Black-box inhomogeneous preconditioning for density-functional theory

Michael F. Herbst, Antoine Levitt

CERMICS, Inria Paris and École des Ponts ParisTech

24th September 2020

→ `https://michael-herbst.com/talks/2020.09.24_ldos_preconditioning.pdf`

Contents

MATHerials Inria École des Ponts ParisTech

Contents

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

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
   - Discretisation: Basis size, k-point mesh
   - Convergence thresholds: SCF, eigensolver, ...
   - Algorithm: SCF guess, preconditioners, mixing, ...
   - Floating-point type

Typical density-functional theory (DFT) workflow

1. Formulate research question
2. Choose DFT model
   - DFT functional
   - Pseudopotential
   - ...
3. Choose numerics
   - Discretisation: Basis size, k-point mesh
   - Convergence thresholds: SCF, eigensolver, ...
   - Algorithm: SCF guess, preconditioners, mixing, ...
   - Floating-point type
4. Run calculation
5. If failure: Tweak numerics, repeat 4

Typical density-functional theory (DFT) workflow

1. Formulate research question
2. Choose DFT model
3. Choose numerics
   - Discretisation: Basis size, k-point mesh
   - Convergence thresholds: SCF, eigensolver, ...
   - Algorithm: SCF guess, preconditioners, mixing, ...
   - Floating-point type
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
7. Physics appropriately modelled?

Typical density-functional theory (DFT) workflow

1. Formulate research question
2. Choose DFT model
3. Choose numerics
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
   - Repeat 4 (and 5) until results converged
7. Physics appropriately modelled?
   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

Typical density-functional theory (DFT) workflow

1. Formulate research question
2. Choose DFT model
3. Choose numerics
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
   - Repeat 4 (and 5) until results converged
7. Physics appropriately modelled?
   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

Typical density-functional theory (DFT) workflow

1. Formulate research question
2. Choose DFT model
3. Choose numerics
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
   - Repeat 4 (and 5) until results converged
7. Physics appropriately modelled?
   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

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 . . .)
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
7. Physics appropriately modelled?
   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

Typical DFT workflow (2)

1. Formulate research question
2. Choose DFT model
3. Choose numerics (thresholds, algorithms . . .)
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
7. Physics appropriately modelled?
   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

Typical DFT workflow (2)

1. Formulate research question
2. Choose DFT model
3. Choose numerics (thresholds, algorithms . . .)
4. Run calculation
5. If failure: Tweak numerics, repeat 4
6. Convergence study
7. Physics appropriately modelled?
   - No: Back to 2 and repeat!
   - Yes: Hooray! Done!

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 preconditioners (this work)
  - Use maths: Error estimates and automatic error balancing

$\Rightarrow$ Requires code base to support developments *and* 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 . . .

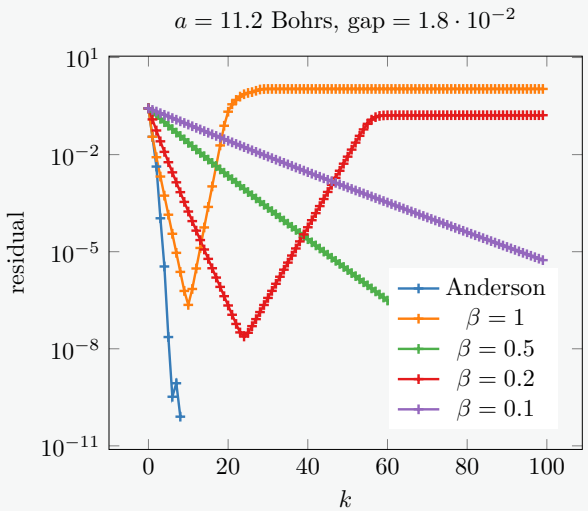
- `https://michael-herbst.com/learn-julia`

DFTK — https://dftk.org

- 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`

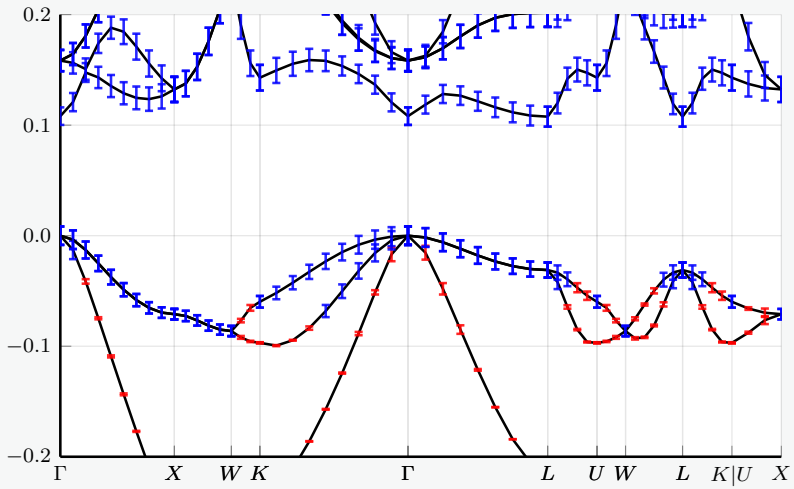
A few recent DFTK projects

Numerical analysis of SCF[1]



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

Error estimates for Kohn-Sham[2]



