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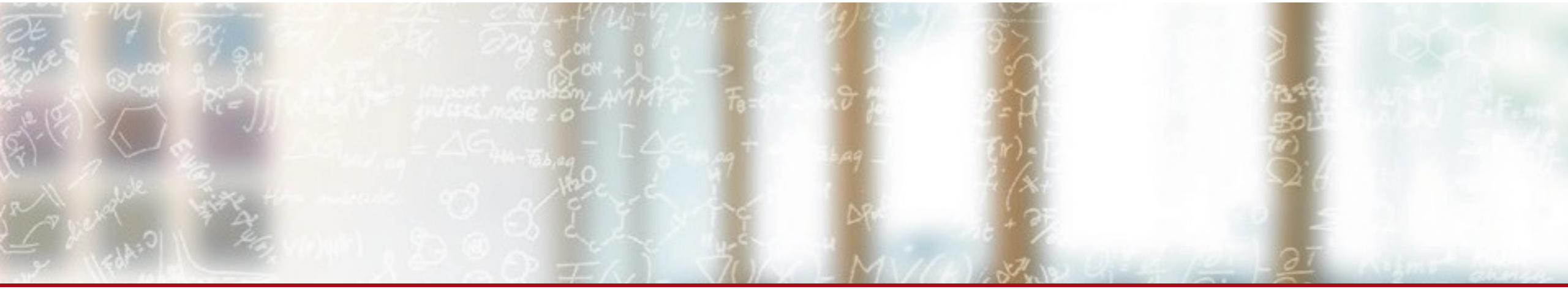

GPU acceleration of plane-wave codes using SIRIUS library

MATERIAL SCIENCE CODES ON INNOVATIVE HPC ARCHITECHTURES: TARGETING EXASCALE

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December 05, 2017

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Introduction

Hybrid supercomputers at CSCS

Tödi
AMD Opteron + NVIDIA K20X
393 Teraflops

October 2011

Hybrid supercomputers at CSCS

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Piz Daint
Intel Sandy Bridge + NVIDIA K20X
7.787 Petaflops

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Piz Daint
Intel Haswell + NVIDIA P100
25.326 Petaflops

