Uncertainty Quantification

Dealing with uncertainties in computational science and engineering

Lorenzo Tamellini

CNR-IMATI, Pavia

The Uncertainty Quantification framework

Parameters $\boldsymbol{y}$ ⟹ PDE/ODE ⟹

- Solution $u(\boldsymbol{x},\boldsymbol{y})$
- Solution functional $F(\boldsymbol{y})$

The Uncertainty Quantification framework

Parameters ***y***
- coefficients
- forcing terms
- Initial cond.
- boundary cond.
- Domain shape

⟹ PDE/ODE ⟹

- Solution *u(**x**,**y**)*
- Solution functional *F(**y**)*
  - Fluxes
  - Drag / lift forces
  - Time of arrival
  - ...

- ***y* are random/uncertain:**
  - experimental error
  - scarcity of data (expensive/difficult measurements)
  - lack of knowledge
  - intrinsic randomness (wind load, rainfall, earthquakes)
- Then, *u(**y**) and F(**y**)* are random quantities
- **What is the variability of *u and F* wrt to *y* ?**

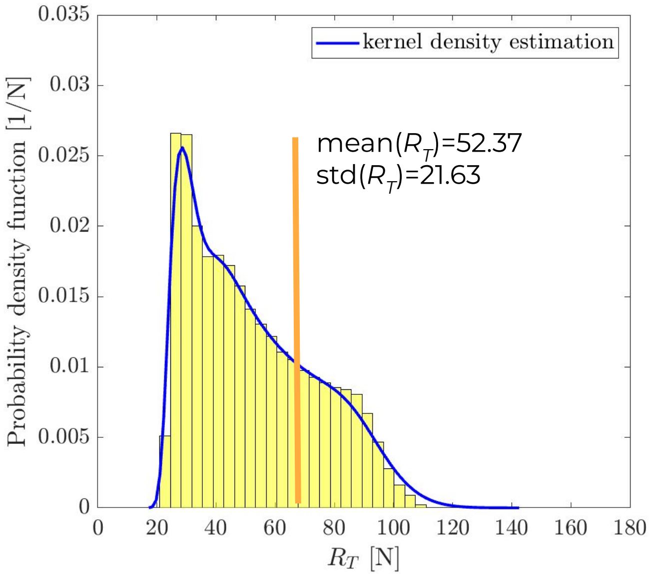
Different kind of analysis are possible

- **Forward UQ:**
  Compute mean, variance, quantiles, probability density function (pdf) of $u(\boldsymbol{y})$

- **Inverse UQ (calibration):**
  Can we reduce the uncertainty on $\boldsymbol{y}$ if we measure u?

Practical example: forward UQ for a ferry

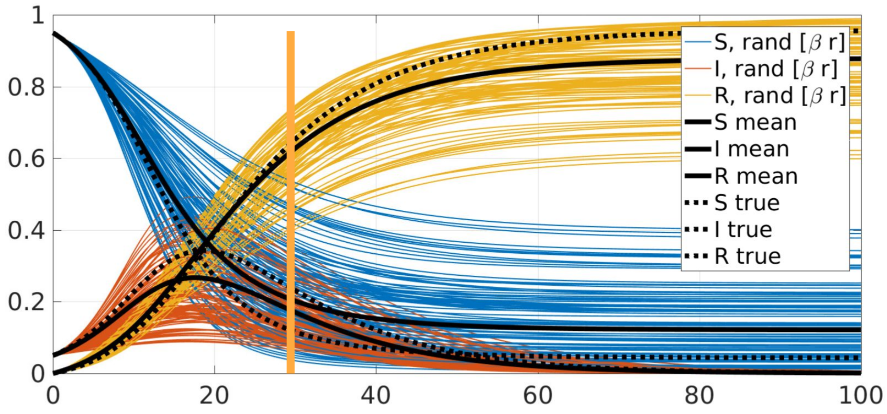
- Two operational **uncertain parameters:**
  - **Speed** within the operational range
  - **Draught** ±10% design (±15% design payload)
- Quantity of interest: resistance to advancement (ship drag)
- PDE: Navier-Stokes (RANS solver)



Practical example: inverse UQ for epidemics

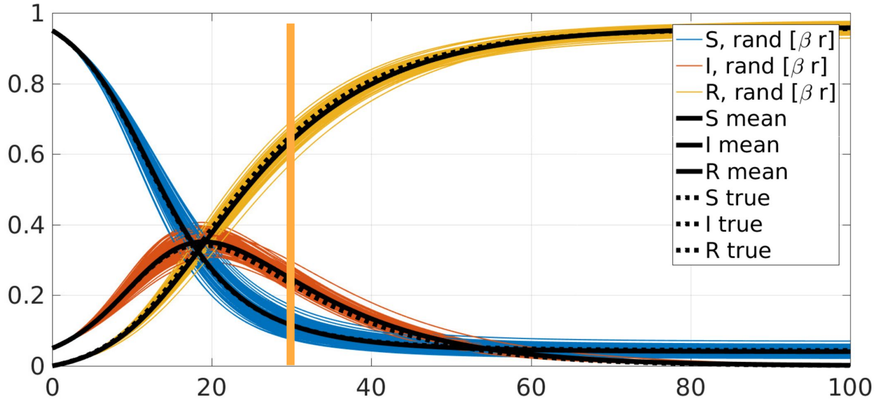
- Two **uncertain parameters**
  - **Contact probability, β**
  - **Recovery time**, r
- ODE: SIR system

no data are available



β in [0.25, 0.35], r in [0.06,0.18] (literature)

with data on I,R up to t=30



β ~ N(0.285,0.80), r ~ N(0.086,0.26)

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Different kind of analysis are possible

- **Forward UQ:**
  Compute mean, variance, quantiles, probability density function (pdf) of $u(\boldsymbol{y})$
  - **Sensitivity Analysis:**
    Which parameters impact the most the variability of u?
  - **Optimization under uncertainty:**
    If $u = u(\boldsymbol{x},\boldsymbol{y},\boldsymbol{p})$ and **p** are under our control, chose **p** that e.g. maximizes the expected value of u, or minimizes the variance
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  - **Identifiability analysis:** Can I actually calibrate $\boldsymbol{y}$ if I measure u?
    - *Structural*: is there a unique $\boldsymbol{y}$ that matches best my data?
    - *Practical*: how sensitive is my calibration to data quality (nb data, noise)?
  - **Design of experiments:**
    What measurement of u are the best to calibrate $\boldsymbol{y}$?

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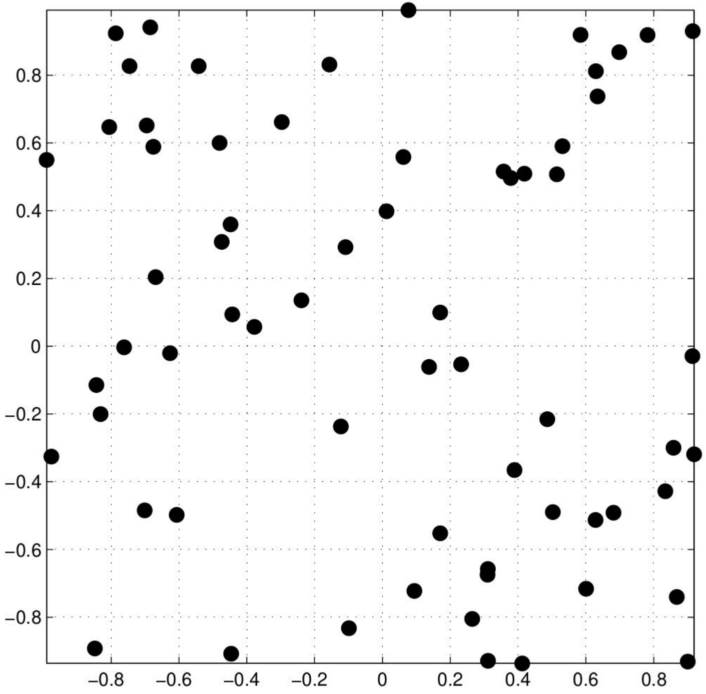
Solve, solve, solve!

- Most techniques boil down to repeatedly solving the ODE/PDE for multiple values of y (**sampling**)
- **How many** samples? For **what values** of y?
    - Alternative 1: **Monte Carlo**
        - Robust but very expensive
        - *Error* $\approx M^{-1/2}$



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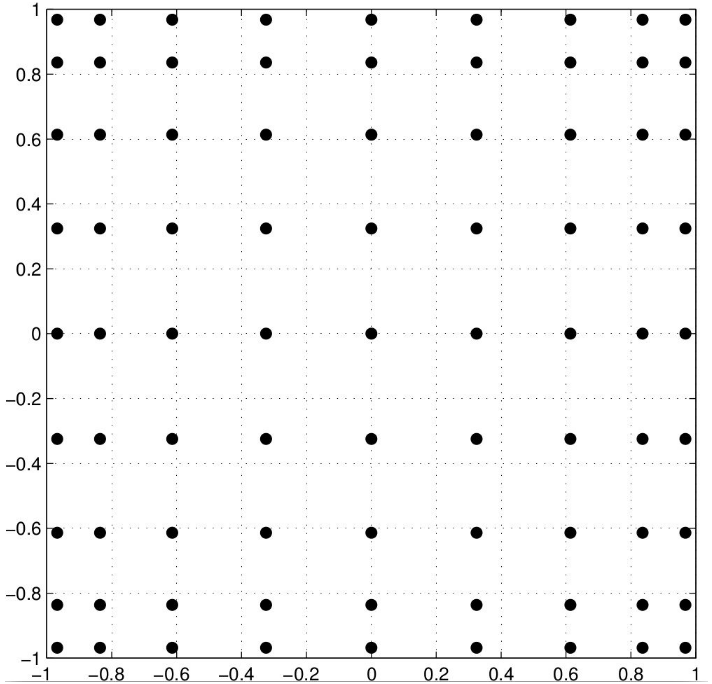
    - More accurate but also expensive
    - $M = M_0^N$



