Parallel research of numerous eigenvalues in ABINIT

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Framework of the problem

- Calculation of the ground-state energy $E^{KS}(\rho)$, for a fixed geometry.

$$\begin{cases} \bar{H}\varphi_i = \varepsilon_i \varphi_i, \ \forall i = 1, \ldots, N, \\ \displaystyle\int_{\mathbb{R}^3} \varphi_i \varphi_j^* = \delta_{ij}. \end{cases}$$

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- Numerical resolution: discretization in a finite dimension basis $\{\chi_j\}_{j=1,\ldots,M}$ (Galerkin method)
$\Rightarrow$ generalized eigenvalue problem

$$\varphi_i = \sum_{j=1}^{M} c_{ji}\chi_j \Rightarrow \tilde{H}\mathbf{c_i} = \varepsilon_i S\mathbf{c_i}, \forall i = 1, \ldots, N$$

$\tilde{H}$: discretized KS Hamiltonian; S: overlap matrix

Numerical resolution

- Direct minimization of $E^{KS}(\rho)$, by nonlinear conjugate gradient (NLCG) algorithm

$$\min \left\{ \sum_{i=1}^{N} (\tilde{H}\psi_i, \psi_i);\ (\psi_i, \psi_j) = \delta_{ij} \right\}$$

$\{\psi_i\}$: wave vectors; $\{\varphi_i\}$: KS orbitals

At SCF convergence:
$Span(\psi_1, \ldots, \psi_N) = Span(\varphi_1, \ldots, \varphi_N)$

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- Complexity (orthogonalization of the ψ_i): $\mathcal{O}(MN^2)$ or $\mathcal{O}(N^3)$. (matrix/vectors products in $\mathcal{O}(N^2 \log N)$)

Specificities of the ABINIT code and difficulties:

- for each SCF loop, calculation of pseudo-eigenvectors (i.e. not converged)
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Goal: propose parallel methods to realize calculations on more complex molecular systems.

New algorithm (1)

- calculation of exact eigenvectors instead of pseudo-eigenvectors $\Rightarrow$ orthogonality of the ψ_i ($\tilde{H}$ symmetric)
  such that

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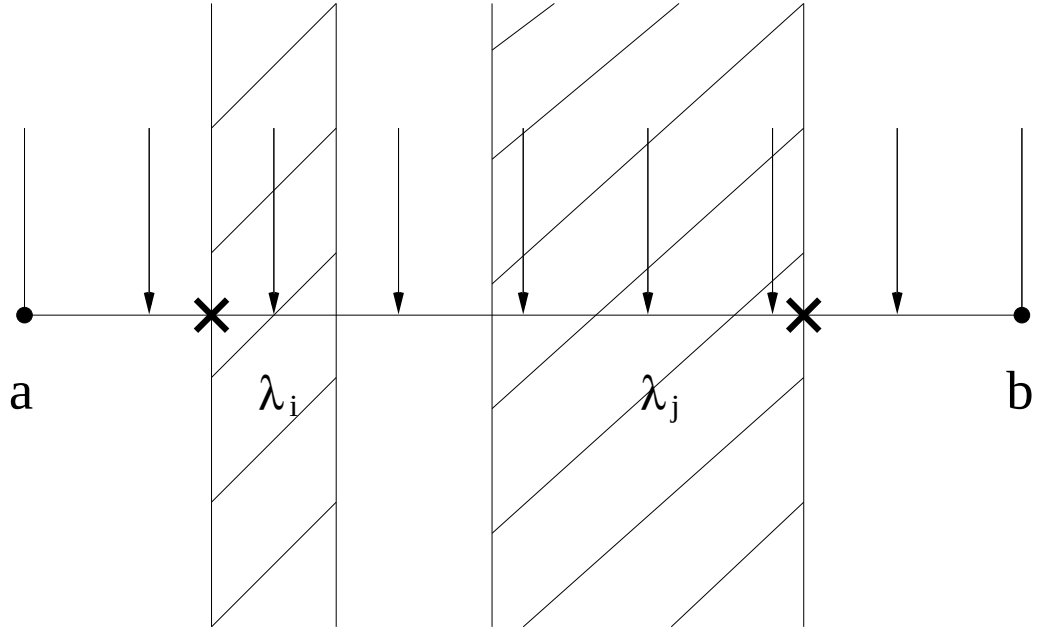
  Proposals for the choice of a and b:

