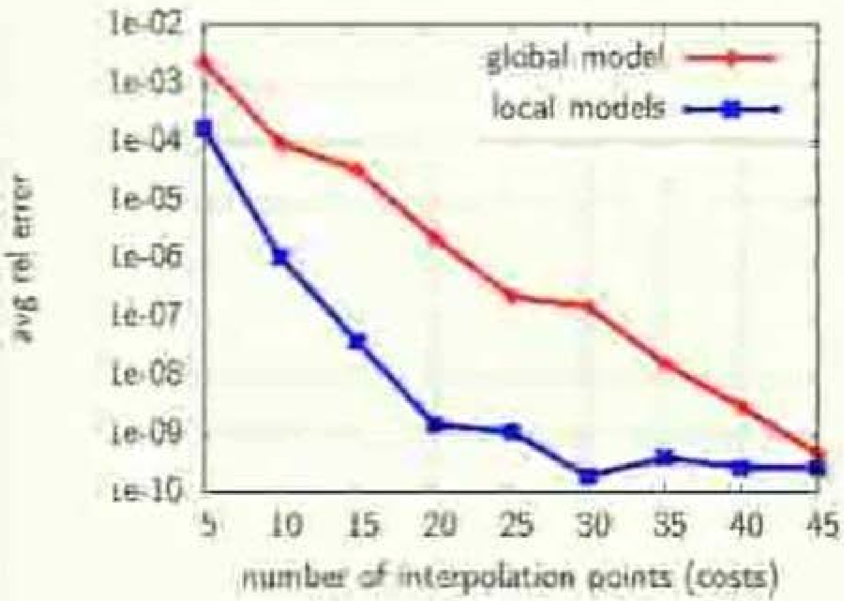
- Governed by convection-diffusion-reaction equation

$$\kappa \Delta \boldsymbol{y} - \nu \nabla \boldsymbol{y} + \boldsymbol{F}(\boldsymbol{y}, \boldsymbol{\mu}) = 0 \quad \text{in } \Omega$$

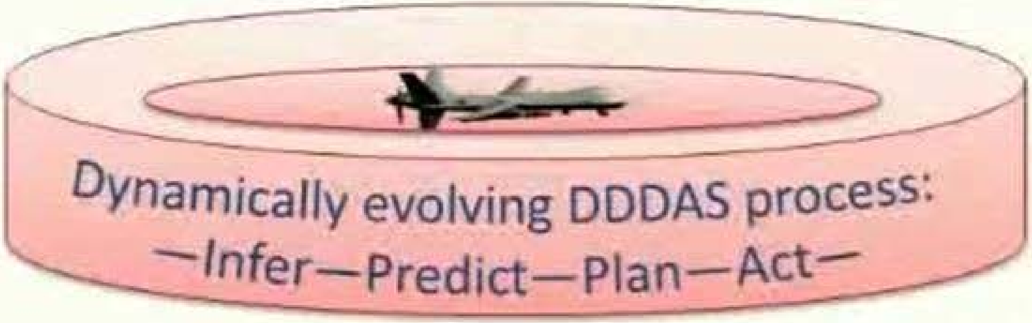
- Exponential nonlinearity (Arrhenius-type source term)
- POD-DEIM reduced model