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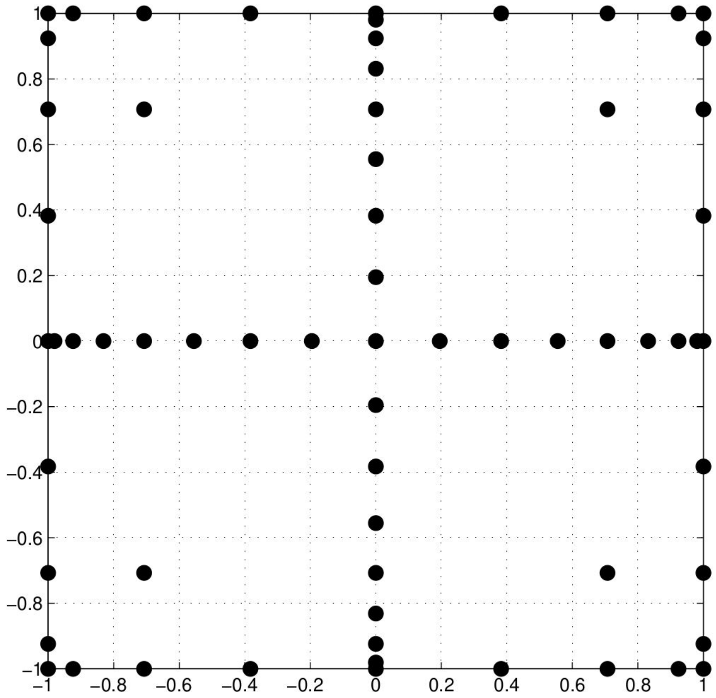
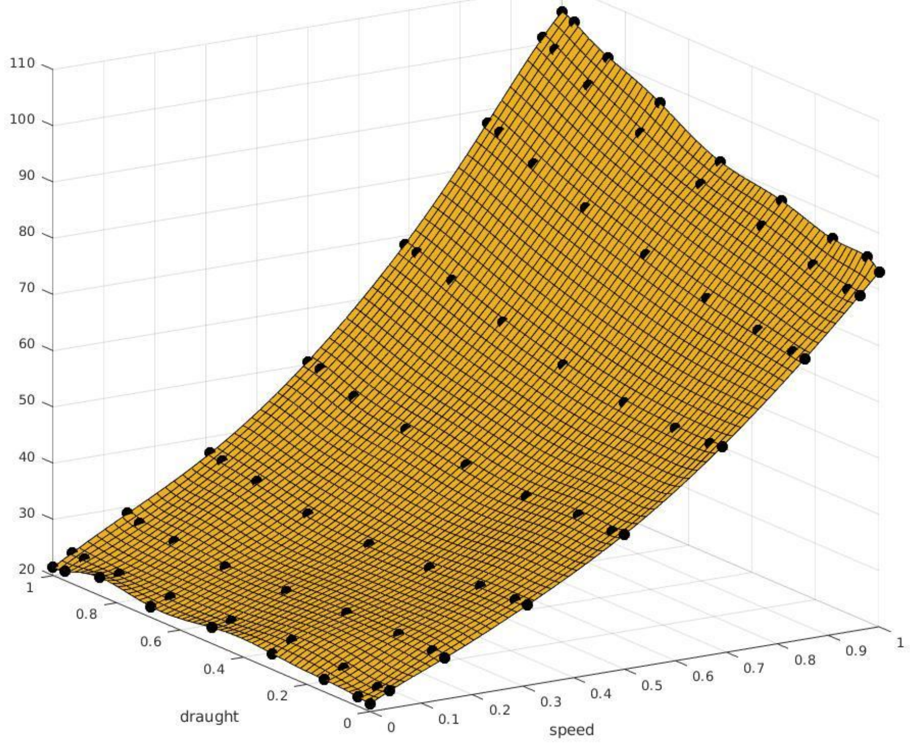
  - Alternative 3: **Sparse grids**, and more...



Make it faster: surrogate modeling

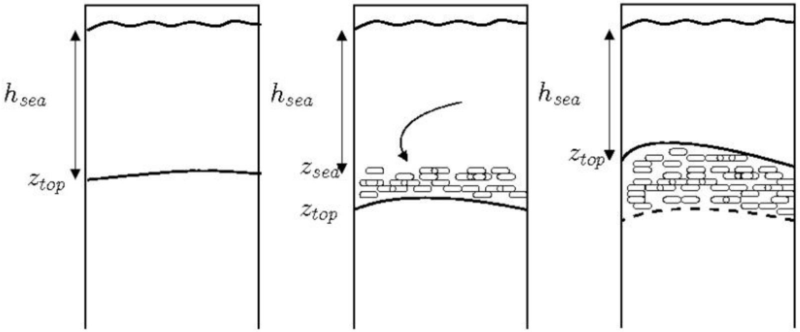
- Instead of solving the PDE for all value of ***y***
    a. Solve for a few “selected” ***y***
    b. “Interpolate” the values of *u*(***y***)
    c. Evaluate the surrogate model: **much cheaper!**
    d. Works for **smooth functions** *u*(***y***)

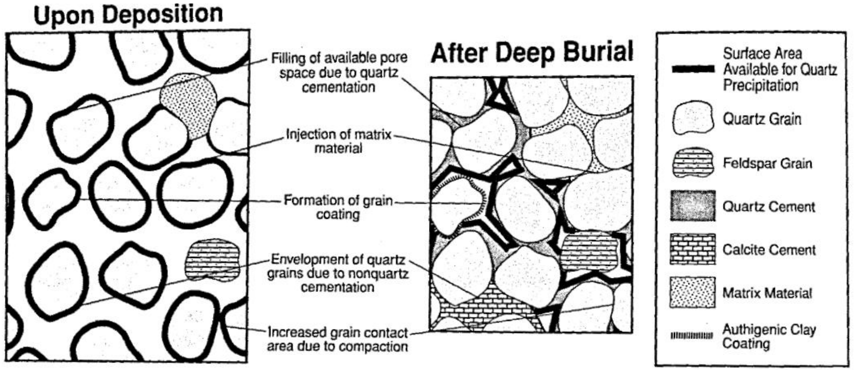


- Many alternatives:
    a. Polynomial Chaos Expansion
    b. Sparse Grids
    c. Reduced Basis
    d. Proper Orthogonal Decomposition
    e. Radial Basis Functions
    f. Gaussian Processes
    g. Neural Networks
    h. …

Example: a geochemical compaction model

How does sand on the bottom of the ocean become rock?





Example: a geochemical compaction model

conservation equations

$$\frac{\partial \phi \rho_l}{\partial t} + \frac{\partial [\phi \rho_l u_l]}{\partial z} = 0$$

water mass conservation law

$$\frac{\partial (1-\phi)\rho_s}{\partial t} + \frac{\partial [(1-\phi)\rho_s u_s]}{\partial z} = q_{qrtz}$$

solid mass conservation law

- q_{qrtz} is the quartz production rate
- h_{sea} is the height of the sea over the basin

$$C_1 \frac{\partial T}{\partial t} + C_2 \frac{\partial T}{\partial z} - \frac{\partial}{\partial z}\left(K_T \frac{\partial T}{\partial z}\right) = q_T$$

energy conservation law

- $C_1 = \phi \rho_l c_l + (1-\phi)\rho_s c_s$
- $C_2 = \phi \rho_l c_l u_l + (1-\phi)\rho_s c_s u_s$
- q_T represents internal heat sources

$$\sigma = \underbrace{-\int_{z_{top}}^{z} [\phi \rho_l + (1-\phi)\rho_s]\, g dz + s_0}_{\text{overburden load}} - p_l$$

force balance

- g is the gravity acceleration
- s_0 is the weight of the sea water column
- σ is resulting effective stress on the solid matrix

constitutive equations

$$K = 10^{k_1 \phi - k_2 - 15}$$

porosity/permeability law

$$\phi(u_l - u_s) = -\frac{K}{\mu_l}\left(\frac{\partial p_l}{\partial z} - \rho_l g\right)$$

Darcy law

- μ_l is the water viscosity

$$K_T(T) = \lambda_l^{\phi}[\lambda_s(T)]^{1-\phi}$$

thermal conductivity of the water/rock system

- $\lambda_s(T) = \lambda_0/(1 + c_0 T)$

$$\frac{d\phi}{dt} = \frac{d\phi_M}{dt} - \frac{d\phi_Q}{dt}, \quad \phi > 0$$

porosity rate of change

- $\frac{d\phi_M}{dt} = -\beta(\phi_0 - \phi_f)\exp(-\beta\sigma)\frac{d\sigma}{dt}$
- $\frac{d\phi_Q}{dt} = \frac{M_Q}{\rho_Q} A_0 \left(\frac{\phi}{\phi_{act}}\right) a\, 10^{bT} \quad T \geq T_c$

parameter	units	lower bound	upper bound
β	$[\mathrm{Pa}^{-1}]$	5×10^{-8}	7×10^{-8}
a	$[\mathrm{mol\ m^{-2}\ s^{-1}}]$	0.5×10^{-18}	3.5×10^{-18}
b	$[{}^\circ\mathrm{C}^{-1}]$	0.020	0.024
T_c	$[{}^\circ\mathrm{C}]$	70	90
h_{sea}	[m]	450	550
k_1	[-]	14.07	14.22
k_2	[-]	1.35	2.38