  - given by the code user
  - Lanczos algorithm
  - estimate of the N^{th} eigenvalue of $\bar{H}$

Spectral partitionning: details

- Iterative algorithm with dynamic allocations of shifts λ_i until $[a, b]$ is completely explored.



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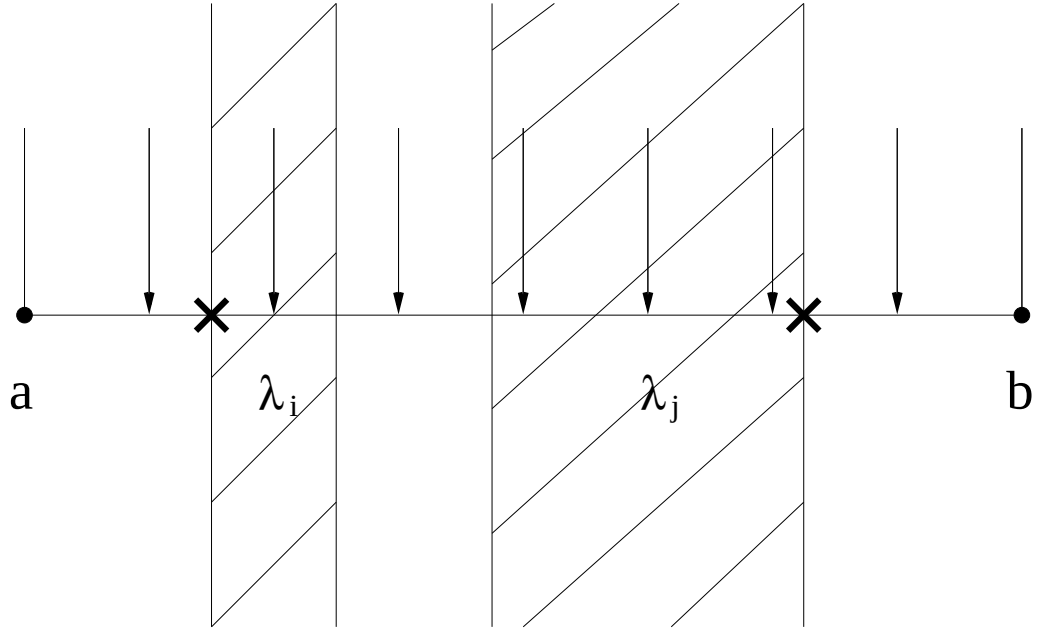

- $k > N$ eigenvalues in $[a, b] \Rightarrow \alpha k$ research of eigenvalues ($3 < \alpha < 4$).

- To take into account of multiple eigenvalues:

$$\min \left\{ \sum_{i=1}^{N_{\boldsymbol{n}}} \sum_{j=1}^{\boldsymbol{n}} \Big((\tilde{H} - \lambda_i I)^2 \psi_{ij}, \psi_{ij} \Big), (\psi_{ij}, \psi_{ik}) = \delta_{jk} \right\},$$

where $N_{\boldsymbol{n}} = \dfrac{N}{\boldsymbol{n}}$ is the number of blocks of $\boldsymbol{n}$ wave vectors ($\boldsymbol{n} \in \{1, 2, 3, 4\}$).

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- Theoretical complexity: $N_{\boldsymbol{n}} \times M\boldsymbol{n}^2 = \boldsymbol{n}MN \Rightarrow \mathcal{O}(N^2)$ sequentially.

