A plane wave and projector augmented wave implementation of DFT+DMFT

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Outline of the presentation

• Choice of the basis and local orbitals.
• The PAW framework
• Description of the actual calculation
• Some tests/examples.
• Conclusion.
Localization of $3d$, $4f$ and $5f$ electrons

$3d$ and $4f$ are orthogonal to other orbitals only through the **angular** part.

![Graphs showing the angular part of $3d$, $4f$, and $5f$ orbitals for $V$, $Nb$, $Ta$, $Ce$, and $Th$.](image-url)
DFT+U and the Dynamical Mean Field Theory (DMFT)

- DFT+U ⇒ To describe interactions in solids with static mean field theory
  Main idea: An electron is described, in the effective field of all the other electrons.
  ⇒ Self-consistent Hartree Fock problem.

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  Main idea: An electron is described, in the effective field of all the other electrons.
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• **DMFT** ⇒ To describe correlation in solids beyond static mean field theory.
  
  Main idea: An atom is isolated (in red), *local correlations are described exactly*, in the effective field of other atoms.
  ⇒ Self-consistent Impurity problem: Anderson model

[see review A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg Rev. Mod. Phys. 68, 13 (1996)]
The DFT+DMFT scheme

\[ \Sigma = G_{\text{imp}}^{-1} - G_{\text{latt}}^{-1} \]

DMFT for fixed \( n(\mathbf{r}) \)

Self-consistency condition

Impurity problem

\[ G_0^{-1} = \Sigma + G_{\text{imp}}^{-1} \]

\( \langle \chi_{\mathbf{k}m}^R | \psi_{\mathbf{k}\nu} \rangle \)

DFT+DMFT Loop over density

DFT Hamiltonian is built and diagonalized: new KS eigenvalues and eigenfunctions are extracted. A special care is taken to obtain the new KS bands with a good accuracy for each new electronic density. Wannier functions are built for the next DMFT loop. KS eigenvalues are also used to compute the Green function using Eq. 2.5.

Peculiarities of the PAW formalism for the computation of the electronic density are described in Appendix A.

2.3. Calculation of Internal Energy in DFT+DMFT

The DFT+DMFT formalism can be derived from a functional of both the local density and the local Green’s function. The internal energy can be derived and one obtains the general...
DMFT in the Kohn Sham basis

- Let’s choose the Bloch basis as the basis for one electron quantities.
- One electron Hamiltonian:

\[
H_{KS} = \sum_{\nu,k} |\Psi_{k\nu}\rangle \varepsilon_{k\nu} \langle \Psi_{k\nu}|
\]

- A basis set for one electron quantities: \(|B_{k\alpha}\rangle\).
- The matrix element on the Hamiltonian can thus be computed as:

\[
H_{KS,\alpha\alpha'}(k) = \langle B_{k\alpha} | H_{KS} | B_{k\alpha'} \rangle = \sum_{\nu} \langle B_{k\alpha} | \Psi_{k\nu} \rangle \varepsilon_{k\nu} \langle \Psi_{k\nu} | B_{k\alpha'} \rangle.
\]

- A definition for d/f local orbitals, let’s call them \(|\chi_{k}^{R}\rangle\). (m is an angular momentum index)
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- The matrix element on the Hamiltonian can thus be computed as:

\[ H_{KS,\nu\nu'}(k) = \langle \Psi_{k\nu}|H|\Psi_{k\nu}\rangle = \varepsilon_{k\nu} \delta_{\nu,\nu'} \]

- A definition for d/f local orbitals, let’s call them \( |\chi_{km}\rangle \). (m is an angular momentum index)
DMFT in the Kohn Sham basis (2)

- All one electron quantities can be expressed in the basis set $|\Psi_{k\nu}\rangle$.
- Let's define projectors:

  Projections: $P_{mn\nu}^{R}(k) \equiv \langle \chi_{km}^{R} | \Psi_{k\nu} \rangle$, $P_{mn\nu}^{R}(k)^{*} \equiv \langle \Psi_{k\nu} | \chi_{km}^{R} \rangle$.

