Challenges and prospects of a posteriori error estimation in density-functional theory

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→ https://michael-herbst.com/talks/2020.10.14_aposteriori_error.pdf

Contents

1. High-throughput DFT and DFTK
2. Overview of *a posteriori* error analysis for DFT
3. *A posteriori* error for linear Kohn-Sham

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Typical density-functional theory (DFT) workflow

1. Formulate research question
   - Start with structure / lattice
   - Select quantities of interest:
     - Free energy, band gap, excitation energies, ...
2. Choose DFT model
   - DFT functional
   - Pseudopotential
   - ...
3. Choose numerics
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study

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   - Algorithm: SCF guess, preconditioners, mixing, ...
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   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

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High-throughput DFT applications

- High-throughput screening: Systematic computation
- Narrow down 10k candidates to $\mathcal{O}(10)$

$\Rightarrow$ Preselect for later investigation

- Applications:
  - *In silico* design of novel materials
  - Catalysis, battery research, structure determination

$\Rightarrow$ Reduce expensive experiments / manual work

$\Rightarrow$ Requires high degree of automation

Typical DFT workflow (2)

1. Formulate research question
2. Choose DFT model
3. Choose numerics (thresholds, algorithms . . .)
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Obstacles for high-throughput screening

- Accuracy-related parameters chosen by experience
- Empirical balance: Accuracy *versus* speed *versus* reliability

$\Rightarrow$ Need to reduce number of parameters:

  - Use physics: Reliable black-box SCF algorithms
  - Use maths: Error estimates and error balancing (this work)

$\Rightarrow$ Need code base to support mathematical developments *and* scale-up to the level of applications

Demands for interdisciplinary software

- **Mathematicians:** Toy models and unphysical edge cases
- **High-performance person:** Exploit hardware specialities
- **Scientist:** Design new models, not tweak numerics
- **Practitioner:** Reliable, black-box code, high-level interface

- julia for multidisciplinary research:
  - *Walks like Python, talks like Lisp, runs like FORTRAN*
  - Rich ecosystem (Optimisation, PDEs, stochastic processes, GPUs, Machine-Learning, Statistics, Linear Algebra . . .)
  - No two-language problem (high-level, compiled and hackable)

  $\Rightarrow$ Write code once, re-use for many back ends / machines . . .

- `https://michael-herbst.com/learn-julia`

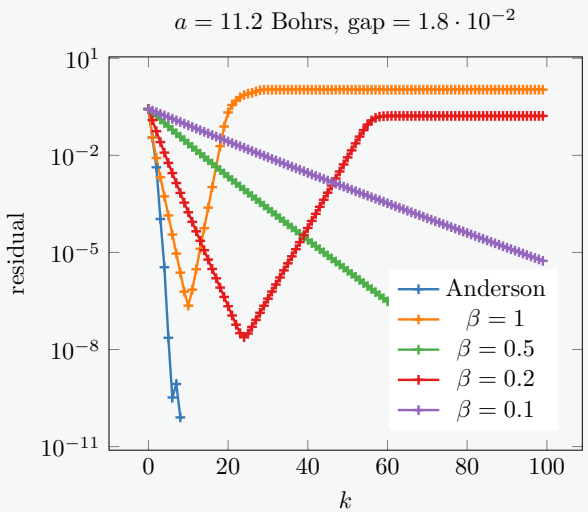
DFTK — https://dftk.org

- 17 months of development, ≈ 5500 lines of julia
- Sizeable feature list (see `https://docs.dftk.org`):
  - Ground state and a bit of response theory (new including spin)
  - Multitude of SCF approaches (> 800 electrons possible)
  - Compose your model (e.g. analytic potentials, . . .)
  - 1D / 2D / 3D systems
  - Arbitrary floating point type
  - Integration with materials-related python modules
- Performance: Within factor 2 of established codes

- Documentation and examples: `https://docs.dftk.org`

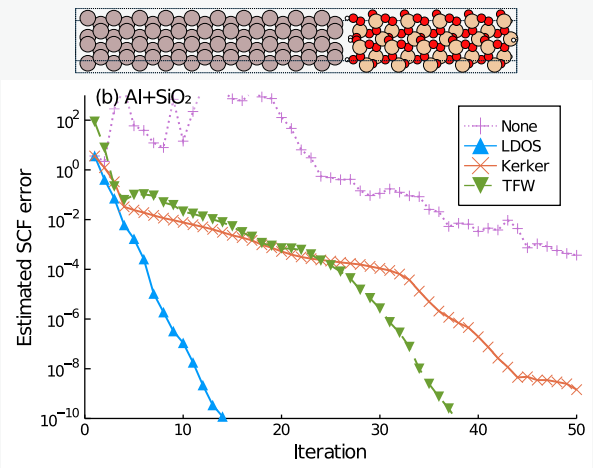
A few recent DFTK projects

Numerical analysis of SCF[1]



