Large scale electronic structure calculations with the LOBPCG method

François Bottin\textsuperscript{1}, Stéphane Leroux\textsuperscript{1}, Andrew Knyazev\textsuperscript{2}, Gilles Zérah\textsuperscript{1}

\textsuperscript{1} Département de Physique Théorique et Appliquée, CEA-DAM Ile de France
\textsuperscript{2} Department of Mathematical Sciences, University of Colorado at Denver

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Parallelization: one of the main computational tasks

- Large supercell *ab initio* calculations are very time consuming.
- Increase of the power and number of processors of supercomputers

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<td>Cluster, Xeon</td>
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- **Aim:** to use and to be efficient on these supercomputers.
Large scale electronic structure calculations with the LOBPCG method

1. Theoretical background
   - The Norm-Conserving method (NC)
   - The Projector Augmented-Wave method (PAW)
   - The self-consistent loop (SCF)
   - Locally Optimal Block Preconditioned Conjugate Gradient method (LOBPCG)
   - LOBPCG method versus CG

2. BandFFT parallelization
   - Implementation

3. BandFFT Results
   - Benchmarks
   - Norm-conserving Results
   - PAW results
   - Adding k-points parallelization

4. Tests with LOBPCGII
   - Avoiding the 3mX3m RR
   - LobpcgII: discussion
   - LOBPCGI method versus LOBPCGII

5. Conclusion – Prospects
   - Conclusion
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The Norm-Conserving method (NC)

Hamiltonian

\[ \tilde{H} = -\frac{\Delta}{2} + v_{\text{loc}} + \sum_{I} \sum_{lm \in I} \frac{\langle \tilde{P}_{lm}^{I} | \tilde{P}_{lm}^{I} \rangle}{\langle \tilde{P}_{lm}^{I} | \tilde{\Phi}_{lm}^{I} \rangle} \quad \text{with} \quad \tilde{H} \tilde{\Psi}_{nk} = \epsilon_{nk} \tilde{\Psi}_{nk} \]

Density

\[ \tilde{n}(r) = \sum_{nk} f_{nk} |\tilde{\Psi}_{nk}(r)|^2 \]
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The Projector Augmented-Wave method (PAW)

**Hamiltonian**

\[ \hat{H} = -\frac{\Delta}{2} + v_{\text{loc}} + \sum_{I} \sum_{ij \in I} |\tilde{P}_i^I\rangle D_{ij}^I \langle \tilde{P}_j^I| \quad \text{with} \quad \hat{H}\tilde{\Psi}_{nk} = \epsilon_{nk} O\tilde{\Psi}_{nk} \]

**Densities – Overlap operator**

\[ \tilde{n}(r) \quad \text{and} \quad \rho_{ij}^I = \sum_{nk} f_{nk} \langle \tilde{\Psi}_{nk} | \tilde{P}_i^I \rangle \langle \tilde{P}_j^I | \tilde{\Psi}_{nk} \rangle \]

\[ O = I + \sum_{I} \sum_{ij \in I} |\tilde{P}_i^I\rangle (\langle \Phi^I_i|\Phi^I_j\rangle) - (\langle \tilde{\Phi}^I_i|\tilde{\Phi}^I_j\rangle) \langle \tilde{P}_j^I| \]

\[ n(r) = \tilde{n}(r) + \sum_{I} (n^{1,I}(r) - \tilde{n}^{1,I}(r)) \]
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**SCF loop**

\[ \tilde{\Psi}_n(\mathbf{r}) = \sum_G c_n(\mathbf{G}) e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} \]

\[ \tilde{\Psi}_n(\mathbf{r}) = [\tilde{n} + \hat{n}](\mathbf{r}) \text{ and } \rho_{ij} \leftarrow \{c_n(\mathbf{G}); \epsilon_n\} \]

\[ \mathbf{v}_{\text{loc}}(\mathbf{r}) \text{ and } \mathbf{v}_{\text{nl}}(\mathbf{r}) \]

\[ \langle e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} | \hat{H} | \tilde{\Psi}_n \rangle = \epsilon_n \langle e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} | \mathcal{O} | \tilde{\Psi}_n \rangle \]

\[ | \hat{H} - \epsilon_n \mathcal{O} | = 0 \]
Large scale electronic structure calculations with the LOBPCG method

SCF loop

\[ \tilde{\Psi}_n(r) = \sum_G c_n(G)e^{i(k+G)\cdot r} \]

\[ [\hat{n} + \hat{\rho}](r) \quad \text{and} \quad \rho_{ij} \quad \leftrightarrow \quad \{c_n(G); \epsilon_n\} \]

\[ v_{\text{loc}}(r) \quad \text{and} \quad v_{\text{nl}}(r) \]

\[ \langle e^{i(k+G)\cdot r} | \tilde{\mathcal{H}} | \tilde{\Psi}_n \rangle = \epsilon_n \langle e^{i(k+G)\cdot r} | \mathcal{O} | \tilde{\Psi}_n \rangle \]

Time consuming parts

- The non-local like terms.
Large scale electronic structure calculations with the LOBPCG method