October 2011

Novembre 2013

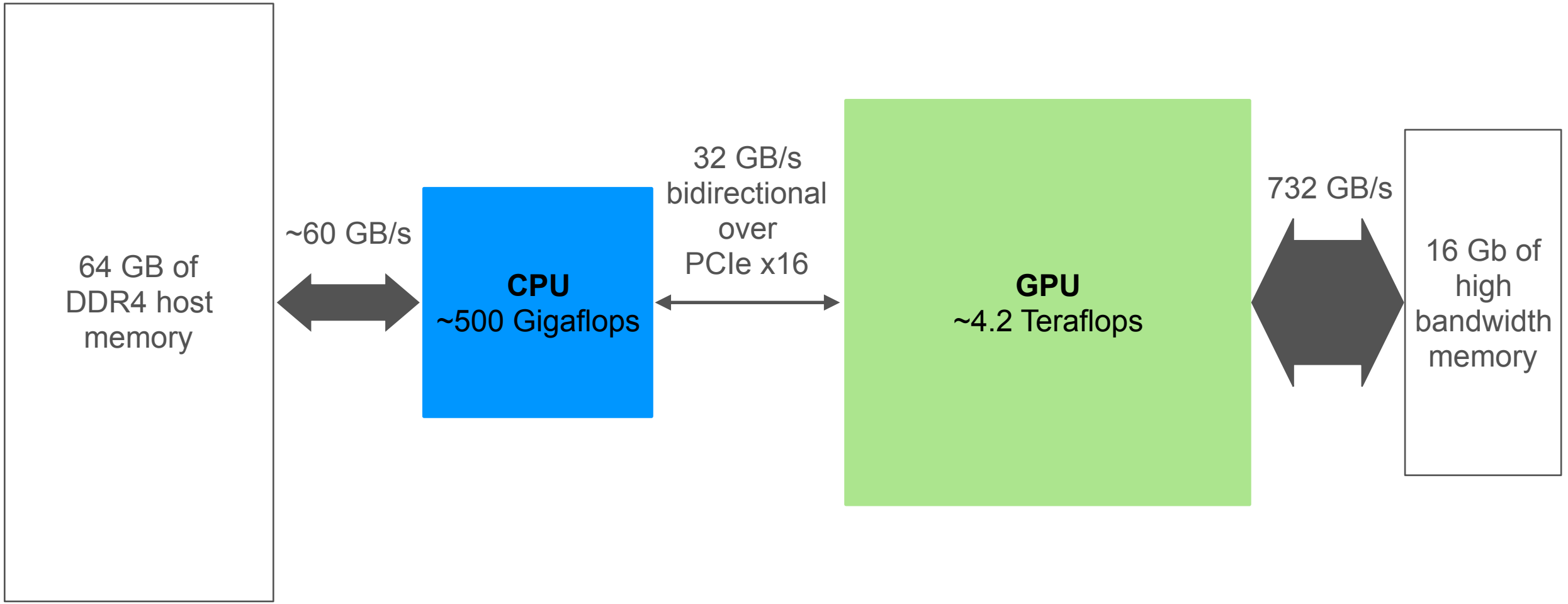
Novembre 2016

Piz Daint: #3 supercomputer in the world

Cray XC50, 5320 nodes

Intel Xeon E5-2690v3 12C, 2.6GHz, 64GB + NVIDIA Tesla P100 16GB
4.761 Teraflops / node

Piz Daint node layout



Porting codes to GPUs

No magic “silver bullet” exists!

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Usual steps in porting codes to GPUs

Porting codes to GPUs

No magic “silver bullet” exists!

Usual steps in porting codes to GPUs

- cleanup and refactor the code
- (possibly) change the data layout
- fully utilize CPU threads and prepare code for node-level parallelization
- move compute-intensive kernels to GPUs

Porting codes to GPUs

- CUDA (C / C++ / Fortran)

```
__global__ void add_pw_ekin_gpu_kernel(int num_gvec__,
                                       double alpha__,
                                       double const* pw_ekin__,
                                       cuDoubleComplex const* phi__,
                                       cuDoubleComplex const* vphi__,
                                       cuDoubleComplex* hphi__)
{
    int ig = blockIdx.x * blockDim.x + threadIdx.x;
    if (ig < num_gvec__) {
        cuDoubleComplex z1 = cuCadd(vphi__[ig], make_cuDoubleComplex(alpha__ * pw_ekin__[ig] * phi__[ig].x,
                                                                     alpha__ * pw_ekin__[ig] * phi__[ig].y));
        hphi__[ig] = cuCadd(hphi__[ig], z1);
    }
}
```

- OpenCL

```
__kernel void vector_add(const int n, __global float *a, __global float *b, __global float *c) {
  const int i = get_global_id(0);
  if (i < n) {
    c[i] = a[i] + b[i];
  }
}
```

- OpenACC

```
      acc = 0
      !$acc parallel present(x)
      !$acc loop reduction(+:acc)
      do i = 1, N
          acc = acc + x(i) * x(i)
      enddo
      !$acc end parallel
      call mpi_allreduce(acc, accglobal, 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD, err)
```

- OpenMP 4.0

```
#pragma omp target data map(tofrom: x[0:n],y[0:n])
{
    #pragma omp target
    #pragma omp for
    for (int i = 0; i < n; i++)
        y[i] += a * x[i];
}
```

Porting codes to GPUs

- CUDA (C / C++ / Fortran)

```
__global__ void add_pw_ekin_gpu_kernel(int num_gvec__,
                                       double alpha__,
                                       double const* pw_ekin__,
                                       cuDoubleComplex const* p
                                       cuDoubleComplex const* v
                                       cuDoubleComplex* hphi__)
{
    int ig = blockIdx.x * blockDim.x + threadIdx.x;
    if (ig < num_gvec__) {
        cuDoubleComplex z1 = cuCadd(vphi__[ig], make_cuDoubleCo

        hphi__[ig] = cuCadd(hphi__[ig], z1);
    }
}
```

- OpenCL

```
__kernel void vector_add(const int n, __global float *a, __global float *b, __global float *c) {
    id(0);
```

- OpenACC

```
      acc = 0
      !$acc parallel present(x)
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          acc = acc + x(i) * x(i)
      enddo
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```

4.0

```
arget data map(tofrom: x[0:n],y[0:n])