- $P$ matrix is in general nonsquare.
- The Self energy is a local quantity in DMFT, thus:

$$
\Sigma = \sum_{mm'} \sum_{T} |\chi_{Tm}^{R}\rangle \sum_{mm'}^{\text{Imp}} \langle \chi_{Tm'}^{R} | \Sigma^{R}_{mm'}_{T} | \chi_{Tm'}^{R}\rangle
$$
Thus

\[ \Delta \Sigma_{\alpha \alpha'}(\mathbf{k}, i\omega_n) = \langle \Psi_{k\nu} | \Sigma(\mathbf{k}) | \Psi_{k\nu} \rangle = \sum_{mm'} P^R_{m\nu}(\mathbf{k})^{*} \Sigma^R_{mm'} P^R_{m'\nu}(\mathbf{k}). \]

The lattice Green’s function \( G_{\alpha,\alpha'}(\mathbf{k}, i\omega_n) \) can be expressed in the complete Bloch Basis \( \Psi_{k\nu} \), and projected to compute the local (impurity) Green’s function.

\[ G^\text{imp}_{mm'}(i\omega_n) = \sum_{\mathbf{k}} \sum_{\nu\nu'} P^R_{m\nu}(\mathbf{k}) P^R_{m'\nu'}(\mathbf{k})^{*} \times \]

\[ \times \left\{ [(i\omega_n + \mu - \varepsilon_{k\nu}) \mathbf{I} - \Delta \Sigma(\mathbf{k}, i\omega_n)]^{-1} \right\}_{\nu\nu'}. \]
Choice of the basis set and local orbitals

- The local atomic-like orbitals $\chi_{km}^R$ will in general have a decomposition involving all Bloch bands (closure relation)

$$|\chi_{km}^R\rangle = \sum_\nu \langle \Psi_{k\nu} | \chi_{km}^R \rangle |\Psi_{k\nu}\rangle = \left[ \sum_\nu |\Psi_{k\nu}\rangle \langle \Psi_{k\nu}| \right] |\chi_{km}^R\rangle$$

- If the basis set is restricted to a limited number of KS states in the window energy $\mathcal{W}$:

$$|\tilde{\chi}_{km}^R\rangle \equiv \sum_{\nu \in \mathcal{W}} \langle \Psi_{k\nu} | \chi_{km}^R \rangle |\Psi_{k\nu}\rangle = P_{m\nu}^R(k)^* |\Psi_{k\nu}\rangle$$

- $|\tilde{\chi}_{km}^R\rangle$ need to be orthonormalized to give true Wannier functions $|w_{km}^R\rangle$.

$$O_{m,m'}^{R,R'}(k) = \langle \tilde{\chi}_{km}^R | \tilde{\chi}_{km'}^{R'} \rangle = \sum_\nu P_{m\nu}^R(k) P_{m'\nu}^{R'}(k)^*$$
Choice of the basis set and local orbitals

• $|w^{R}_{km}\rangle$ is thus obtained though:

$$
|w^{R}_{km}\rangle = \sum_{R',m'} \left\{ [O(k)]^{-1/2} \right\}_{m,m'}^{R,R'} |\tilde{\chi}^{R'}_{km'}\rangle
$$

⇒ Projections accordingly renormalized.

⇒ The localized basis $|w^{R}_{km}\rangle$ depends on the energy windows $\mathcal{W}$.

• $|w^{R}_{km}\rangle$ less localized than initial $\chi^{R}_{km}$ since the basis has a smaller energy range.

• If $|w^{R}_{km}\rangle$ is chosen (through the window of energy), the whole framework is exact: There is no finite basis effect.
  • $\langle w^{R}_{km} | \Psi_{kn} \rangle = 0$ if $\nu \notin \mathcal{W}$.
  ⇒ No convergence as a function of the size of the basis.
A reminder: hybridization in a diatomic molecule (oversimplified)
An oversimplified derivation for the diatomic molecule VO

\[ \Psi_1 = \alpha \phi_O + \beta \phi_V \quad \beta \ll \alpha \]

\[ \Psi_2 = \beta \phi_O - \alpha \phi_V \quad \beta \ll \alpha \]

Two windows of energy are possible to compute

\[ |\chi\rangle = \sum_{\mathcal{W}} \langle \Psi_i | \phi_V \rangle |\Psi_i\rangle \]

- If only \( \varepsilon_2 \) is included, the correlated wavefunction is
  \[ |\chi\rangle = |\Psi_2\rangle = \beta |\phi_O\rangle - \alpha |\phi_V\rangle \]
  and contains an Oxygen contribution

