Numerical methods for surrogate modeling

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KTH Royal Institute of Technology, Stockholm

Stockholm University – January 17, 2025

Objectives

Numerical methods for surrogate modeling

Get the slides:

- Get acquainted with my research and **surrogate modeling** in general
- Critical thinking: **reflect** on whether your research can profit from surrogate modeling

A broad overview

Trends in scientific computing

Numerical simulations are crucial in many applications:

- to study large & complex systems

Trends in scientific computing

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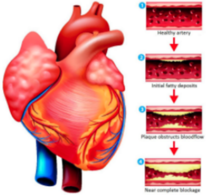
- to take smarter clinical decisions



Trends in scientific computing

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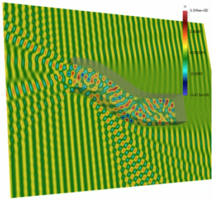
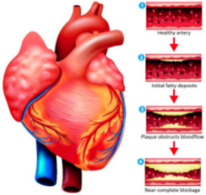
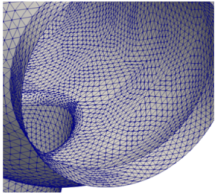
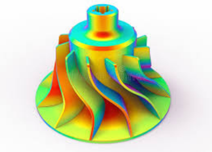
High accuracy comes at a price...

- complex model & implementation
- computational resources

$\rightarrow$ high simulation time



How to speed up simulations?

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- Develop faster and better methods & algorithms
  - huge challenge in most cases
  - chances of success?

Surrogate modeling

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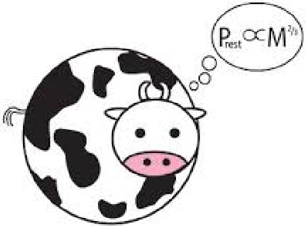
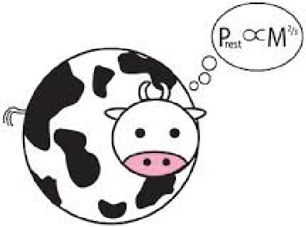
  - huge challenge in most cases
  - chances of success?
- Simplify model
  - **quantify modeling error**?

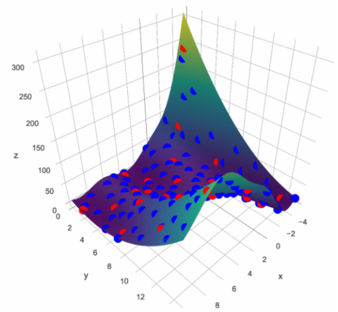


Surrogate modeling

How to speed up simulations?

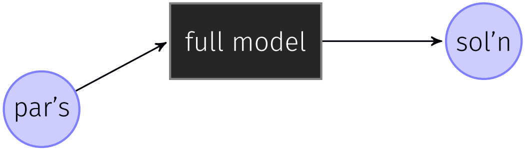
- Develop faster and better methods & algorithms
  - huge challenge in most cases
  - chances of success?
- Simplify model
  - quantify modeling error?
- Surrogate modeling
  - systematic
  - relies on numerical methods to speed up numerical simulations





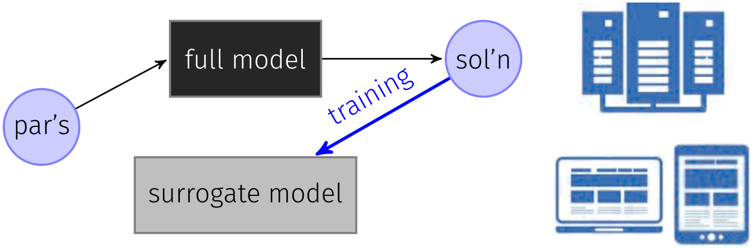
A broad overview

Surrogate modeling



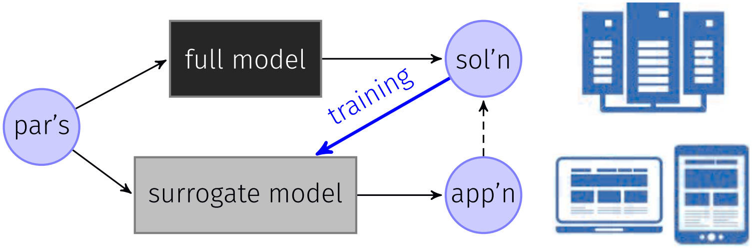
Process data coming from **expensive** simulations