Temperature field of flame for different parameter configurations



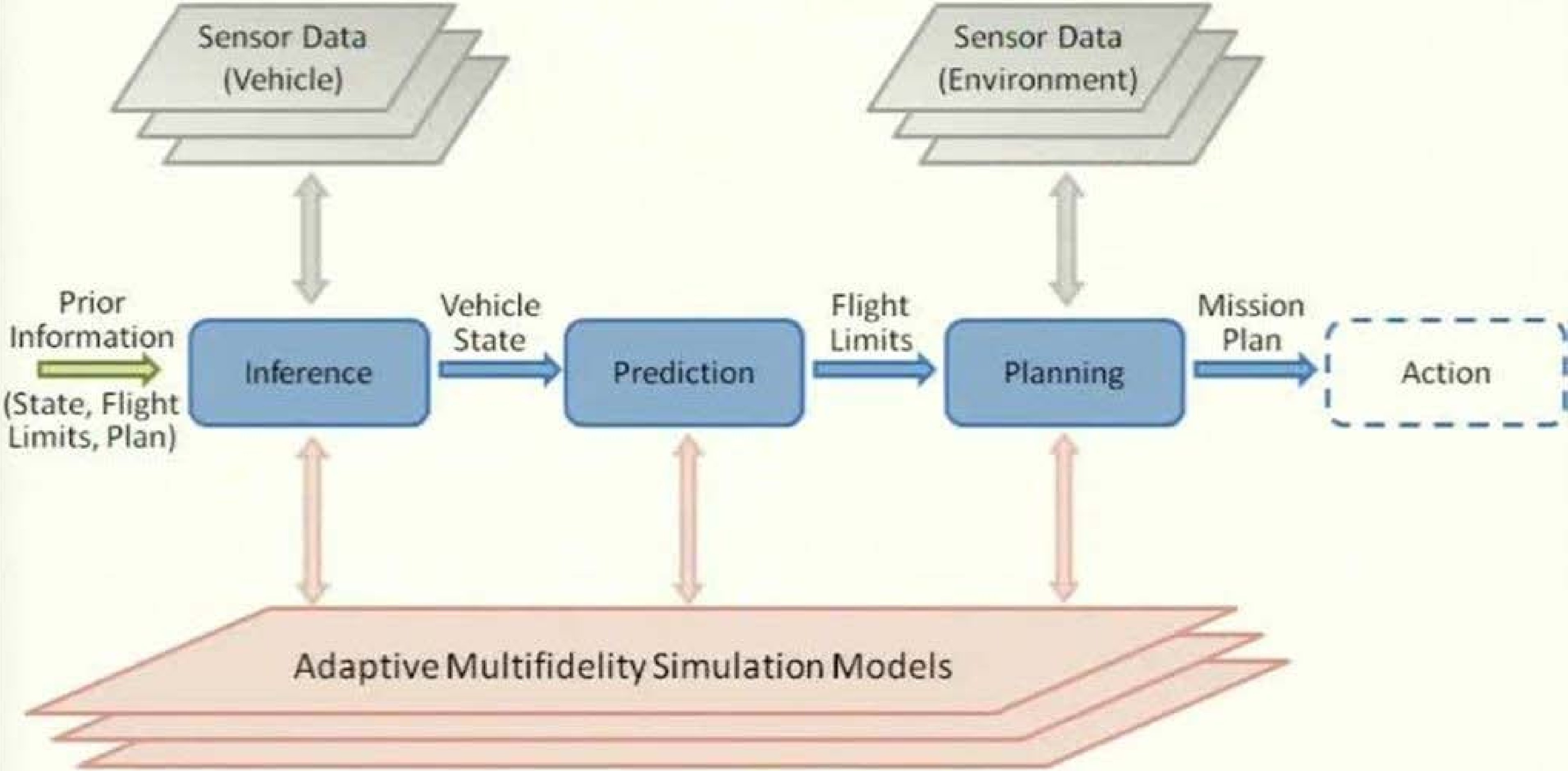
Combining **4 local models** with machine-learning-based model management achieves **accuracy improvement by up to two orders of magnitude** compared to a single, global model