Results and conclusions:

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- calculation of exact eigenvalues by NLCG can be very hard. The difficulties are:

$$\begin{cases} \cdot \text{ numerical: } \text{cond}(\psi_k) = \dfrac{\lambda_{\max}}{\min\limits_{j \neq k} |\lambda_j - \lambda_k|} \\ \cdot \text{ physical: spectrum of Hamiltonians has not a regular distribution} \end{cases}$$

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- E^{KS} and ρ are invariant under any unitary tranformation

$\Rightarrow$ proposal of a new algorithm (2) with calculations of clusters of eigenvalues.

New algorithm (2)

- Calculation of eigensubspaces with local reorthog. by

$$\begin{cases} \cdot \text{ NLCG on } (\tilde{H} - \lambda_i I)^2 \\ \cdot \text{ Lanczos on } (\tilde{H} - \lambda_i I)^{-1} \end{cases}$$

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- Hierarchy of algorithms:

Original ABINIT, full reorthog. $\mathcal{O}(N^3)$
$\Rightarrow$ SCF convergence

$\updownarrow$

algo. (2), with partial reorthog.
$\Rightarrow$ convergence of eigenspaces

$\updownarrow$

algo. (1), without reorthog. $\mathcal{O}(\frac{N^2}{N_{proc}})$
$\Rightarrow$ bad convergence of eigenvectors

- Numerical property of NLCG for eigensubspaces calculation:

Proposition 1. *Let A be a matrix of order M and $\{u_j, \lambda_j\}$ its eigenstates such that $|\lambda_1 - \mu| < \ldots < |\lambda_M - \mu|$. Then the convergence factor of the approximated eigenspace of dimension m is $\mathcal{O}\left(\left|\frac{\lambda_m - \mu}{\lambda_{m+1} - \mu}\right|\right)$ (subspace iteration algorithm).*

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- $\Rightarrow$ if $m_\mu =$ dimension of the closest cluster near μ then:

$$\begin{cases} \cdot\ m < m_\mu\text{: very slow convergence} \\ \cdot\ m = m_\mu\text{: optimal convergence} \\ \cdot\ m > m_\mu\text{: it depends of the } \exists \text{ of other clusters} \end{cases}$$

- Exemple: A diagonal, $\dim(A) = 20$, concentrated spectrum:

$$\text{sp}(A) = \{0.99, 1.02, 1.03, 1.04, 1.05, \ldots, 3.99, 4.02, 4.03, 4.04, 4.05\}$$

