

# Data and Models - Introductory Comments

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## 1 What is this about?

- Prelude
- Examples

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## 2 Two Worlds

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- Discrete  $\leftrightarrow$  continuous ( $\infty$ -dimensional) settings;
- nonlinear and adaptive concepts;
- optimization

# Playgrounds

Data (-Science): extract information from observations/measurements ...

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- atomistic models (micro-scale)
- kinetic models (meso-scale)
- continuum models, balance laws (macro-scale)
- multiscale models

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Quantify information/prediction accuracy



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Examples:  $\rightsquigarrow$  "Small-Data Problem"

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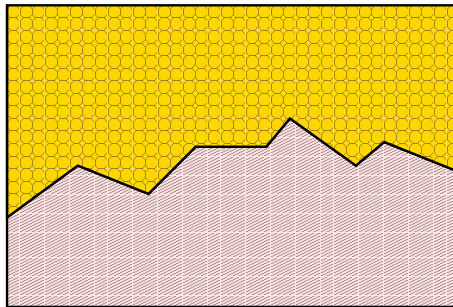
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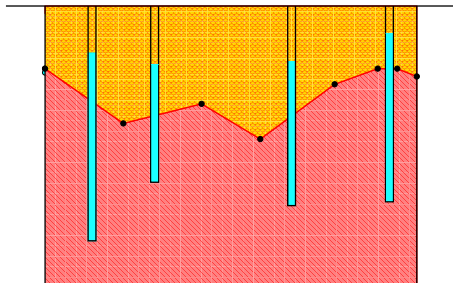
# Porous Media Flow



Model:

$$-\operatorname{div}(a(y)\nabla u) = f \quad (+b.c.'s)$$

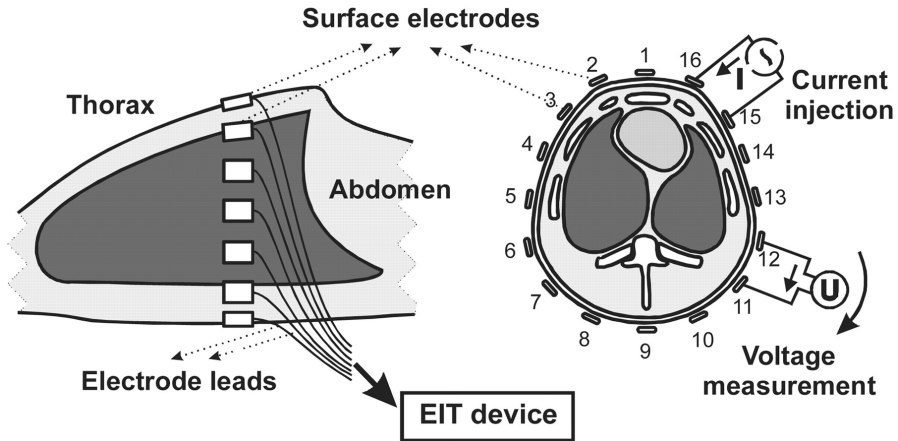
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## EIT



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# Data Driven Approaches

## Big Data Problem

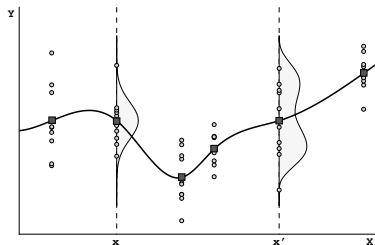
- Given data/observations/measurements

$$\mathcal{Z}_n = \{(z_i = (x_i, y_i) : i = 1, \dots, n)\} \subset \mathbb{X} \times \mathbb{Y}$$

learn "functional law":  $f : \mathbb{X} \rightarrow \mathbb{Y}$ ,  $f(x_i) \approx y_i$ , explaining the data

- Stochastic model:  $z_i$  i.i.d. with respect to (often) **unknown** probability density  $\rho$  on  $\mathbb{X} \times \mathbb{Y}$
- Typical goal: find an **estimator**  $\hat{f}_{\mathcal{Z}_n} : \mathbb{X} \rightarrow \mathbb{Y}$  that approximates  $f$  in a certain sense
- $\mathbb{Y} = \text{continuum} \rightsquigarrow$  regression
- $\#\mathbb{Y} < \infty \rightsquigarrow$  classification

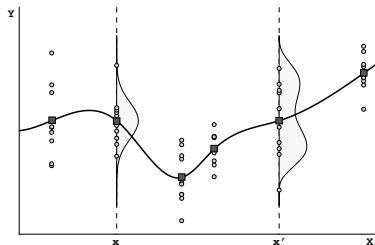
# Regression



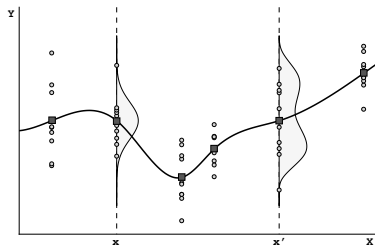


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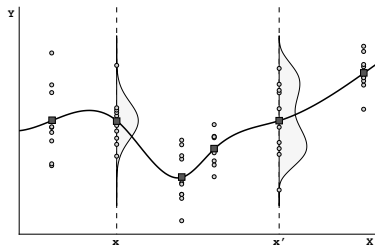


