A posteriori error estimation for the non-self-consistent Kohn-Sham equations

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→ https://michael-herbst.com/talks/2020.09.03_faraday_error_nonscf_kohn_sham.pdf

Aim of *a posteriori* error analysis

- Starting point: Problem has been solved numerically
- Question: How good is the answer?

- Annotate *guaranteed* upper bound on numerical error
  - $\simeq$ Error bars of experimental science
- Balance sources of error:
  - Bigger basis? Tighter convergence criterion? Double precision?
  - $\Rightarrow$ **Aim:** Automatic selection of accuracy parameters

$\Rightarrow$ Need accurate and computable bounds on errors

Sources of error in Kohn-Sham density-functional theory

Model error	DFT method
Discretisation error	Brillouin-zone sampling Finite basis size
Algorithm error	Convergence threshold for iterative procedures
Arithmetic error	Finite floating-point precision
Programming error	Bugs, implementation mistakes
Hardware error	Error in CPU, RAM, etc.

- Ignore non-linear terms (drop Hartree and XC)

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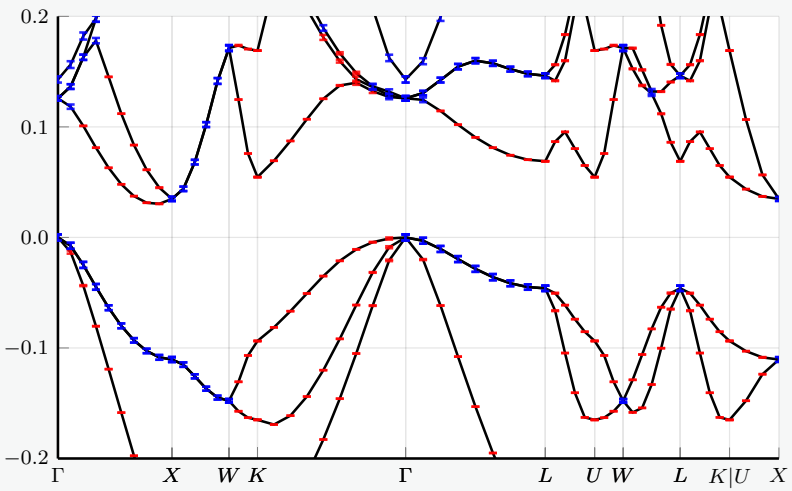
Quantity of interest, models and results

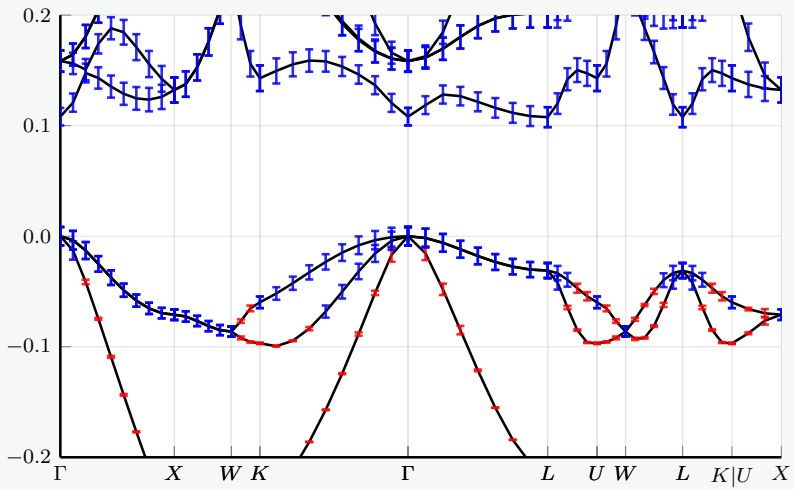
- Band structure, i.e. eigenpairs $H_{\mathbf{k}}\psi = \varepsilon\psi$ per $\mathbf{k}$-point
- Plane-wave discretisation
- Implementation: **DFTK**, `https://dftk.org`

Cohen-Bergstresser Silicon



- Fitted model potential
- Finite range in Fourier space

non-self-consistent Silicon



- XC, Hartree dropped
- Goedecker-Teter-Hutter pseudos

- 16 months of development, ≈ 5000 lines of julia
- Sizeable feature list (see `https://docs.dftk.org`):
  - Ground state and a bit of response theory
  - Compose your model: Gross-Pitaevskii, analytic potentials ...
  - Multitude of SCF approaches (> 800 electrons possible)
  - Multi-level threading
  - 1D / 2D / 3D systems
  - Arbitrary floating point type
  - Integration with materials-related python modules
- Performance: Within factor 2 of established codes
- Platform for multidisciplinary collaboration
- Documentation and examples: `https://docs.dftk.org`