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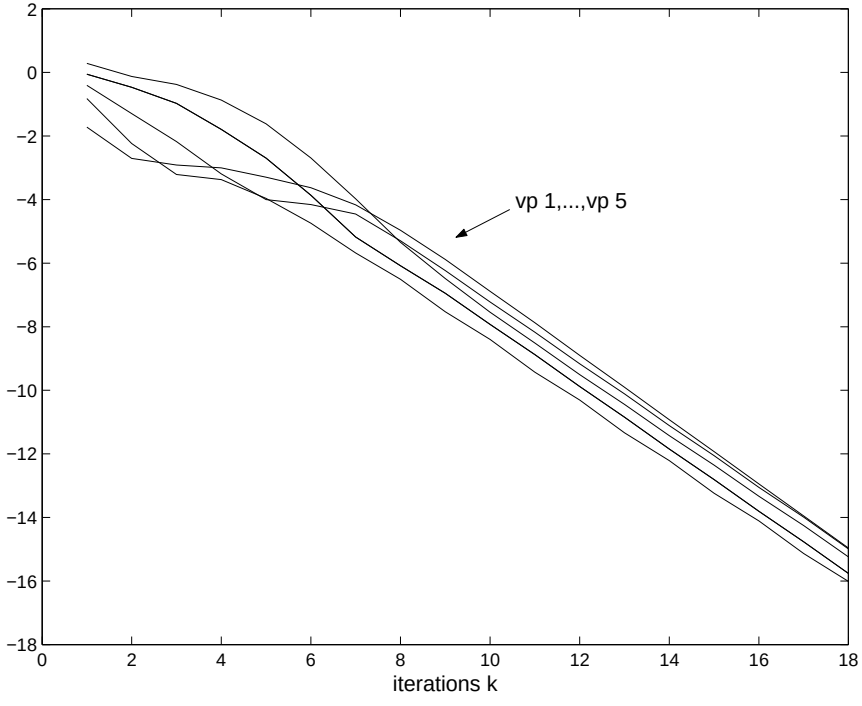
