M2:SIAM (2019-2020)

Model exploration for approximation of complex high-dimensional problems.

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Overview

What is a model?

What is a complex high-dimensional problem?

How to build an approximation?

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What is a **model**?

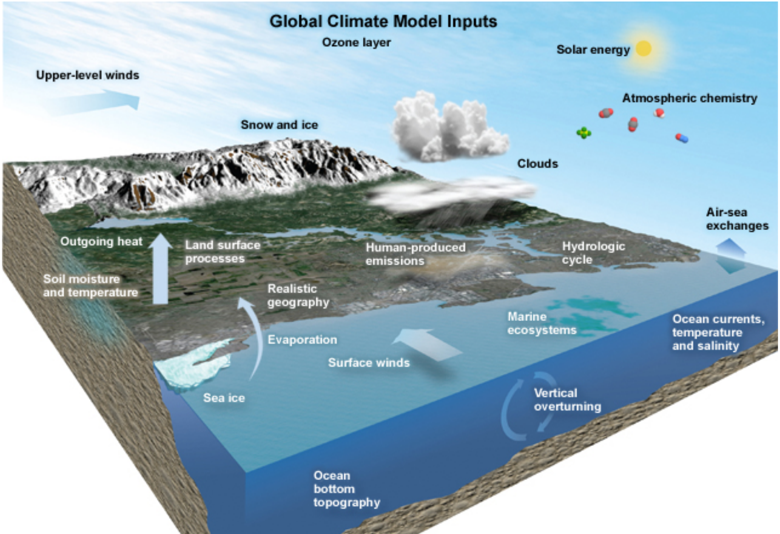
George Box: "All models are **wrong** but some are **useful**."

- Abstract (mathematical) representation of a phenomenon
- Useful for prediction, help better understand a problem at hand...
- Supercomputers gives the computational power to deal with complex models
- **Numerical models** as an input-output relationship:

$$\boxed{\text{Input parameter}} \xrightarrow{\text{Model}} \boxed{\text{Output of interest}}$$

Example: **climate change** simulation

Input



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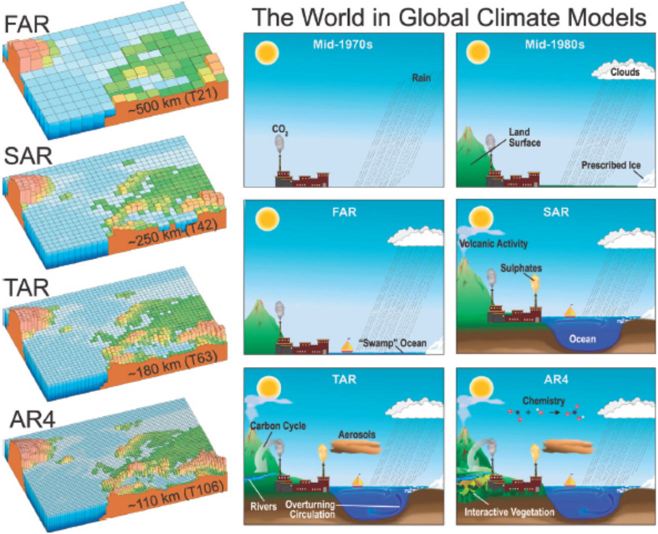
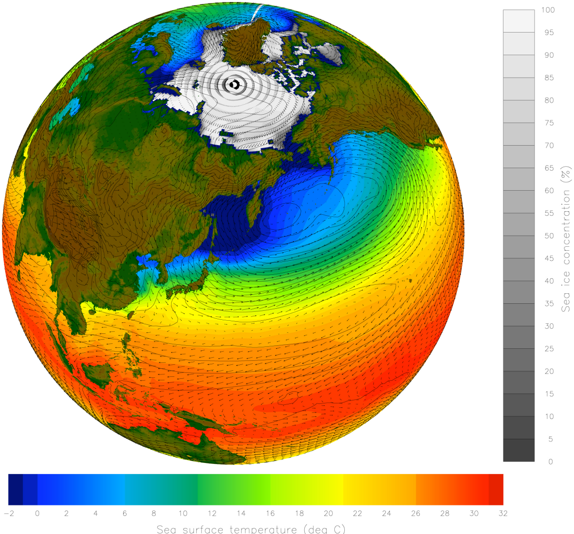
Input →



