A Parallel and Scalable Iterative Solver for Sequences of Dense Eigenproblems Arising in FLAPW

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Abstract

In one of the most important methods in Density Functional Theory – the Full-Potential Linearized Augmented Plane Wave (FLAPW) method – dense generalized eigenproblems are organized in long sequences. Moreover each eigenproblem is strongly correlated to the next one in the sequence. We propose a novel approach which exploits such correlation through the use of an eigensolver based on subspace iteration and accelerated with Chebyshev polynomials. The resulting solver, parallelized using the Elemental library framework, achieves excellent scalability and is competitive with current dense parallel eigensolvers.

1 Introduction

We present a methodological approach to solve for eigenpairs of sequences of correlated dense eigenproblems arising in Density Functional Theory (DFT). The novelty of this approach resides in the use of approximate solutions in combination with a simple block eigensolver based on polynomially accelerated subspace iteration. When parallelized for distributed memory architectures this iterative method is a viable alternative to conventional dense eigensolvers both in terms of scalability and performance. Ultimately our approach will enable the DFT specialists to simulate larger and more complex physical systems.

Within the realm of condensed-matter physics, DFT is considered the standard model to run accurate simulations of materials. The importance of these simulations is two-fold: on the one hand they are used to verify the correctness of the quantum mechanical interpretation of existing materials. On the other hand, simulations constitute an extraordinary tool to verify the validity of new atomistic models which may ultimately lead to the invention of brand new materials.

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Each simulation consists of a series of self-consistent cycles; within each cycle a fixed number $N_k$ of independent eigenvalue problems is solved. Since dozens of cycles are necessary to complete one simulation, one ends up with $N_k$ sequences made of dozens of eigenproblems. The properties of these eigenproblems depend on the discretization strategy of the specific DFT method of choice. In this paper we will exclusively consider the Full-Potential Linearized Augmented Plane Waves method (FLAPW). This DFT method gives rise to dense hermitian generalized eigenproblems (DGEVP) with matrix size typically ranging from 2,000 to 20,000.

In FLAPW only a fraction of the lowest part of the eigenspectrum is required. The eigenvalues inside this fraction correspond to the energy levels below Fermi energy and their number never falls below 3% or exceeds 20% of the eigenspectrum. The relatively high number of eigenpairs in combination with the dense nature and the size of the eigenproblems inevitably lead to the choice of direct eigensolvers. Direct eigensolvers follow a constrained path of linear transformations starting from the generalized eigenproblem and arriving to a tridiagonal one. In turn, the tridiagonal problem is solved iteratively using one of the two methods available for computing just a fraction of the spectrum, namely bisection inverse iteration (BXINV) [1] and multiple relatively robust representations (MRRR) [2,3].

Until very recently, the computational strategy on parallel distributed memory architecture favored the use of ScaLAPACK [4] implementation of BXINV. Modern and efficient dense libraries, like ELPA [5] and EleMRRR [6], improve the performance but do not change the overall computational strategy: each problem in the sequence is solved in complete independence from the previous one. The latter choice is based on the view that problems in the sequence are apparently only loosely connected. In this paper we propose a completely different strategy which tries to maximally exploit the sequence of eigenproblems using an iterative eigensolver as opposed to a direct one.

The novelty of our approach, in spite of the assumed loose connection between eigenproblems, is in the use of the solutions of one problem in the sequence as input when solving the next one. By its inherent nature only an iterative method would be able to accept eigenvectors as input. On the other hand not all such methods are capable of maximally exploiting the information inputed. In this regards one of the most effective methods is Subspace Iteration (SI). We have implemented a version of this method accelerated with Chebyshev polynomials. The end result is an algorithm (ChFSI) whose bulk of computations is performed making use of the highly optimized Basic Linear Algebra Subroutines (BLAS) library and can be easily parallelized on shared and distributed memory architectures. In this paper we present preliminary results for a distributed memory version of ChFSI implemented using the Elemental library framework [20].

2 FLAPW Simulations on Large Parallel Architectures

Every DFT method is based on a variational principle stemming from the fundamental work of Kohn and Hohenberg [7], and its practical realization [8]. Central to DFT is the solution of a large number of coupled one-particle Schrödinger-like equations known as Kohn-Sham
Due to the dependence of the effective potential $V_{\text{eff}}$ on the charge density $n(r)$, in itself a function of the orbital wave functions $\phi_i(r)$, the KS equations are non-linear and are generally solved self-consistently.