- A posteriori estimates for non-self-consistent Kohn-Sham
- Estimation of arithmetic error
- Elevated floating-point type
- Time to publication: 10 weeks

[1] E. Cancès, G. Kemlin, A. Levitt. arXiv 2004.09088 (2020)

[2] M. F. Herbst, A. Levitt and E. Cancès. Faraday Discuss. *In press.* (2020)

Algorithm selection in self-consistent field iterations

- Screening studies: Crash of SCF not acceptable
  - What about challenging systems: Disorder, spin, . . . ?
  - Black-box and reliable SCF methods?
  - Systems with new physics can be the tough ones!
- Focus of this work: Algorithm selection for SCF
- Preconditioning of SCF iterations $\equiv$ mixing

Contents

The essence of density-functional theory

$$\gamma_0 = \arg\min_{\gamma \in \mathcal{P}_N} \mathcal{E}_{\mathsf{DFT}}(\gamma)$$

- Energy functional (LDA)

$$\mathcal{E}_{\mathsf{DFT}}(\gamma) = \mathrm{tr}_{L^2}\left(-\frac{1}{2}\Delta\gamma\right) + \int \rho_\gamma(\underline{\boldsymbol{r}}) V_{\mathsf{Nuc}}(\underline{\boldsymbol{r}})\,\mathrm{d}\underline{\boldsymbol{r}} + \frac{1}{2}\int \rho_\gamma(\underline{\boldsymbol{r}}) v_C(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') \rho_\gamma(\underline{\boldsymbol{r}}')\,\mathrm{d}\underline{\boldsymbol{r}}\,\mathrm{d}\underline{\boldsymbol{r}}' + E_{\mathsf{xc},\rho_\gamma}$$

- Density matrix $\gamma \in \mathcal{P}_N$
- Density $\rho_\gamma(\underline{\boldsymbol{r}}) = \gamma(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}})$
- Coulomb kernel $v_C(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') = 1/\left\|\underline{\boldsymbol{r}} - \underline{\boldsymbol{r}}'\right\|$
- Exchange-correlation energy $E_{\mathsf{xc},\rho_\gamma}$
- XC potential $V_{\mathsf{xc},\rho}(\underline{\boldsymbol{r}}) = \frac{\mathrm{d}E_{\mathsf{xc},\rho}}{\mathrm{d}\rho(\underline{\boldsymbol{r}})}$ and kernel $f_{\mathsf{xc},\rho}(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') = \frac{\mathrm{d}^2 E_{\mathsf{xc},\rho}}{\mathrm{d}\rho(\underline{\boldsymbol{r}})\,\mathrm{d}\rho(\underline{\boldsymbol{r}}')}$

The self-consistent field procedure

- Euler-Lagrange equations (LDA):

$$\begin{cases} \gamma_0 = f_{\varepsilon_F}\left(-\frac{1}{2}\Delta + V_{\gamma_0}\right) & \text{with } \varepsilon_F \text{ s.t. } \gamma_0 \in \mathcal{P}_N \\ V_\gamma = V_{\text{Nuc}} + \int (v_C \rho_\gamma) + V_{\text{xc},\rho_\gamma}, \\ \rho_\gamma(\underline{\boldsymbol{r}}) = \gamma(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}), \gamma \in \mathcal{P}_N \end{cases}$$

where

$$f_{\varepsilon_F}\left(\hat{\mathcal{F}}\right) = \sum_n f\left(\frac{\varepsilon_n - \varepsilon_F}{T}\right) |\psi_n\rangle \langle\psi_n| \qquad \text{with} \qquad \hat{\mathcal{F}}\psi_n = \varepsilon_n \psi_n$$

- Fermi-Dirac distribution

$$f(x) = \frac{1}{1 + \exp(x)}$$

The self-consistent field procedure

- Euler-Lagrange equations (LDA):

$$\begin{cases} \gamma_0 = f_{\varepsilon_F}\left(-\frac{1}{2}\Delta + V_{\gamma_0}\right) & \text{with } \varepsilon_F \text{ s.t. } \gamma_0 \in \mathcal{P}_N \\ V_\gamma = V_{\text{Nuc}} + \int (v_C \rho_\gamma) + V_{\text{xc},\rho_\gamma}, \\ \rho_\gamma(\underline{\boldsymbol{r}}) = \gamma(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}), \gamma \in \mathcal{P}_N \end{cases}$$

  where

$$f_{\varepsilon_F}\left(\hat{\mathcal{F}}\right) = \sum_n f\left(\frac{\varepsilon_n - \varepsilon_F}{T}\right) |\psi_n\rangle \langle\psi_n| \qquad \text{with} \qquad \hat{\mathcal{F}}\psi_n = \varepsilon_n \psi_n$$

- Self-consistent field procedure:
  (1) Guess initial ρ_γ
  (2) Build Kohn-Sham Hamiltonian $-\frac{1}{2}\Delta + V_\gamma$
  (3) Diagonalise it to get new $\{\psi_i\}_i$
  (4) Build new ρ_γ, go to (2).