- If only \( \varepsilon_1 \) and \( \varepsilon_2 \) is included, the correlated wavefunction is
  \[ |\chi\rangle = \sum_i \langle \Psi_i | \phi_V \rangle |\Psi_i\rangle = |\phi_V\rangle \]
  and is much more localized.
• LMTO ASA \( |\chi_{1,l',m,m'}(k)\rangle \) (Andersen 1975).
  • LMTO’s are an optimized atomic orbital Bloch basis.
  • The local correlated subspace is thus a subset of the LMTO basis \( B_{k\alpha} \).
    • \( |\chi_{1=2,l'=2,m,m'}(k)\rangle \) for d orbitals.
  • First implementation in DMFT: Lichtenstein and Katsnelson 1998, Anisimov et al 1997
  • Fast, efficient, but method dependent.
The Projector-Augmented Wave (PAW) method: introduction

• Norm conserving pseudopotentials
  • Electronic density is erroneous.
  • Transferability might be thus questionnable
  • High number wave needed.

• A solution
  • A better description of all electron wavefunctions nodes

\[ |\Psi\rangle = |\widetilde{\Psi}\rangle + \sum_i c_i (|\phi_i\rangle - |\widetilde{\phi}_i\rangle) \text{ with } c_i = \langle \widetilde{p}_i | \Psi \rangle \]

• Relax the constraints over norm of pseudopotentials ("ultrasoft")

• **PAW** Blöchl PRB 1994
  • No pseudopotential approximation
  • Use an augmentation around atoms to have a correct shape for wavefunctions near the nucleus.
  • Keep frozen core approximation (can be controlled)
The Projector Augmented Wave Method

Wavefunction:
\[
|\psi_n\rangle = |\tilde{\psi}_n\rangle + \sum_i (|\phi_i\rangle - |\tilde{\phi}_i\rangle) \langle \tilde{p}_i | \tilde{\psi}_n \rangle = \tau |\tilde{\psi}_n\rangle
\] (1)

PAW

- Efficiency with respect to usual plane wave calculations.
- Accuracy: nodal structure of valence wfc are reproduced.
- Flexibility: energy of several structures can be compared with the same basis.
- Frozen core approximation can be controlled.

From M. Torrent and F. Jollet Torrent, Jollet, Bottin, Zerah, Gonze CMS 2008
How to construct atomic data for PAW

- Solve All Electrons Atomic problem $\Rightarrow \varphi_i(r)$
- Pseudize local pseudopotential $V_{\text{loc}}$.
- Pseudize partial wave $\tilde{\varphi}_i(r)$.
- Build projectors $p_i(r)$.
Solve All Electrons Atomic problem $\Rightarrow \varphi_i(r)$

- Solve atomic Schrödinger equation to compute electronic density. Get $V_{ae}(r)$
- Choose an energy set $\epsilon_i$ and solve the Schrödinger equation. Get $\varphi_i(r)$ for each $\epsilon_i$
Compute pseudo functions

\[ l=1 \text{ and } r_{\text{paw}} = 1.5 \text{ au} \]
Check transferability.
Check transferability.

$1 = 1$ and $r_{\text{paw}} = 1.5$ au

- AE
- PAW with one projector

First ref energy (AE eigenvalue)
Check transferability.

\[ l=1 \text{ and } r_{\text{paw}} = 1.5 \text{ au} \]

- **AE**
- **PAW with two projectors**

1\textsuperscript{st} ref energy
(AE eigenvalue)

2\textsuperscript{nd} ref energy
The DFT+DMFT scheme (1): a practical calculation

- First step: Make a converged DFT calculation.
- Wavefunctions $\Psi_{k\nu}$ and Eigenvalues $e_{k\nu}$ are available.
- Unoccupied wavefunctions must be accurately computed in order to be used in the DMFT calculation.
Diagonalise the Hamiltonian

- Solve DFT self-consistently
- Diagonalize the Hamiltonian with empty states
- Get Eigenvalues and eigenvectors.
Calculation of projections within PAW

Projections: \( P_{m\nu}^{R}(k) \equiv \langle \chi_{km}^{R} | \Psi_{k\nu} \rangle \), \( P_{m\nu}^{R}(k)^\ast \equiv \langle \Psi_{k\nu} | \chi_{km}^{R} \rangle \).