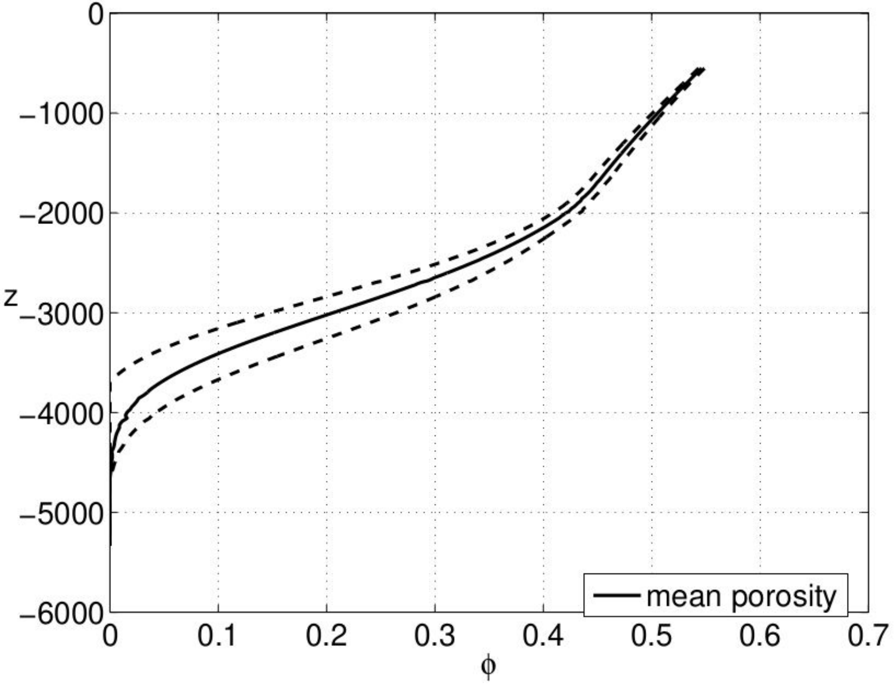
Forward UQ for:

- Porosity
- Temperature
- Pressure

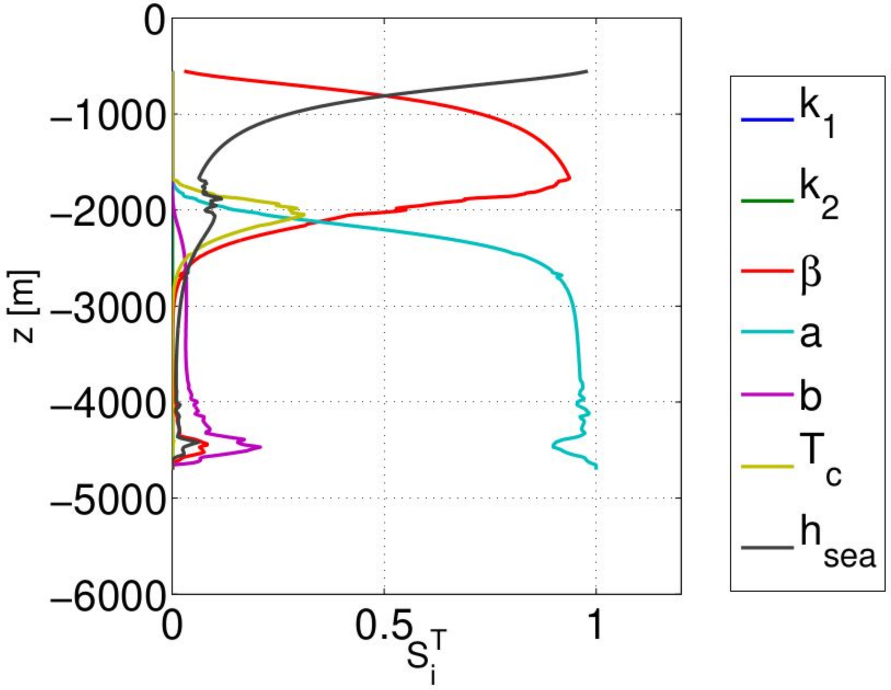
Applications:

- Groundwater management
- Oil and mineral extraction

Example: a geochemical compaction model

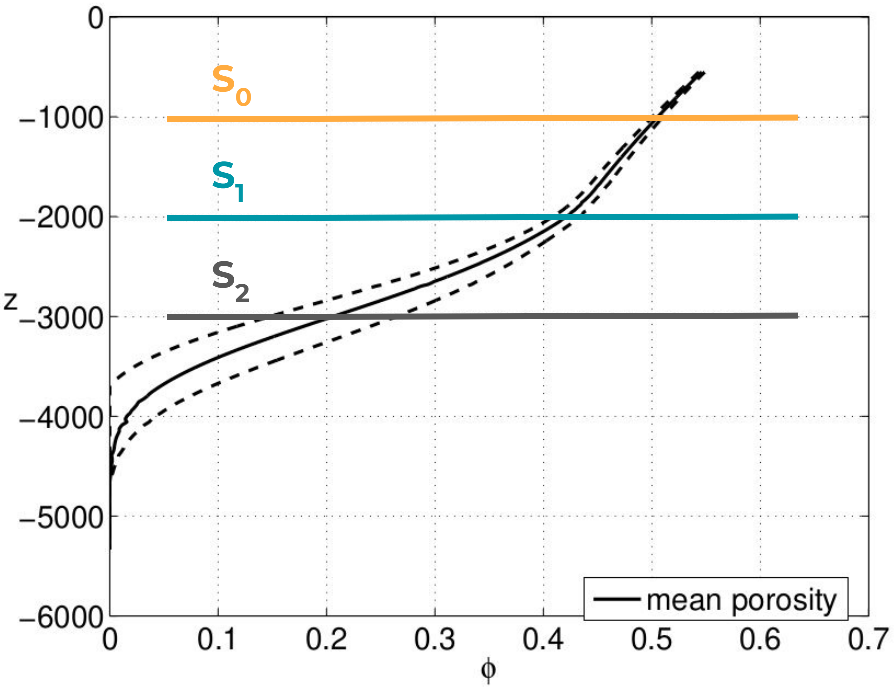


Mean ± std for porosity (forward UQ)



Porosity sensitivity analysis

Example: a geochemical compaction model



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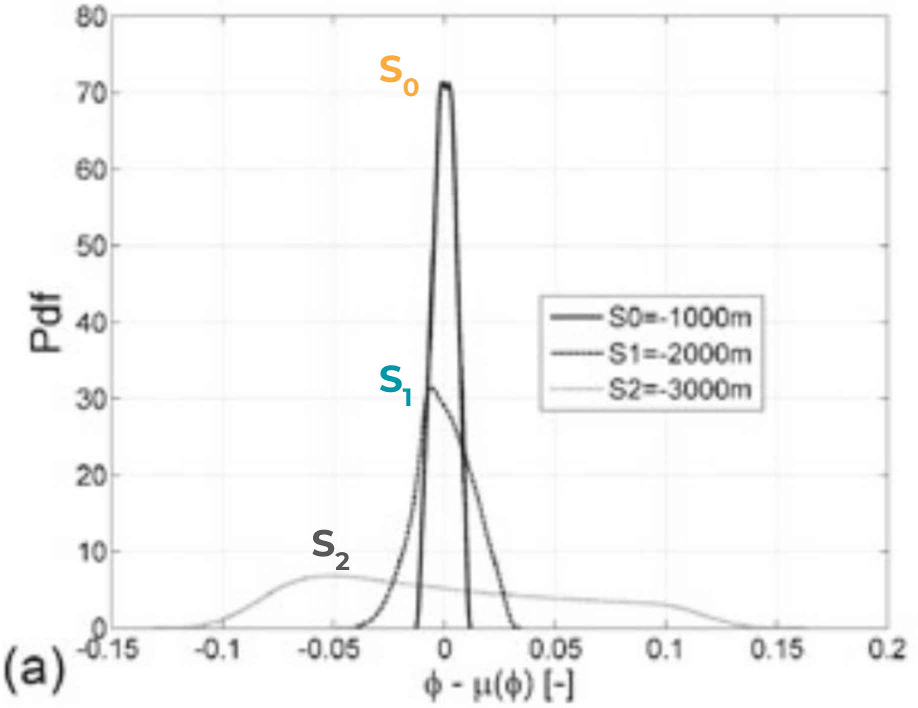


Porosity pdf at three depths

Example: a geochemical compaction model

	Monte Carlo (s)	Sparse grids (s)
Method creation	$1.46 \cdot 10^{-1}$	$0.27 \cdot 10^{-1}$
Realizations	$1.24 \cdot 10^{7}$	$7.30 \cdot 10^{4}$
Moments	$6.67 \cdot 10^{4}$	$3.82 \cdot 10^{2}$
Sobol indices		$4.20 \cdot 10^{3}$
MC of PCE		$1.22 \cdot 10^{5}$
Total	$1.25 \cdot 10^{7}$	$2.00 \cdot 10^{5}$

Surrogate model 100x faster
(600 sparse grids samples vs 1e5 MC samples)