mp target
#pragma omp for
for (int i = 0; i < n; i++)
    y[i] += a * x[i];
}
```

Electronic-structure codes

Electronic structure codes

Basis functions for KS states / Atomic potential treatment	Periodic Bloch functions (plane-waves or similar)	Localized orbitals
Full-potential	FLEUR Wien2K Exciting Elk	FHI-aims FPLO
Pseudo-potential	VASP CPMD Quantum ESPRESSO Abinit Qbox	CP2K SIESTA OpenMX

Atomic total energies with LAPW

	Hydrogen	Helium	Lithium	Beryllium	Boron	Carbon	Nirogen	Oxygen	Fluorine	Neon
NIST	-0.478671	-2.834836	-7.343957	-14.447209			-54.136799			-128.233481
LAPW	-0.478671	-2.834835	-7.343958	-14.447209	-24.356062	-37.470324	-54.136792	-74.531333	-99.114324	-128.233477
MADNESS	-0.478671	-2.834836	-7.343957	-14.447209	-24.356065	-37.470329	-54.136798	-74.531345	-99.114902	-128.233481
NWCHEM					-24.356064	-37.470328	-54.136799	-74.531344	-99.114901	
	$1s^1$	$1s^2$	$2s^1$	$2s^2$	$2s^2p^1$	$2s^2p^2$	$2s^2p^3$	$2s^2p^4$	$2s^2p^5$	$2s^2p^6$

Linearized augmented plane-wave method (LAPW):

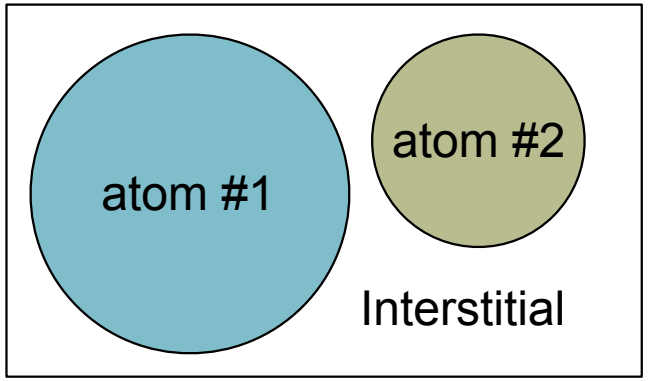
- provides a very high accuracy of the DFT total energy