\[
\Psi = |\tilde{\Psi}\rangle + \sum_{i} \langle \tilde{p}_{i} | \tilde{\Psi} \rangle |\varphi_{i}\rangle - \sum_{i} \langle \tilde{p}_{i} | \tilde{\Psi} \rangle |\tilde{\varphi}_{i}\rangle
\]

\[
P_{m\nu}(k) = \langle \chi_{m} | \tilde{\Psi}_{k\nu} \rangle + \sum_{i} \langle \tilde{p}_{i} | \tilde{\Psi}_{k\nu} \rangle (\langle \chi_{m} | \varphi_{i} \rangle - \langle \chi_{m} | \tilde{\varphi}_{i} \rangle)
\]

However, atomic d or f wavefunctions are mainly localized inside spheres.

\[
P_{m\nu}(k) = \sum_{n_{i}} \langle \tilde{p}_{n_{i}} | \tilde{\Psi}_{k\nu} \rangle \langle \chi_{m} | \varphi_{n_{i}} \rangle
\]

- Check completeness during contraction of atomic data.
- Check that PAW radius is not too small.
- Logarithmic derivatives
- Basis completeness relative to energy

Data constructed with Atompaw (Holzwarth, Torrent and Jollet 2007.)
The DFT+DMFT scheme (2)

- From $\varepsilon_{k\nu}$, compute DFT (LDA) Green’s function:

$$
G^{\text{Bloch}}_{\nu,\nu'}(i\omega_n, \mathbf{k}) = \left[ (i\omega_n + \mu - \varepsilon_{k\nu}) I \right]^{-1}_{\nu\nu'}
$$

$$
G^{\text{imp}}_{mm'}(i\omega_n) = \sum_k \sum_{\nu\nu'} P^R_{mv}(k) P^R_{m'v'}(k) G^{\text{Bloch}}_{\nu,\nu'}(i\omega_n, \mathbf{k})
$$
The DFT+DMFT scheme (3)

- 1\textsuperscript{st} iteration: DFT LDA Green’s function used as Weiss field
- From Weiss Field $G_{0\,m,m'}$, Anderson Impurity Model is solved to get impurity Green’s function $G_{m,m'}$. 

![Diagram of the DFT+DMFT scheme](image-url)
• Self-energy is computed from Dyson Equation: $\Sigma = G_0^{-1} - G^{-1}$
• The Lattice Green’s function is computed with the self-energy.
• Fermi level adjusted to the number of electrons
• The Impurity Green’s function is obtained by projection.
• Dyson equation is again used to recover new Weiss Field.
The lattice Green’s function \( G_{\nu,\nu'}(k, i\omega_n) \) can be expressed in the complete Bloch Basis \( \Psi_{k\nu} \) and projected to compute the local (impurity) Green’s function.

\[
G_{\nu,\nu'}(k, i\omega_n) = \left\{ \left[ (i\omega_n + \mu - \varepsilon_{k\nu}) I - \Delta\Sigma(k, i\omega_n) \right]^{-1} \right\}_{\nu\nu'},
\]

\[
G_{mm'}^{\text{imp}}(i\omega_n) = \sum_k \sum_{\nu\nu'} P_{m\nu}(k) P_{m'\nu'}(k)^* \times \left\{ \left[ (i\omega_n + \mu - \varepsilon_{k\nu}) I - \Delta\Sigma(k, i\omega_n) \right]^{-1} \right\}_{\nu\nu'},
\]
• The DMFT Loop is done until convergency (of $G$, $\Sigma$).
• Then occupations of electrons inside orbitals have changed, and thus, the local density must be updated.
The self-consistency over electronic density

The number of electron are recovered by a Fourier transform:

\[ f_{\nu,\nu'}(k) = \sum_{i\omega_n} G_{\nu,\nu'}(k, i\omega_n) e^{i\omega_n 0^+} \]

The Green function can be written in real space basis as:

\[ G(r, r') = \sum_{i\omega_n} \langle r | \hat{G}(i\omega_n) | r \rangle e^{i\omega_n 0^+} \]

\[ G(r, r') = \sum_{i\omega_n} \langle r | \left[ \sum_{k, \nu, \nu'} |\Psi_{k\nu}(r)\rangle G_{\nu,\nu'}(k, i\omega_n) \langle \Psi_{k'\nu'} | \right] | r \rangle e^{i\omega_n 0^+} \]