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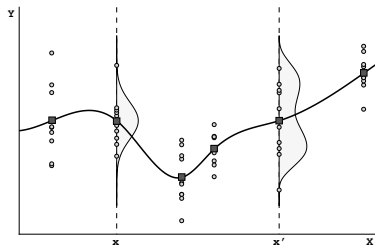
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Risk functional:

$$\mathcal{E}(f) := \int_{\mathbb{X} \times \mathbb{Y}} (y - f(x))^2 d\rho$$

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$$\mathcal{E}(f) = \mathcal{E}(f_\rho) + \|f - f_\rho\|_{L_2(\mathbb{X}, \rho_X)}^2, \quad \|\cdot\| := \|\cdot\|_{L_2(\mathbb{X}, \rho_X)}$$

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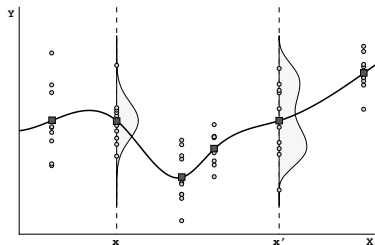
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Ideal desirable performance bound:

$$\mathbb{P}_{\rho^n} \left\{ \mathcal{Z} : \|f_\rho - \hat{f}_{\mathcal{Z}}\| \geq c(d) \left( \frac{\log n}{n} \right)^{\frac{s}{2s+1}} \right\} \leq Cn^{-\beta}$$

$$d\rho(x, y) = d\rho(y|x)d\rho_X(x)$$

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Applications: imaging, spectral imaging, learning noise models

# Model Based Approaches

**Modeling:** Physical, technological process described by  $u$ : find "balance law" describing  $u$

$$F(u, f) = 0$$

where  $F(u, f) = G(u, \partial_t u, \partial_x^\alpha u) - f$  is a PDE, integral equation, etc.

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**Issues:**

- **fixed** discretization: efficient solvers, preconditioning

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**Issues:**

- **optimize** discretization, adaptive solvers



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- high-dimensionality



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**Forward problem:** given  $f \in \mathbb{F} = ???$  (and  $y$ ), find  $u \in \mathbb{U} = ???$  s.t.

$$F(u, f) = 0 \quad \text{is well conditioned}$$

**Discretization:** Contrive a discrete model

$$F_h(u_h, y, f) = 0 \quad y \in \mathcal{Y}$$

**Issues:**

- choice of  $\mathbb{U}, \mathbb{F}$  finite  $\leftrightarrow$  infinite-dimensional problem



# Ideal Stability

$F(u, f) = 0$  :  $\bar{u}$  approximation to  $u$  - would like to have:

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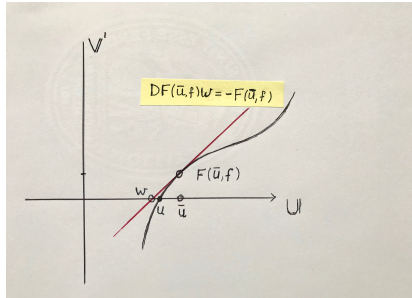
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inf-sup condition  $\rightsquigarrow$  DPG framework

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**inf-sup condition**  $\rightsquigarrow$  DPG framework
- A posteriori error indicators that drive **adaptive** refinements
- Residuals  $\rightsquigarrow$  surrogates for greedy constructions of **reduced bases**

# Example: Flooded City

Courtesy of Nils Gerhard and Siegfried Müller, RWTH Aachen, Germany

Reference:	Experiment in a Channel
Computational Domain:	$36 \times 3.6 \text{ m}^2$
Size of the Buildings:	$0.3 \times 0.3 \text{ m}^2$
Width of Streets between Buildings:	$0.1 \text{ m}$
# Buildings:	25

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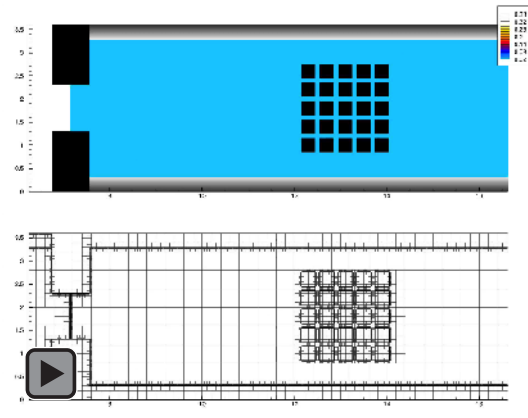
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# mesh cells:	13,271,040
# of D.o.Fs in Uniform Discretization:	79,626,240
maximal # of cells in Adaptive Mesh:	623,025 (4,7% of Reference Method)
# of Time Steps:	ca 1,000,000
CPU Time:	48 Hours on 320 CPUs (Intel Xeon Cluster)

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(click video to play)



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# The Role of Reduced Models

- Parametric family of PDEs:  $F(u, \mathbf{y}, f) = 0$ ,  $\mathbf{y} \in \mathcal{Y}$ ,  $\mathcal{M} = \{u(\mathbf{y}) : \mathbf{y} \in \mathcal{Y}\}$

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- Frequent parameter queries (design tasks, optimal control, calibration, parameter estimation, etc.)

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- Frequent parameter queries (design tasks, optimal control, calibration, parameter estimation, etc.)
- Given  $\epsilon > 0$ , find **possibly small** space  $\mathbb{U}_\epsilon \subset \mathbb{U}$  such that

$$\sup_{\mathbf{y} \in \mathcal{Y}} \inf_{w \in \mathbb{U}_\epsilon} \|u(\mathbf{y}) - w\|_{\mathbb{U}} =: \text{dist}(\mathcal{M}, \mathbb{U}_\epsilon) \leq \epsilon$$



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This workshop:

- foundational aspects of reduced models, data assimilation, state estimation
- structural imaging, optimization
- DPG - a framework for well conditioned variational formulations