- designed for crystalline solids
- considered as a gold standard for electronic structure simulations

Delta DFT codes effort

Code	Version	Basis	Electron treatment	Δ-value	Authors
WIEN2k	13.1	LAPW/APW+lo	all-electron	0 meV/atom	S. Cottenier [16]
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic atomic_zora scalar)	0.2 meV/atom	ASE [2,16]
Exciting	development version	LAPW+xlo	all-electron	0.2 meV/atom	Exciting [10,16]
Elk	3.1.5	APW+lo	all-electron	0.3 meV/atom	Elk [14,16]
Quantum ESPRESSO	5.1	plane waves	SSSP Accuracy (mixed NC/US/PAW potential library)	0.3 meV/atom	QuantumESPRESSO [12,16]
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic zora scalar 1e-12)	0.3 meV/atom	ASE [2]
VASP	5.2.12	plane waves	PAW 2015 GW-ready (5.4)	0.3 meV/atom	K. Lejaeghere [16]
ABINIT	7.8.2	plane waves	PAW JTH v1.0	0.4 meV/atom	F. Jollet and M. Torrent
FLEUR	0.26	LAPW (+lo)	all-electron	0.4 meV/atom	FLEUR [9,16]

Full-potential linearized augmented plane-wave method

- Unit cell is partitioned into “muffin-tin” spheres and interstitial region