The KS equations need to be “discretized” in order to be solved numerically. Intended in its broadest numerical sense, the discretization translates the KS equations in a non-linear eigenvalue problem. Eigenproblems generated by distinct discretization schemes have numerical properties that are often substantially different; for sake of simplicity we can group most of the schemes in three classes. The first and the second classes make respectively use of plane waves and localized functions to expand the one-particle orbital wave functions $\phi_i(r)$ appearing in the KS equations

$$
\phi_i(r) \rightarrow \phi_{k,i}(r) = \sum_G c_{k,i}^G \psi_G(k, r).
$$

Methods in the third class do not use an explicit basis for the $\phi_i(r)$’s but discretize the KS equations on a grid in real space using finite differences.

The eigenvalue problems emerging from the first two discretization classes consist of dense matrices of small-to-moderate size while, within real space methods, one ends up with very large sparse matrices. Due to the dramatically different set of properties of the eigenproblems, each DFT method uses a distinct strategy in solving for the required eigenpairs. For instance it is quite common that methods based on plane waves (ABINIT, VASP, PARATEC, Castep, . . . ) use direct eigensolvers while real space methods (PARSEC, GPAW, Octopus, . . . ) make use of iterative eigensolver based on Krylov- or Davidson-like subspace construction. From the point of view of software packages for distributed memory architectures, the choice between direct or iterative eigensolvers leads respectively to the use of traditional parallel libraries like ScaLAPACK or PARPACK [9].

In this paper we deal with a specific instance of a plane wave method which splits the basis functions support domain: in a spherical symmetric area around each atom, $\psi_G$ receive contributions by augmented radial functions, while plane waves are supported in the interstitial space between atoms. This discretization of the KS equations – known as FLAPW – translates in a set of $N_k$ quite dense DGEVP

$$
\sum_{G'} (A_k)_{GG'} c_{k,i}^{G'} = \lambda_{k,i} \sum_{G'} (B_k)_{GG'} c_{k,i}^{G'},
$$

each one labeled by a value of the plane wave vector $k$. The role of eigenvectors is played by the $n$-tuple of coefficients $c_{k,i}^G$ expressing the orbital wave functions $\phi_i$ in terms of the basis wave functions $\psi_G$.

The entries of each DGEVP matrix are initialized by evaluating numerically a series of expensive multiple integrals involving the $\psi_G$s. Since we are dealing with non-linear eigenvalue problems, each DGEVP has to be solved in a chain of self-consistent cycles

$$
A_k c_{k,i} = \lambda_{k,i} B_k c_{k,i} \rightarrow P_{k}^{(\ell)}: A_k^{(\ell)} c_{k,i}^{(\ell)} = \lambda_{k,i}^{(\ell)} B_k^{(\ell)} c_{k,i}^{(\ell)} \quad (\ell = 1, \ldots, N).
$$
All along the sequence the solutions of all $P_k^{(\ell-1)}$ are used to initialize the new eigenproblems $P_k^{(\ell)}$. In particular the eigenvectors $c_{k,i}^{(\ell-1)}$ are used to derive the orbital functions $\phi_{k,i}^{(\ell-1)}$ which in turn contribute to the charge density $n^{(\ell-1)}(r)$. At the next cycle $n^{(\ell-1)}(r)$ contributes to modify the potential $V_{\text{eff}}$ which causes the functional form of the $\psi_G$’s to change. These new basis function set directly determines the initialization of the entries of $A_k^{(\ell)}$ and $B_k^{(\ell)}$ and indirectly the new eigenvectors $c_{k,i}^{(\ell)}$. The result is a sequence $\{P_k^{(1)} \ldots P_k^{(N)}\}$ for each $k$ where the eigenpairs $(\lambda_{k,i}^{(N)}, c_{k,i}^{(N)})$ converged within tolerance to the solution of the original non-linear problem. In theory the chain of computations that goes from $P_k^{(\ell-1)}$ to $P_k^{(\ell)}$ implies a connection between eigenvectors of successive eigenproblems. In practice there is no known mathematical formalism that makes this connection explicit. Correlation between the eigenvectors becomes evident only numerically [10].

