Electronic-structure simulations using julia

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→ `https://michael-herbst.com/talks/2019.10.17_dftk_julia_paris.pdf`

Why care about electronic structures?

- Electrons glue the world together
- Electrons keep the world apart

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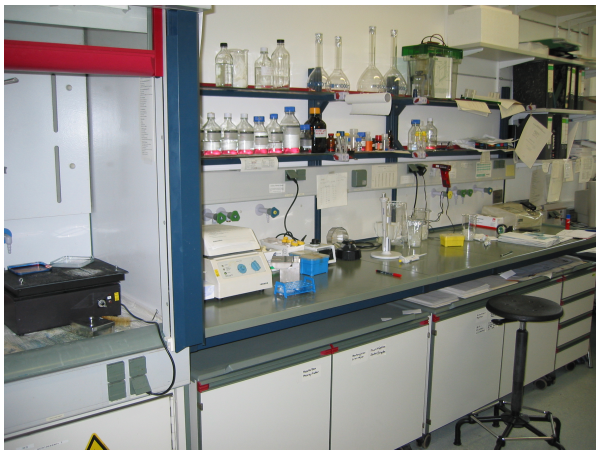
Materials and semiconductors

CC-by-3.0 https://en.wikipedia.org/wiki/File:Silicon.jpg

Chemical and pharmaceutical industry



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Simulating electronic structures

- Overall goals:
  - Model properties
  - Compare with experiments
- Sketching the approach:
  - Regime of quantum mechanics
  - System: Hamiltonian $\hat{\mathcal{H}}$ differential operator
  - Minimisation problem: Ground state Ψ with energy

$$E = \min_{\Psi} \int_{\mathbb{R}^{3N}} \Psi\left(\underline{\boldsymbol{r}}_1, \underline{\boldsymbol{r}}_2, \ldots, \underline{\boldsymbol{r}}_N\right) \hat{\mathcal{H}} \Psi\left(\underline{\boldsymbol{r}}_1, \underline{\boldsymbol{r}}_2, \ldots, \underline{\boldsymbol{r}}_N\right) \mathrm{d}\underline{\boldsymbol{r}}_1 \cdots \mathrm{d}\underline{\boldsymbol{r}}_N$$

  - Properties: Derivatives of the energy

Density-functional theory

$$E = \min_{\Psi} \int_{\mathbb{R}^{3N}} \Psi\left(\underline{\boldsymbol{r}}_1, \underline{\boldsymbol{r}}_2, \ldots, \underline{\boldsymbol{r}}_N\right) \hat{\mathcal{H}} \Psi\left(\underline{\boldsymbol{r}}_1, \underline{\boldsymbol{r}}_2, \ldots, \underline{\boldsymbol{r}}_N\right) \mathrm{d}\underline{\boldsymbol{r}}_1 \cdots \mathrm{d}\underline{\boldsymbol{r}}_N$$

Challenges:

- Challenge: Size of N
- 2 Silicon atoms: $N = 28 \Rightarrow \mathbf{2}^{84} \approx 2 \cdot 10^{25}$ quadrature points

$\Rightarrow$ Finished in 1 year:

$\Rightarrow$ Density-functional theory (DFT) approximation

- Effective one-particle model ($N = 1$)
- May construct DFT model for specific context
- Discretisation basis: Build known physics into model

Density-functional theory

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Questions related to reliability / high-throughput

- Challenge: Mass screening of materials
  - Reliable, black-box codes
  - Accuracy vs. computational effort
- Elevated / reduced precision?
- Reliable, mathematically proven algorithms?
- Leverage GPU and other accelerators?
- Distributed computing?

$\Rightarrow$ Difficult to address in existing (large) codes

$\Rightarrow$ Interdisciplinary setting

Demands for interdisciplinary software

- **Mathematicians:** Toy models and unphysical edge cases
- **Scientist:** Wants to focus on science, not numerics
- **High-performance:** Exploit all hardware specialities
- **Practitioner:**
  - Reliable, black-box, high-level for setup and data analysis

- Everything in one project?
- Still keep a minimalistic code base?
- Need good compromise *and* suitable programming language

DFTK (mid-term) goals

- DFTK: density-functional toolkit
  - Minimalistic code base: Use existing libraries and codes
  - Rapid extension and development
- Explore mathematics
  - Numerical experiments assisting proof
- High-performance computing
  - Laptop-level parallelism
  - GPU acceleration
- Allow novel methodologies
  - Mixed precision
  - Elevated precision and interval arithmetic
  - Automatic differentiation

Requirements from julia

- Algorithms
  - ☐ Nonlinear solvers
  - ☐ Reliable eigensolver
  - ☐ Fast Fourier transforms
- Infrastructure
  - ☐ Interoperability with legacy code (Python, FORTRAN)
  - ☐ Tooling for debugging / testing
  - ☐ Community and ecosystem
- Special methodologies
  - ☐ Extensibility to HPC / GPU
  - ☐ Automatic differentiation
  - ☐ Use of elevated or special floating point types

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DFTK goals (after 10 months)

- DFTK: density-functional toolkit
  - ☑ Minimalistic code base: < 3000 lines
  - ☑ Rapid extension and development (10 months!)
- Explore mathematics
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DEMO

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Show-casing DFTK

Outlook

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Questions?

DFTK: `https://github.com/mfherbst/DFTK.jl`


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