- Inside MT spheres spherical harmonic expansion is used
- In the interstitial region functions are expanded in plane-waves



Full-potential linearized augmented plane-wave method

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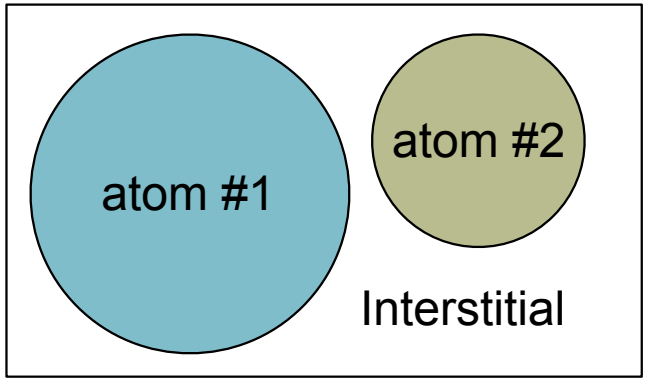
Basis functions:

$$\varphi_{\mathbf{G}+\mathbf{k}}(\mathbf{r}) = \begin{cases} \sum_{\ell m} \sum_{\nu=1}^{O_\ell^\alpha} A_{\ell m \nu}^\alpha(\mathbf{G}+\mathbf{k}) u_{\ell\nu}^\alpha(r) Y_{\ell m}(\hat{\mathbf{r}}) & \mathbf{r} \in \mathrm{MT}\alpha \\ \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{G}+\mathbf{k})\mathbf{r}} & \mathbf{r} \in \mathrm{I} \end{cases}$$



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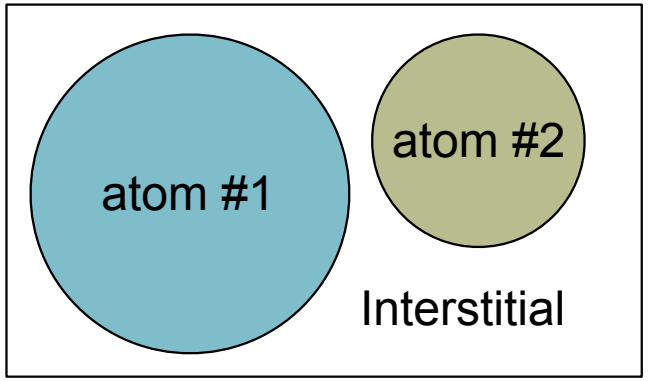


Potential and density:

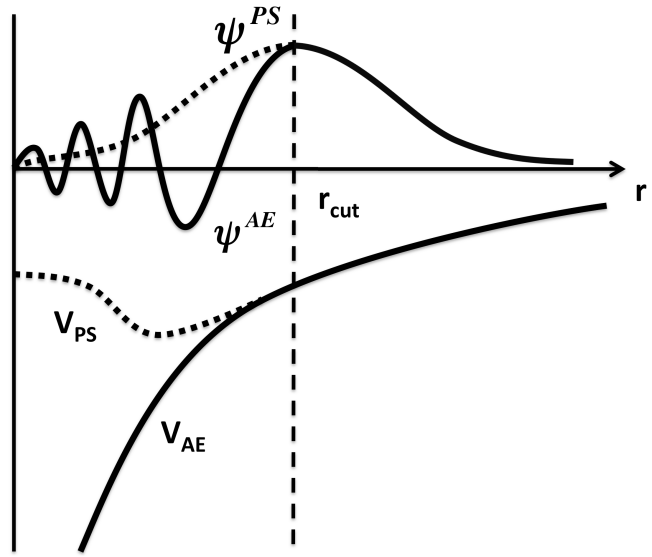
$$V(\mathbf{r}) = \begin{cases} \sum_{\ell m} V_{\ell m}^\alpha(r) Y_{\ell m}(\hat{\mathbf{r}}) & \mathbf{r} \in \mathrm{MT}\alpha \\ \sum_{\mathbf{G}} V(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}} & \mathbf{r} \in \mathrm{I} \end{cases} \qquad \rho(\mathbf{r}) = \begin{cases} \sum_{\ell m} \rho_{\ell m}^\alpha(r) Y_{\ell m}(\hat{\mathbf{r}}) & \mathbf{r} \in \mathrm{MT}\alpha \\ \sum_{\mathbf{G}} \rho(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}} & \mathbf{r} \in \mathrm{I} \end{cases}$$

Full-potential linearized augmented plane-wave method

- No approximation to atomic potential
- Core states are included
- Number of basis functions: ~100 / atom
- Number of valence states: ~15-20% of the total basis size
- Large condition number of the overlap matrix
- Full diagonalization of dense matrix is required (iterative subspace diagonalization schemes are not efficient)
- Atomic forces can be easily computed
- Stress tensor can’t be easily computed (N-point numerical scheme is required)

Pseudopotential plane-wave method

- Unit cell is mapped to a regular grid
- All functions are expanded in plane-waves
- Atomic potential is replaced by a pseudopotential $\hat{V}_{\mathrm{PS}} = V_{loc}(\mathbf{r}) + \sum_{\alpha} \sum_{\xi\xi'} |\beta_{\xi}^{\alpha}\rangle D_{\xi\xi'}^{\alpha} \langle\beta_{\xi'}^{\alpha}|$



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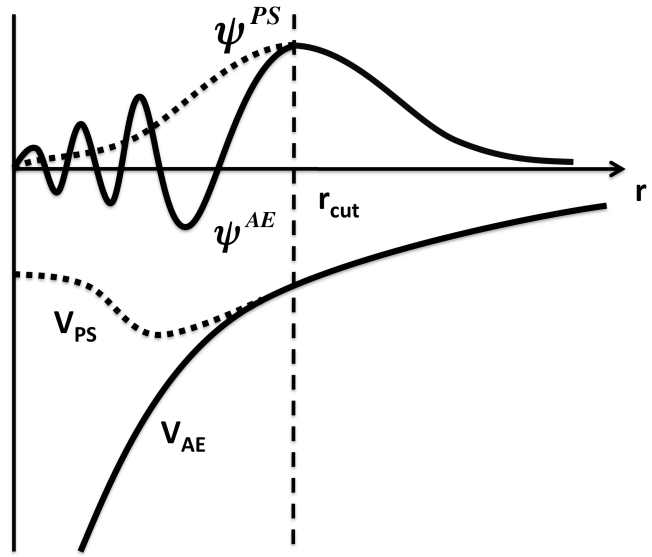
Basis functions:

$$\varphi_{\mathbf{G}+\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{G}+\mathbf{k})\mathbf{r}}$$



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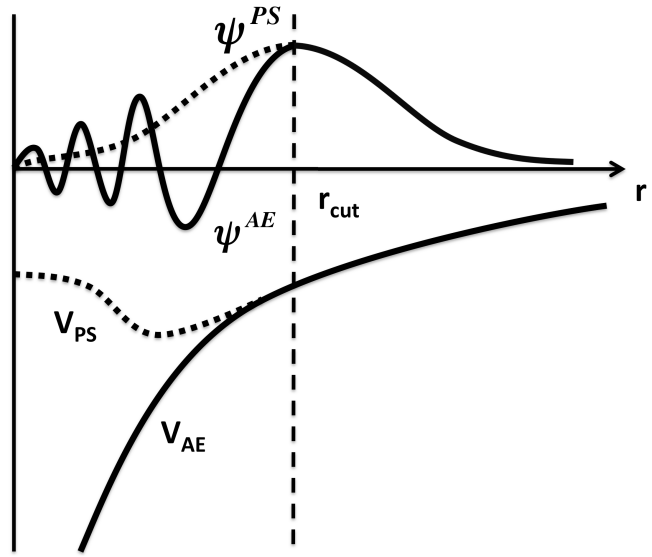

Potential and density:

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}} \qquad \rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}}$$

Pseudopotential plane-wave method

- Approximation to atomic potential
- Core states are excluded
- Number of basis functions: ~1000 / atom
- Number of valence states: ~0.001 - 0.01% of the total basis size
- Efficient iterative subspace diagonalization schemes exist
- Atomic forces can be easily computed
- Stress tensor can be easily computed

Common features of the FP-LAPW and PP-PW methods

- Definition of the unit cell (atoms, atom types, lattice vectors, symmetry operations, etc.)
- Definition of the reciprocal lattice, plane-wave cutoffs, **G** vectors, **G+k** vectors
- Definition of the wave-functions
- FFT driver
