New implementation of Chebyshev filtering inside ABINIT

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Chebyshev filtering algorithm

- Eigenvalues of Eigenproblem $H\psi = \lambda S\psi$ can be represented by Λ, and eigenvectors can be represented by P
- In that case eigenproblem notation becomes $HP = SP\Lambda$ or $S^{-1}H = P\Lambda P^{-1}$
- Spectral filter T_n can be used to filter eigencomponents as given in formula: $T_n(S^{-1}H)\psi = PT_n(\Lambda)P^{-1}\psi$
- Rayleigh-Ritz procedure is used to separate the individual eigenvectors and eigenvalues, and iterate until convergence

Chebyshev filtering algorithm

- Input: a set of $N_{pw} \times N$ bands wavefunctions Ψ
- Output: the updated wave-functions Ψ
  - Locate eigenvalue spectrum
    - Compute Rayleigh quotients for every band, and set λ_- equal to the largest one
    - Set λ_+ to be an upper bound of the spectrum
    - Compute the filter center and radius $c = (\lambda_+ + \lambda_-)/2$, $r = (\lambda_+ - \lambda_-)/2$
  - Compute Chebyshev polynomial for each eigenvector
    - for each band ψ do
      - Set $\psi^0 = \psi$, and $\psi^1 = 1/r * (S^{-1} H\psi^0 - c\psi^0)$
      - for $i = 2, \ldots, n_{inner}$ do
        - $\psi^i = 2/r * (S^{-1} H\psi^{i-1} - c\psi^{i-1}) - \psi^{i-2}$
      - end for
    - end for
  - Apply Rayleigh-Ritz procedure
    - Compute the subspace matrices $H_\psi = \Psi^T H\Psi$, and $S_\psi = \Psi^T S\Psi$
    - Solve the dense generalized **eigenproblem** $H_\Psi X = S_\Psi X\Lambda$, where Λ is a diagonal matrix of **eigenvalues**, and X is the S_Ψ - orthonormal set of **eigenvectors**
    - Do the subspace rotation $\Psi \leftarrow \Psi X$

Abinit abstract layer (xg datatypes – developed by Jordan Bieder[2])

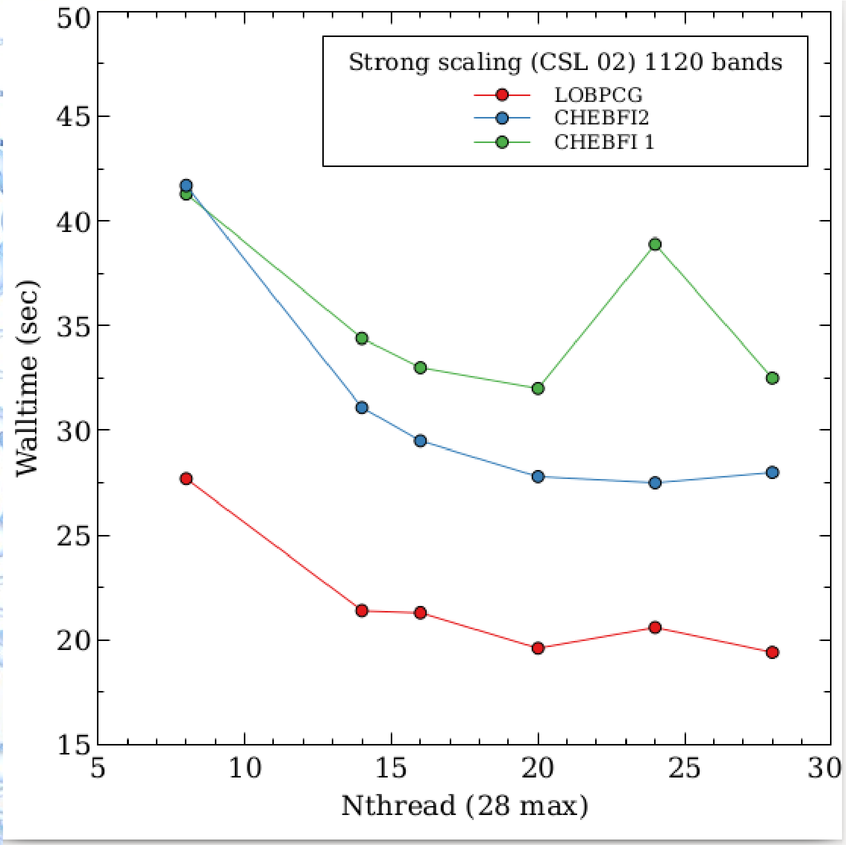
- Highly efficient multi-threaded wrapper module for BLAS/LAPACK (level-1 and level 2) routine calls
- Module is used to help developer use 2D arrays and their subblocks with ease (by xgBlock pointer objects)
- It contains sub-module used for MPI matrix transpositions (all-to-all and all-gether)
- New functions added during Chebfi2 development:
  - xgBlock_colwiseDivision
  - xgBlock_saxpy
- XG provided smooth translation of CB1 code into CB2 without worrying about particular details of BLAS or LAPACK function parameters, Fortran pointers or OpenMP pragmas and variables