The SCF procedure as a fixed-point problem

- Euler-Lagrange equations (LDA)

$$\begin{cases} \gamma_0 = f_{\varepsilon_F}\left(-\frac{1}{2}\Delta + V_{\gamma_0}\right) \quad \text{with } \varepsilon_F \text{ s.t. } \gamma_0 \in \mathcal{P}_N \\ V_\gamma = V_{\text{Nuc}} + \int (v_C \rho_\gamma) + V_{\text{xc},\rho_\gamma}, \\ \rho_\gamma(\underline{\boldsymbol{r}}) = \gamma(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}), \gamma \in \mathcal{P}_N \end{cases}$$

- Define the potential-to-density map F by

$$F(V)(\underline{\boldsymbol{r}}) = \left[f_{\varepsilon_F}\left(-\frac{1}{2}\Delta + V\right)\right](\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}})$$

and the density-to-potential map by

$$\mathcal{V}(\rho) = V_{\text{Nuc}} + \int (v_C \rho_\gamma) + V_{\text{xc},\rho_\gamma}$$

$\Rightarrow$ SCF solves $\rho = F(\mathcal{V}(\rho))$

The SCF Jacobian

- SCF solves $\rho = F(\mathcal{V}(\rho))$
- Consider damped fixed-point scheme:

$$\rho_{n+1} = \rho_n + \alpha \left[F(\mathcal{V}(\rho_n)) - \rho_n\right]$$

- Near a fixed-point the error goes as

$$e_{n+1} \simeq \left[1 - \alpha\epsilon^\dagger\right] e_n$$

  where $\epsilon^\dagger = 1 - \chi_0(v_C + f_{\text{xc},\rho})$

- χ_0: Independent-particle susceptibility (derivative of F)

$\Rightarrow$ Jacobian $J_\alpha = 1 - \alpha\epsilon^\dagger$ determines SCF convergence

- $\epsilon = 1 - (v_C + f_{\text{xc},\rho})\chi_0$ is the dielectric matrix

$\Rightarrow$ Convergence of SCF linked to dielectric properties of material

Dielectric matrix and SCF instabilities

- Dielectric adjoint: $\epsilon^\dagger = 1 - \chi_0(v_C + f_{\text{xc},\rho})$
- $f_{\text{xc},\rho}$ usually small. If ignored $\epsilon^\dagger \simeq 1 - \chi_0 v_C$ is positive.

$\Rightarrow$ Dampened iteration

$$\rho_{n+1} = \rho_n + \alpha\left[F(\mathcal{V}(\rho_n)) - \rho_n\right] \qquad J_\alpha = 1 - \alpha\epsilon^\dagger$$

converges for small enough $\alpha > 0$.

- But: Required α can be painfully small if
  - $\epsilon^\dagger$ has small eigenvalues (e.g. symmetry breaking)
  - χ_0 has large eigenvalues (localised states)
  - Large charge-sloshing modes of v_C are uncompensated by χ_0.
- This work: Only charge-sloshing

Charge sloshing and mixing

- In Fourier space: $\widehat{(v_C \rho)}(\underline{\boldsymbol{q}}) = \frac{4\pi\hat{\rho}(\underline{\boldsymbol{q}})}{|q|^2}$
- Smallest $q \sim 1/L$ where L is crystal length

$\Rightarrow \lambda_{\text{max}}(v_C) \sim L^2$

$\Rightarrow$ condition number (roughly) grows as L^2 (charge sloshing)

- Can imply $\lambda_{\text{max}}(\epsilon^\dagger) \sim L^2$ (e.g. in metals, next slide)

$\Rightarrow$ Infeasible to do some large systems with damped SCF

- Mixing schemes: Preconditioned quasi-Newton updates

$$\rho_{n+1} = \rho_n + \alpha P^{-1} \left[F(\mathcal{V}(\rho_n)) - \rho_n \right]$$

where $P^{-1} \approx \left(\epsilon^\dagger\right)^{-1}$.

Construction of preconditioners: Bulk metals

- To prevent charge-sloshing need model in small-q regime
- $\lim_{q\to 0} \chi_0(\underline{\boldsymbol{q}}) \simeq -D$ with density of states $D > 0$
- Approximate dielectric:

$$\epsilon(\underline{\boldsymbol{q}}) = \frac{4\pi D + |q|^2}{|q|^2} \quad \lambda_{\mathsf{max}}(\epsilon) \sim L^2$$

- Kerker mixing ($k_{\mathsf{TF}} > 0$)

$$P^{-1}(\underline{\boldsymbol{q}}) = \frac{|q|^2}{|q|^2 + k_{\mathsf{TF}}^2}$$

- Based on Thomas-Fermi theory (where $k_{\mathsf{TF}} = \sqrt{4\pi D}$)

Preconditioners: Bulk insulators / semiconductors

- $\lim_{q\to 0} \chi_0(\underline{\boldsymbol{q}}) \simeq -\underline{\boldsymbol{q}}^T \sigma_0 \underline{\boldsymbol{q}}$ where σ_0 is polarisability tensor
- Approximate dielectric:

$$\lim_{q\to 0} \epsilon(\underline{\boldsymbol{q}}) = 1 + 4\pi \frac{\underline{\boldsymbol{q}}^T \sigma_0 \underline{\boldsymbol{q}}}{|q|^2}$$