The local density can be written as

\[ n(r) = G(r, r) \]

\[ n(r) = \sum_{k, \nu, \nu'} \Psi_{k\nu}^*(r) f_{\nu,\nu'}(k) \Psi_{k'\nu'}(r') \]
Then, using the fundamental relation (11) of Bloechl PRB 1994 for the operator $|r\rangle\langle r|$, we have three part in the expression of the total density:

$$n(r) = \tilde{n}'(r) + n^{1'}(r) - \tilde{n}^{1'}(r)$$  \hspace{1cm} (22)

and

$$\rho'_{ij} = \sum_{\nu,\nu',k} f_{\nu,\nu',k} \langle \tilde{\Psi}_\nu,k | \tilde{p}_j \rangle \langle \tilde{p}_i | \tilde{\Psi}_{\nu',k} \rangle.$$  \hspace{1cm} (22)
The DFT+DMFT scheme (6)

From total density, the Hamiltonian $H[n(\mathbf{r})]$ is diagonalized and new KS wavefunctions, projectors, and eigenvalues are computed for the next DMFT loop.

At convergence of the electronic density $n(\mathbf{r})$, the calculation is stopped.
Analysis of DMFT calculations

• Spectral Function
  • Impurity spectral function: From Green’s function projected over local correlated orbitals
  • Bloch states spectral function (k-resolved or sum): Green’s function of Kohn Sham states.

• Self-energy
• Total energy
Formalism: Spectral function of SrVO$_3$

Full orbitals.
⇒ The position of O$_p$ bands vs V$_d$

Redefinition of local orbitals
⇒ More localized

Anisimov, Kondakov, Kozhevnikov, Nekrasov et al PRB (2005)
Functionals

A functional is built from the partition function (Kotliar and Savrasov (2004)):

\[
\begin{align*}
\Omega[\rho(r), G_{ab}; v_{KS}(r), \Delta \Sigma_{ab}]_{LDA+DMFT} &= -\text{tr} \ln[i\omega_n + \mu + \frac{1}{2}\nabla^2 - v_{KS}(r) - \chi^* \cdot \Delta \Sigma \cdot \chi] \\
&- \int dr (v_{KS} - v_c)\rho(r) - \text{tr}[G \cdot \Delta \Sigma] + \frac{1}{2} \int dr dr' \rho(r)U(r-r')\rho(r') + E_{xc}[\rho(r)] \\
&+ \sum_R \left( \Phi_{imp}[G_{ab}^{RR}] - \Phi_{DC}[G_{ab}^{RR}] \right)
\end{align*}
\]

minimisation $\Rightarrow$ equations of LDA+DMFT.

$\Rightarrow$ Total energy.

\[
E_{LDA+DMFT} = E_{DFT} - \sum_{\lambda} \varepsilon_{\lambda}^{LDA} + \langle H_{KS} \rangle + \langle H_{U} \rangle - E_{DC}
\]

The one electron part of DFT is replaced by one electron part of DMFT, and DMFT interaction terms are added.

Amadon, Biermann, Georges and Aryasetiawan (2006)
Total energy: first, reminder of total energy in DFT

\[ E_{\text{DFT}} = T_0^{\text{DFT}} + E_{\text{xc+Ha}}[n(r)] + \int d\mathbf{r} \nu_{\text{ext}}(\mathbf{r}) n(\mathbf{r}) \]

Alternatively

\[ E_{\text{DFT}} = \sum_{\nu,k} f_{\nu,k}^{\text{DFT}} \epsilon_{\nu,k}^{\text{DFT}} + E_{\text{DFT DC}}[n(\mathbf{r})] \]

with \( E_{\text{DFT DC}}[n(\mathbf{r})] = -E_{\text{Ha}}[n(\mathbf{r})] + E_{\text{xc}}[n(\mathbf{r})] - \int \nu_{\text{xc}} n(\mathbf{r}) d\mathbf{r} \)
Thus, we have the following expression for the total energy in DFT+DMFT:

\[
E_{\text{DFT+DMFT}}^2 = T_{0 \text{DFT+DMFT}} + E_{\text{xc+Ha}}[n(r)] + \int dr v_{\text{ext}}(r)n(r) + \langle H_U \rangle - E_{\text{DC}}
\]

with \( T_{0 \text{DFT+DMFT}} = - \sum_{\nu,\nu',k} f_{\nu,\nu',k} \int \Psi_{k\nu}^* \nabla^2 \Psi_{k\nu'} \)

