

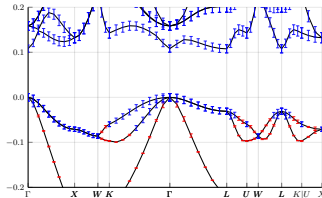
Error control in scientific modelling

(with a focus on eigenvalue problems)

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Mathematics for Materials Modelling (matmat.org), EPFL

11 September 2025



All computation is wrong, only some is useful.

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

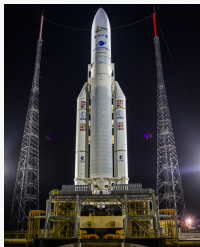
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So far so obvious, but to what extent should one care?

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

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Build an oil rig



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

Intercept a missile



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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

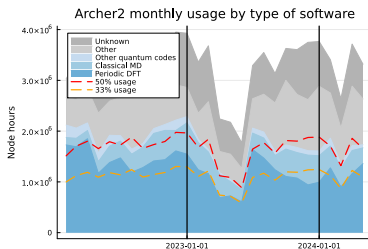
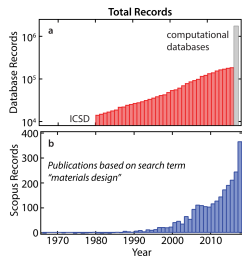
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Brainstorming: Sources of error in scientific simulations

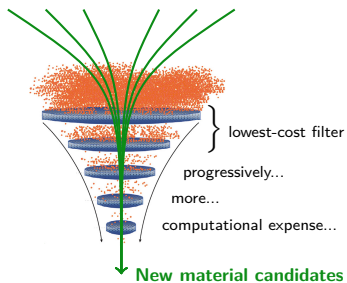
- Model
- Numerics (discretisation / basis set, algorithm, arithmetic)
- Implementation
- Hardware (CPUs have bugs!)

Motivation in the group

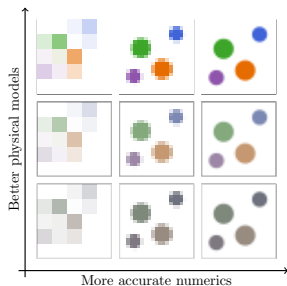
- 21st century challenges:
 - Renewable energy, green chemistry, health care ...
- Current solutions limited by properties of available materials
⇒ Innovation driven by **discovering new materials**
- Crucial tool: **Computational materials discovery**
 - Systematic simulations on $\simeq 10^4 - 10^6$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



Does everything need to be equally accurate ?

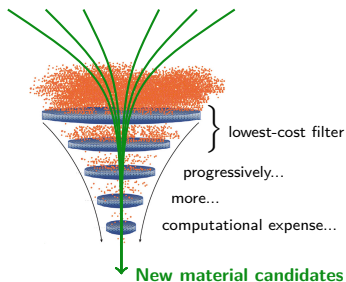


Computational materials design funnel
Involved data-driven multi-physics workflows

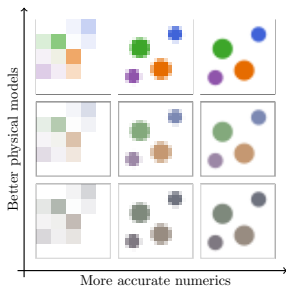


Multitude of modelling choices
How should we spend our efforts best ?

Does everything need to be equally accurate ?



Computational materials design funnel
Involved data-driven multi-physics workflows

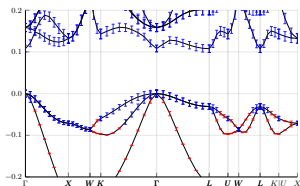


Multitude of modelling choices
How should we spend our efforts best ?

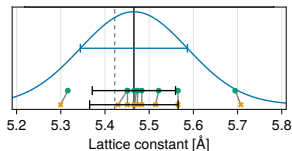
Goal in ~~M~~tMat group: Error-controlled robust algorithms

- Many parameters to choose (algorithms, tolerances, models)
- Need balance: Too expensive \leftrightarrow Insufficient reliability
- \Rightarrow Trial and error process !