### SCF loop

\[
\tilde{\Psi}_n(r) = \sum_G c_n(G)e^{i(k+G).r} \\
[\tilde{n} + \hat{n}](r) \quad \text{and} \quad \rho_{ij} \quad \leftarrow \quad \{c_n(G); \epsilon_n\} \\
v_{\text{loc}}(r) \quad \text{and} \quad v_{n1}(r) \quad \quad \quad \quad |\tilde{H} - \epsilon_n \mathcal{O}| = 0 \\
\langle e^{i(k+G).r} | \tilde{H} | \tilde{\Psi}_n \rangle = \epsilon_n \langle e^{i(k+G).r} | \mathcal{O} | \tilde{\Psi}_n \rangle
\]

### Time consuming parts

- The non-local like terms.
- The resolution of the KS equations (LOBPCG).
Large scale electronic structure calculations with the LOBPCG method

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**Time consuming parts**

- The non-local like terms.
- The resolution of the KS equations (LOBPCG).
- The diagonalisation within the sub-space.
Theory
NC
PAW
SCF
LOBPCG
LOBPCG VS
CG
Implementation
Principles
Results
Benchmarks
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k-points
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Conclusion
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Large scale electronic structure calculations with the LOBPCG method

SCF loop

\[ \tilde{\Psi}_n(\mathbf{r}) = \sum_G c_n(G) e^{i(\mathbf{k} + G) \cdot \mathbf{r}} \]

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Time consuming parts

- The non-local like terms.
- The resolution of the KS equations (LOBPCG).
- The diagonalisation within the sub-space.
- The calculation of the density and local potential (FFT).
Large scale electronic structure calculations with the LOBPCG method

**SCF loop**

\[ \tilde{\Psi}_n(r) = \sum_G c_n(G)e^{i(k+G) \cdot r} \]

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**Possible Parallelizations**

- over the k-points.
- over the plane-waves → require a parallel 3dim-FFT \(^a\).
- over the bands → require a block eigensolver.

Algorithm 1 LOBPCG

**Require:** $\Psi^0 = \{\Psi_1^0, \ldots, \Psi_m^0\}$ close to the minimum and $K$ a preconditioner; $P = \{P_1^{(0)}, \ldots, P_m^{(0)}\}$ is initialized to 0.

1: for $i=0,1,\ldots,\kappa$ do
2: $\Upsilon^{(i)} = \Upsilon(\Psi^{(i)})$
3: $R^{(i)} = \mathcal{H}\Psi^{(i)} - \Upsilon^{(i)} \mathcal{O}\Psi^{(i)}$
4: $W^{(i)} = KR^{(i)}$
5: The Rayleigh-Ritz method is applied within the subspace $\Xi = \{P_1^{(i)}, \ldots, P_m^{(i)}, \Psi_1^{(i)}, \ldots, \Psi_m^{(i)}, W_1^{(i)}, \ldots, W_m^{(i)}\}$
6: $\Psi^{(i+1)} = \Delta^{(i)}\Psi^{(i)} + \Lambda^{(i)}W^{(i)} + \Gamma^{(i)}P^{(i)}$
7: $P^{(i+1)} = \Lambda^{(i)}W^{(i)} + \Gamma^{(i)}P^{(i)}$
8: end for

More efficient than CG in many cases

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Large scale electronic structure calculations with the LOBPCG method

Carbon in its Diamond phase, Plutonium in its alpha phase

We compare also the use of different blocksizes: blocksize=1 and blocksize=\textit{nband}

- The convergence is linear up to a higher precision for lobpcg, but blocksize=\textit{nband} yields better results
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Implementation

\[ \tilde{\Psi}_n(r) = \sum_G c_n(G) e^{i(k+G) \cdot r} \]

\[ [\hat{n} + \hat{n}](r) \quad \text{and} \quad \rho_{ij} \quad \leftarrow \quad \{c_n(G); \epsilon_n\} \]

\[ v_{\text{loc}}(r) \quad \text{and} \quad v_{n1}(r) \]

| \[ \begin{bmatrix} \hat{H} - \epsilon_n \mathcal{O} \end{bmatrix} = 0 \]

| \[ \langle e^{i(k+G) \cdot r} \mid \hat{H} \mid \tilde{\Psi}_n \rangle = \epsilon_n \langle e^{i(k+G) \cdot r} \mid \mathcal{O} \mid \tilde{\Psi}_n \rangle \]

In LOBPCG: blocks of size m

| \begin{bmatrix} c_{1:m}(g_{11}) & c_{1:m}(g_{12}) & \cdots & c_{1:m}(g_{1p}) \\ c_{1:m}(g_{21}) & c_{1:m}(g_{22}) & \cdots & c_{1:m}(g_{2p}) \\ \vdots & \vdots & \ddots & \vdots \\ c_{1:m}(g_{m1}) & \cdots & \cdots & c_{1:m}(g_{mp}) \end{bmatrix} |
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... which can be transposed...