When solving for an eigenvalue problem the first high level choice is between direct and iterative eigensolvers. The first are in general used to solve for a large portion of the eigenspectrum of dense problems. The latter are instead the typical choice for sparse eigenproblems or used to solve for just few eigenpairs of dense ones. In FLAPW the hermitian matrices $A_k$ and $B_k$ are quite dense, have size not exceeding 20,000, and each $P_k^{(\ell)}$ is solved for a portion of the lower spectrum not bigger than 20%. Consequently, when each DGEVP is singled out from the rest of the sequence, direct solvers are unquestionably the method of choice. Currently, most of the codes based on FLAPW methods [11–13] use the algorithms BXINV or MRRR directly out of the ScaLAPACK or ELPA library.

If the use of direct solvers is the obvious choice when each $P_k^{(\ell)}$ is solved in isolation, the same conclusion may not be drawn when we look at a the entire sequence of $\{P_k^{(\ell)}\}$. In [10] it is shown how the correlation between eigenvectors of successive DGEVPs becomes manifest in the evolution of the angles $\theta_{k,i}^{(\ell)} = \langle c_{k,i}^{(\ell-1)}, c_{k,i}^{(\ell)} \rangle$. In particular the $\theta_{k,i}^{(\ell)}$ decrease almost monotonically as a function of cycle index $\ell$, going from $\sim 10^{-1}$ down to $\sim 10^{-8}$ towards the end of the sequence.

The empirical evolution of the eigenvectors suggests that they can be “reused” as approximate solutions, and inputed to the eigensolver at the successive cycle. Unfortunately no direct eigensolver is capable of accepting vectors as approximate solutions. Therefore if we want to exploit the progressive collinearity of vectors as the sequence progresses, we are lead to consider iterative solvers; these solvers by their own nature build approximate eigenspaces by manipulating approximate eigenvectors. In particular we need a block iterative eigensolver that accepts at the same time many vectors as input. Among the many choices of block solvers, the Chebyshev Filtered Subspace Iteration method (ChFSI) showed the highest potential to take advantage of approximate eigenvectors [14](see also Fig. 1(b)). Since the core of the algorithm is based on the repetitive use of matrix-matrix multiplications, the use of the BLAS 3 library makes it very efficient and easy to scale.
The data in this figure refers to eigenproblems of distinct sizes $n$ relative to the same physical system $Au_{98}Ag_{10}$. Plot (a) represents the computing fractions of EleChFSI’s main algorithmic steps w.r.t. the total computing time. Plot (b) shows the speed-up of EleChFSI when inputed approximate solutions as opposed to random vectors.

3 The Parallel Chebyshev Subspace Iteration

Subspace Iteration complemented with a Chebyshev polynomial filter is a well known algorithm in the literature [15]. A version of it was recently developed for a real space discretization of DFT by Chelikowsky et al. [16,17] and included in the PARSEC code [18].

SI is probably one of the earliest iterative algorithms to be used as numerical eigensolver. It is by definition a block solver since it simply attempts to build an invariant eigenspace by multiplying a block of vectors with the operator to be diagonalized. It is a known fact that any implementation based on subspace iteration converges very slowly. By using a polynomial filter on the initial block of inputed vectors the method experiences a high rate of acceleration. Unfortunately the block of vectors spanning the invariant subspace could easily become linearly dependent. In order to avoid such an occurrence SI is usually complemented with some re-orthogonalization procedure.

Our ChFSI algorithm is a slightly more sophisticated version of the basic SI and is specifically tailored for DFT-like eigenproblems. The whole algorithm is illustrated in the Algorithm 1 scheme. Notice that the initial input is not the initial $P^\ell$ but its reduction to standard form $H^\ell = L^{-1}A^\ell L^{-T}$ where $B^\ell = LL^T$, and $\hat{Y}^{(\ell-1)}$ are the eigenvectors of $H^{(\ell-1)}$. ChFSI uses few Lanczos iterations (line 1) so as to estimate the upper limit of the eigenproblem spectrum [19]. This estimate is necessary for the correct usage of the filter based on Chebyshev polynomials [15]. After the Chebyshev filter step (line 3) the resulting block of vectors is re-orthonormalized using a simple QR algorithm (line 4) followed by a Rayleigh-Ritz procedure (line 5). At the end of the Rayleigh-Ritz step eigenvector
Algorithm 1 Chebyshev Filtered Subspace Iteration with locking