Surrogate modeling



Process data coming from **expensive** simulations to build a **cheap** surrogate model that can give **useful** information,

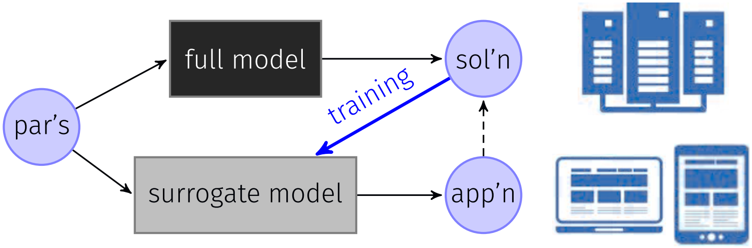
Surrogate modeling



Process data coming from **expensive** simulations to build a **cheap** surrogate model that can give **useful** information, with **"enough" accuracy**

A broad overview

Surrogate modeling



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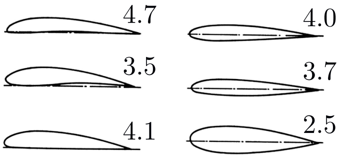
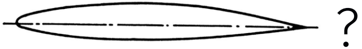
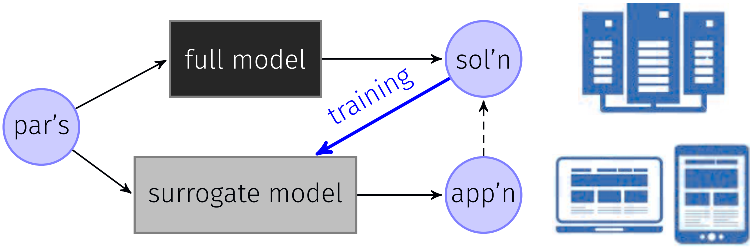
Database



New query





- First papers in computational mechanics in the '80s
- Mathematical momentum since the '00s

[Baur, Benner, Breiten, Cohen, Farhat, Feng, Glas, Haasdonk, Himpe, Huynh, Iapichino, Kramer, Maday, Manzoni, Mula, Nouy, Ohlberger, Panzer, Patera, Peherstorfer, Quarteroni, Rozza, Schwab, Smetana, Stykel, Urban, Veroy-Grepl, Volkwein, Willcox, Zimmermann, ...]

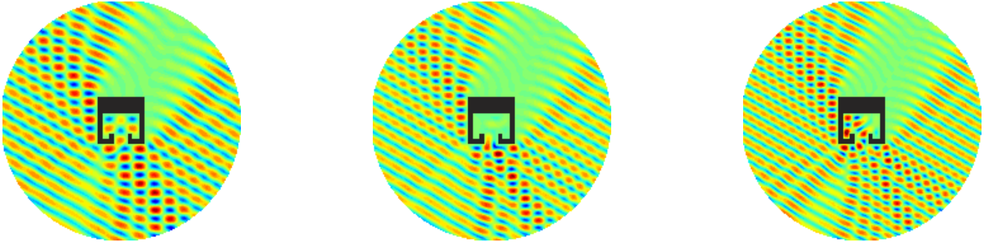
Most contributions are for "nice" problems, where* the solution **depends smoothly on the parameters**

A motivating example

- A broad overview
- A motivating example
- The not-so-nice problems
- Conclusions

