Error control in scientific modelling

(with a focus on eigenvalue problems)

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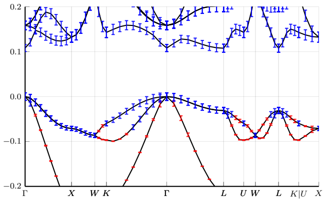

Leading thought

All computation is wrong, only some is useful.

So far so obvious, but to what extend should one care?

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So far so obvious, but to what extend should one care?

Or: Why should I devote a full semester to this topic?

Why care ? Let's say your future job involves to . . .

Launch a rocket

Build an oil rig

Intercept a missile

Why care ? Let's say your future job involves to ...

Launch a rocket

- June 1996
- Ariane 5 test
- 500 million dollar

Build an oil rig

- August 1991
- Sleipner A offshore platform
- 1 billion dollar

Intercept a missile

- February 1991
- Patriot missile failure
- 28 soldiers killed, 100 injured

Launch a rocket

- June 1996
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- floating point conversion error

Build an oil rig

- August 1991
- Sleipner A offshore platform
- 1 billion dollar
- Too crude discretisation

Intercept a missile

- February 1991
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- See website of Douglas N. Arnold for more details: `https://www-users.cse.umn.edu/~arnold/disasters/disasters.html`

Ok, so these are the extreme cases, right?

Brainstorming: Sources of error in scientific simulations

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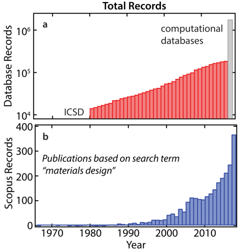
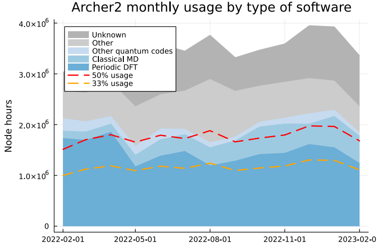
Brainstorming: Sources of error in scientific simulations

- Model
- Numerics (discretisation / basis set, algorithm, arithmetic)
- Implementation
- Hardware (CPUs have bugs!)

Motivation in the MXtMat group

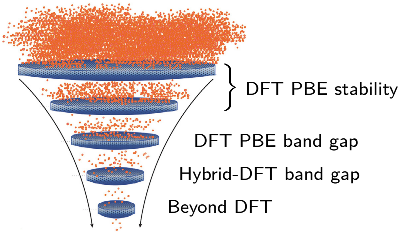
- 21st century challenges:
  - Renewable energy, green chemistry, health care . . .
- Current solutions limited by properties of available materials
  - $\Rightarrow$ Innovation driven by discovering new materials
- Crucial tool: Computational materials discovery
  - Systematic simulations on $\simeq 10^4 - 10^6$ compounds
  - Complemented by data-driven approaches
  - Noteworthy share of world's supercomputing resources



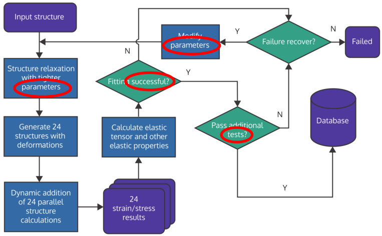


K. Alberi *et. al.* J. Phys. D, **52**, 013001 (2019).

Sketch of high-throughput workflows



Design funnel for photovoltaic materials



Workflow for computing elasticity tensors

- Many parameters to choose (algorithms, tolerances, models)
  - Elaborate heuristics: Failure rate $\simeq 1\%$
  - Still: Thousands of failed calculations
  - $\Rightarrow$ Wasted resources & increased human attention (limits througput)
- **Goal** in MatMat group: Self-adapting black-box algorithms
  - Transform empirical wisdom to built-in convergence guarantees
  - Requires: Uncertainty quantification & error estimation
  - $\Rightarrow$ Understand where and how to spend efforts best

G. Hautier Comput. Mater. Sci. **164**, 108 (2019); L. Himanen *et. al.* Adv. Science **6**, 1900808 (2019).

Broader vision: Robust & error-controlled simulations

- Error control = Track simulation uncertainties:
  - Self-adapting simulations with mathematical guarantees
  - Integrate with error propagation efforts for surrogates[1]
  - ⇒ Byproducts: Data quality control, accelerated design
- Error control = Learn missing physics:
  - Data-enhanced models, active learning
  - Integration with experiment (autonomous discovery)
  - ⇒ Exploit high-fidelity experimental, beyond-DFT data
- Error control = Leverage inexactness:
  - Error balancing: Optimal adaptive parameter selection
  - Randomised methods, selective precision (16-bit, FPGA)
  - Multi-fidelity approaches (reduced basis, surrogates)

⇒ Understand where and how to spend efforts best

⇒ Realm of mathematical research

[1] F. Musil, A. Grisafi *et. al.* J. Chem. Theo. Comput. **15**, 2 (2019).

Questions ?

Focus of the course: Eigenvalue problems

- Eigenvalue problems are ubiquitous, e.g.