**Input:** Matrix $H^{(ℓ)}$ of the DGEVP reduced to standard form, approximate eigenvectors $\hat{Y}^{(\ell-1)} := [\hat{y}_1^{(\ell-1)}, \ldots, \hat{y}_{nev}^{(\ell-1)}]$ and eigenvalues $\lambda_1^{(\ell-1)}$ and $\lambda_{nev+1}^{(\ell-1)}$.

**Output:** Wanted eigenpairs $(\Lambda, Y)$.

1: Estimating the largest eigenvalue. ▷ **Lanczos**
2: repeat
3: Filtering the vectors $\hat{Y} = C_m(\hat{Y})$. ▷ **Chebyshev filter**
4: Re-orthonormalizing $\hat{Y}$. ▷ **QR algorithm**
5: Computing Rayleigh quotient $G = \hat{Y}^TH^{(\ell)}\hat{Y}$. ▷ **Rayleigh-Ritz (Start)**
6: Solving reduced problem $G\hat{w} = \lambda\hat{w}$ giving $(\hat{\Lambda}, \hat{\mathbf{W}})$. ▷ **Rayleigh-Ritz (End)**
7: Computing $\hat{Y} = \hat{Y}\hat{\mathbf{W}}$. ▷ **Rayleigh-Ritz (End)**
8: for $i = \text{converged} \rightarrow \text{nev}$ do ▷ **Deflation & Locking (Start)**
9: if $\text{Res}(\hat{Y}(;i), \hat{\Lambda}(i)) < \text{TOL}$ then
10: $\Lambda \leftarrow [\Lambda \hat{\Lambda}(i)]$
11: $Y \leftarrow [Y \hat{Y}(;i)]$
12: end if
13: end for ▷ **Deflation & Locking (End)**
14: until converged $\geq \text{nev}$

residuals are computed, converged eigenpairs are deflated and locked (line 13) while the non-converged vectors are sent again to the filter to repeat the whole procedure.

The Chebyshev polynomial filter is at the core of the algorithm. The vectors $\hat{Y}$ are filtered exploiting the 3-terms recurrence relation which defines Chebyshev polynomials of the first kind

$$C_{m+1}(\hat{Y}) = 2H C_m(\hat{Y}) - C_{m-1}(\hat{Y}) \quad ; \quad C_m(\hat{Y}) \overset{\text{def}}{=} C_m(H) \cdot \hat{Y}. \quad (2)$$

This construction implies all operations internal to the filter are executed through the use of ZGEMM, the most performant among BLAS 3 routines. Since roughly 90% of the total CPU time is spent in the filter (see pie chart in Fig. 1), the massive use of ZGEMM makes ChFSI quite an efficient algorithm and potentially a very scalable one.

The parallel MPI version of ChFSI (EleChFSI) is implemented within the Elemental library, a framework for distributed memory dense linear algebra. The core of the library is the two-dimensional cyclic element-wise (“elemental” or “torus-wrap”) matrix distribution (default distribution hereafter). The $p$ MPI processes involved in the computation are logically viewed as a two-dimensional $r \times c$ process grid with $p = r \times c$. The matrix $A = [a_{ij}] \in \mathbb{F}^{n \times m}$ is distributed over the grid in such a way that the process $(s,t)$ owns the matrix

$$A_{s,t} = \begin{pmatrix}
        a_{\gamma,\delta} & a_{\gamma,\delta+c} & \cdots \\
        a_{\gamma+r,\delta} & a_{\gamma+r,\delta+c} & \cdots \\
        \vdots & \vdots & \ddots
    \end{pmatrix},$$
where $\gamma \equiv (s + \sigma_r) \mod r$ and $\delta \equiv (t + \sigma_c) \mod c$, and $\sigma_r$ and $\sigma_c$ are arbitrarily chosen alignment parameters.