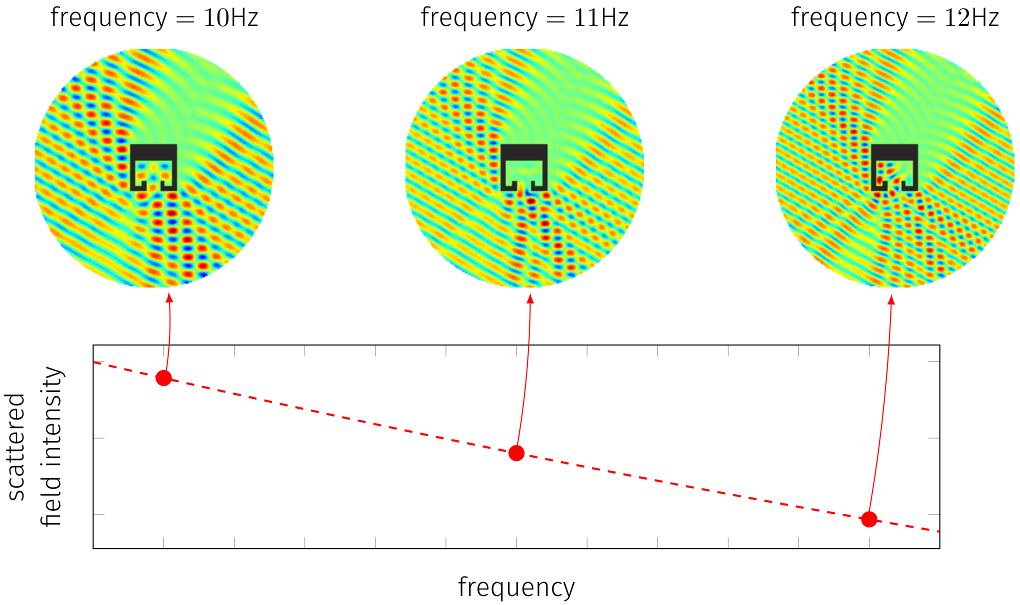
Scattering (EM/acoustic) has applications in engineering, communications, warfare, etc.

frequency $= 10\text{Hz}$ frequency $= 11\text{Hz}$ frequency $= 12\text{Hz}$

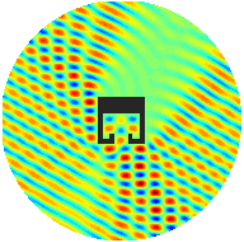


A motivating example

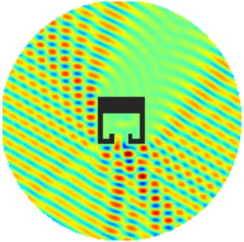
EM scattering



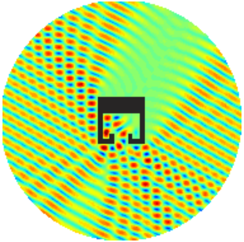
frequency = 10Hz

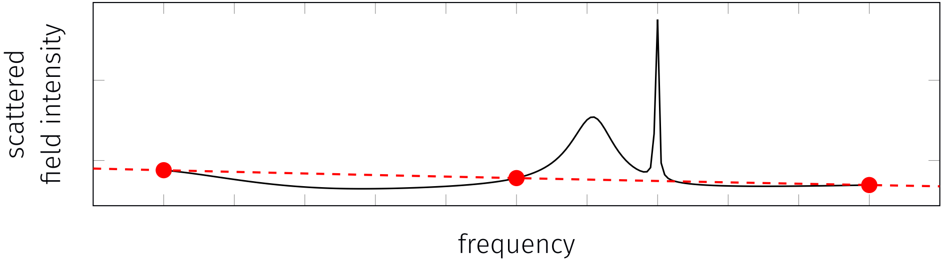


frequency = 11Hz



frequency = 12Hz





Challenges

Given the three expensive data points,

- what is the **best** surrogate model we can **build**? $\rightarrow$ best approximation class
- can we estimate the **approximation error** we are committing? $\rightarrow$ model certification

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If we can afford more samples,

- where to place the 4^{th} sample to **get the most information**? → optimal information
- how many samples to **achieve a user-prescribed error tolerance**? → adaptivity

Challenges

Given the three expensive data points,

- what is the [covered] can **build**? → **best approximation class**
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for "nice" problems these have been well understood since the seminal papers in '00s

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- where to place the 4^{th} sample to **get the most information**? → **optimal information**
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Can we remain agnostic of the discretization? → **non-intrusiveness**

The not-so-nice problems

- A broad overview
- A motivating example
- The not-so-nice problems
- Conclusions