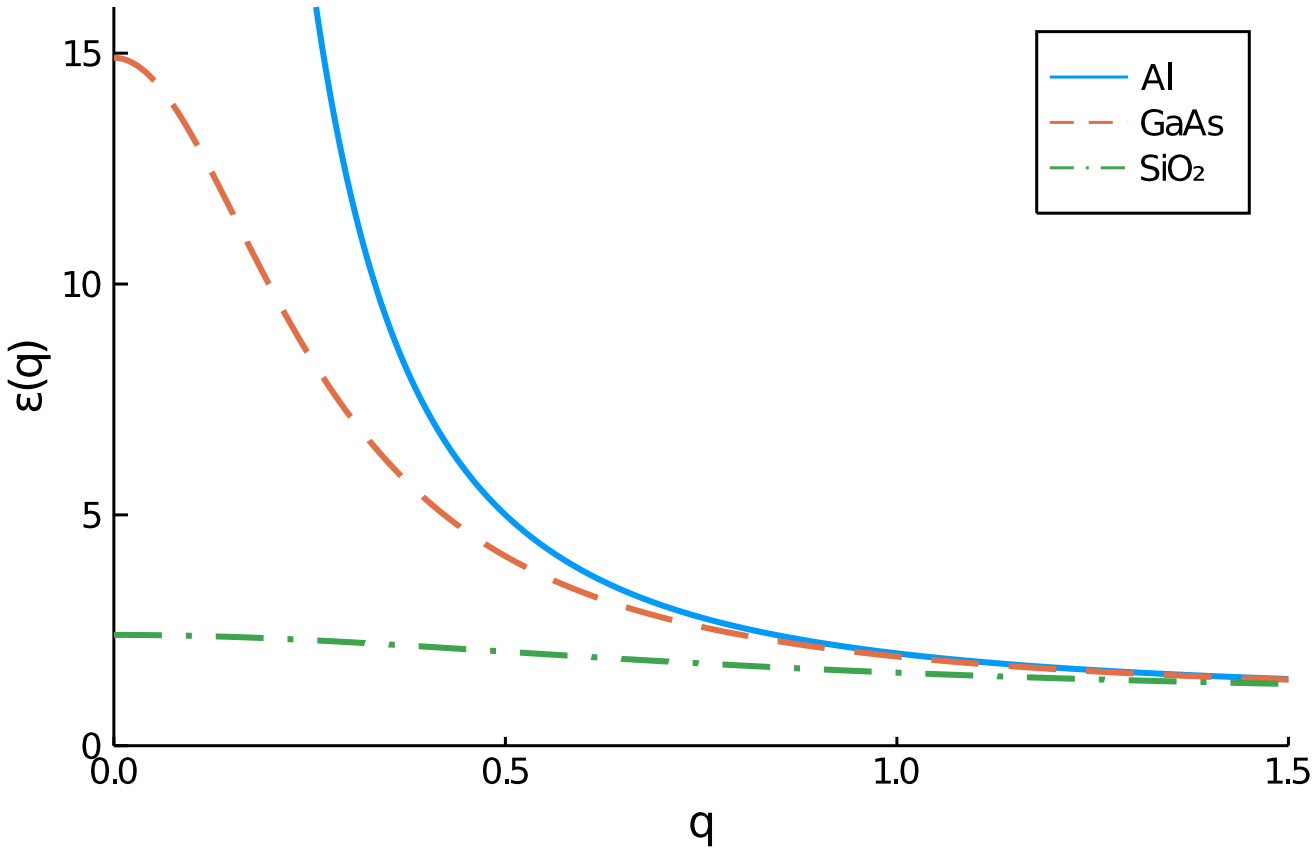
- σ_0 isotropic: $\epsilon(0) = 1 + 4\pi\sigma_0 \equiv \varepsilon_r$, i.e. dielectric constant
- For larger q: Empirically interpolate to known behaviour $q \to \infty$[1]:

$$\epsilon(\underline{\boldsymbol{q}}) = \frac{\varepsilon_r + (\varepsilon_r - 1)\frac{|q|^2}{k_{\mathrm{TF}}^2}}{1 + (\varepsilon_r - 1)\frac{|q|^2}{k_{\mathrm{TF}}^2}}$$

$\Rightarrow$ Construct Dielectric mixing

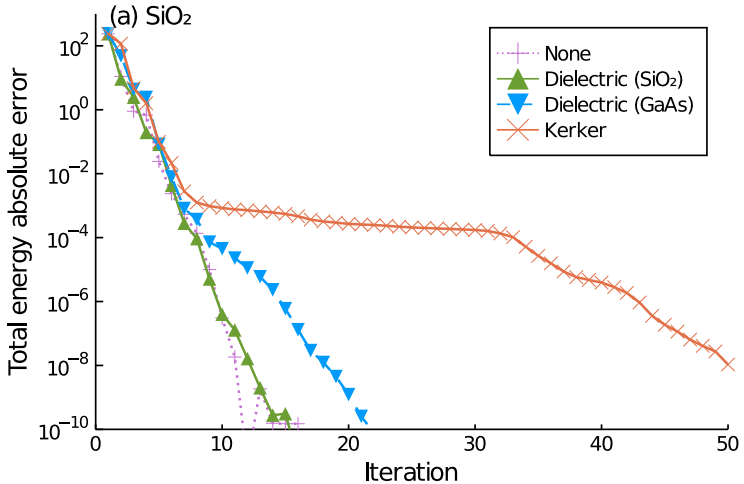
[1] M. F. Herbst, A. Levitt. arXiv 2009.01665 (2020)

