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JÜLICH FORSCHUNGSZENTRUM

A knowledge-based approach to high-performance computing in ab initio simulations.

AICES Advisory Board Meeting. July 14th 2014 | Edoardo Di Napoli

Academic background

Laurea in Physics
Università di Roma I "La Sapienza".

Ph.D. in Physics
University of Texas at Austin.

Postdoctoral Research Associate
University of North Carolina at Chapel Hill.

Head of the Simulation Laboratory *ab initio*
Jülich Supercomputing Centre.

Junior Research Group Leader
Aachen Institute for Advanced Study in Computational Engineering Science.

High-performance simulations

Two Observations

- Often software libraries are used as **black boxes**.
- Very **little information** coming from the physics of the specific application is exploited by scientific computing codes.

High-performance simulations

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One Objective

Exploiting physical information extracted from the simulations in order to:

- increase the performance of large legacy codes;
- improve the computational paradigm on which the codes are based.
- enabling access to more physics

Main active projects

HPC and scalable eigensolvers tailored to Density Functional Theory (DFT)

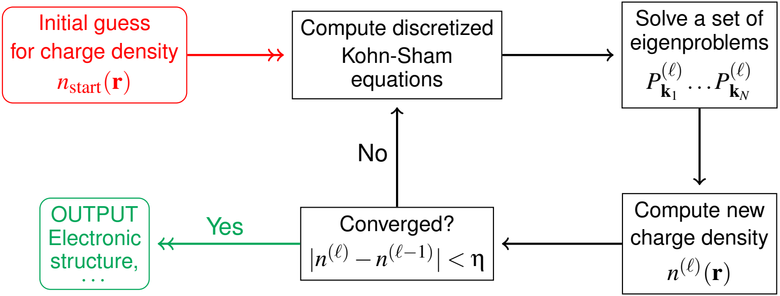
- **Chebyshev Filtered Subspace Iteration** – Development of a block iterative eigensolver tailored to sequences of *dense eigenvalue* problems arising in DFT methods based on the LAPW basis set.
  Collaboration with M. Berljafa (University of Manchester)
- **Spectrum-slicing methods** – Development of a integral-based iterative eigensolver for sparse generalized hermitian eigenvalue problems appearing in real-space DFT methods.
  Collaboration with Y. Saad (U. of Minnesota) and E. Polizzi (U. of Massachussets).

HPC Tensor algebra

Development of taxonomy rules and tailored kernels for high-performance multi-contraction operations between high dimensional tensors for quantum chemistry.
Collaboration with P. Bientinesi (AICES) and J. Hammond (Intel)

Density Functional Theory simulations

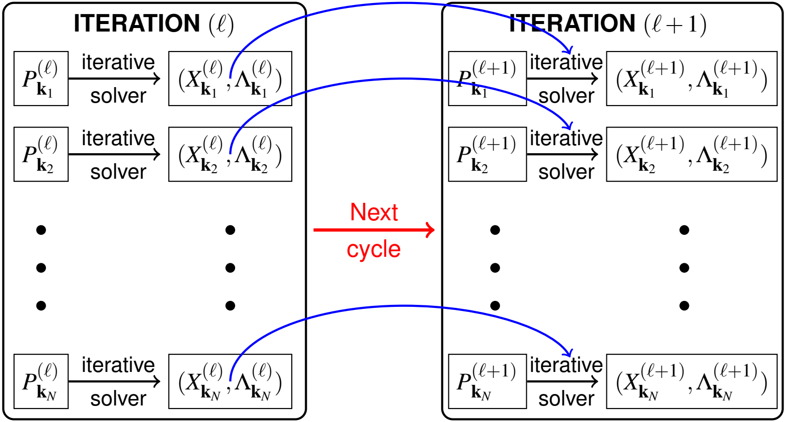
General framework



1. every $P^{(\ell)}_{\mathbf{k}} : A^{(\ell)}_{\mathbf{k}} x = B^{(\ell)}_{\mathbf{k}} \lambda x$ is a generalized eigenvalue problem;
2. A and B are hermitian (B is positive definite);
3. required: lower $2 \div 10$ % of eigenpairs;
4. k-vector index: $\mathbf{k} = 1 : 10 \div 100$;
5. iteration cycle index: $\ell = 1 : 20 \div 50$.