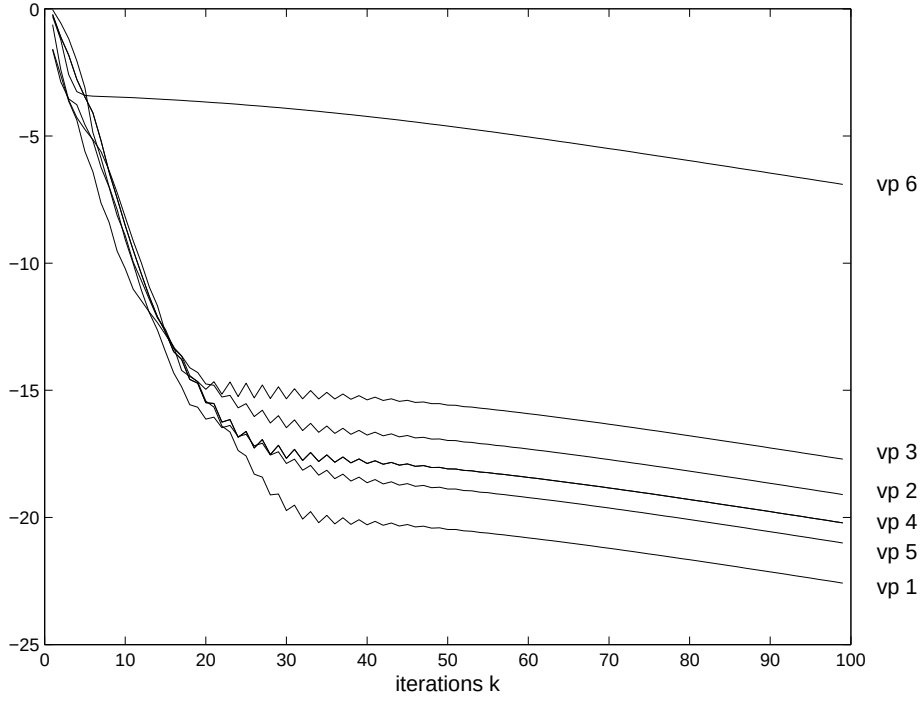
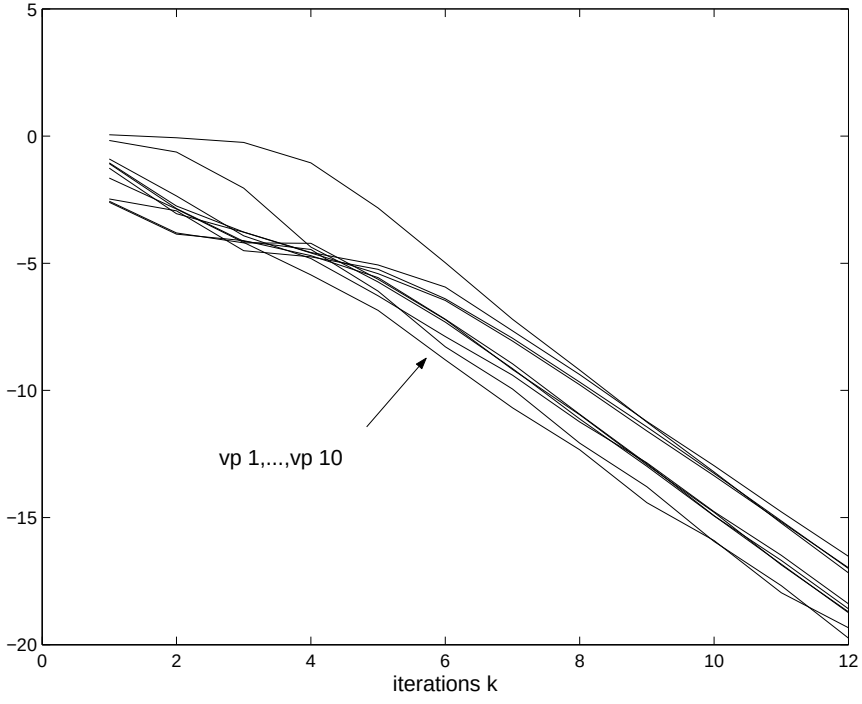
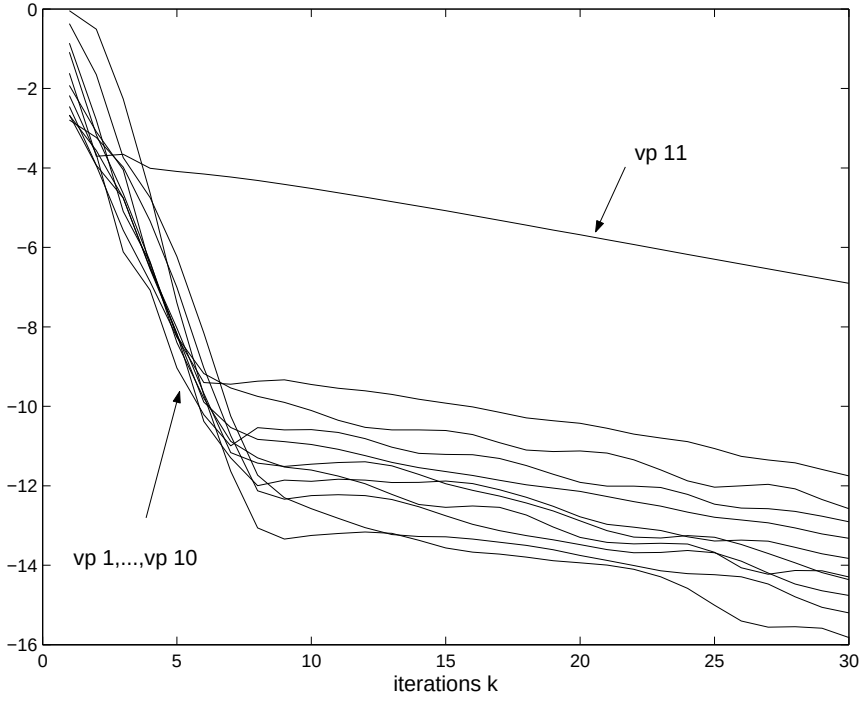