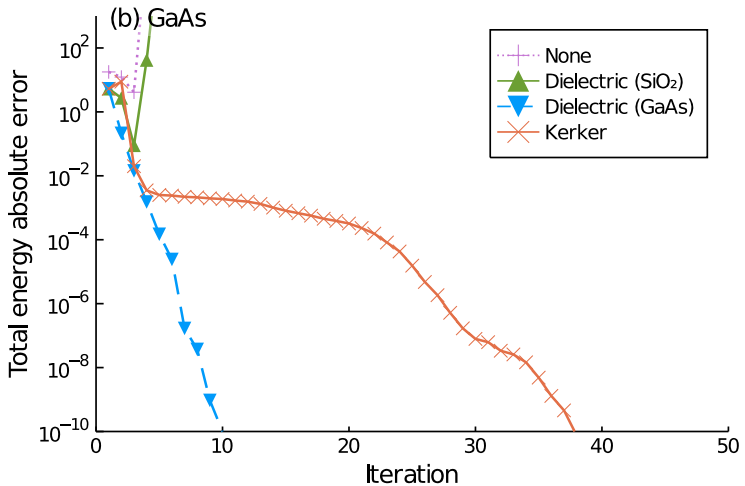
Comparison of model dielectric functions

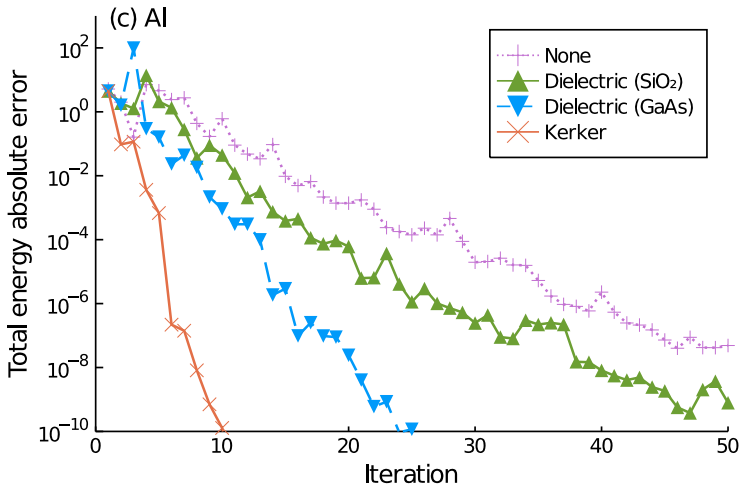


- Differing behaviour for small q
- Different preconditioning for each required

Convergence results for bulk materials[1]







- silica (SiO_2) insulator
- gallium arsenide (GaAs) semiconductor
- aluminium (Al) metal

- 40 randomised repeats
- Optimal damping
- Anderson acceleration

[1] M. F. Herbst, A. Levitt. arXiv 2009.01665 (2020)

Problems with the discussed approaches

- Preconditioner / mixing scheme manually chosen
- What is in screening study material properties change?
- How to deal with unknown material?
- How to deal with inhomogeneous materials?