Example: **climate change** simulation

Input ⟶ Output



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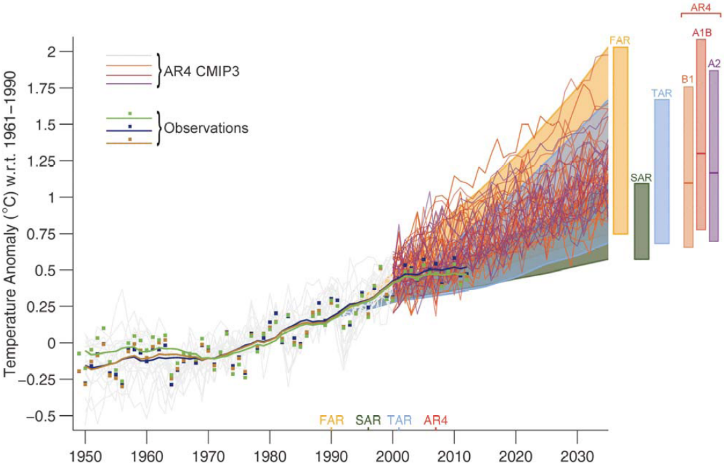
Input ⟶ Output



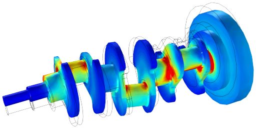
Example: **mechanical structure** simulation

$\boxed{\text{Input}} \longrightarrow \boxed{\text{Output}}$

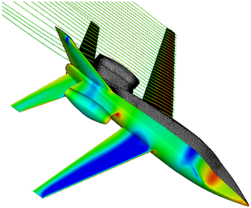
- Geometry
- External forcing
- Material properties
- ...

- VonMises stress field
- Probability of failure
- Lifespan
- ...

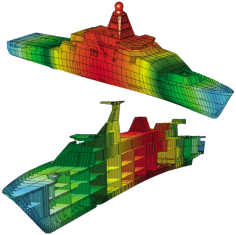
Cars



Airplanes



Ships



Example: **mechanical structure** simulation

Input $\longrightarrow$ Output

Input:

- **Geometry**
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- Material properties
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Output:

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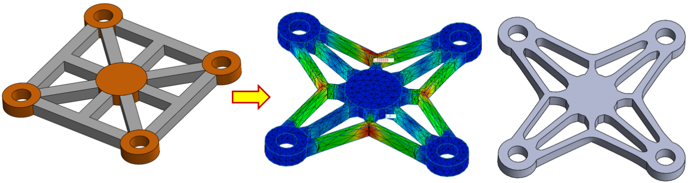

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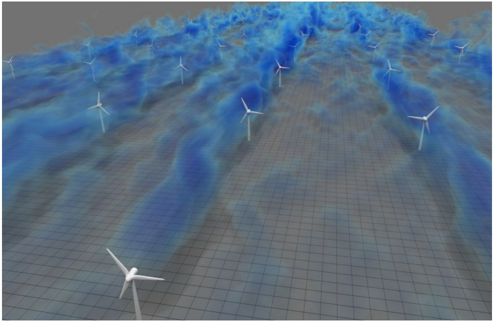

Example: **mechanical structure** simulation

Input $\longrightarrow$ Output

Input

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- **Material properties**
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Output

- VonMises stress field
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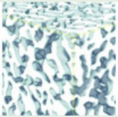
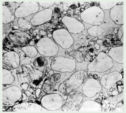
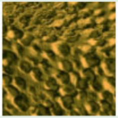
Snow



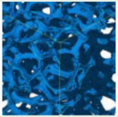
Sand



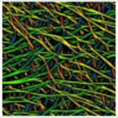
Composites



Foam



Polymers



Concrete

Overview

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How to build an approximation?

What is a **complex**, **high-dimensional** problem?

Gather the **input parameters** in a high-dimensional vector

$$x = (x_1, \dots, x_d), \quad d \gg 1$$

and denote by $u(x)$ the **output** of the model. The input-to-output map

$$\begin{aligned} u : \mathcal{P} &\to V \\ x &\mapsto u(x) \end{aligned}$$

is expensive to evaluate (*e.g.* requires the solution of a complex PDE).