- SCF and direct minimisation
- Convergence wrt. spectral gap
- Numerical tests in DFTK

SCF for inhomogeneous systems[2]



- SCFs for large inhomogeneous materials hard to converge
- Black-box and parameter-free mixing scheme (unlike other approaches)

$\Rightarrow$ Platform for multidisciplinary collaboration

[1] E. Cancès, G. Kemlin, A. Levitt. arXiv 2004.09088 (2020)
[2] M. F. Herbst, A. Levitt. arXiv 2009.01665 (2020)

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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
  - $\not\simeq$ Statistical error
- Prospect: Automatic selection of accuracy parameters
- Challenges: Error bounds are useless unless . . .
  - . . . they are computable
  - . . . they are sharp / accurate
- Better error bounds $\Rightarrow$ Restricted scope
  - Basis type, quantity of interest, . . .

Errors everywhere . . .

1. Formulate research question, define quantity of interest
2. Choose DFT model (Model error)
3. Choose numerics
   - Discretisation: Basis size, k-point mesh (Discretisation error)
   - Convergence thresholds: SCF, eigensolver, . . . (Algorithm error)
   - Algorithm: SCF guess, preconditioners, mixing, . . .
   - Floating-point type (Arithmetic error)
4. Run calculation (Programming error, hardware error)
5. . . .

$\Rightarrow$ Error terms known $\Rightarrow$ Identify accuracy-limiting parameters

$\Rightarrow$ Automatically deduced refined setup

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A posteriori error estimation

- Hamiltonian H, eigenstates (ε, u), quantity of interest q
- Calculation yields approximations $\tilde{\varepsilon}$, $\tilde{u}$, $\tilde{q}$ (at current parameter set)

- Error $\|q - \tilde{q}\|_V$ (for some norm V)
  - Examples: $\|\rho - \tilde{\rho}\|_V$, $|E - \tilde{E}|$
- But q is unknown!

$\Rightarrow$ Need residual-error relationship, i.e. find constant C and norms W, s.t.

$$\|q - \tilde{q}\|_V \leq C \|\tilde{r}\|_W \qquad (\textit{a posteriori} \text{ error})$$

- Where $\tilde{r}$ is some residual, e.g. the eigenpair residual

$$\tilde{r} = H\tilde{u} - \tilde{\varepsilon}\tilde{u}$$

- Note: Exact H unknown $\Rightarrow \|\tilde{r}\|_W$ unknown (but easier . . .)

Finding the right norms is not always easy . . .

- Residual-error relationship $\|q - \tilde{q}\|_V \leq C \|\tilde{r}\|_W$
- Which norms to pick? $\|\cdot\|_\infty$ $\|\cdot\|_2$ $\|\cdot\|_{H^1}$ $\|\cdot\|_{H^{-1}}$

$\Rightarrow$ Depends on quantity of interest!

$\Rightarrow$ Error bounds depend on quantity of interest

- Consider linear response problem $Ax = b$
- x should be plotted $\Rightarrow \|\cdot\|_V = \|\cdot\|_\infty$
- Oettli-Prager relation:

$$\|\tilde{x} - x\|_\infty \leq \frac{\|A\tilde{x} - b\|_\infty}{\|A\|_\infty \|\tilde{x}\|_1 + \|b\|_\infty}$$

Status of error estimation in DFT

- A priori error (plane-wave)[1]
- A posteriori (FE, assuming exact solution)[2]
- k-point sampling[3]
- Cluster bounds[4]
- Non-linear eigenproblems[5]

$\Rightarrow$ So far just good building blocks

- Our contribution: Computable bounds for linear KS model[6]

[1] E. Cancès, R. Chakir, Y. Maday. ESIAM: M2AN, **49**, 755 (2015)
[2] H. Chen, X. Dai *et. al.* Mulscale. Model. Sim. **12**, 1828 (2014)
[3] E. Cancès and V. Ehrlacher *et. al.* Numer. Math. **144**, 479 (2020)
[4] E. Cancès, G. Dusson *et. al.* Math. Comp. In print (2020)
[5] E. Cancès, G. Dusson *et. al.* Comp. Rend. Math. **352**, 941 (2014)
[6] M. F. Herbst, A. Levitt, E. Cancès. Faraday Discus. (2020) DOI 10.1039/D0FD00048E