Multi-fidelity

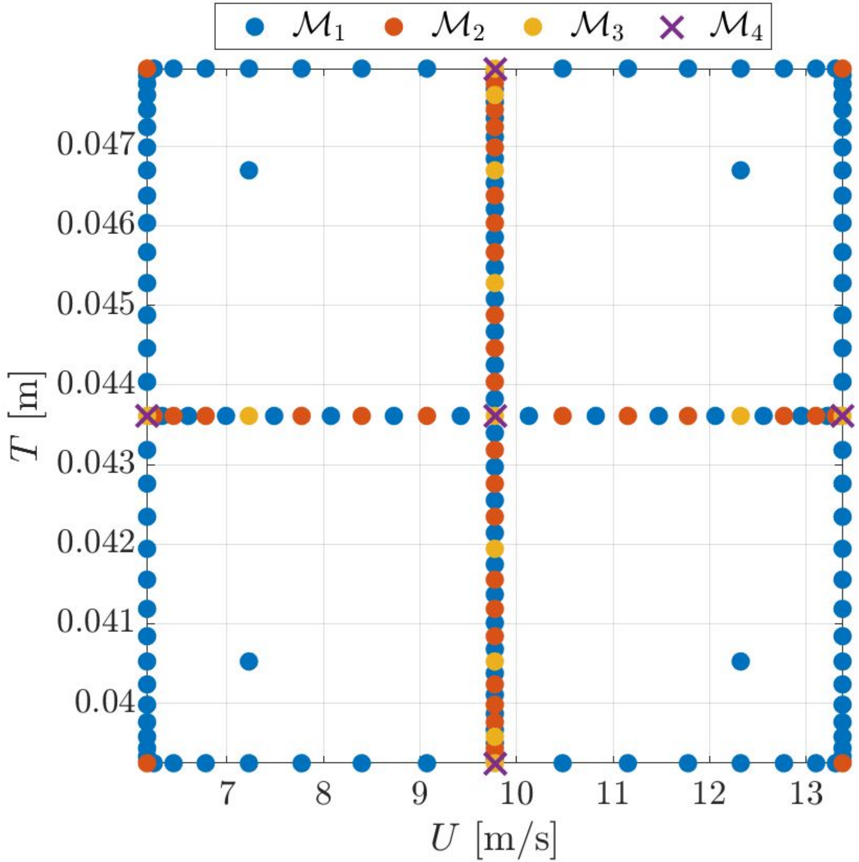
- Consider a **hierarchy of approximations** of the same ODE/PDE:
    a. Different **discretizations**
    b. Different **physics:** Euler / Stokes / RANS / Direct Navier Stokes

- Explore the “bulk” of the variability due to y with **many queries of the cheap models** …

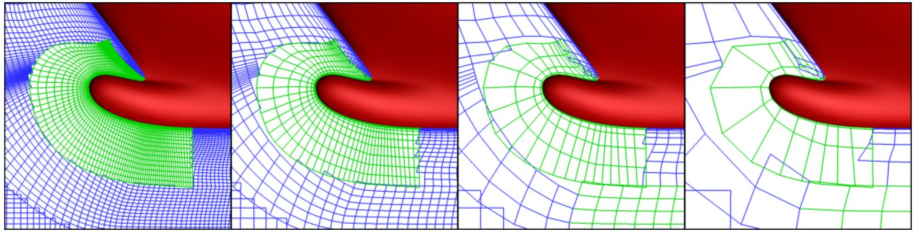
- … and correct with a **handful of queries of the high-fidelity models**

- Can (should) be combined with the **surrogate-modeling** paradigm

Multi-fidelity: back to the ferry problem



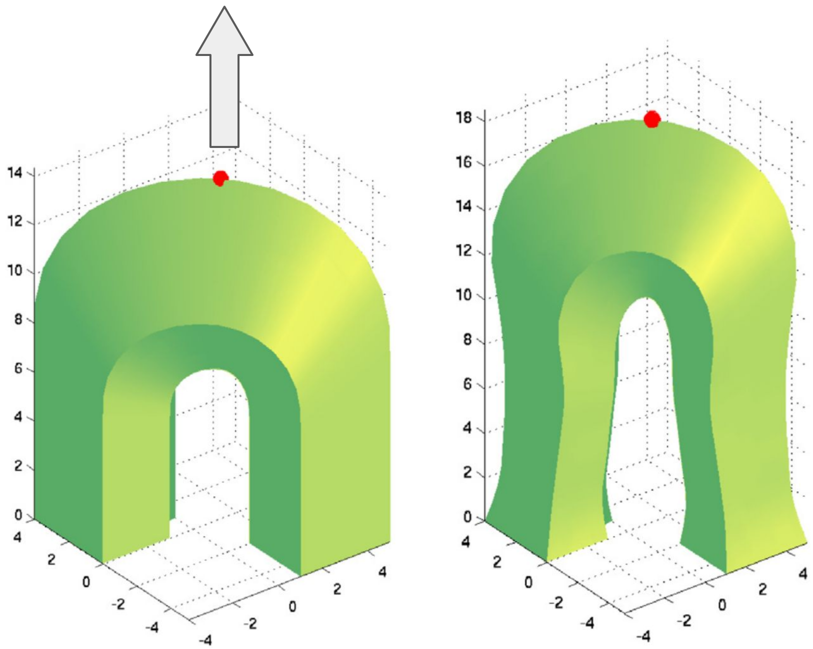
Mesh	Cells	Queries
M_1	11K	~180
M_2	87K	~50
M_3	699K	10
M_4	5.5M	5



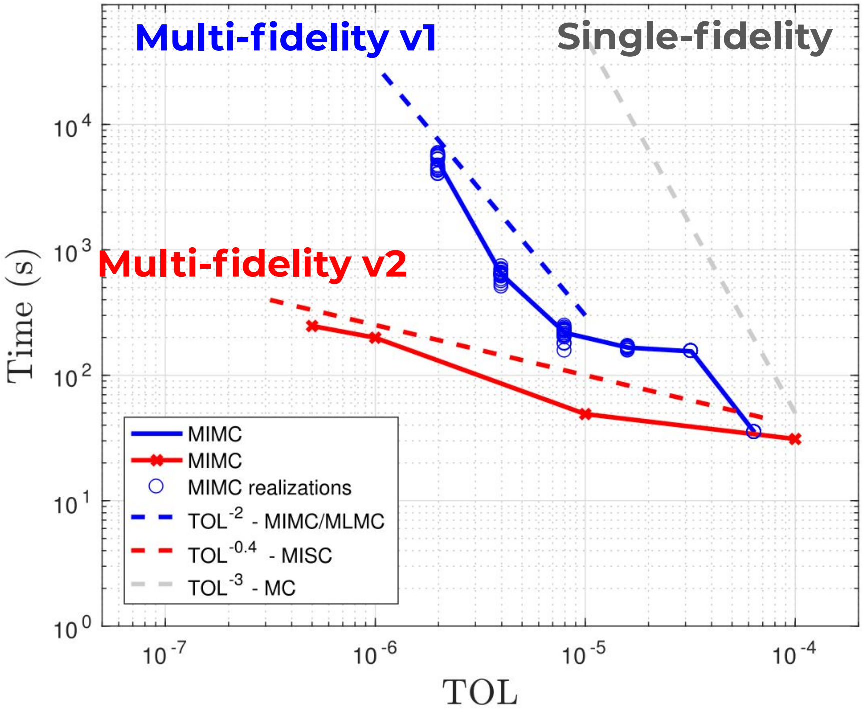
M_4 M_3 M_2 M_1

Multi-fidelity: a 3d-printing problem

- Uncertain *E*, *v* after having 3d printed an object
- mean elongation given a constant pull?
- *E* = [105,120] GPa, *v* = [0.265,0.34] (Ti64, https://www.eos.info/material-m)