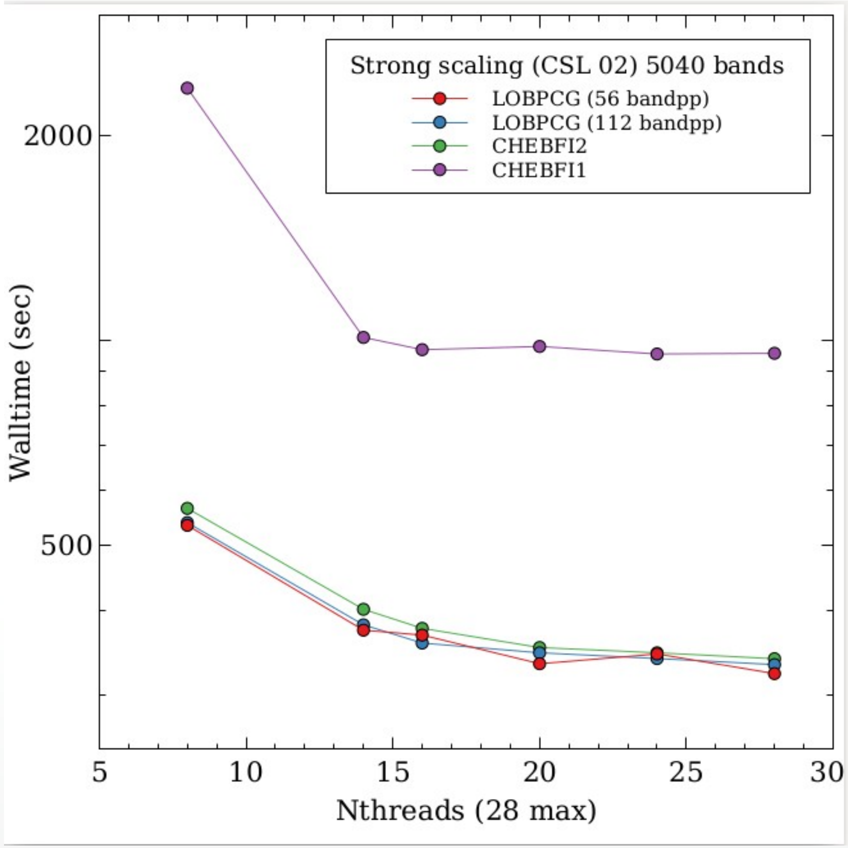
Xg usage example (Chebfi 2 nextOrderPolynom)

```
if (chebfi%paw) then
  !apply matrix inverse function
  call getBm1X(chebfi%xAXColsRows, chebfi%X_next)
else
  !copy xAXColsRows into X_next array
  call xgBlock_copy(chebfi%xAXColsRows,chebfi%X_next, 1, 1)
end if
!scale xXColsRows by center
call xgBlock_scale(chebfi%xXColsRows, center, 1)
!X_next = X_next - xXColsRows
call xgBlock_saxpy(chebfi%X_next, dble(-1.0), chebfi%xXColsRows)
!scale xXColsRows by 1/center
call xgBlock_scale(chebfi%xXColsRows, 1/center, 1)

if (iline == 0) then
  !scale X_next by 1/radius
  call xgBlock_scale(chebfi%X_next, one_over_r, 1)
else
  !scale X_next by 2/radius
  call xgBlock_scale(chebfi%X_next, two_over_r, 1)
  !X_next = X_next - X_prev
  call xgBlock_saxpy(chebfi%X_next, dble(-1.0), chebfi%X_prev)
end if
```

Different solver scaling on Intel Xeon Cascadelake





TODO list and expectations

- TODO:
  - Finalization of MPI transposition
  - Optimization of coding (Hamiltonian application and inverse matrix calculation)
  - Addition of nspinors=2 capability
  - Automation of task distribution
- Expectations:
  - Better MPI scaling of Chebfi2 than LOBPCG2 because Rayleigh-Ritz procedure is done only once (instead of once per iteration) – thus reducing communication
  - Chebfi2 will be available for use as a standalone library