Chebyshev Filtered Subspace Iteration

Alternative solving strategy



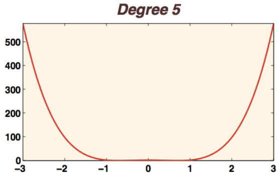
$X \equiv \{x_1, \ldots, x_n\}$ $\quad\quad$ $\Lambda \equiv \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$

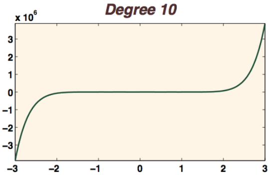
Chebyshev Filtered Subspace Iteration

Chebyshev filter

A generic vector $v = \sum_{i=1}^{n} s_i x_i$ is very quickly aligned in the direction of the eigenvector corresponding to the extremal eigenvalue λ_1

$$
\begin{aligned}
v^m = p_m(A)v &= \sum_{i=1}^{n} s_i p_m(A) x_i = \sum_{i=1}^{n} s_i p_m(\lambda_i) x_i \\
&= s_1 x_1 + \sum_{i=2}^{n} s_i \frac{C_m(\frac{\lambda_i - c}{e})}{C_m(\frac{\lambda_1 - c}{e})} x_i \sim \boxed{s_1 x_1}
\end{aligned}
$$

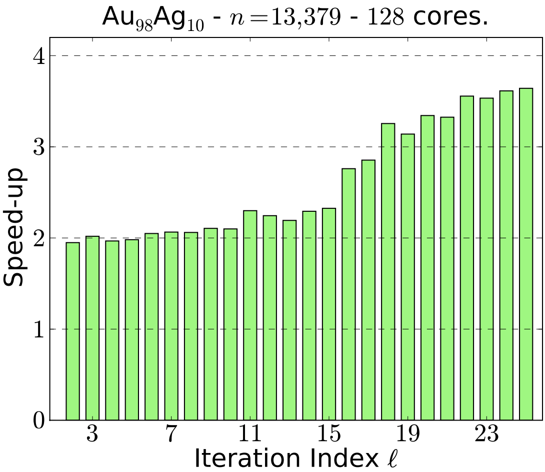




Chebyshev Filtered Subspace Iteration

Speed-up

$$\text{Speed-up} = \frac{\text{CPU time (input random vectors)}}{\text{CPU time (input approximate eigenvectors)}}$$

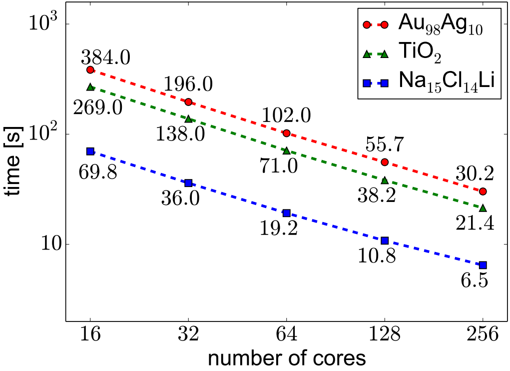


Chebyshev Filtered Subspace Iteration

Strong scalability

Size n of the eigenproblems are kept fixed while the number of cores is progressively increased

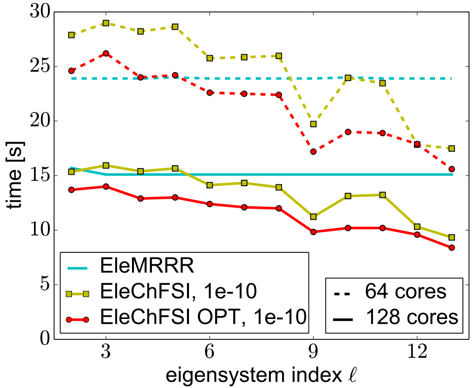
Three systems of size $n = 13,379 - 12,455 - 9,273$.



Chebyshev Filtered Subspace Iteration

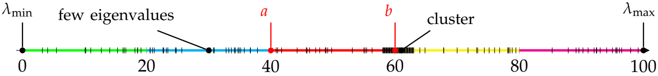
Optimized ChFSI versus direct solvers

For the size of eigenproblems here tested the ScaLAPACK implementation of BXINV or MRRR is on par or worse than EleMRRR. For this reason a direct comparison with ScaLAPACK is not included.