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Setting: Model[1]

- Quantity of interest: Band structure
- Need eigenpairs $Hu = \varepsilon u$ with periodic Kohn-Sham Hamiltonian (treated k point per k point)

$$H = \frac{1}{2}(-i\nabla + k)^2 + V + \cancel{V_{\mathrm{H}}[\{u\}]} + \cancel{V_{\mathrm{xc}}[\{u\}]}$$

- Only support linear terms in KS Hamiltonian (for now)
- Error contributions tackled:
  - Discretisation error due to finite basis size
  - Algorithm error due to convergence threshold
  - Arithmetic error due to floating-point precision

[1] M. F. Herbst, A. Levitt, E. Cancès. Faraday Discus. (2020) DOI 10.1039/D0FD00048E

Setting: Basis functions[1]

- Normalised plane-wave basis (Ω: Unit cell volume):

$$e_G(r) = \frac{1}{\sqrt{|\Omega|}} e^{iG\cdot r}$$

- Basis set determined by finite cutoff E_{cut}:

$$X = \text{span}\left\{ e_G \,\middle|\, \frac{1}{2}|G+k|^2 \leq E_{\text{cut}} \right\}$$

- For this basis:

$$\langle e_G | H e_{G'} \rangle = \frac{1}{2}|G+k|^2 \delta_{GG'} + \langle e_G | V e_{G'} \rangle \qquad G, G' \in X$$

$\Rightarrow$ Kinetic energy is diagonal

[1] M. F. Herbst, A. Levitt, E. Cancès. Faraday Discus. (2020) DOI 10.1039/D0FD00048E

Setting: Potentials[1]

- Goedecker-Teter-Hutter (GTH) pseudopotential
- local & non-local term $V = V_{\text{loc}} + V_{\text{nl}}$ with

$$V = V_{\text{loc}} + V_{\text{nl}}$$
$$\langle e_G | V_{\text{loc}} e_{G'} \rangle = \frac{\hat{v}_{\text{loc}}(G - G')}{|\Omega|}$$
$$\langle e_G | V_{\text{nl}} e_{G'} \rangle = \sum_{Lij} d_{Lij}\, p_{Li}(k+G)\, \overline{p_{Lj}(k+G')}$$

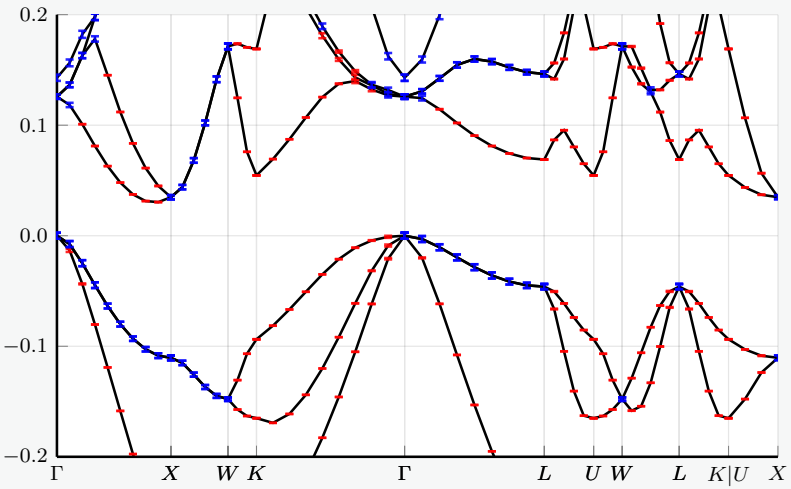
- Local term determined by Fourier coefficients $\hat{v}_{\text{loc}}(\Delta G)$
- Non-local term is sum of projectors $p_{Li}(k+G)$

[1] M. F. Herbst, A. Levitt, E. Cancès. Faraday Discus. (2020) DOI 10.1039/D0FD00048E

Main result: Band structure with error bars

- Fully guaranteed *a posteriori* bounds
- Numerical error proven to be within error bars