For a given number $p > 1$ of processors there are several possible choices for $r$ and $c$ forming different grid shapes $(r, c) \text{ def } r \times c$. Since the grid shape can have a significant impact on the overall performance, careful experiments should be undertaken in order to determine the best choice of $(r, c)$. Another parameter which affects performance is the algorithmic block size. This term refers to the size of blocks of input data and is correlated to the square root of the L2 cache [21]. In practice, the effective size of the algorithmic block not only depends on the algorithm itself, but it is also affected by the architecture. Figure 2 shows that for EleChFSI a block size of 256 is always recommended independently of the number of cores or grid shape. This effect is imputable to the large number of matrix multiplications carried on by the filter.

![The interplay between algorithmic block size and grid shape.](image)

Figure 2: The data in this plot refer to a DGEVP of $\ell = 20$, size $n = 13,379$, and number of sought after eigenpairs $\text{NEV} = 972$, corresponding to the physical system $Au_{98}Ag_{10}$. The eigenproblem was repeatedly solved with EleChFSI using 16, 32, and 64 cores, all possible grid shapes $(r, c)$ and three distinct algorithmic block sizes.

In the EleChFSI algorithm the Hamiltonian and the approximate eigenvectors are distributed using the default distribution over the $r \times c$ grid employing the Elemental library DistMatrix class\(^1\) which internally “hides” the details about the matrix data-type, size, leading dimension, and alignments. The net effect is to lift the user from the burden of passing

\(^1\)The library provides several other matrix distributions [20].
all those attributes to internal routines as it is customary in (P)BLAS and (Sca/P)LAPACK libraries. The resulting separation of concerns allows for the parallelization of the Chebyshev filter in a straightforward fashion by calling the distributed memory implementation of ZGEMM. However, due to the generalization of the 3-term recursive relation, care must be taken with the distribution update of diagonal entries of the Hamiltonian.

The reduced eigenproblem in the Rayleigh-Ritz step is solved using a parallel implementation of the MRRR eigensolver – EleMRRR [6] – which is an integral part of Elemental. The deflation and locking mechanism deserves particular attention. When only a portion of the vectors are locked, the algorithm has to re-filter a number of vectors that may, in general, no longer have the same alignment \( \sigma_c \). To overcome this problem the Elemental interface provides (among others) the routine View, which takes as arguments two distributed matrices \( A \) and \( B \) and four integers \( i, j, \text{height} \) and \( \text{width} \) and makes \( A \) a view of the \( \text{height} \times \text{width} \) submatrix of \( B \) starting at coordinate \( (i, j) \).\(^2\) The View routine works purely on pointers and fully handles the distribution details eliminating the need of allocating additional memory where to copy the data.

![Graph](image)

(a) EleChFSI Strong scalability.

![Graph](image)

(b) EleChFSI Weak scalability.

Figure 3: EleChFSI scalability for an increasing number of cores. In plot (a) the size of the eigenproblems are kept fixed while the number of cores is progressively increased. Eigenproblems of the two bigger system in Table 1 are tested, namely \( n = 13,379 \) and \( n = 9,273 \). In plot (b) all the systems are tested keeping the ratio of data per processor fixed. Times are weighted a posteriori by a factor keeping into account the ratio of operations per data varies in a non-predictable fashion with the size of the system.

The communication for the computations is performed almost entirely in terms of collective communication within rows and columns of the process grid. Such strategy in general implies that a square grid shape is usually the best option [22]. However, since in our case we are solving for a small fraction of the eigenspectrum, the matrix of vectors \( \hat{Y}(\ell) \) is tall and skinny. Consequently we expect that a narrow rectangular grid shape will do a better job than a

\(^2\)The function is overloaded, and there are thus other different definitions.
square and wider one. This deduction is confirmed by Fig. 2 independently of the number of cores the optimal grid shape is either \((2^m, 4)\) or \((2^{m+1}, 2)\), where \(m > 2\).