DYNAMIC DATA-DRIVEN DECISIONS VIA ADAPTIVE REDUCED MODELS

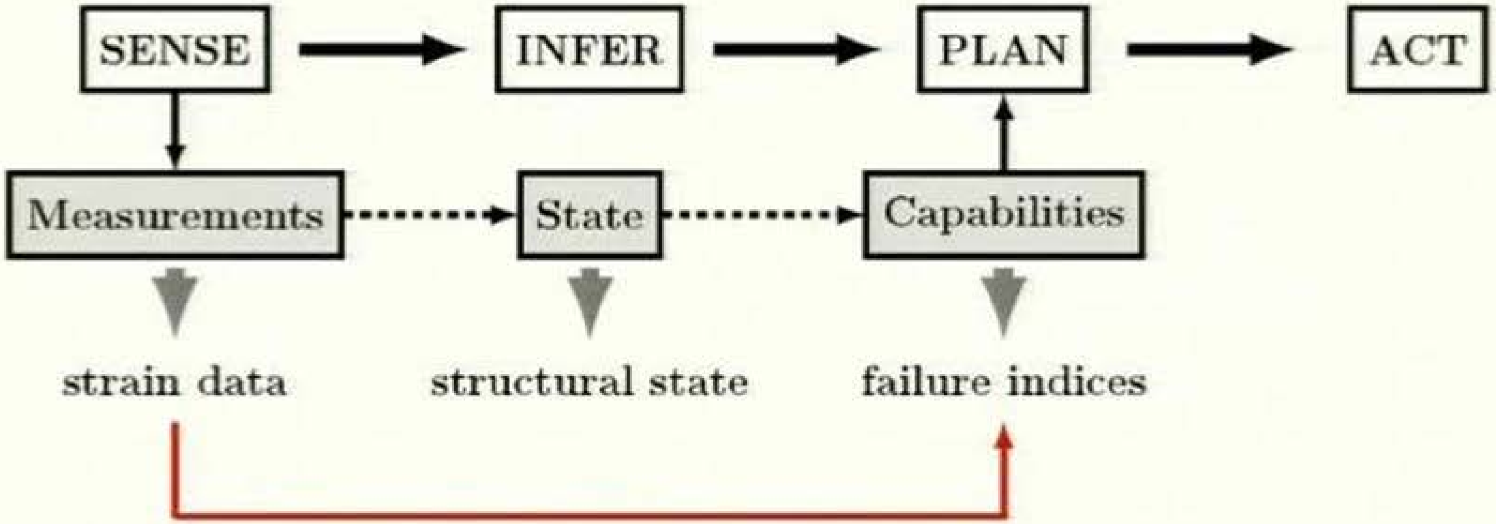
Motivating application: Dynamic data-driven decisions

- A **self-aware aerospace vehicle** can dynamically adapt the way it performs missions by gathering information about itself and its surroundings and responding intelligently



Dynamic data-driven structural assessment

[Mainini & W., AIAA 2015]