- **Real time** simulation (e.g. weather forecasting for tomorrow should take less than 1 day!)
- **Optimization** problems (e.g. shape optimization)

$$\boxed{\min_x J\big(u(x)\big)}$$

- **Inverse problems**: knowing $u(x)$, can we find the corresponding x?

$$\boxed{u(x) \quad \rightsquigarrow \quad x}$$

- One often consider the parameter x as a realization of a random variable
$$X = (X_1, \ldots, X_d)$$
  - The parameter is **intrinsically random** (e.g. wind)
  - **Lack of knowledge** of the parameter (e.g. material properties): epistemic uncertainties

The goal of **uncertainty propagation** is to compute statistics (mean, variance, probability of failure...) of

$$\boxed{Y = u(X)}$$

Computational strategy

- Limited budget = only a few number of model runs is possible:

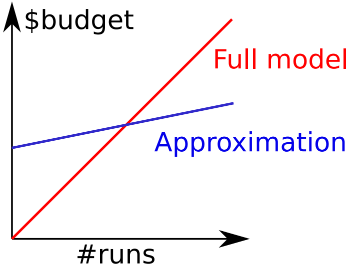
$$u(x^1), u(x^2), u(x^3), u(x^4).$$

- Offline-online strategy:

Allocate a part of the computational budget (**offline**) to build an approximation

$$\widetilde{u}(x) \approx u(x)$$

whose evaluation $x \mapsto \widetilde{u}(x)$ is much cheaper than the one of $x \mapsto u(x)$ (**online**).



- Then replace $u(x)$ by $\widetilde{u}(x)$ (not the only option!).

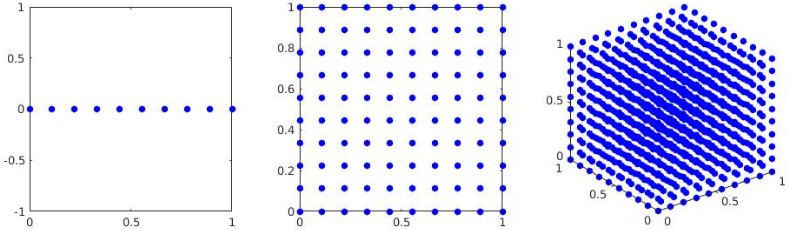
Limitations: the "**curse of dimensionality**" [Bellman1957]

Build an approximation by **learning** from u (sampling). The naive exploration of a d-dimensional space requires

$$\mathcal{O}(\exp(d))$$

point evaluations, and each evaluation if (very) expensive.

d=1 d=2 d=3



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Exploiting an **underlying structure** the function can have

- Assume that the function is **linear**:

$$u(x) = a^T x,$$

but a is unknown. How many evaluations of $x \mapsto u(x)$ do we need to recover $a \in \mathbb{R}^d$?

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- Same question, but with **quadratic** functions:

$$u(x) = \frac{1}{2} x^T A x + b^T x,$$

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- **Other options**:
  - Anisotropy,
  - Sparsity,
  - Small Kolmorogov width
  - Low-rank structure
  - Low-effective dimension
  - ...

To be or not to be "**intrusive**"? (not an easy notion to define...)

We'll see that some methods require more **intrusive coding** than other.

black box

Input parameter $\longrightarrow$

$\longrightarrow$ Output of interest

- There are some code you **cannot touch** at all (ultra specific and optimized codes, generally industrial codes)

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grey box

Input parameter →

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- Sometime you **have access to a lot**: gradients, residuals etc (recent codes or codes that are developed in academia)

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intrusive

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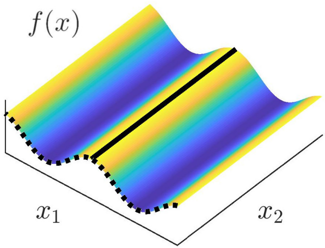
- Sometime you **have access to a lot**: gradients, residuals etc (recent codes or codes that are developed in academia)
- Some you can do **anything** (generally it's your code!)

Part I: Exploiting the "low-effective dimension"

Seek a **ridge** approximation

$$\boxed{u(x) \approx \widetilde{u}(x) = f(Ax) \quad \text{where} \begin{cases} A \in \mathbb{R}^{m\times d} \\ f : \mathbb{R}^m \to V \end{cases}}$$

- Sensitivity analysis and screening
- Active subspace
- Sliced Inverse Regression
- Ridge function recovery



Part II: Exploiting the “low-rank” structure

Seek a r-**term** approximation

$$\boxed{u(x) \approx \widetilde{u}(x) = \sum_{i=1}^{r} u_i \phi_i(x) \quad \text{where} \left\{ \begin{array}{l} u_r \in V \\ \phi_i : \mathbb{R}^d \to \mathbb{R} \end{array} \right.}$$

- Projection-based approximation
  - Proper Orthogonal Decomposition (POD)
  - Reduced Basis (RB)
- Least square via Polynomials
- Interpolation using Kernel functions
- ...

References

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