The paradigm

Tame the problem

↓

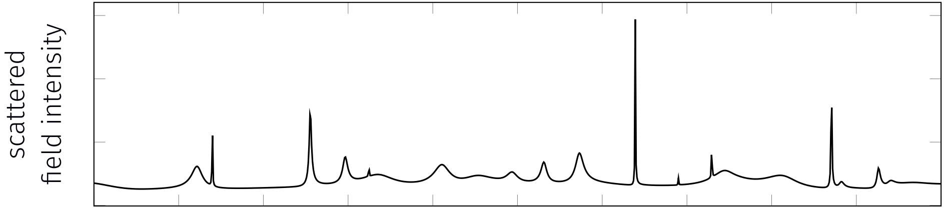
Handle the approximation

↓

Apply surrogate modeling

The not-so-nice problems

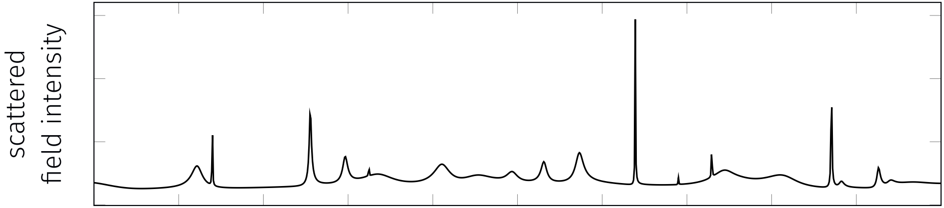
Taming the problem



Task: understand the cause of the spikes

Tools: spectral theory of operators, perturbation theory, complex analysis, PDE theory

Taming the problem



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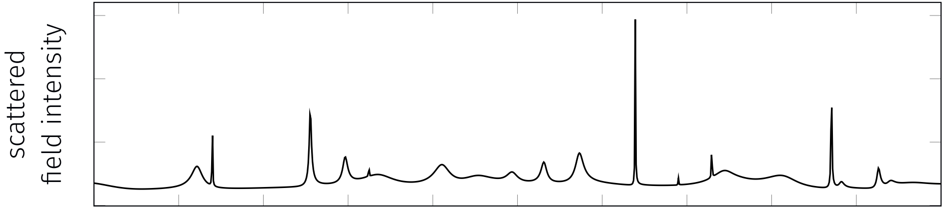
Answer (simplified): if a problem depends **smoothly** on parameters, its solution depends **meromorphically** on parameters

$$\underbrace{\mathcal{L}(\mu)}_{\text{smooth}}{}^{-1} = \underbrace{\mathcal{H}(\mu)}_{\text{smooth}} + \sum_i \frac{\mathcal{P}_i}{(\mu - \lambda_i)^{\alpha_i}}$$

Taming the problem



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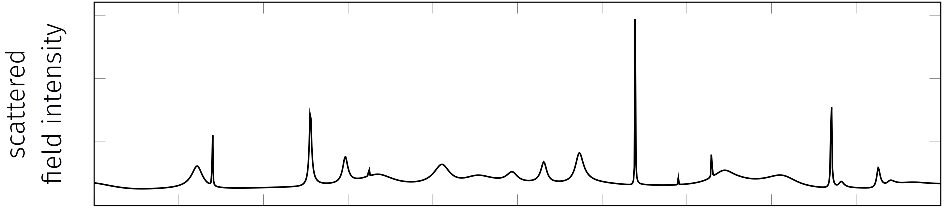
Outcome: seek the **surrogate model** within **meromorphic functions**!