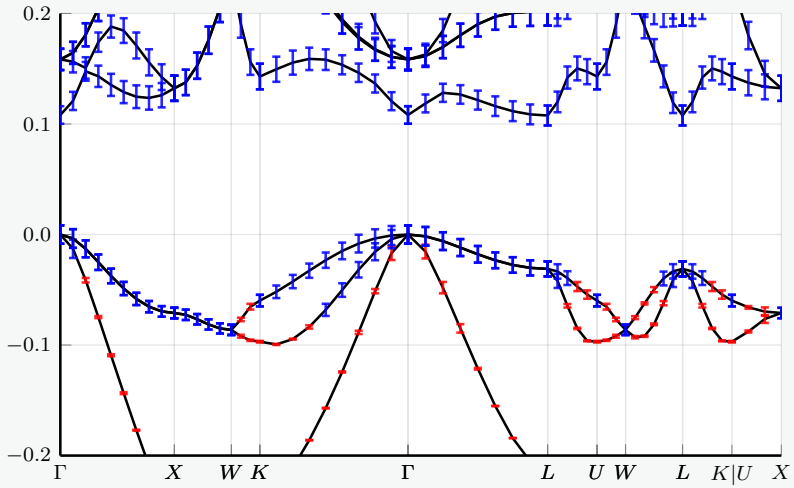
Cohen-Bergstresser Silicon



- Simple model: $V_{\text{nl}} = 0$, only finite non-zero $\hat{v}_{\text{loc}}(\Delta G)$

$\Rightarrow$ H is known exactly

non-self-consistent Silicon



- XC, Hartree dropped
- GTH pseudos

$\Rightarrow$ H *not* known exactly

Assumptions for our error estimate[1]

- Plane-wave basis set $\Rightarrow$ kinetic energy is diagonal
- Fourier coefficients $\hat{v}_{\text{loc}}(G)$ decay for $|G| > q_{\text{min}}$
  - (i.e. $v_{\text{loc}}(r)$ sufficiently regular)
- The GTH projectors $p_{Li}(k+G)$ decay for $|G+k| > q_{\text{min}}$
- Potential V can be computed on extended basis

$$Y = \text{span}\left\{ e_G \,\middle|\, \frac{1}{2}|G+k|^2 \leq E_{\text{cut}}^{(2)} \right\}$$

with $E_{\text{cut}}^{(2)} \geq \frac{1}{2} q_{\text{min}}^2 > E_{\text{cut}}$

  - (i.e. until decay sets in)

$\Rightarrow$ Satisfied for GTH pseudos / Cohen-Bergstresser model

[1] M. F. Herbst, A. Levitt, E. Cancès. Faraday Discus. (2020) DOI 10.1039/D0FD00048E

Algorithm and discretisation error: Overview

- Residual $\tilde{r} = H\tilde{u} - \tilde{\varepsilon}\tilde{u}$
- Possible residual-error relationships:

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

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

- Strategy:
  - Need lower bound on gap δ
  - Need upper bound on $\|\tilde{r}\|$

Estimating the residual

- P_X: Projector into X basis
- Split up residual into contributions:

$$\|\tilde{r}\| = \|P_X \tilde{r}\| + \|P_{X^\perp} \tilde{r}\| = \|P_X H \tilde{u} - \tilde{\varepsilon}\tilde{u}\| + \|P_{X^\perp} V \tilde{u}\|$$

(Use $P_X \tilde{u} = \tilde{u}$ and diagonal kinetic operator)

- $\|P_X \tilde{r}\|$: Residual inside X (algorithm error)
- $\|P_{X^\perp} \tilde{r}\|$: Residual outside X (discretisation error)

Estimating the residual (2)

- Dual-basis approach:
  - X is discretisation basis (used for main computation)
  - $Y \supset X$: Basis on which V can be computed
- Second split:

$$\|P_{X^\perp} V\tilde{u}\| = \|P_{X^\perp \cap Y} V\tilde{u}\| + \|P_{Y^\perp} V\tilde{u}\|$$

- First term computable, second term is

$$\|P_{Y^\perp} V\tilde{u}\|^2 = \sum_{G \in Y^\perp} \left| \sum_{G' \in X} \langle e_G | V e_{G'} \rangle \, \tilde{u}(G') \right|^2$$