Contents

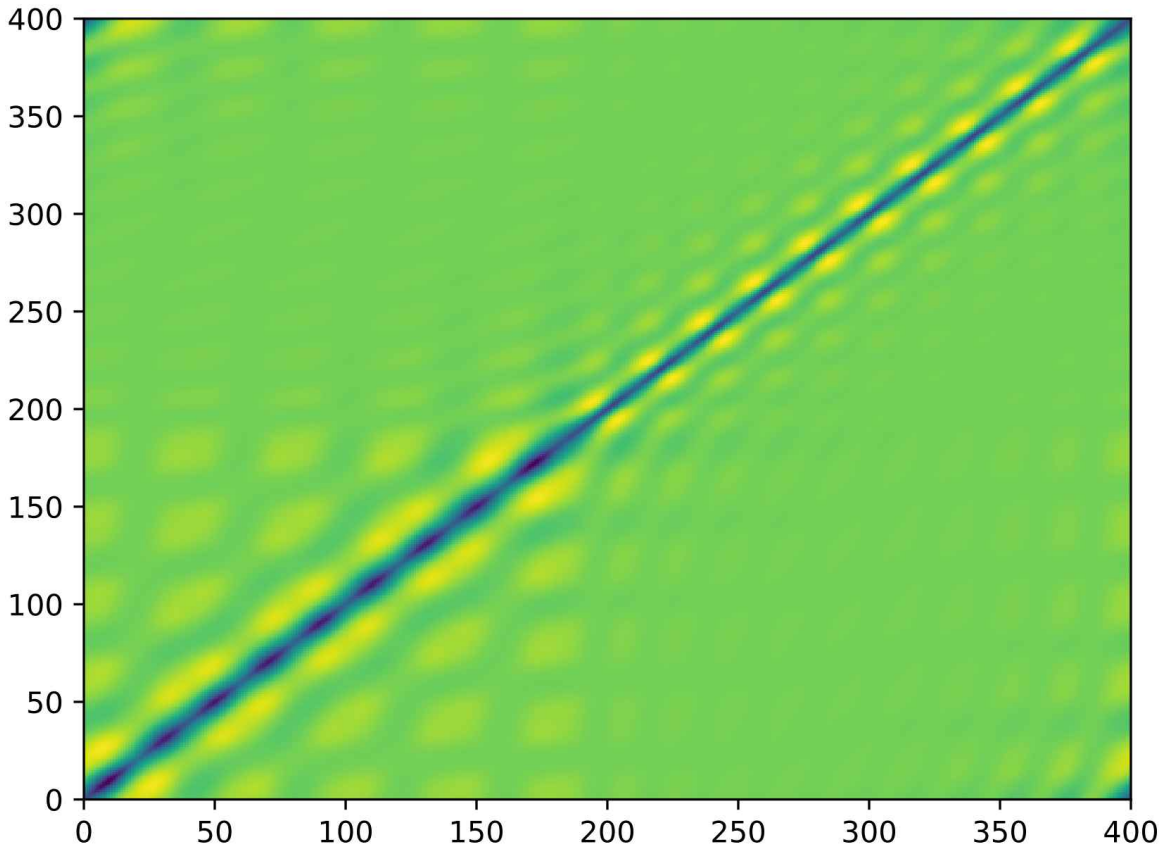
Approximating χ_0

- $\epsilon^\dagger = 1 - \chi_0(v_C + f_{\text{xc},\rho})$
- So far:
  - Closed-form approximation for $\epsilon(\underline{\boldsymbol{q}})$
  - Neglect of local field effects

  $\Rightarrow$ Closed form $P^{-1}(\underline{\boldsymbol{q}}) \simeq \left(\epsilon(\underline{\boldsymbol{q}})\right)^{-1}$ in q
- Now: Approximate χ_0 directly
- Try a *non-local* approximation $\widetilde{\chi_0}(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') \simeq \chi_0(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}')$
- Obtain iteratively

$$P^{-1}\delta\rho = \left(1 - \widetilde{\chi_0} v_C\right)\right)^{-1} \delta\rho$$

Plot of (exact) χ_0



- 1D system (Chain of 10 Sodium atoms and 10 helium atoms)

Local density of states (LDOS)

- Kohn Sham eigenpairs (ε_n, ψ_n), Fermi-Dirac distribution f, temperature T, Fermi level ε_F
- Occupations and occupation derivative:

$$f_n = f\left(\frac{\varepsilon_n - \varepsilon_F}{T}\right) \qquad f'_n = \frac{1}{T} f'\left(\frac{\varepsilon_n - \varepsilon_F}{T}\right)$$

- Local density of states

$$D_{\text{loc}}(\underline{\boldsymbol{r}}) = -\sum_n f'_n |\psi_n(\underline{\boldsymbol{r}})|^2$$

- Satisfies $\int_\Omega D_{\text{loc}}(\underline{\boldsymbol{r}})\,\mathrm{d}\underline{\boldsymbol{r}} = D$

LDOS approximation for χ_0[1]

- Adler-Wiser formula

$$\chi_0(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') = \sum_{n,m} \frac{f_n - f_m}{\varepsilon_n - \varepsilon_m} \psi_n(\underline{\boldsymbol{r}}) \psi_m^*(\underline{\boldsymbol{r}}) \psi_m(\underline{\boldsymbol{r}}') \psi_n^*(\underline{\boldsymbol{r}}') + \frac{D_{\text{loc}}(\underline{\boldsymbol{r}}) D_{\text{loc}}(\underline{\boldsymbol{r}}')}{D}$$