Spectrum-slicing methods

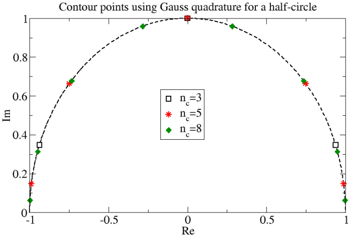
Integral based projector



$$P = -\frac{1}{2i\pi}\int_\Gamma (A - zB)^{-1} B \, dz \quad \equiv \sum_{\lambda_i \in [a\ b]} u_i u_i^T B$$

Approximation

$$P \approx \chi_{n_c}(A,B) = \sum_{j=1}^{n_c} w_j (A - z_j B)^{-1} B$$



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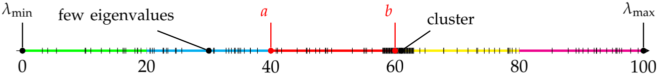


Integral-based Subspace Iteration

$$\textbf{While}\{\text{CONV} < \text{NEV}\} \quad Q_i = PQ_{i-1} \approx \chi_{n_c}(A,B) = \sum_{j=1}^{n_c} w_j (A - z_j B)^{-1} B Q_{i-1}$$

Core problems

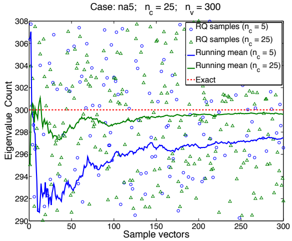
1. Relies on good estimates of number $\mu_{[a\ b]}$ of eigenvalues in $[a\ b]$
2. Solve for multiple right-hand side linear systems per integration node
3. Accuracy depends on the quadrature method used

Spectrum-slicing methods

Under investigation

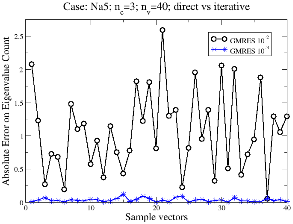
Stochastic estimator

$$\mathrm{Trace}(P) \approx \frac{n}{n_v} \sum_{j=1}^{n_c} \gamma_j \sum_{k=1}^{n_v} v_k^T (A - \sigma_j I)^{-1} v_k$$



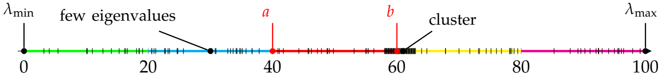
Sparse linear systems

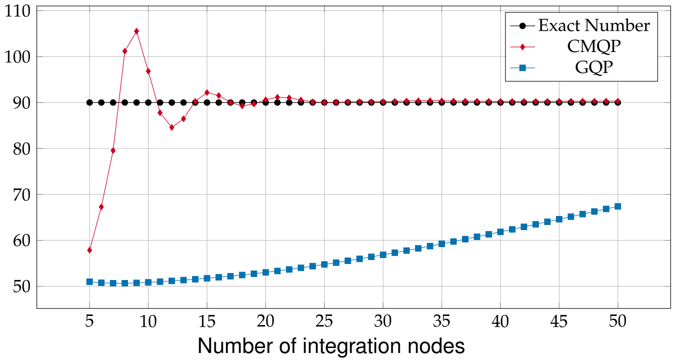
- Solving with Generalized Minimal Residual method (GMRES)
- Exploiting rational Krylov methods



Spectrum-slicing methods

Under investigation





Other active projects

Matrix structure exploitation

Analysis of structure variations in Hamiltonians and Overlap matrices across sequences of DFT eigenproblems. Re-use of data stored in Householder projectors in combination with tailored Jacobi rotations.
Collaboration with P. Bientinesi (AICES)

Data generation in LAPW-based methods

Analisys of matrix entries generation in the FLEUR code with the aim of setting alternative strategies enabling modularity, flexibility and scalability.
Collaboration with P. Bientinesi (AICES) and D. Wortmann (FZJ)

Ab initio nanoscale interfacial heat transfer modeling

Development of a method incorporating ab initio calculations in classical non-equilibrium molecular dynamics (NEMD) modeling. Aim at providing a detailed picture of phonon transport across interfaces from quantum physics simulations.
Collaboration with M. Hu (AICES)

Thank you!

For more information

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