- Vibrations of structures
  - Tacoma narrows bridge collapse 1940
  - London millennium bridge construction flaw

- Quantum states (details follow)

- Tight relation to linear problems & PDEs
  - Convergence analysis (CG, iterative methods)
  - Quantum mechanics
  - Close relation to solving PDEs (details follow)

Structure of the course

- Moodle: `https://go.epfl.ch/error-control`
- Lectures split into two rough segments
  - First half: Matrix eigenvalue problems & floating-point error
  - Second half: Operator theory & discretisation error
- Attendance of exercises is expected (introduces new material!)
  - Discussion follows weekly exercise sheet
- Evaluation:
  - Marked semester project ($1/3$ of grade)
  - Project interview & oral exam ($2/3$ of grade)
  - Project done in teams of $2 - 3$ students.
  - Interdisciplinary teams are highly recommended
- Working on the projects requires substantial time outside class

  $\Rightarrow$ We will setup survey in week 2 to aid formation of groups

Details on the exercises & problem sheets

- One problem sheet per week from moodle:
  `https://go.epfl.ch/error-control`
- Handing in of exercise sheets is optional
  - Submission can only be done in the project group
  - Tutors give feedback on submitted sheets
- Initial exercises classes will be denser
- Later exercise classes provide time to work on the project

Details on the projects

- Each project is essentially a larger problem sheet
- One joint solution is submitted by each group
- Responsibilities should be shared equally.

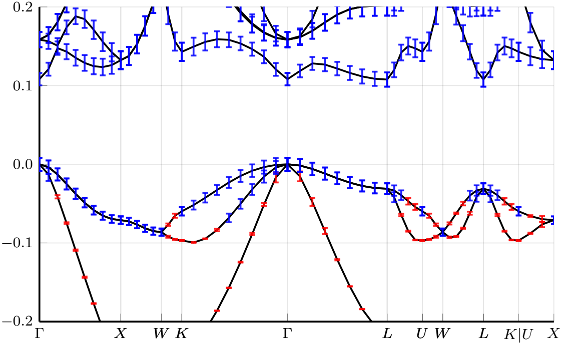
- During the oral exam (about half the time)
  - Presentation of the problem sheet by student
  - Targeted follow-up questions

- Evaluation criteria:
  - See document on moodle

- Each group member obtains an individual mark.

Semester project

- Topic: Band structures with guaranteed error bars
  - Handout: 21st October (tentative)
  - Duration: 2 months, i.e. projected deadline: **20th December**



- Let's have a brief look at last year's projects ...

Questions ?

Your background and prior knowledge

Vector spaces

Which of the following things is a vector space over $\mathbb{R}$

1. $\mathbb{R}^n = \{(x_1, \ldots, x_n)^T, x_i \in \mathbb{R}\}$
2. $\mathcal{F}(D, \mathbb{R}) = \{f : D \to \mathbb{R}\}$, the set of all functions from D to $\mathbb{R}$.
3. $\mathbb{R}^{n \times n}$: The set of all matrices

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Answer: All of them!

Inner products

Given vectors x, y, z from an $\mathbb{C}$-vector space V. What makes an inner product?

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- $\langle x, x\rangle \geq 0$
- $\langle x, y\rangle = \overline{\langle y, x\rangle}$
- $\langle x, \alpha y + \beta z\rangle = \alpha\langle x, y\rangle + \beta\langle x, z\rangle$

Examples:

- $\langle x, y\rangle = x^H y = \overline{x^T} y = \sum_{x=1}^{n} \overline{x_i} y_i$ for vectors $x, y \in \mathbb{C}^n$
- $\langle A, B\rangle_F = A^H B = \mathrm{tr}(A^H B)$ for matrices $A, B \in \mathbb{C}^{n\times n}$

Norms

Which of these statements is true:

1. If $\langle x, y\rangle$ is an inner product, then $\|x\| = \sqrt{\langle x, x\rangle}$ is a norm
2. If $\langle x, y\rangle$ is an inner product and $\|x\| = \sqrt{\langle x, x\rangle}$, then
$$\langle x, y\rangle < \|x\| \, \|y\|$$
3. If $\|x\|$ is a norm, there exists an inner product $\langle x, y\rangle$, such that $\|x\| = \sqrt{\langle x, x\rangle}$
4. Every norm satisfies the triangle inequality
$$\|x + y\| \leq \|x\| + \|y\|$$

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Answer: 1 and 4 are true, 2 and 3 are false. 2 is almost true the correct version is

$$\langle x, y \rangle \leq \|x\| \, \|y\| \qquad \text{Cauchy-Schwarz}$$

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Which iterative diagonalisation algorithms do you know?

Who has studied before:

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- Rayleigh-quotient iteration

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Which iterative diagonalisation algorithms do you know?

Who has studied before:

- Power method
- Inverse power method
- Rayleigh-quotient iteration
- LOPCG

I need a volunteer

- **Your job:** Take pictures of blackboards