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\begin{pmatrix}
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\[ \tilde{\Psi}_n(\mathbf{r}) = \sum_{\mathbf{G}} c_n(\mathbf{G}) e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} \]

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Benchmarks – Test cases

- Gold system with 108 atoms, 648 bands, $108^3$ FFT grid, 1 $k$-point and $E_{\text{cut}}=24$ Ha.
- We stop the SCF for $\text{nstep}=15$
- A two-dimensional grid of processors with $n\text{proc}=1, 4, 18, 36, 54, 108, 162$ and 216.
- Example: for $n\text{proc}=108$, we can choose $m \times p=108 \times 1, 54 \times 2, 36 \times 3, 27 \times 4, 18 \times 6, 12 \times 9, 9 \times 12, 6 \times 18, 4 \times 27$ and $3 \times 36$
- Tests are performed on 2 supercomputers:

<table>
<thead>
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<th>Supercomputer</th>
<th>Node</th>
<th>Interconnection</th>
</tr>
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<tbody>
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<td>Tantale (CCRT)</td>
<td>4-procs AMD OPTERON 2.4 GHz</td>
<td>Infiniband</td>
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<tr>
<td>TERA-10 (CEA/DIF)</td>
<td>Novascale 16-procs Intel Itanium</td>
<td>Quadrics</td>
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Large scale electronic structure calculations with the LOBPCG method

Norm-conserving Results

108 atoms, 648 bands, $108^3$ FFT grid, 1 $k$-point and $E_{\text{cut}}=24$ Ha.

- In sequential: 90 000 sec. (with 90% in LOBPCG).
- Linear scaling up to 100 for ABINIT and 200 for LOBPCG.
Large scale electronic structure calculations with the LOBPCG method

**PAW results (with 2 projectors per angular momentum)**

108 atoms, 648 bands, $72^3$ FFT grid, 1 k-point and $E_{\text{cut}}=12$ Ha.

- In sequential: 75 000 sec. (with 90% in LOBPCG).
- Due to non-local like and spherical terms.
Large scale electronic structure calculations with the LOBPCG method

The triple nkG parallelization (in ABINIT 5.5.x)

108 atoms, 648 bands, $108^3$ FFT grid, 10 $k$-point and $E_{\text{cut}}=24$ Ha.
Large scale electronic structure calculations with the LOBPCG method

1. Theoretical background
   - The Norm-Conserving method (NC)
   - The Projector Augmented-Wave method (PAW)
   - The self-consistent loop (SCF)
   - Locally Optimal Block Preconditioned Conjugate Gradient method (LOBPCG)
   - LOBPCG method versus CG

2. BandFFT parallelization
   - Implementation

3. BandFFT Results
   - Benchmarks
   - Norm-conserving Results
   - PAW results
   - Adding k-points parallelization

4. Tests with LOBPCGII
   - Avoiding the 3mX3m RR
   - LobpcgII: discussion
   - LOBPCGI method versus LOBPCGII

5. Conclusion – Prospects
   - Conclusion
Large scale electronic structure calculations with the LOBPCG method

**Algorithm 2 LOBPCGI**

**Require:** $\Psi^0 = \{\Psi_1^0, \ldots, \Psi_m^0\}$ close to the minimum and $K$ a pre-conditioner; $P = \{P_1^0, \ldots, P_m^0\}$ is initialized to 0.

1: for $i=0,1,\ldots,\kappa$ do
2: \[ \Upsilon^{(i)} = \Upsilon(\Psi^{(i)}) \]
3: \[ R^{(i)} = H\Psi^{(i)} - \Upsilon^{(i)}\Omega\Psi^{(i)} \]
4: \[ W^{(i)} = KR^{(i)} \]
5: The Rayleigh-Ritz method is applied within each subspace $\Xi_j = \{P_1^{(i)}, \Psi_1^{(i)}, W_1^{(i)}\}$
6: \[ \hat{\Psi}_j^{(i+1)} = \Delta_j^{(i)}\Psi_j^{(i)} + \Lambda_j^{(i)}W_j^{(i)} + \Gamma_j^{(i)}P_j^{(i)} \]
7: \[ P_j^{(i+1)} = \Lambda_j^{(i)}W_j^{(i)} + \Gamma_j^{(i)}P_j^{(i)} \]
8: Apply RR on the subspace $\{\hat{\Psi}_1^{i+1}, \ldots, \hat{\Psi}_m^{i+1}\}$
9: end for

Computes a smaller Ritz matrix. Now the $P$ are somewhat inconsistent with the $\Psi$
LobpcgII: discussion

- Eigenvalues are sometimes running away
- This is due to the lack of orthogonalization step
- To remain in the spirit of CG eigensolvers the $P$ must be modified
- A good approximation is to impose
  \[ \text{span}(\Psi_{j+1}^i, \Psi_j^i) = \text{span}(\Psi_{j+1}^i, P_{j+1}^i) \]
Large scale electronic structure calculations with the LOBPCG method

**LOBPCGI vs LOBPCGII**

We compare also the use of different block sizes: blocksize=1 and blocksize=nband
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Conclusion

- LOBPCG is responsible for the superlinear behaviour and scales perfectly up to 200 processors.
- ABINIT scales linearly up to 100 processors in NC and slightly underneath in PAW.
- LOBPCG-II could yield an even greater gain in scalability, by avoiding the orthogonalization step.
- This is the object of our current studies.