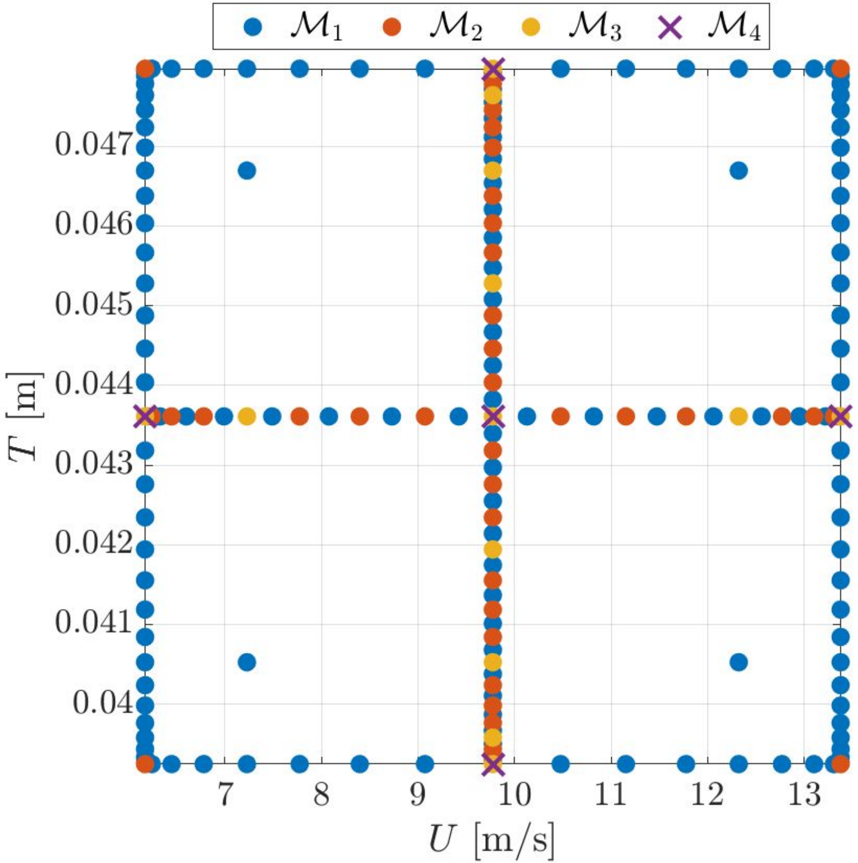
Multi-fidelity: a 3d-printing problem



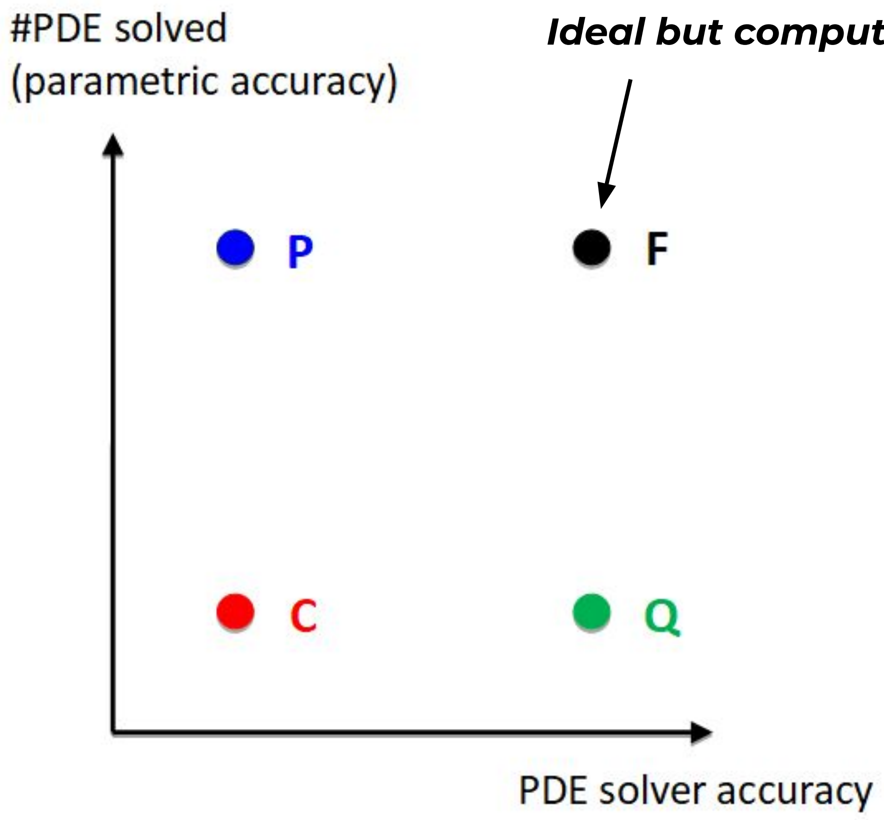
Multi-fidelity methods run faster!

… and now, some details on multi-fidelity

- Our multi-fidelity method is called **Multi-Index Stochastic Collocation** (MISC)
- It uses a **sparse grid** sampling for each fidelity (roughly)
- It creates a multi-fidelity **surrogate** model
- Solvers can be used in a **black-box** way, embarrassingly **parallel**
- Based on the so-called **“sparsification principle”**



MISC: the sparsification principle



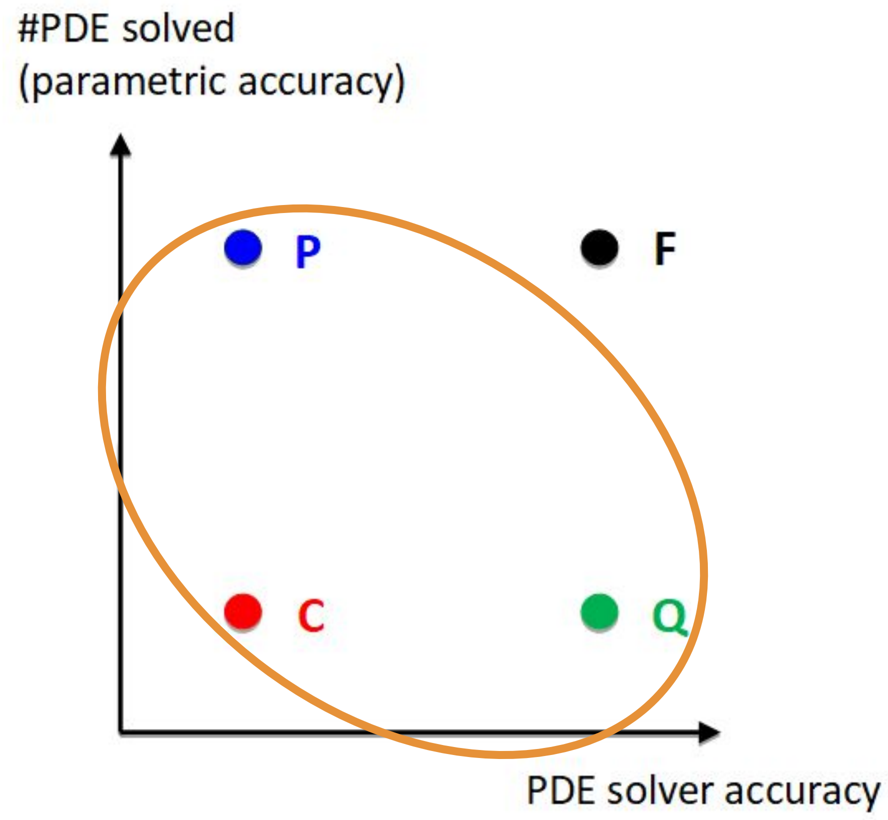
C: coarse discretization (coarse mesh, few samples)

Q: refine PDE mesh

P: add more samples in the parameter space

F: take both actions

MISC: the sparsification principle



Write a **telescopic equality**

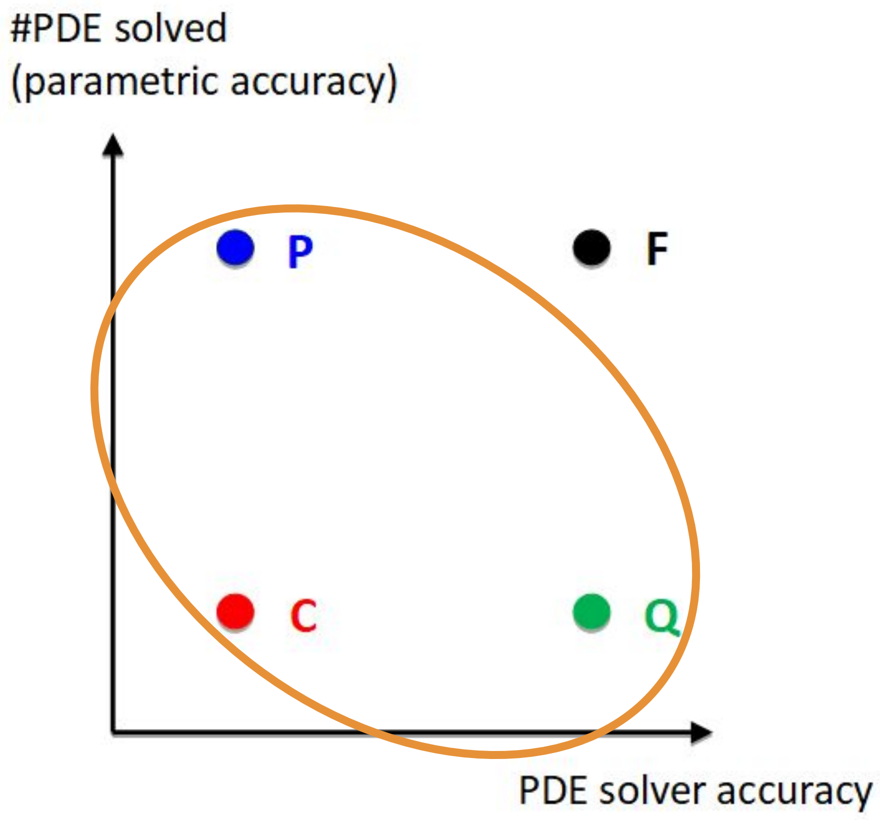
$$
\begin{aligned}
F = F &+ C - C \\
&+ C - C \\
&+ P - P \\
&+ Q - Q
\end{aligned}
$$

Rearrange to put in evidence three corrections

$$
\begin{aligned}
F = {} & \cancel{C} \\
&+ P - \cancel{C} \\
&+ Q - C \\
&+ \cancel{F - P - Q + C}
\end{aligned}
$$

2nd order correction,
small but expensive!