$$\mu = -1.0,\ \log(|\lambda_i^{(k)} - \lambda_i|) = f(k),\ m = 5 \text{ et } 6.$$





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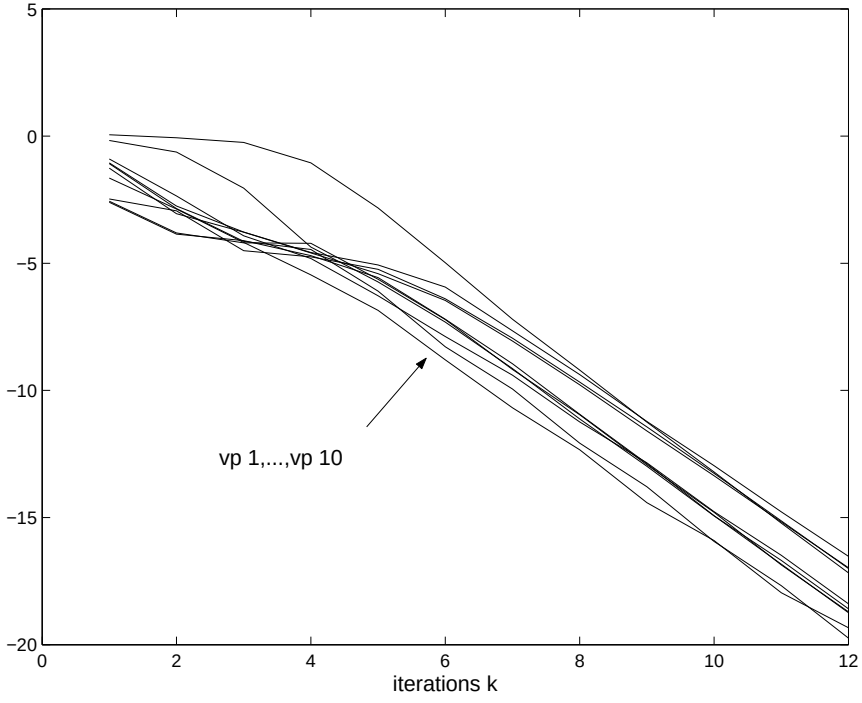

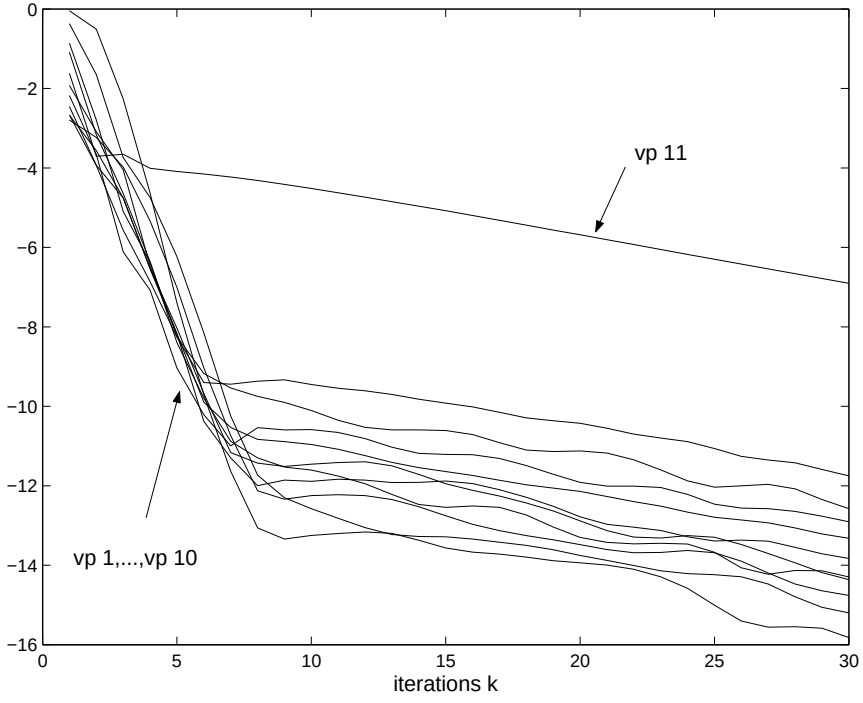

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- $\Rightarrow$ convergence of sub-clusters of eigenvalues gives another criterium of partitionning of $[a, b]$, related to physical properties.

- In a few words:

(1) - Spectral slice of an energy band with bounds to be chosen
(2) - Filling of energy regions via calculations of eigensubspaces, with local reorthog. Two ways:

$\left\{ \right.$ (2.1) - Lanczos on $(\tilde{H} - \lambda_i I)^{-1}$
$\Rightarrow$ “Classical” partitionning.
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- “Long distance orthogonality”: theorems quantifying the speed of orthog. between 2 vectors for different algorithms (numerical and theoretical studies).