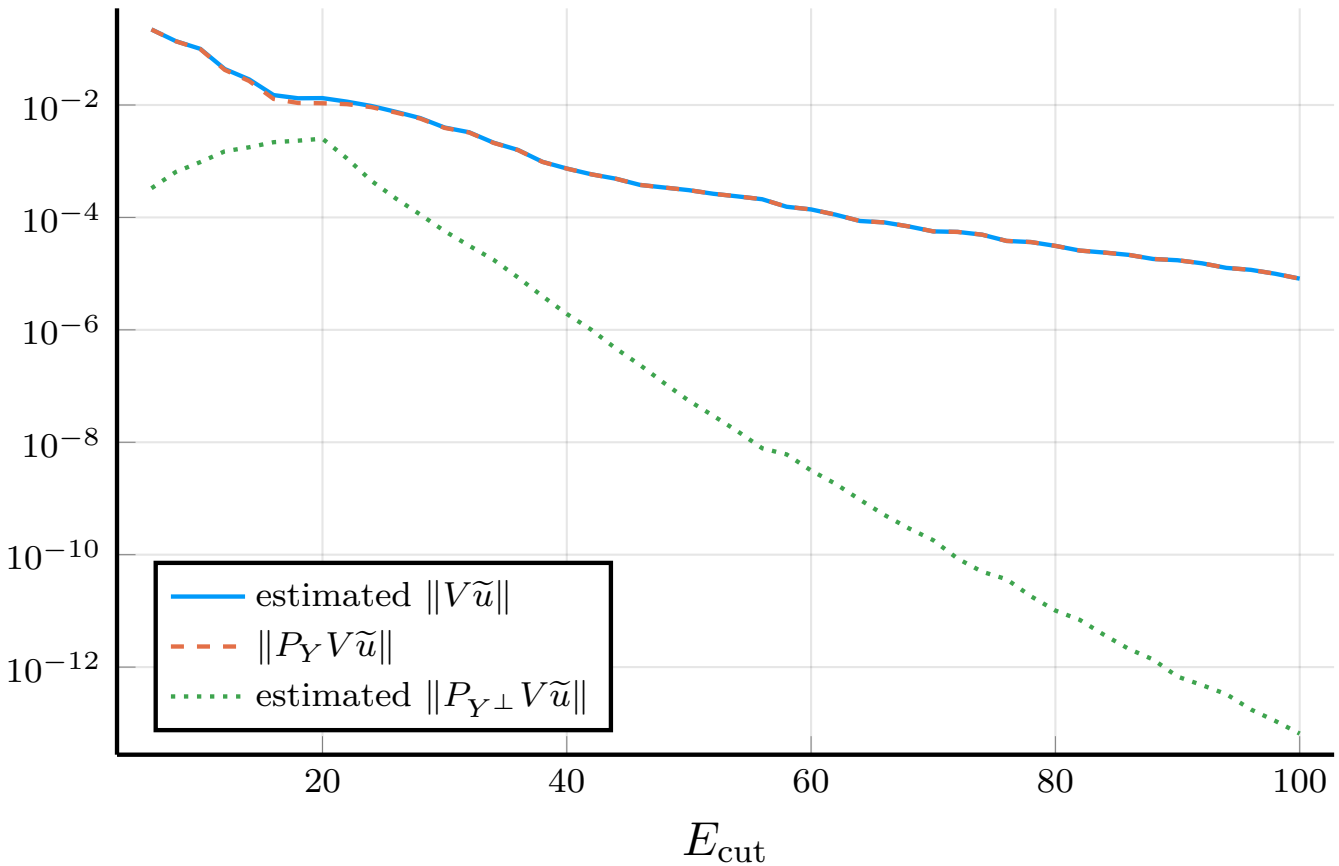
- By construction: $\hat{v}_{\text{loc}}(G)$ and $p_{Li}(k+G)$ decay outside Y

$\Rightarrow$ Elements $\langle e_G | V e_{G'} \rangle$ coupling X and $Y^\perp$ are small!

$\Rightarrow$ Can derive upper bound for $\|P_{Y^\perp} V\tilde{u}\|$

Numerical results for residual estimate

- $E_{\text{cut}}^{(2)}$ (and thus Y) fixed empirically to $4E_{\text{cut}}$



Estimating the gap

- Assume there is a gap (i.e. no degeneracy)
  - If not use Bauer-Fike
- Lower bound on gap δ for eigenvalue ε_n

  $\Rightarrow$ Lower bound on $\varepsilon_{n+1} - \varepsilon_n$ and on $\varepsilon_n - \varepsilon_{n-1}$

  $\Rightarrow$ Upper bound on ε_n and ε_{n-1} / lower bound on ε_{n+1} and ε_n
- Upper bounds are easy (variational principle):

$$\varepsilon_n \leq \tilde{\varepsilon}_n$$

- Rigorous lower bounds are more tricky ...