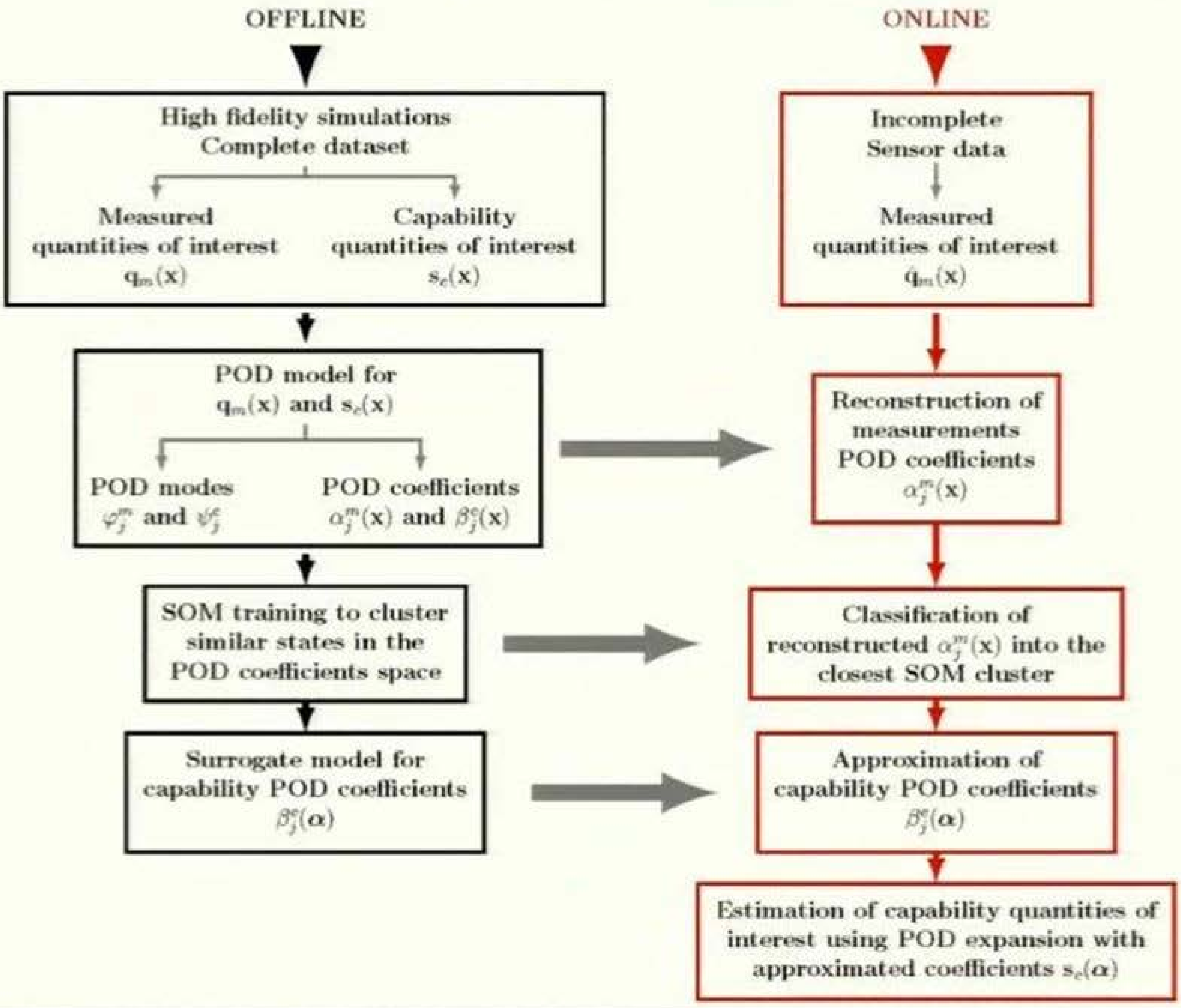


We want to:

use sensed structural data
└→ estimate the structural state
└→ update the flight capabilities
└→ dynamically re-plan the mission

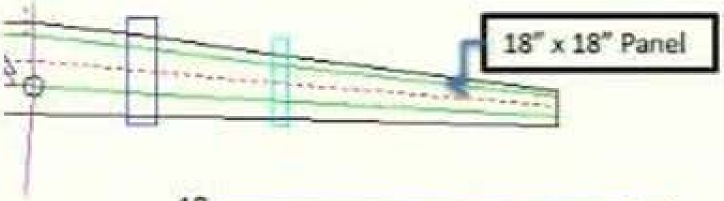
adaptive surrogate modeling to map from sensed data to capabilities