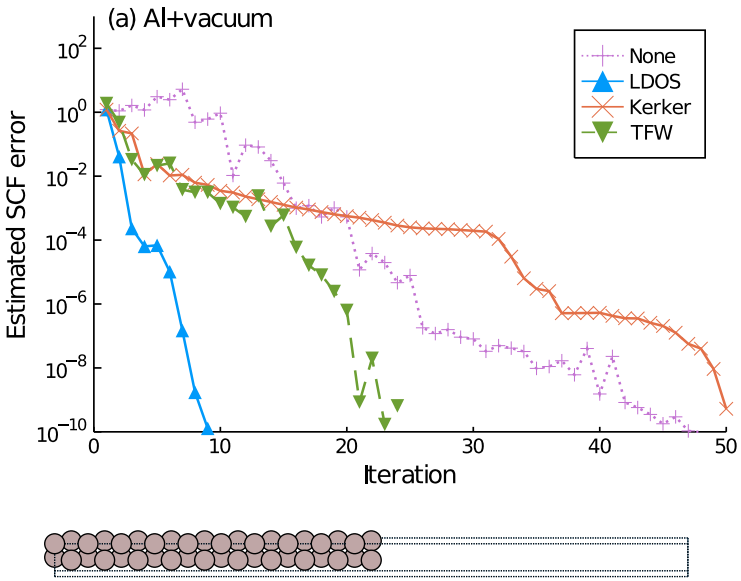
- Main interest: Large-scale variations

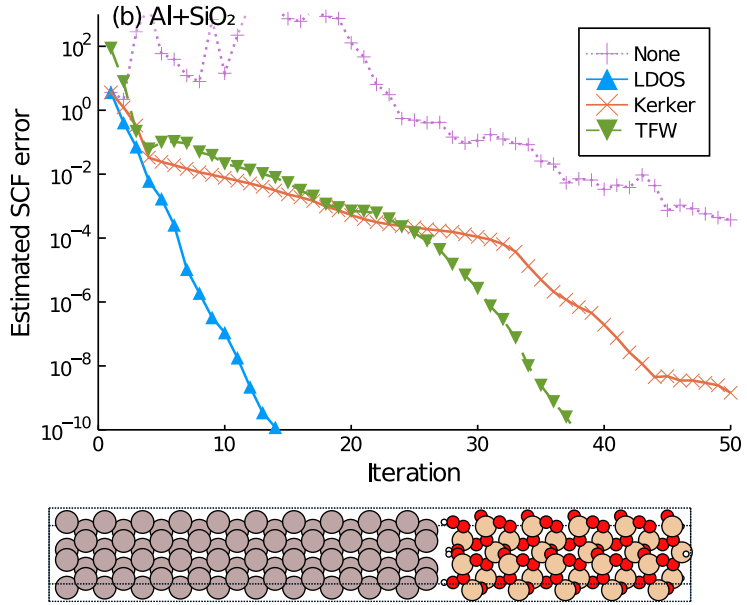
$\Rightarrow$ Argue $\underline{\boldsymbol{r}}' \mapsto \chi_0^{(1)}(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}')$ more localised around $\underline{\boldsymbol{r}}$ than $V(\underline{\boldsymbol{r}})$:

$$\begin{aligned}
\int \chi_0^{(1)}(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') V(\underline{\boldsymbol{r}}') \, \mathrm{d}\underline{\boldsymbol{r}}' &\simeq V(\underline{\boldsymbol{r}}) \int \chi_0^{(1)}(\underline{\boldsymbol{r}}, \underline{\boldsymbol{r}}') \, \mathrm{d}\underline{\boldsymbol{r}}' \\
&= V(\underline{\boldsymbol{r}}) \sum_{n,m} \frac{f_n - f_m}{\varepsilon_n - \varepsilon_m} \psi_n(\underline{\boldsymbol{r}}) \psi_m^*(\underline{\boldsymbol{r}}) \delta_{mn} \\
&= V(\underline{\boldsymbol{r}}) D_{\text{loc}}(\underline{\boldsymbol{r}})
\end{aligned}$$

[1] M. F. Herbst, A. Levitt. arXiv 2009.01665 (2020)

LDOS preconditioning (examples)



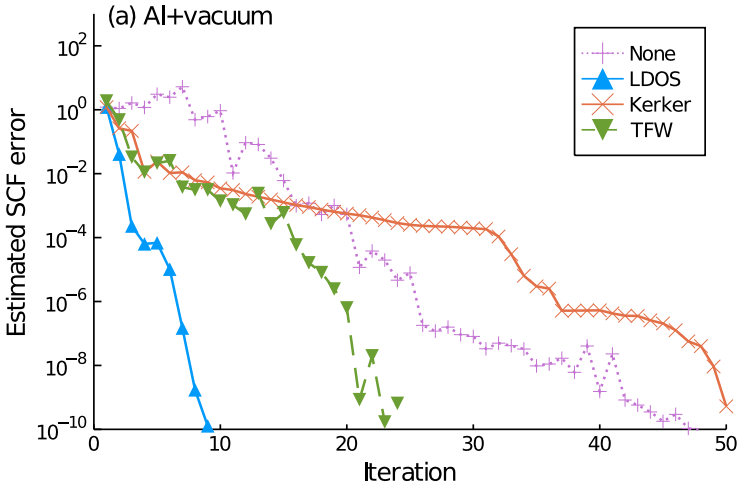


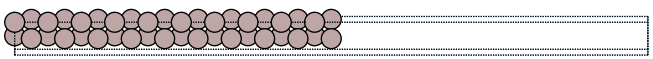
- 20 repeats of aluminium + 20 repeats vacuum / silica
- TFW: local Thomas-Fermi-von Weizsäcker mixing[1]
- LDOS automatically interpolates between Kerker mixing (in the metallic region) and no mixing (insulating region)

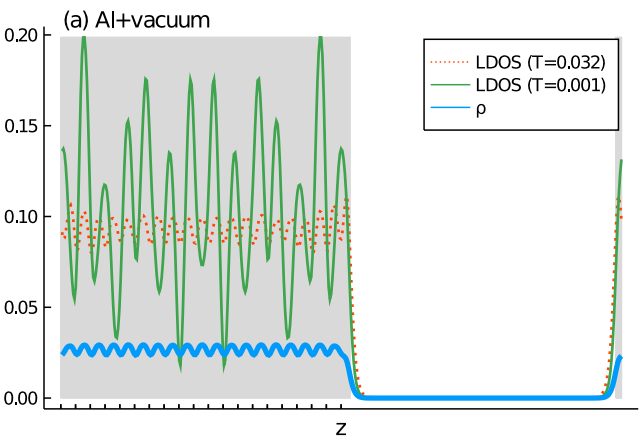
$\Rightarrow$ Parameter-free and black-box

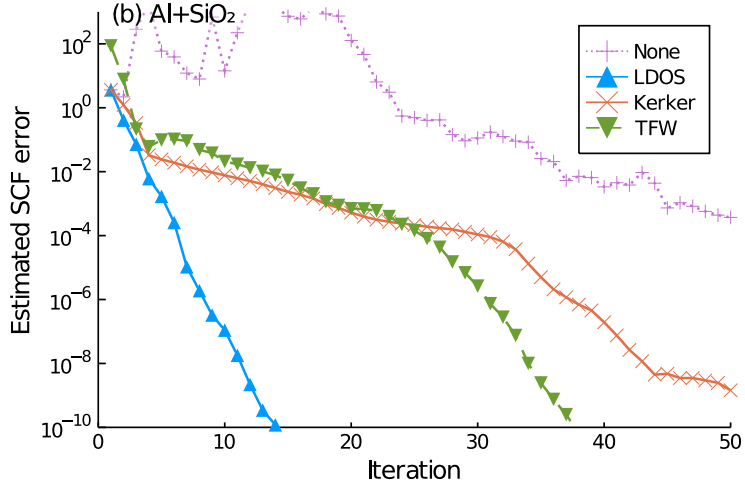
[1] D. Raczkowski, A. Canning, L. W. Wang, Phys. Rev. B. **64**, 121101 (2001).