Lower bounds on eigenvalue ε_{n+1}

- Imagine we knew a μ with $\varepsilon_n \leq \mu \leq \varepsilon_{n+1}$

  $\Rightarrow$ It were a good lower bound to ε_{n+1}

- For such a μ we had $\sigma_-(H - \mu) = n$, i.e. $H - \mu$ had exactly n negative eigenvalues

- Partition shifted H into part in X and outside:

$$H - \mu = \begin{pmatrix} H_{XX} - \mu & V_{XX^\perp} \\ V_{X^\perp X} & H_{X^\perp X^\perp} - \mu \end{pmatrix} \quad \text{(kin. op. diagonal)}$$

- Haynsworth inertia additivity formula:

$$\sigma_-(H - \mu) = \sigma_-(H_{XX} - \mu) + \sigma_-(S_\mu)$$

  where the Schur complement

$$S_\mu = (H_{X^\perp X^\perp} - \mu) - V_{X^\perp X} \left(H_{XX} - \mu\right)^{-1} V_{XX^\perp}$$

Lower bounds on eigenvalue ε_{n+1} (2)

- Now take $\mu \in (\tilde{\varepsilon}_n, \tilde{\varepsilon}_{n+1})$ as a reasonable guess
- For such a μ by construction: $\sigma_-(H_{XX} - \mu) = n$
- Therefore: $\sigma_-(S_\mu) = 0 \Leftrightarrow \sigma_-(H - \mu) = n \Leftrightarrow \mu \leq \varepsilon_{n+1}$

$\Rightarrow$ Remaining job is to adjust μ such that it is guaranteed:

$$(H_{X^\perp X^\perp} - \mu) - V_{X^\perp X} \left(H_{XX} - \mu\right)^{-1} V_{X X^\perp} = S_\mu \geq 0$$

- Now:
  - By construction of X: Kinetic part of $H_{X^\perp X^\perp}$ is bounded from below by E_{cut}
  - Operator norm $\|V\|_{\text{op}}$ is upper bound to eigenvalues of V

$\Rightarrow$ $H_{X^\perp X^\perp} - \mu \geq E_{\text{cut}} + \|V_{X^\perp X^\perp}\|_{\text{op}} - \mu$

Lower bounds on eigenvalue ε_{n+1} (3)

$$(H_{X^\perp X^\perp} - \mu) - \underbrace{V_{X^\perp X} \left(H_{XX} - \mu\right)^{-1} V_{X X^\perp}}_{=B_\mu} = S_\mu \geq 0$$

- Compute a dense eigendecomposition $H_{XX} = \tilde{U}\tilde{\Lambda}\tilde{U}^\dagger$
- Then using the larger grid Y:

$$\begin{aligned}
-B_\mu &\geq -\left\| \left(V_{X^\perp X}\tilde{U}\right) \left(\tilde{\Lambda} - \mu\right)^{-1} \left(V_{X^\perp X}\tilde{U}\right)^\dagger \right\|_{\text{op}} \\
&\geq -\left\| \left(V_{X^\perp \cap Y, X}\tilde{U}\right) \left(\tilde{\Lambda} - \mu\right)^{-1} \left(V_{X^\perp \cap Y, X}\tilde{U}\right)^\dagger \right\|_{\text{op}} \\
&\quad - 2\left\| \left(V_{X^\perp \cap Y, X}\tilde{U}\right) \left(\tilde{\Lambda} - \mu\right)^{-1} \right\|_{\text{op}} \left\| V_{X, Y^\perp} \right\|_{\text{op}} - \frac{\|V_{XY^\perp}\|_{\text{op}}^2}{\tilde{\varepsilon}_n - \mu}
\end{aligned}$$