MISC: the sparsification principle



Rearrange terms, obtain MISC formula

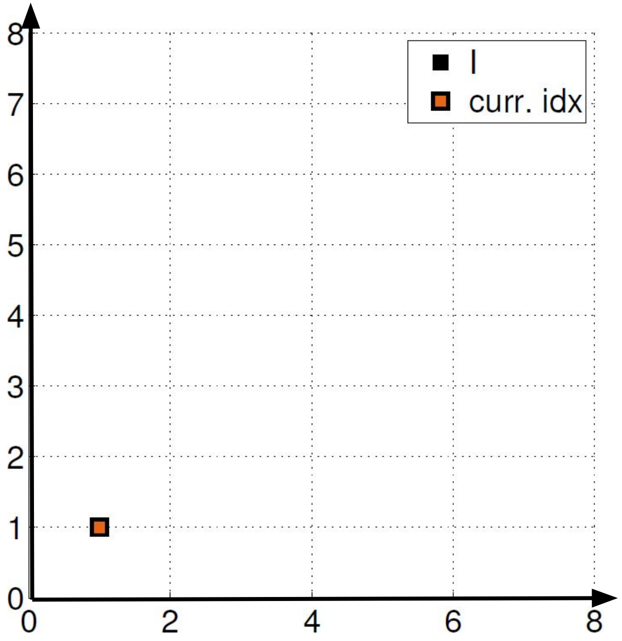
F ≈ **P** + **Q** − **C**

i.e., a **linear combination of three different (cheap) approximations**

Each of them requires fixing a mesh for the PDE and the samples in the parameter space

MISC: an adaptive algorithm

 # PDE solved
(param. accuracy)



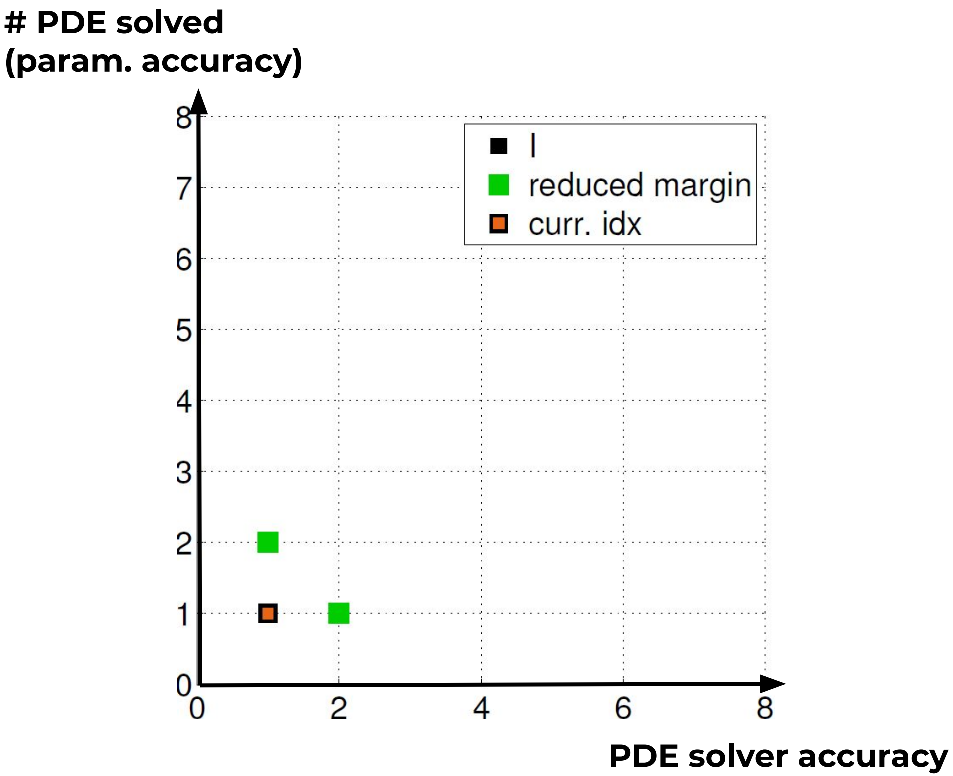
PDE solver accuracy

1. Add "**neighboring refinements**"
2. Choose the one that gave the **best improvement**:

   Δ[Expected value] / cost

3. Repeat

MISC: an adaptive algorithm



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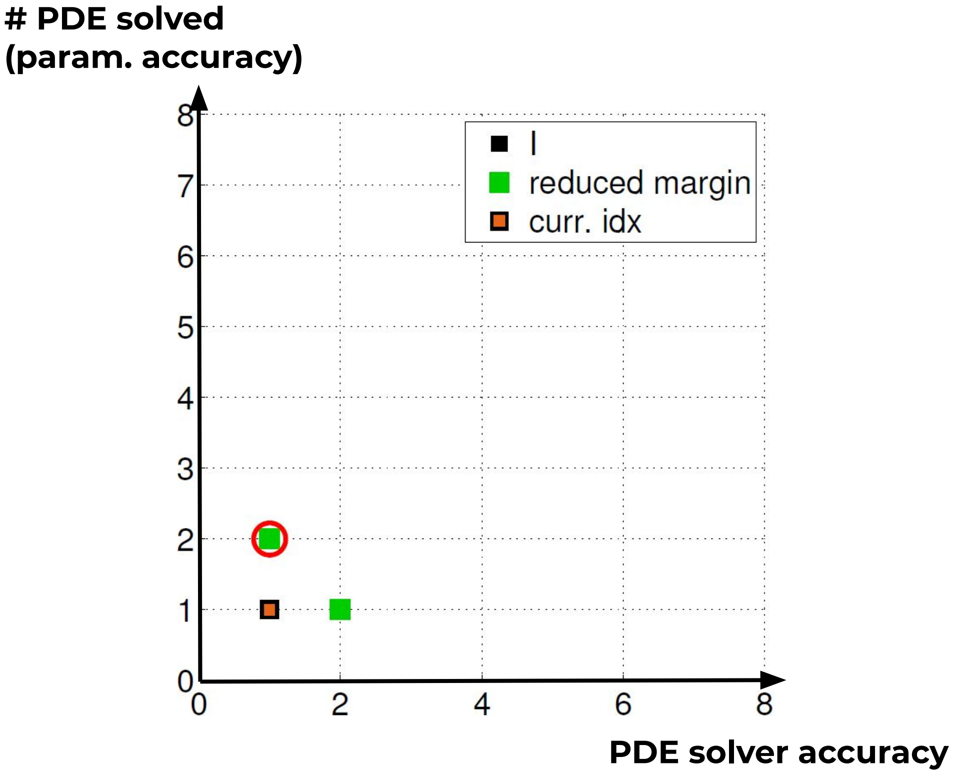

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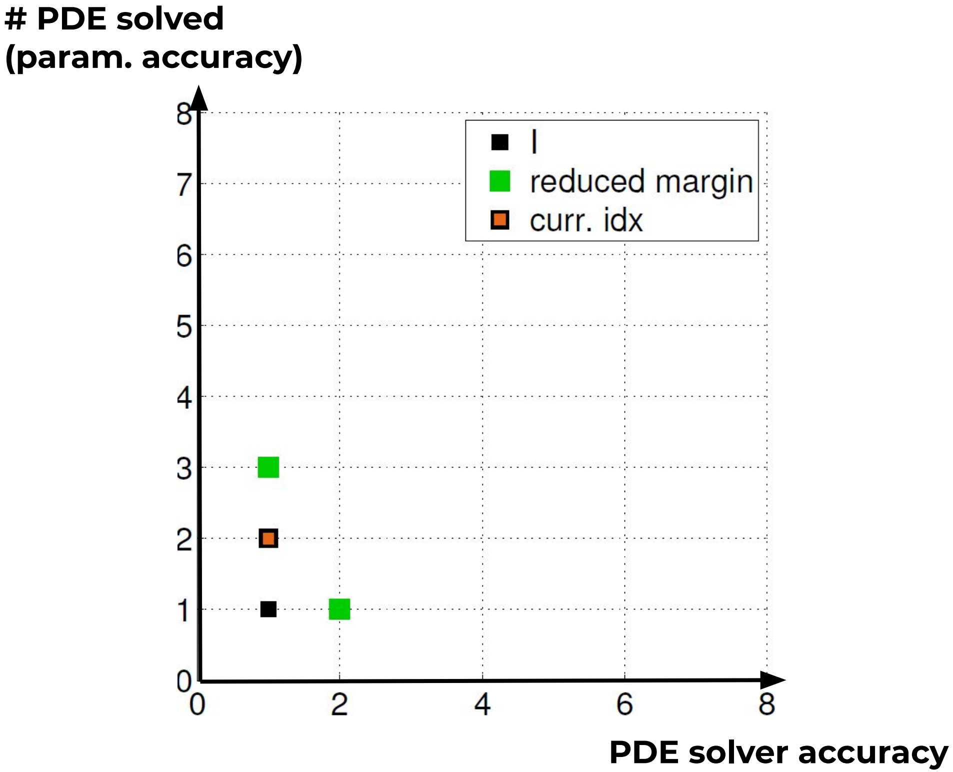

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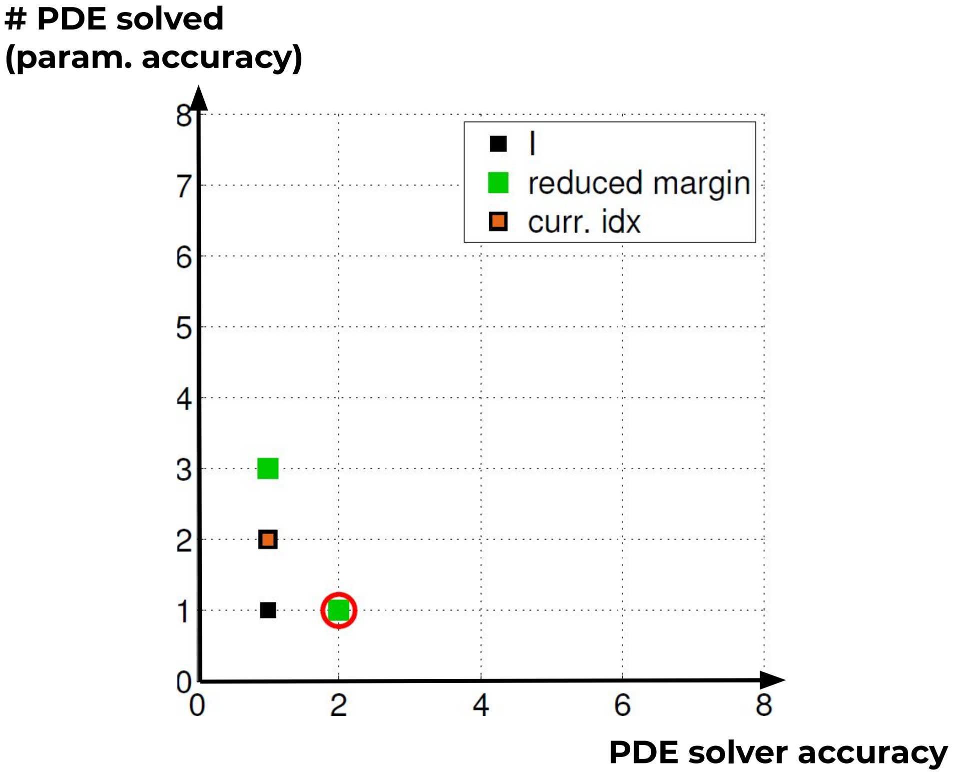