Algorithm and discretisation error

- Residual $\tilde{\mathbf{r}} = H\tilde{\psi} - \tilde{\varepsilon}\tilde{\psi}$ related to error:

$$|\tilde{\varepsilon} - \varepsilon| \leq \|\tilde{\mathbf{r}}\| \qquad \text{Bauer-Fike}$$

$$|\tilde{\varepsilon} - \varepsilon| \leq \frac{\|\tilde{\mathbf{r}}\|^2}{\delta} \qquad \text{Kato-Temple,} \quad \text{gap } \delta$$

- Two-grid approach:
  - $(\tilde{\varepsilon}, \tilde{\psi})$ solved on basis X
  - Assume H computable on extended basis $Y \supset X$

  $\Rightarrow$ Compute $\|P_Y \tilde{\mathbf{r}}\|$, get upper bound for $\|P_{Y^\perp} \tilde{\mathbf{r}}\|$

  $\Rightarrow$ Get lower bound for δ

- Algorithm error: In-basis $\|P_X \tilde{\mathbf{r}}\|$
- Discretisation error: Out-of-basis $\|P_{X^\perp} \tilde{\mathbf{r}}\|$

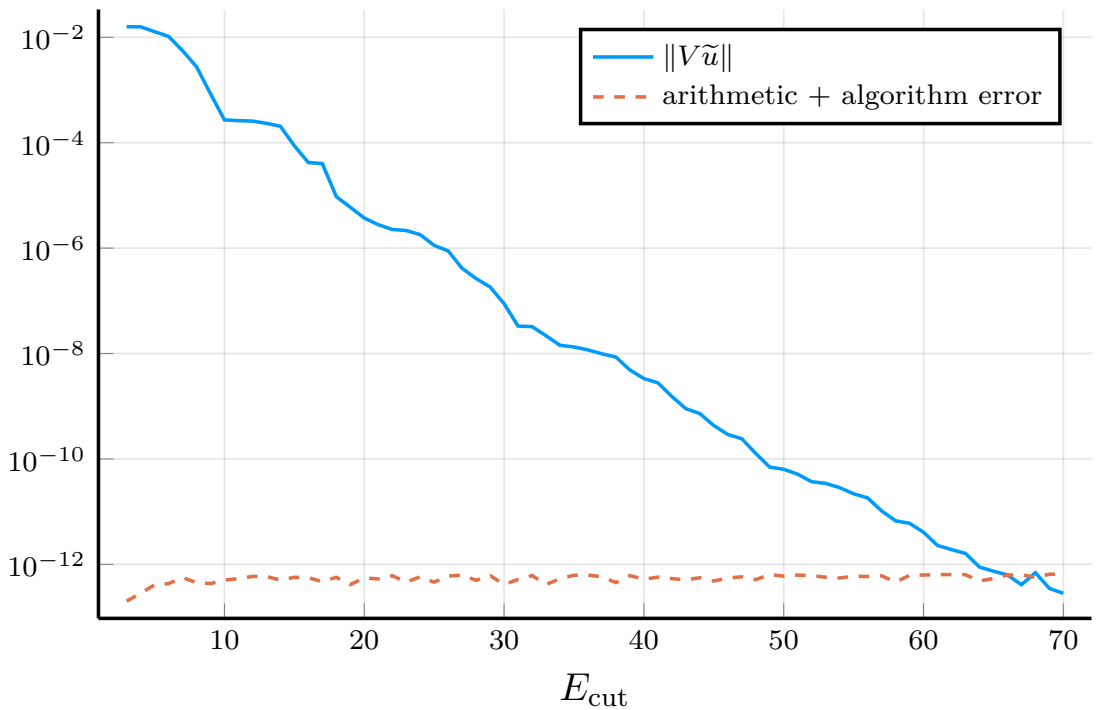
Arithmetic error

- Interval arithmetic: Represent $x \in \mathbb{R}$ by interval

$$[a, b] \quad a, b \in \mathrm{DP}, \quad a \leq x \leq b$$

- Can be used as floating-point type in DFTK

$\Rightarrow$ By computing in-basis $\|P_X \tilde{\mathbf{r}}\|$: Arithmetic + algorithm error

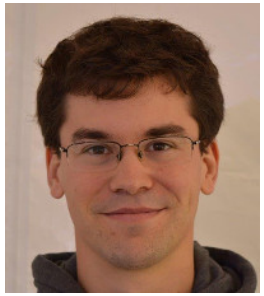


Outlook

- Other quantities of interest:
  - Eigenvectors, density, forces, response, ...
- Extend to non-linear Kohn-Sham DFT (with Hartree and XC)
  - Preliminary work on BZ integration and Gross-Pitaevskii
- Automatic balancing of accuracy parameters
  - User chooses target accuracy
  - Code chooses basis cutoff, convergence threshold and floating-point precision
  - Dynamic selection *while SCF converges*

$\Rightarrow$ Fully black-box modelling

Acknowledgements



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Questions?

DFTK `https://dftk.org`

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