$\rightarrow$ best approximation class & inference

[Bonizzoni&Nobile&Perugia&**P**'20]$\times 2$, [**P**'20], [Bonizzoni&**P**&Ruggeri'23],
[Huwiler&**P**&Schiffmann'24], [**P**&Borghi'24], [Hiptmair&Perugia&**P**'25+]



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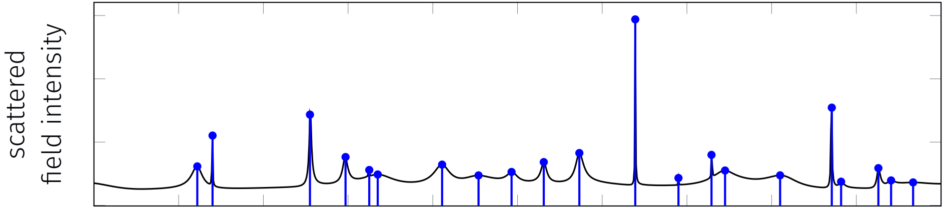
Challenges: nonlinear operators, high number of parameters

The not-so-nice problems

Handling the approximation



Issue: the approximation task is **nonlinear**

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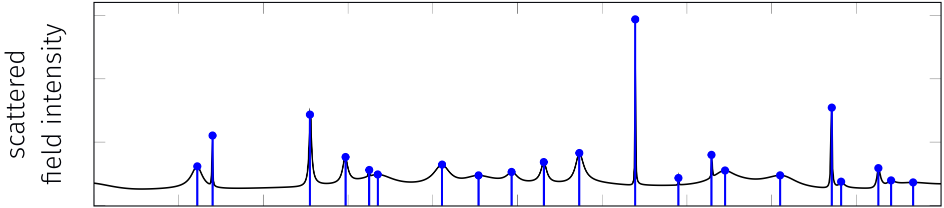


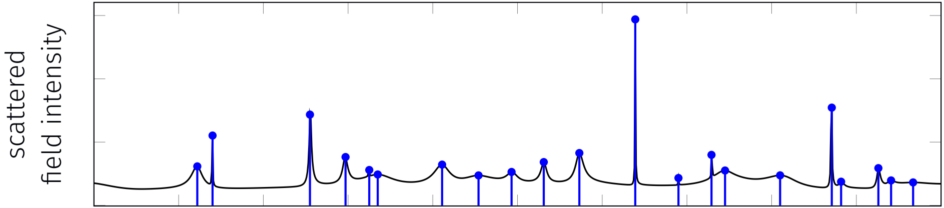
Issue: the approximation task is nonlinear

Tools: rational approximation, “machine” learning, adaptive sampling

$$\sum_j \frac{v_j}{x - x_j} \Big/ \sum_j \frac{w_j}{x - x_j}$$

Rich literature from approximation theory & control theory

Handling the approximation



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[**P**’20], [**P**&Nobile’21], [**P**&Nobile’22], [**P**’23], [**P**&Borghi’24], [**P**&Gosea&Heiland’25+]

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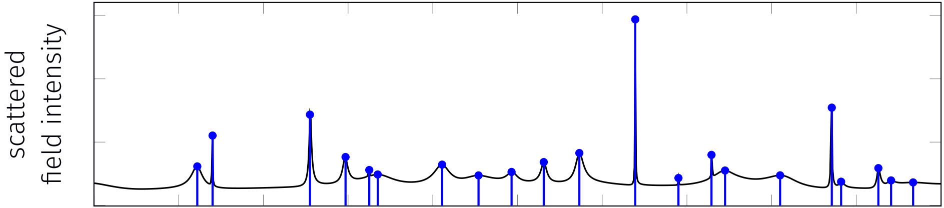

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Challenges: put user first, high number of parameters

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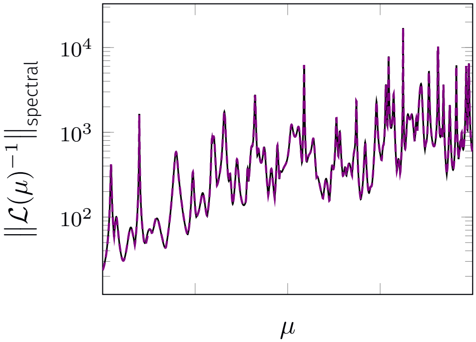
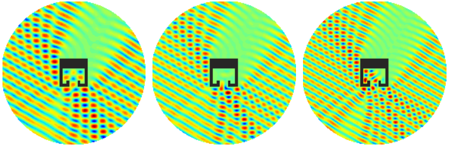
Applying surrogate modeling – Scattering amplification factor (w/ R. Hiptmair & I. Perugia)