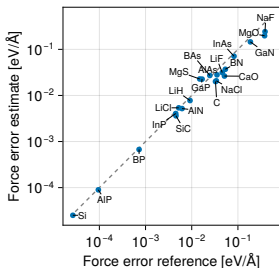
- Transform empirical wisdom to built-in convergence guarantees
- Requires: Uncertainty quantification & error estimation
- \Rightarrow Understand where and how to spend efforts best



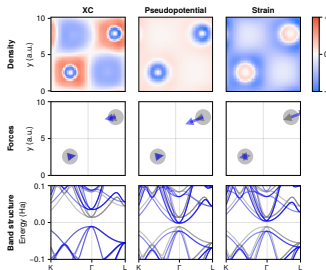
Band structure with **guaranteed error bars**¹



DFT lattice constant **error distribution**²



Plane-wave **basis error estimates** at 20Ha^{2,3}

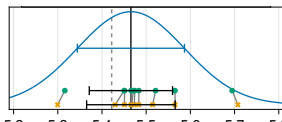
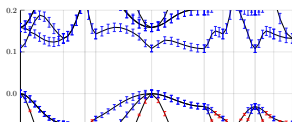


DFT quantity vs. **parameter sensitivities**²

¹MFH, A. Levitt, E. Cancès. Faraday Discuss. **223**, 227 (2020).

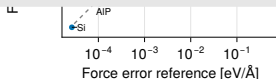
²N. Schmitz, B. Ploumhans, MFH, *in preparation*.

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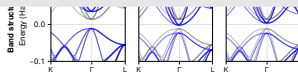


Towards **inexact computation without harm**:

- Error remains controllable
- Challenge: Turning **mathematical analysis into practical tool**
 - Needs performance tuning, heuristics, best practices, ...
- **Opportunities**:
 - Track simulation uncertainties
 - Learn missing physics
 - Leverage inexactness



Plane-wave **basis error estimates** at $20\text{Ha}^{2,3}$



DFT quantity vs. **parameter sensitivities**²

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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>
- **ED Forum:** Announcements & **student-driven** discussion
- Lectures split into two rough segments
 - **First half:** Matrix eigenvalue problems & floating-point error
 - **Second half:** Operator theory & discretisation error
 - **Addendum:** Statistical method for error control (if time)
 - **Notes:** <https://teaching.matmat.org/error-control>
- Attendance of exercises is **expected** (introduces new material!)
 - Discussion follows weekly exercise sheet

Course 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**
 - ⇒ 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>
- Exercise sheets: Not handed in or marked
 - Project groups **take turns to present sheet**
 - **Not marked**; group just presents status of their work
 - Class/tutors give feedback on presented results
- Initial exercises classes will be denser
- Later exercise classes provide time to work on the project
- **Important:**
 - **Bring your laptop** to the exercise sessions
 - **Install  julia** programming language **beforehand**

⇒ See **instructions on moodle**

Details on the project

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

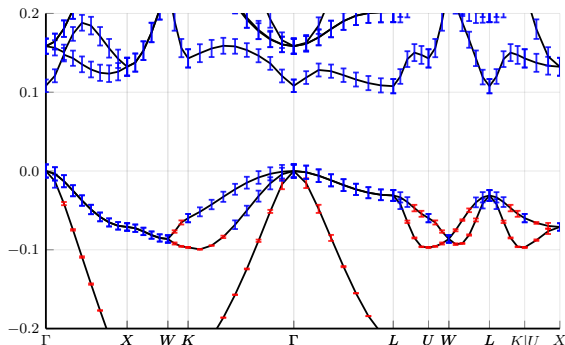
- During the oral exam (about half the time)
 - Presentation of the problem sheet by student
 - Targeted follow-up questions
 - (The other half of the oral is about general course understanding)

- Project evaluation criteria:
 - See document on moodle

- Each group member obtains an **individual mark**.

Topic of the semester project

- Topic: **Band structures with guaranteed error bars**
 - Handout: 24st October (tentative)
 - Duration: 2 months, i.e. projected deadline: **19 December**



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

Group dynamics and mediation

- Team work involves people
- People means tensions
 - ... and potentially unfair distribution of work
 - This is not unusual in academic and industry teams !
- Additional **learning goals of this course:**
 - Learning to distribute work
 - Learning to coordinate as a team
 - Learning to resolve conflicts
- **You are not on your own**
 - We can provide support and mediate
 - Survey around **week 4**: All good ? (y/n)
- **But** we cannot assist you if you don't reach out
Hint: After the exam is too late

Questions ?

Your background and prior knowledge

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

- 1 $\mathbb{R}^n = \{(x_1, \dots, x_n)^T, x_i \in \mathbb{R}\}$
- 2 $\mathcal{F}(D, \mathbb{R}) = \{f : D \rightarrow \mathbb{R}\}$, 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?

Inner products

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

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

Examples:

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

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

Diagonalisation algorithms

Which iterative diagonalisation algorithms do you know?

Who has studied before:

Diagonalisation algorithms

Which iterative diagonalisation algorithms do you know?

Who has studied before:

- Power method

Diagonalisation algorithms

Which iterative diagonalisation algorithms do you know?

Who has studied before:

- Power method
- Inverse power method

Diagonalisation algorithms

Which iterative diagonalisation algorithms do you know?

Who has studied before:

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

Diagonalisation algorithms

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