Alternatively, one can write:

\[
E_{\text{DFT+DMFT}}^1 = \sum_{\nu,k} f_{\nu,k}^{\text{DFT+DMFT}} \epsilon_{\nu,k}^{\text{KS-DFT}} + E_{\text{DFT DC}}[n(r)] + \langle H_U \rangle - E_{\text{DC}}
\]

with \( E_{\text{DFT DC}}[n(r)] = - E_{\text{Ha}}[n(r)] + E_{\text{xc}}[n(r)] - \int \nu_{\text{xc}} n(r) dr \)

Should give the same results at convergence.
Lattice parameter $a$ and Bulk modulus $B_0$ of $\gamma$ Cerium according to experimental data and calculations

<table>
<thead>
<tr>
<th></th>
<th>$a$ (a.u.)</th>
<th>$B_0$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp[Jeong 2004]</td>
<td>9.76</td>
<td>19/21</td>
</tr>
<tr>
<td>PAW/LDA+U</td>
<td>9.58</td>
<td>32</td>
</tr>
<tr>
<td>PAW/LDA+DMFT NSCF (H-I)</td>
<td>9.41</td>
<td>38</td>
</tr>
<tr>
<td>PAW/LDA+DMFT SCF (H-I)</td>
<td>9.58</td>
<td>36</td>
</tr>
<tr>
<td>ASA/LDA+DMFT NSCF (H-I)</td>
<td>9.28</td>
<td>50</td>
</tr>
<tr>
<td>ASA/LDA+DMFT SCF (H-I)</td>
<td>9.31</td>
<td>48</td>
</tr>
</tbody>
</table>
Results: Spectral function of Ce$_2$O$_3$

LMTO-ASA + DMFT

PAW + DMFT
B. Amadon JPCM 2012
Results: Spectral function of Ce$_2$O$_3$

Spectral function of Ce$_2$O$_3$, in LDA+DMFT (Hubbard I).
### Results: Structural parameters of Ce$_2$O$_3$

<table>
<thead>
<tr>
<th>Method/Model</th>
<th>$a$ (Å)</th>
<th>$B_0$ (Mbar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp (Barnighausen 1985)</td>
<td>3.89</td>
<td>1.11</td>
</tr>
<tr>
<td>PAW/LDA+U (AFM) (Da Silva 07)</td>
<td>3.87</td>
<td>1.3</td>
</tr>
<tr>
<td>PAW/LDA+U (AFM)</td>
<td>3.85</td>
<td>1.5</td>
</tr>
<tr>
<td>PAW/LDA+DMFT (H-I) NSCF</td>
<td>3.76</td>
<td>1.7</td>
</tr>
<tr>
<td>PAW/LDA+DMFT (H-I) SCF</td>
<td>3.83</td>
<td>1.6</td>
</tr>
<tr>
<td>ASA/LDA+DMFT (H-I) NSCF (Pourovskii 2007)</td>
<td>3.79</td>
<td>1.6</td>
</tr>
<tr>
<td>ASA/LDA+DMFT (H-I) SCF (Pourovskii 2007)</td>
<td>3.81</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Lattice parameter $a$ and Bulk modulus $B_0$ of Ce$_2$O$_3$. 
Results: Converged Electronic Density.

Difference between electronic densities computed in the LDA+U (left)/LDA+DMFT (right) and in LDA for Ce$_2$O$_3$.

Blue (resp. green-red) area corresponds to positive (resp negative) value of the difference.
In the Hubbard one implementation, the most expensive task is the calculation and integration of Green’s function.

\[ G_{\nu,\nu'}(k, i\omega_n) = \left\{ \left[ (i\omega_n + \mu - \varepsilon_{k\nu})I - \Delta \Sigma(k, i\omega_n) \right]^{-1} \right\}_{\nu\nu'}, \]

This part is thus parallelized over logarithmic frequencies.

Computed on a log frequency
CTQMC Strong coupling (Werner et al 2006) implemented by Jordan Bieder.
Conclusion

- DFT+DMFT physical choices
  - Interactions U, J
  - Definition of local correlated orbitals: Wannier functions
- Technical choices
  - Basis for the one electron Green function: KS in Abinit
- In Abinit
  - PAW+DMFT - Hubbard I
  - Spin-orbit
  - CT-Quantum Monte Carlo (not yet distributed)
- Details of the Abinit implementation can be found in