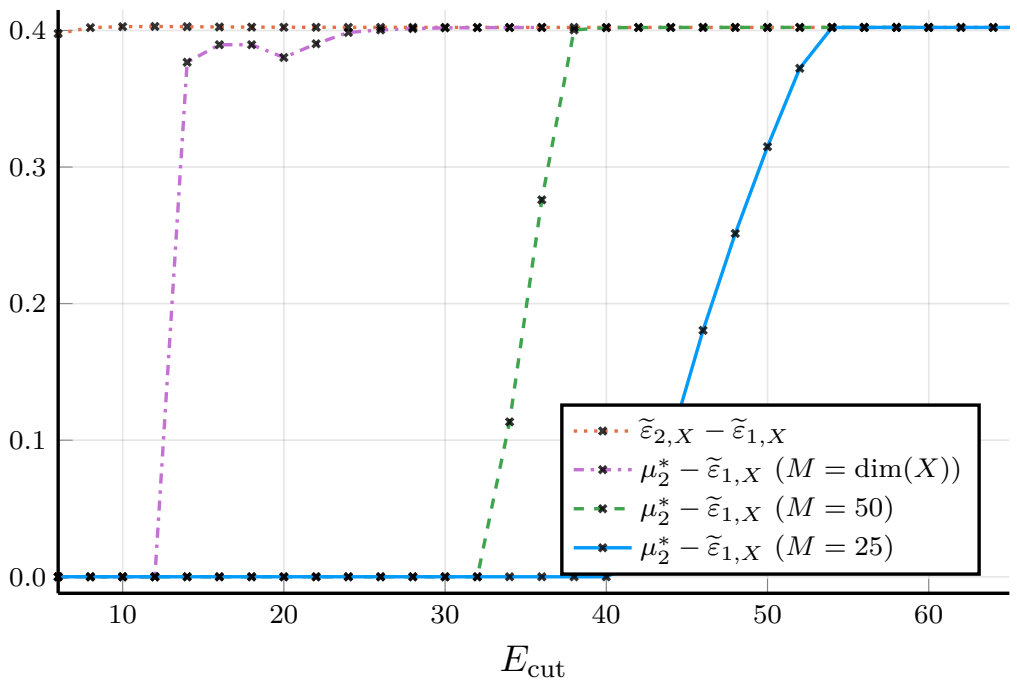
$\Rightarrow$ Bound on $\|V_{X^\perp X^\perp}\|_{\text{op}}$ and $\|V_{XY^\perp}\|_{\text{op}}$, rest computable

Lower bounds on eigenvalue ε_{n+1} (4)

- Strategy to find μ:
  - Guess $\mu \in (\widetilde{\varepsilon}_n, \widetilde{\varepsilon}_{n+1})$
  - Use computed bounds to find largest μ such that

$$E_{\text{cut}} + \|V_{X^\perp X^\perp}\|_{\text{op}} - \mu - B_\mu \geq 0$$

$\Rightarrow$ If exists, proves that μ is guaranteed lower bound to δ

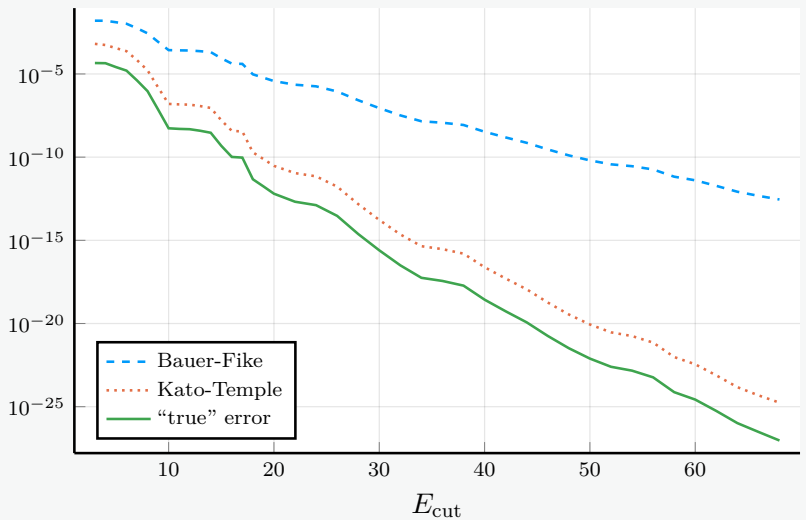


Discretisation error: What I did not tell you . . .

- There are ways to get bound on δ without a full diagonalisation
- Bounds on $\|V_{X^\perp X^\perp}\|_{\text{op}}$, $\|V_{X X^\perp}\|_{\text{op}}$ and $\|V_{X Y^\perp}\|_{\text{op}}$
  - Again uses that $\hat{v}_{\text{loc}}(G)$ and $p_{iL}(k+G)$ decay outside Y
- Some tricks how to compute things fast . . .