Tame: piecewise-meromorphic (kinks may happen)

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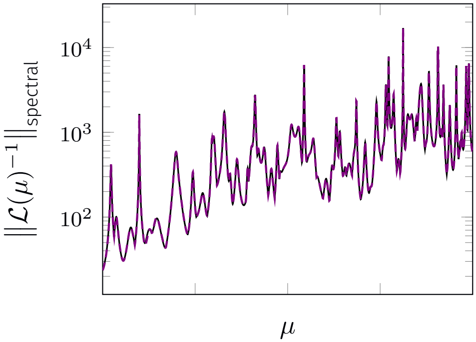

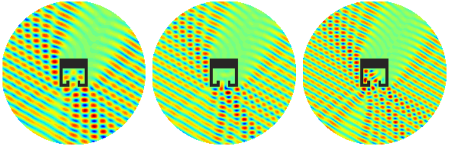

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Handle: **non-intrusive fully adaptive piecewise-rational** approximation

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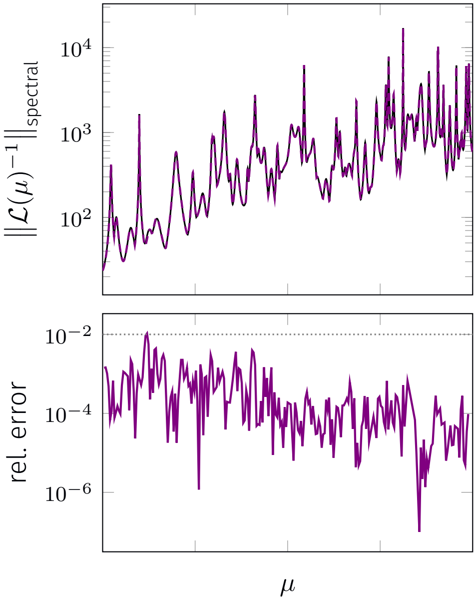

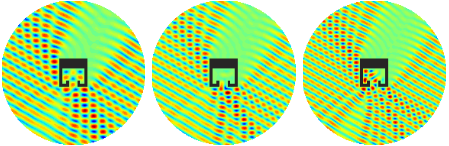

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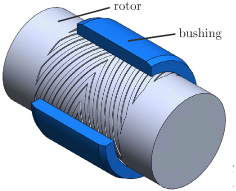
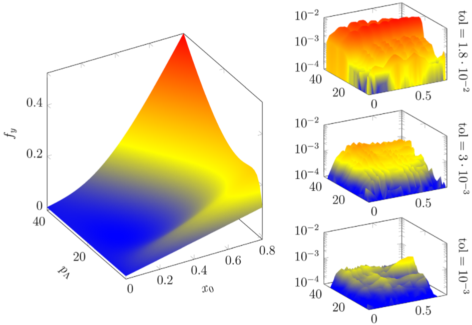
Solve: versatile user-friendly open-source algorithm (only input: tol!); computational **speed-up of 3 OoMs**!

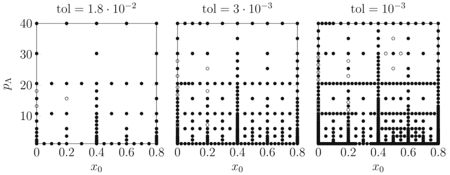
The not-so-nice problems

Applying surrogate modeling – Stiffness parameters of nonlinear bearing (w/ P. Huwiler & J. Schiffmann)



Tame: 7D cw-meromorphic; (closed-source) problem is fully nonlinear in μ





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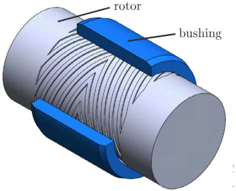
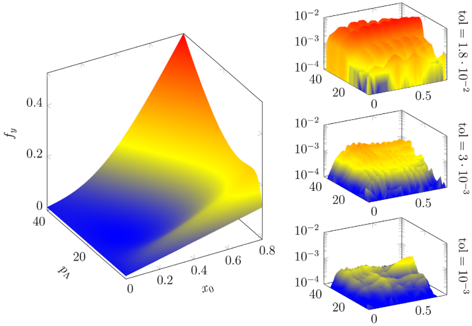
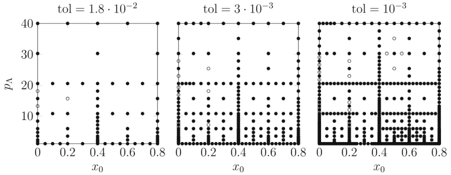