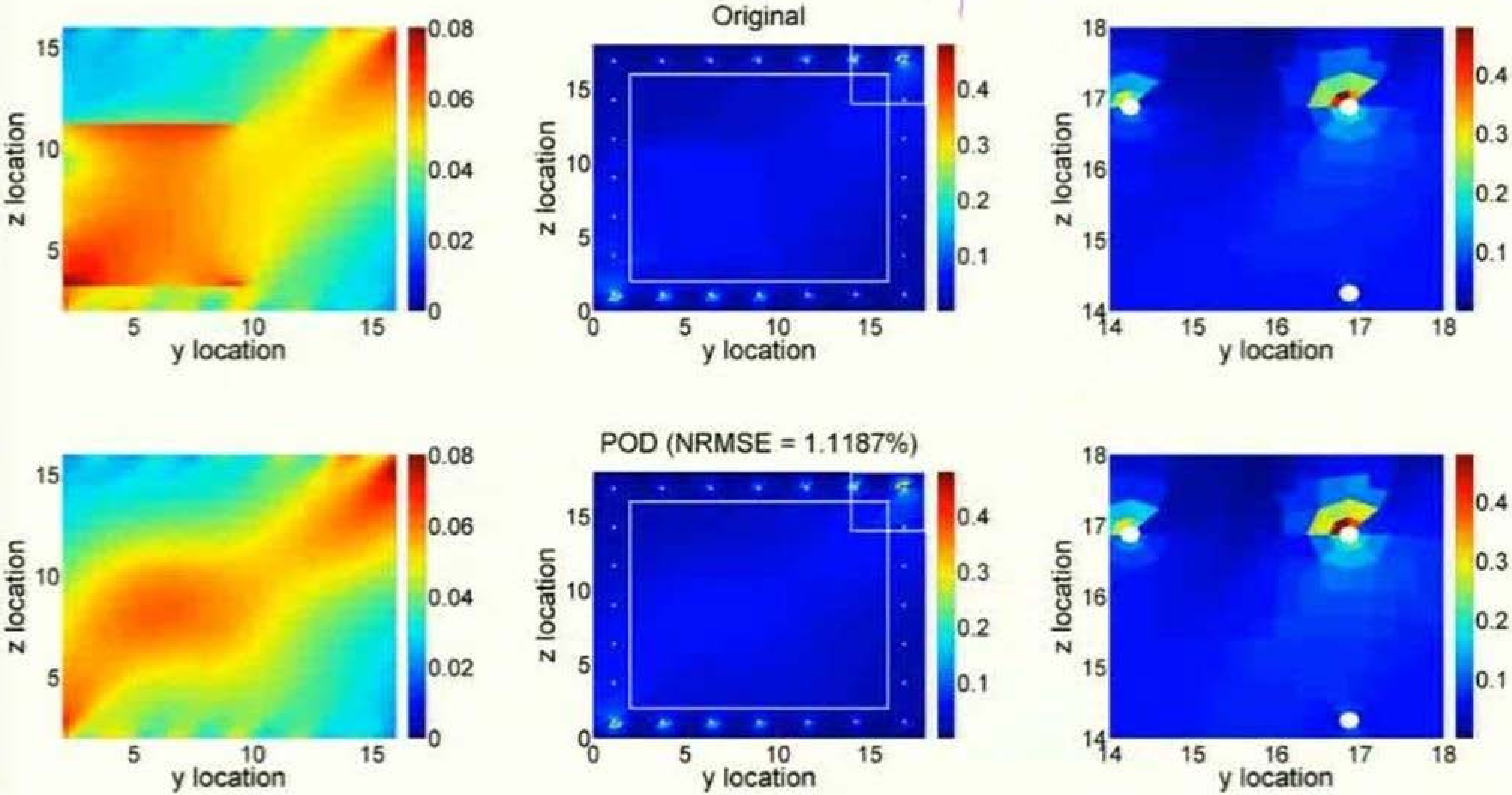
Localization and adaptation using POD and self-organizing maps



Dynamic data-driven structural assessment

Damage: 7.85 x 9.91 in^2, at (5.47, 7.15), ply 4 to 6





measure strain data → POD + SOM models → estimate Failure Index (FI)

$$\pi(p|d) \sim L(d|p)\, \pi_0(p)$$

DATA-DRIVEN REDUCED MODELS FOR INVERSE PROBLEMS

SUMMARY

Data-driven reduced models: Summary

Data-driven reduced models via adaptation, where data could be:

- Sensor data collected online (e.g., structural sensors on board an aircraft)
- Simulation data collected online (e.g., over the path to an optimal solution)

Achieve adaptation in a variety of ways:

- Adapt the basis
  - Data-driven reduced models for inverse problems *(Cui et al., 2014)*
- Adapt the way in which nonlinear terms are approximated
  - Adaptive DEIM *(Peherstorfer, MS260 Wed 1210)*
- Adapt the reduced model itself
  - Low-rank updates *(Peherstorfer & W., in review)*
- Construct localized reduced models; adapt through model choice *(Peherstorfer et al., 2014; Mainini & W., 2015; Mainini MS55)*

Conclusions

- The next generation of complex engineered systems will be endowed with sensors and computing capabilities that enable new modes of decision-making
- New opportunities for model reduction and surrogate modeling, in particular through data-driven reduced models that exploit the synergies of physics-based computational modeling and physical data
  - different sources of information (models, sensors, etc.) tell us different things about the decision problem, with the collective information they provide being greater than the individual parts
  - need methods that leverage complementary perspectives from physics-based modeling and data-driven approaches