4 Numerical Results and Conclusions

The set of numerical tests presented here were performed on two distinct physical systems using three different sizes for the volume of the reciprocal space defining the range of the vector \(\mathbf{G}\) appearing in (1). Consequently we obtained three sequences of eigenproblems for each physical systems. The data of the sequences of eigenproblems are summarized in Table 1. All our numerical tests were performed on JUROP A, a large general purpose cluster where each node is equipped with 2 Intel Xeon X5570 (Nehalem-EP) quad-core processors at 2.93 GHz and 24 GB memory (DDR3, 1066 MHz). The nodes are connected by an Infiniband QDR network with a Fat-tree topology. The tested routines were compiled using the Intel compilers (ver. 12.0.3) with the flag -O3 and linked to the ParTec’s ParaStation MPI library (ver. 5.0.26). The Elemental library was used in conjunction with Intel’s MKL BLAS (ver 11.0). All CPU times were measured by running each test multiple times and taking the average of the results. Eigenproblems were solved by EleChFSI by requiring the eigenpairs residuals to be lower than \(10^{-10}\).

| Material   | NEV | \(\ell_{\text{max}}\) | \(n\) | Material   | NEV | \(\ell_{\text{max}}\) | \(n\) |
|------------|-----|-----------------|-----|------------|-----|-----------------|-----|
| Au\(_{98}\)Ag\(_{10}\) | 25  | 5,638           |     | Na\(_{15}\)Cl\(_{14}\)Li | 13  | 3,893           |     |
|            | 25  | 8,970           |     |            | 13  | 6,217           |     |
|            | 25  | 13,379          |     |            | 13  | 9,273           |     |

As already mentioned in the previous sections, Fig. 2 shows unequivocally the great advantage EleChFSI obtains from the use of the eigenvectors \(\hat{Y}^{(\ell-1)}\) as input in solving the next eigenproblem \(H^{(\ell)}\) in the sequence. This behavior is independent of the physical system or spectral properties of the eigenproblems: EleChFSI experiences speed-ups higher that 2X and often well above 3X towards the end of the sequence. Figure 2 also illustrate which is the optimal choice of grid shape and algorithmic block size. The remaining numerical tests were performed using exclusively the strategies outlined above.

Fig. 3 illustrate the scalability, both strong and weak, of EleChFSI. Plot (a) shows a steady decrease of CPU time as the number of cores increases. The rate of reduction is practically the same for both systems despite their size differ by more than 30%. This plot shows that EleChFSI is extremely efficient even when the ratio of data per processor is not optimal. The weak scalability plot makes manifest the great potential of this algorithm for eigenproblems originating from FLAPW methods. The almost flatness of the two lines implies that large size eigenproblems can greatly exploit large supercomputing architectures. In other words EleChFSI has the potential of allowing the users of FLAPW-based codes to generate more complex physical systems made of thousands of atoms as opposed to just few hundreds.
Figure 4: Comparing EleChFSI with EleMRRR on eigenproblems of increasing self-consistent cycle index $\ell$. For the size of eigenproblems here tested the ScaLAPACK implementation of BXINV is comparable with EleMRRR [6]. For this reason a direct comparison with the BXINV solver is not included here.

Compared to direct solvers, EleChFSI promises to be quite competitive. Depending on the number of eigenpairs computed, our algorithm is on par or even faster than EleMRRR. In plot (a) of Fig. 4 EleChFSI appears to fall behind the direct solver when using just 64 cores. The situation improves substantially with 128 cores and at the end of the sequence both algorithms are on par. The situation is even more favorable in plot (b) where EleChFSI is already faster than EleMRRR for half of the eigenproblems in the sequence (64 cores). When the tests are repeated with 128 cores EleChFSI is unequivocally the faster of the two algorithms. Since the fraction of the spectrum computed in plot (a) and (b) is respectively $\sim 7\%$ and $\sim 3\%$, Fig. 4 shows that EleChFSI scales better than EleMRRR and is more performant when the number of eigenpairs is not too high.

In conclusion, not only EleChFSI showed to take the greatest advantage from the progressive collinearity of eigenvectors along the sequence, but it proved to easily adapt to parallel architectures. We showed how such an algorithm, parallelized for distributed memory architectures, scales extremely well over a range of cores commensurate to the size of the eigenproblems. Compared to direct eigensolvers, EleChFSI is competitive with routines out of ScaLAPACK and Elemental. Eventually the use of EleChFSI in FLAPW-based codes will enable the final user to access larger physical systems which are currently out of reach.

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