Tame: **7D cw-meromorphic**; (closed-source) problem is **fully nonlinear** in μ

Handle: **non-intrusive fully adaptive hybrid smooth-rational** approximation





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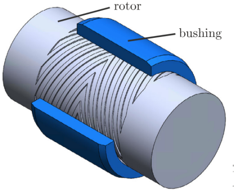

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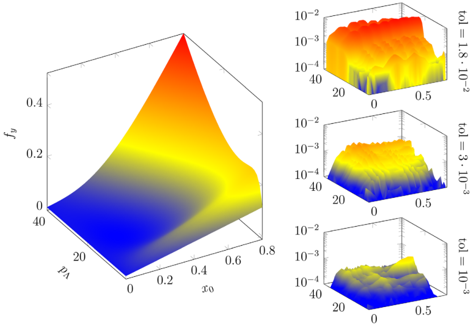
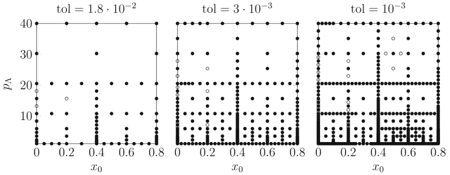
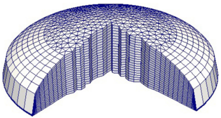


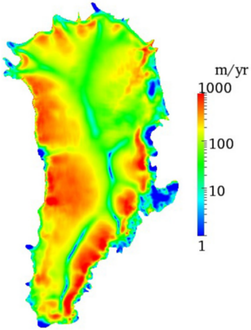


The not-so-nice problems

Applying surrogate modeling? – Ice sheet modeling [Ahlkrona et al.'16]

$$\begin{cases} \nabla \cdot (\alpha(u)\nabla u) = \nabla p \\ \nabla \cdot u = 0 \end{cases}$$





Tame?: expensive nonlinear

Stokes equation

The not-so-nice problems

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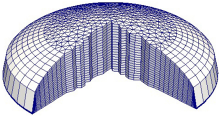

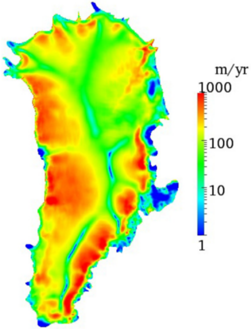

Tame?: expensive nonlinear Stokes equation

Which features are important?

→ inf-sup stability?

→ not a “nice” problem?

→ multi-scale features?

Handle?: what approximation strategy is best to keep such important features?

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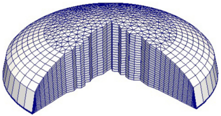

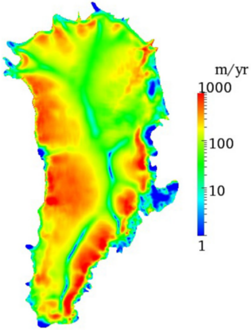

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Just in the last two months on arXiv:

[Ye et al., "Reconstructing MODIS normalized difference snow index product on Greenland ice sheet using spatiotemporal extreme gradient boosting model"]

[Liu et al., "Multi-branch spatio-temporal gNN for efficient ice layer thickness prediction"]

[Aretz et al., "Multifidelity uncertainty quantification for ice sheet simulations"]

Conclusions

- A broad overview
- A motivating example
- The not-so-nice problems
- Conclusions

Summary

Surrogate modeling = developing numerical methods for numerical methods

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Recipe

- Tame complex behavior by understanding its root causes
- Handle non-linear approximation task by effective adaptive numerical methods
- Apply surrogate modeling to challenging real-life applications

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Take-home

- What can surrogate modeling do for *your* problem?

The end?

Thanks to my collaborators!

Thank you all for your attention!

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