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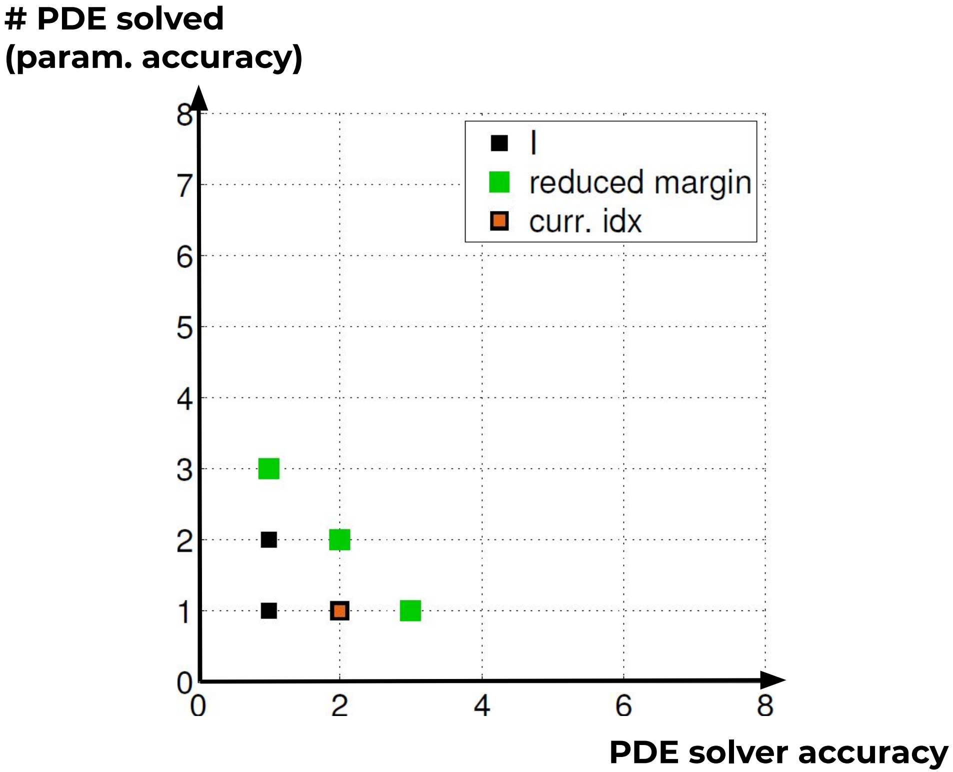

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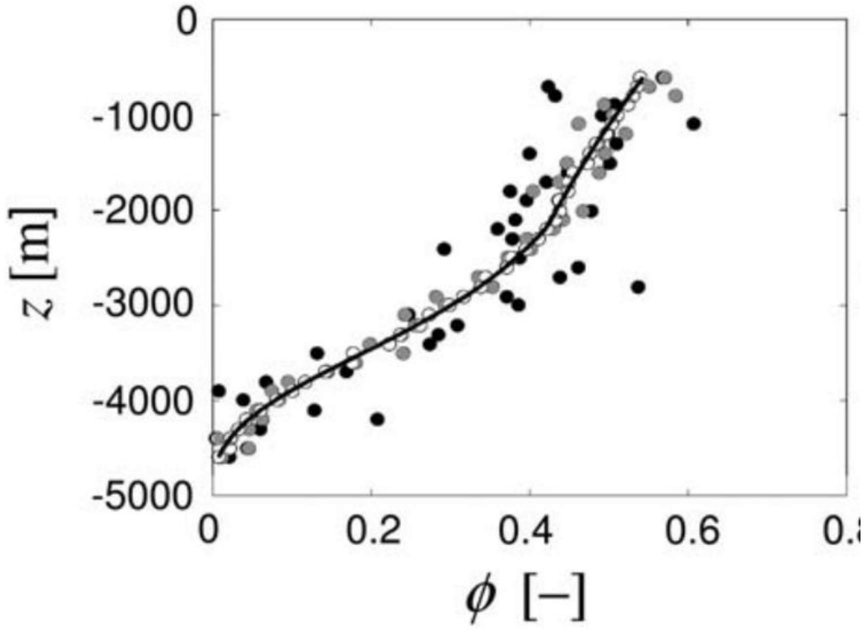
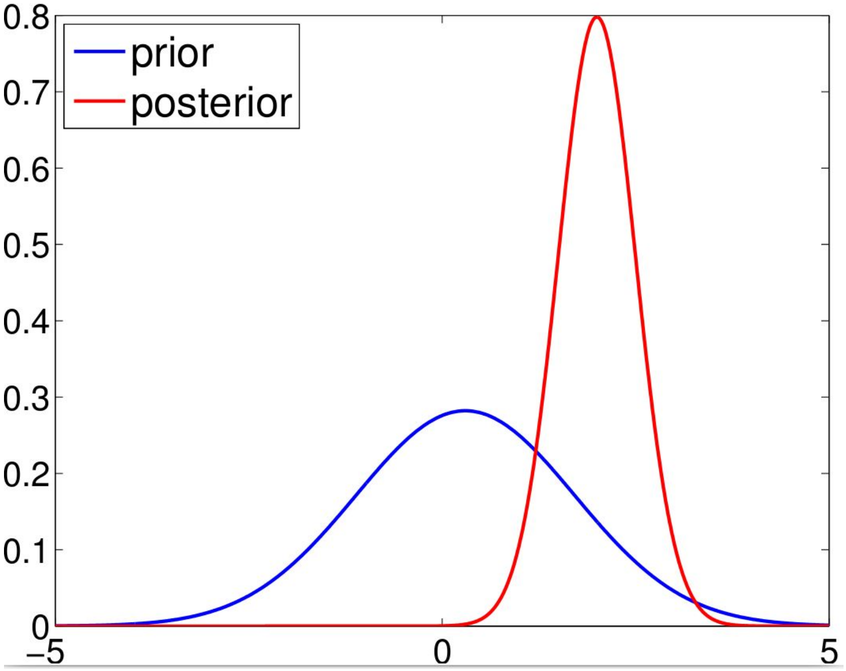
Last but not least: inverse UQ / calibration

Maximum Likelihood and **Bayesian inversion** provide formulas to “update the statistical description” of ***y*** given noisy measures of *u* (posterior pdf of ***y***). It’s a “calibration with uncertainty”





Last but not least: inverse UQ / calibration

- Easiest setting:
  - uniform prior for y
  - gaussian noise
  - “informative data”
- Then, there is a **close** relation to **least squares**: $\min_{\mathbf{y}} \sum_{i=1}^{M} [u_i(\mathbf{y}) - \mathrm{data}_i]^2$

Last but not least: inverse UQ / calibration

- Easiest setting:
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- Then, there is a **close** relation to **least squares**: $\min_{\mathbf{y}} \sum_{i=1}^{M} [u_i(\mathbf{y}) - \mathrm{data}_i]^2$
  *The updated pdf (posterior) of **y** is gaussian with*
  - **Mean** = least squares estimate
  - **St. dev**. = inverse of eigenvalues of Hessian of least squares functional

- Requires optimization, i.e., multiple evaluations of u(**y**)! Surrogate models will help