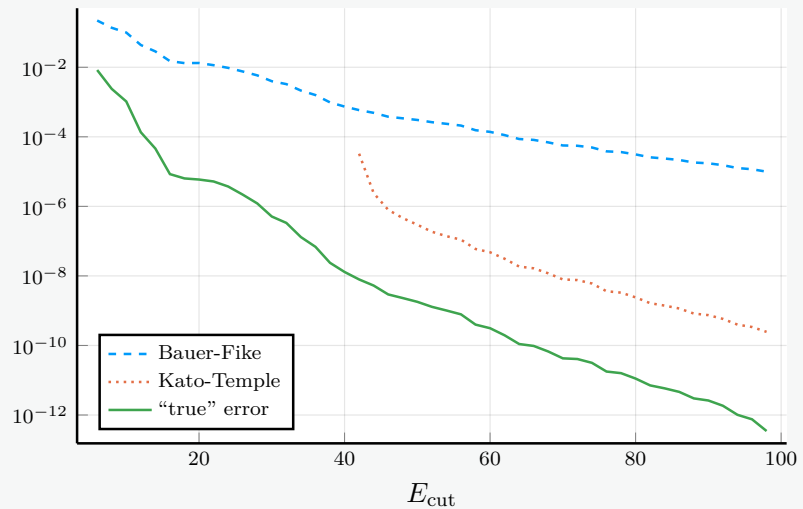
Numerical results for discretisation error

Cohen-Bergstresser Silicon



- Using elevated precision in DFTK

GTH Silicon



- Gap only found from $E_{\text{cut}} = 40$

- Shown for the first eigenvalue ε_1
- Kato-Temple clearly the better bound

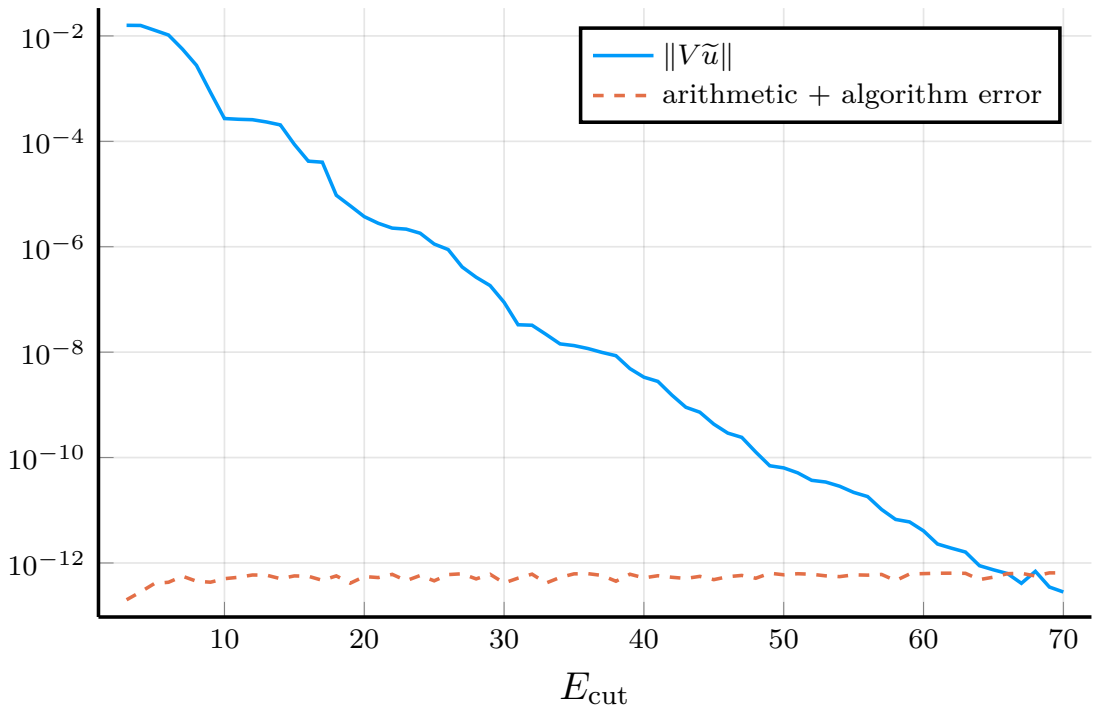
Arithmetic error

- 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

$\Rightarrow$ Compute in-basis $\|P_X \tilde{r}\|$: Sum arithmetic + algorithm error



Extension to other basis functions

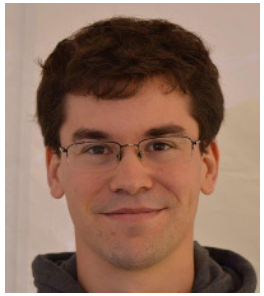
- For the residual: Need estimates $\left\| H_{X^\perp, X} \tilde{u} \right\|$
  - Plane-waves
  - Gaussians
- For the gap: Need estimates $\|H_{X^\perp X^\perp}\|_{\text{op}}$ and $\|H_{X^\perp X}\|_{\text{op}}$
  - Not so easy for Gaussians

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?

https://dftk.org

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