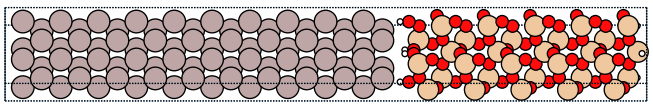
LDOS preconditioning (examples)

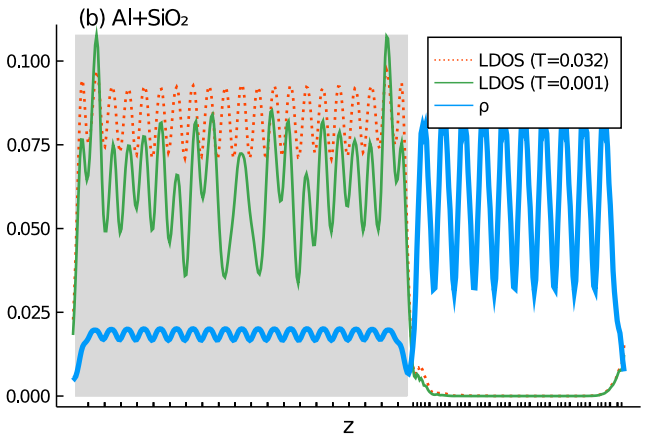












LDOS preconditioning

- Advantages
  - Parameter-free, adaptive mixing for inhomogeneous systems
  - For metals, insulators and vacuum
  - Great for high-throughput studies on surfaces
- Disadvantages
  - Cannot treat semiconductors properly yet
  - LDOS quality depends on BZ / temperature (ok in practice)
- Ok-ish solution for semiconductors:
  - Just add models: $\widetilde{\chi_0} = \chi_0^{\text{LDOS}} + \chi_0^{\text{dielectric}}$
  - Introduces ε_r as a parameter (via Dielectric model)

LDOS preconditioning results

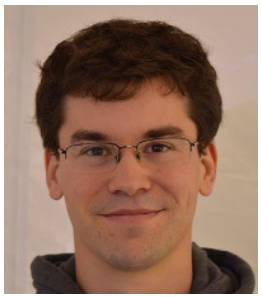
		None		Dielectric		Kerker		LDOS		LDOS+ Dielectric	
	$\mathcal{N}$	it	κ	it	κ	it	κ	it	κ	it	κ
SiO_2+vacuum	10	11	3.3	26	19.7	50	95.7	11	3.3	26	19.7
	20	12	3.4	30	24.4	n.c.	351.5	12	3.4	30	21.7
GaAs+vacuum	10	17	13.4	18	6.2	23	67.0	17	12.4	18	10.4
	20	20	15.5	22	12.9	n.c.	312.2	20	15.5	22	12.9
Al+vacuum	10	19	51.5	24	44.3	22	64.4	9	3.7	16	10.3
	20	47	170.8	49	168.5	n.c.	323.9	9	3.5	20	10.5
GaAs+SiO_2[a]	10	45	13.7	19	8.9	34	52.4	45	13.4	19	8.8
	20	n.c.	18.2	20	10.2	n.c.	170.1	n.c.	18.2	20	10.2
Al+SiO_2	10	43	93.1	29	33.6	30	50.9	17	6.1	20	9.2
	20	n.c.	316.6	n.c.	118.4	n.c.	159.4	14	5.4	20	10.1
Al+GaAs	10	n.c.	144.0	24	22.4	16	9.0	15	7.2	11	3.5
	20	n.c.	485.0	40	59.0	26	28.8	26	21.4	13	5.0
Al+GaAs+SiO_2	10	n.c.	149.5	34	50.4	36	62.9	26	21.5	19	9.0

- Coloured: Condition number κ less than doubled on doubling system size

Summary and outlook

- LDOS preconditioner:
  - Adaptive preconditioning for inhomogeneous systems
  - Parameter-free $\Rightarrow$ Highly suitable for high-throughput
- **DFTK** usage:
  - First develop LDOS scheme on test systems (1D, toy problems)
  - Test scheme on > 800 electrons (in the same code!)
- Next steps for a full black-box SCF preconditioner:
  - Spin / XC term
  - Black-box model for semiconductors
  - Localised states

Acknowledgements



Antoine Levitt

Eric Cancès
Xavier Gonze
Phil Hasnip
Lin Lin
Chao Yang

Other DFTK contributors:
`@gkemlin`, `@ssirajdine`, `@louisponet`

Questions?

DFTK https://dftk.org

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

mfherbst

https://michael-herbst.com/blog

michael.herbst@inria.fr