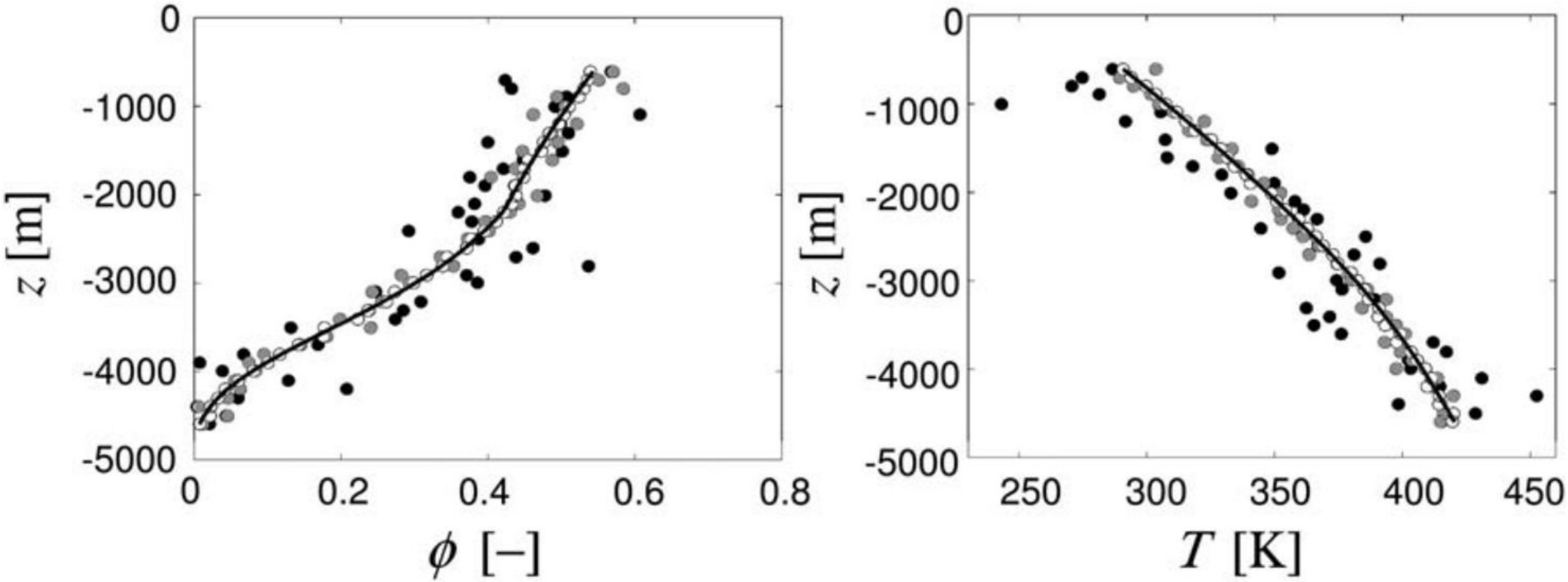
- Can use data from multiple sources

- Alternative methods: **Markov Chain Monte Carlo** (MCMC), **Kalman filter**, …

- Beware of identifiability!
  - **Structural:** is there a unique set of parameters that matches best my data / is the posterior pdf unimodal?
  - **Practical:** How sensitive is the procedure to data quality?

Example: a geochemical compaction model

Calibrate parameters from noisy measurements of porosity and/or temperature.
What data are more informative?

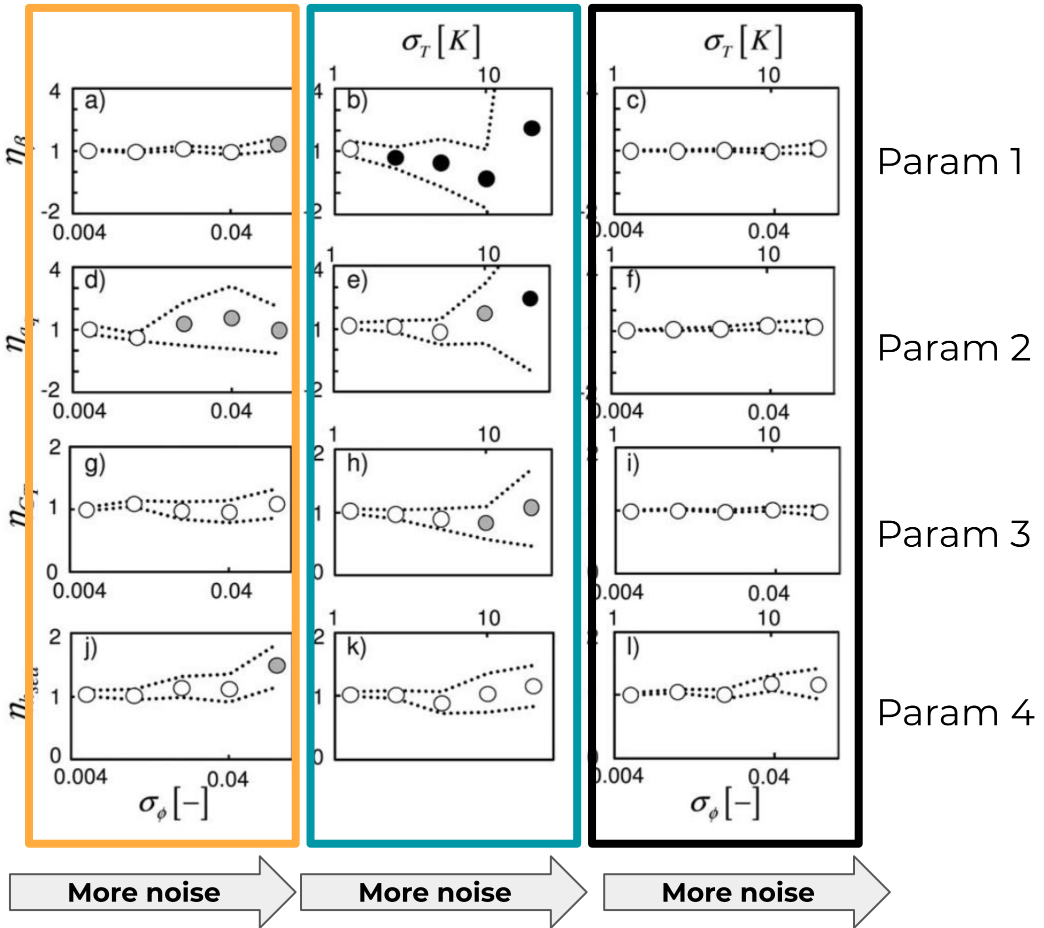


Example: a geochemical compaction model

Porosity data only

Temp. data only

Both data



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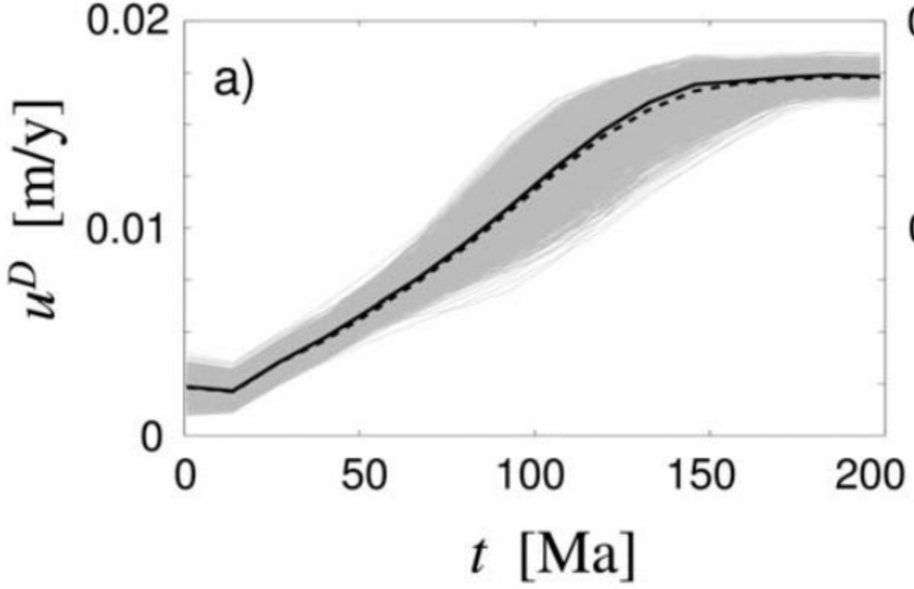

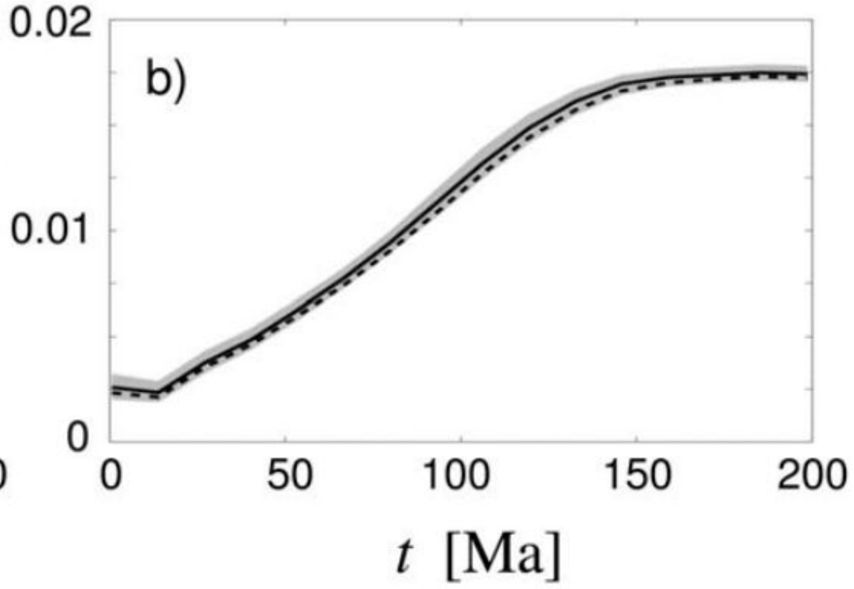

Prior-based predictions

Posterior-based predictions

Conclusions

- UQ is a broad set of techniques to deal with **uncertainties** in computational sciences and engineering
- **forward** UQ, **inverse** UQ, optimization under uncertainty…
- Strong links with approximation theory, statistics, machine learning
- It boils down to repeatedly solving the ODE/PDE at hand: **expensive**!
  - Choose wisely the **sampling** scheme
  - **Surrogate** modeling
  - **multi-fidelity** paradigm
- Examples:
  - Ferry
  - Geochemical compaction
  - 3d-printing
  - SIR system

PhD course on UQ @ UniPV

- April 12 - May 26
- Classes: Monday 11am/1pm
- Lab session: Thursday 9:30am/11:30am
- https://sites.google.com/view/phd-course-uq-tamellini

Bibliography

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Thanks for your attention