- Generation of the charge density on the regular grid
- Generation of the XC-potential
- Symmetrization of the density, potential and occupancy matrices
- Low-level numerics (spherical harmonics, Bessel functions, Gaunt coefficients, spline interpolation, Wigner D-matrix, linear algebra wrappers, etc.)

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SIRIUS library

Motivation for a common domain specific library

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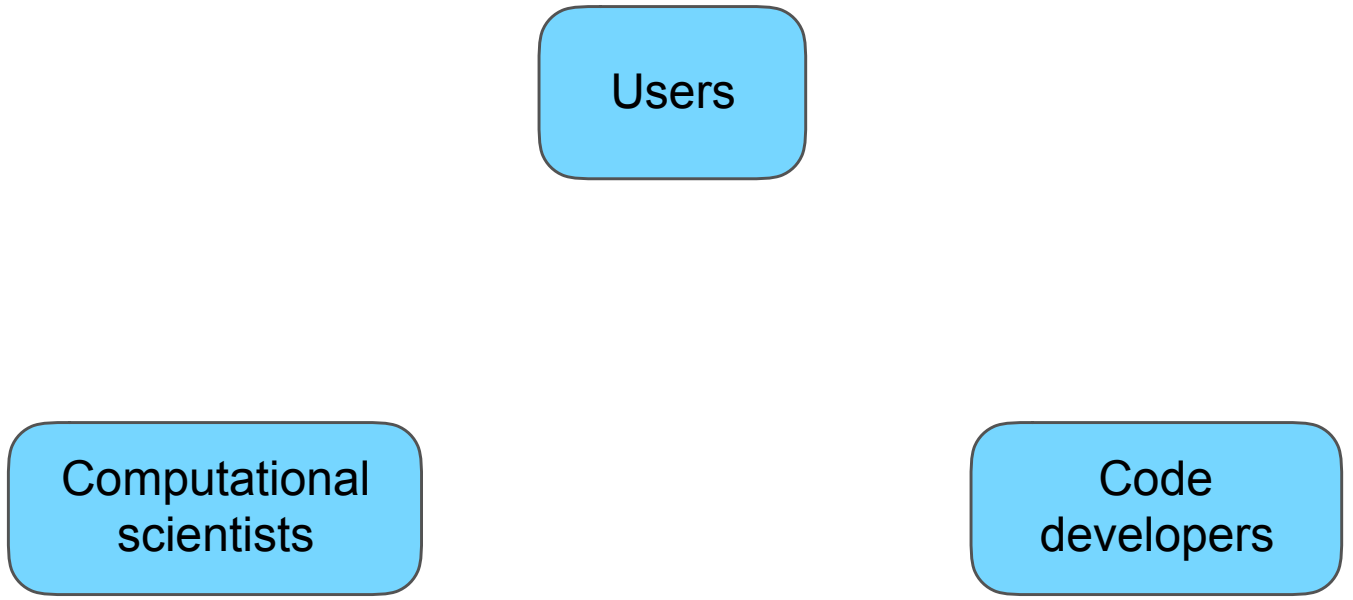
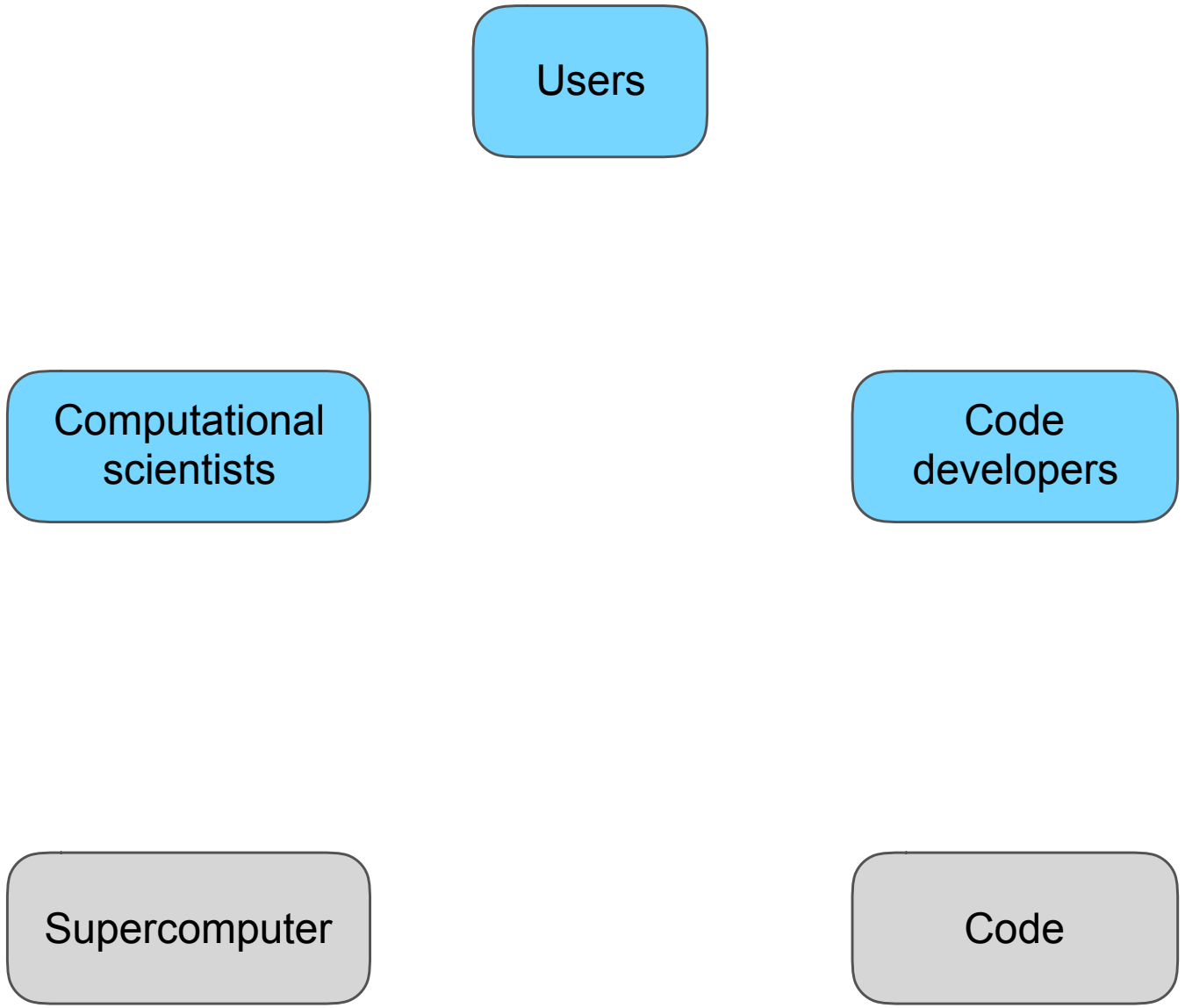


Motivation for a common domain specific library



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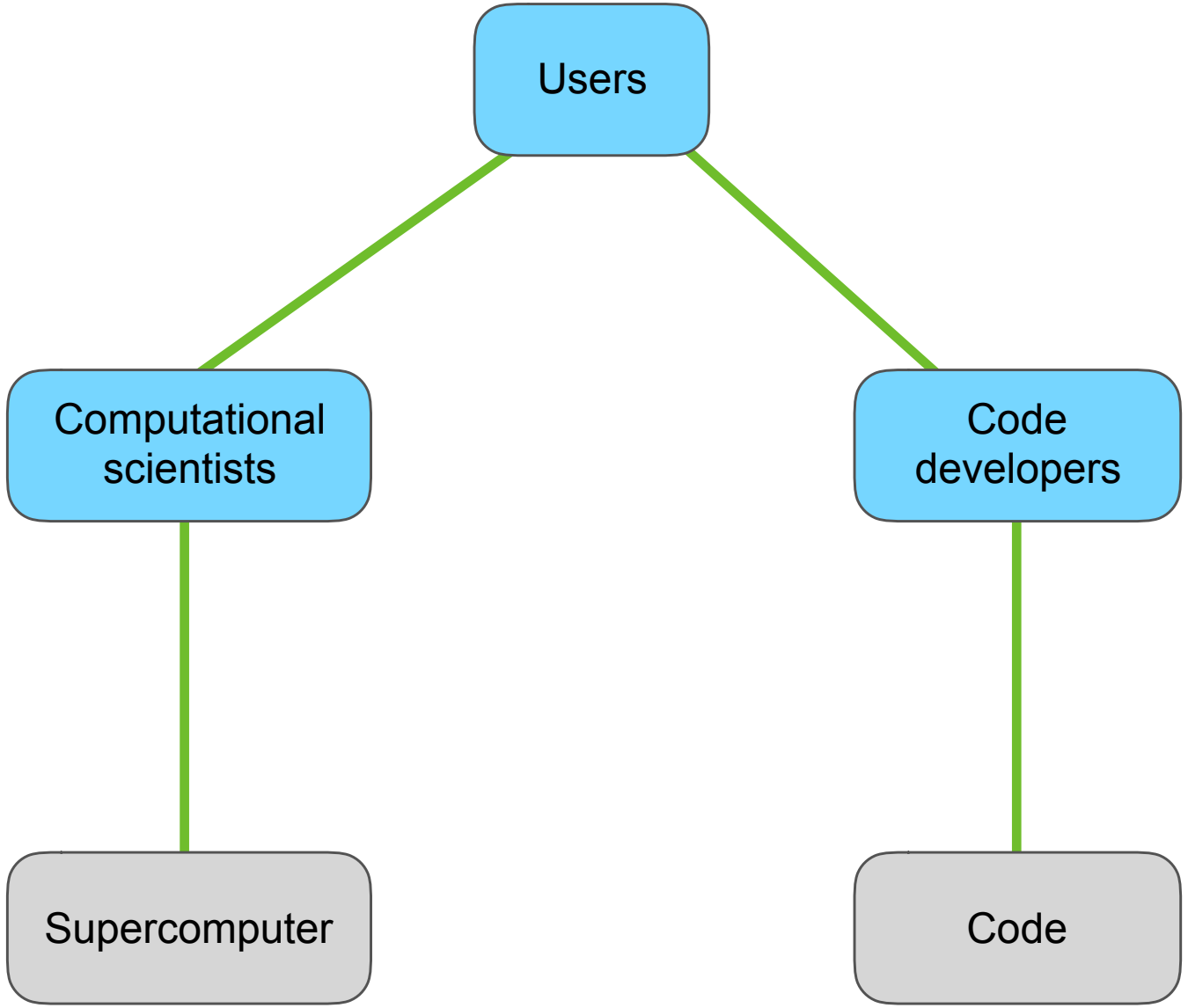

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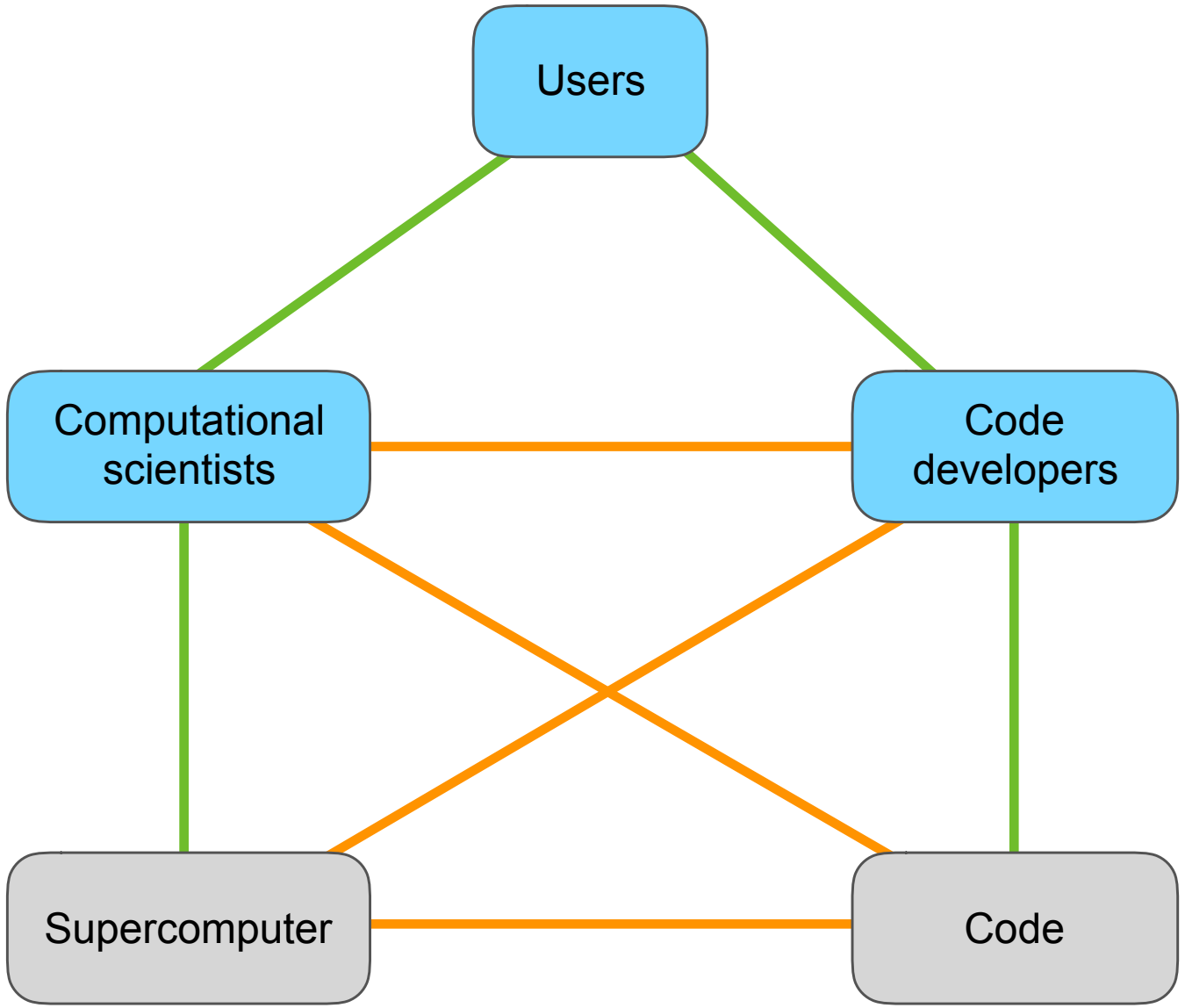
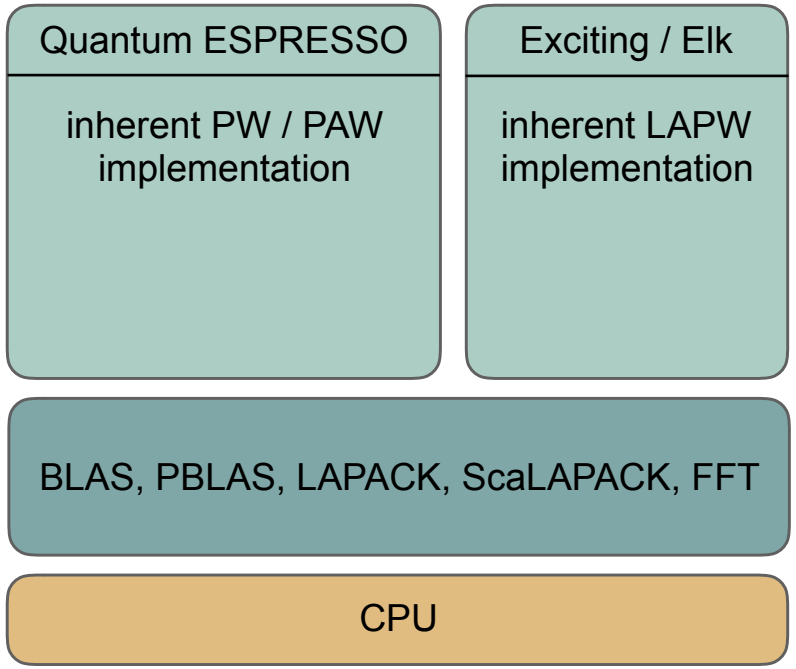


Motivation for a common domain specific library

Extend the legacy Fortran codes with the API calls to a domain-specific library which runs on GPUs and other novel architectures.



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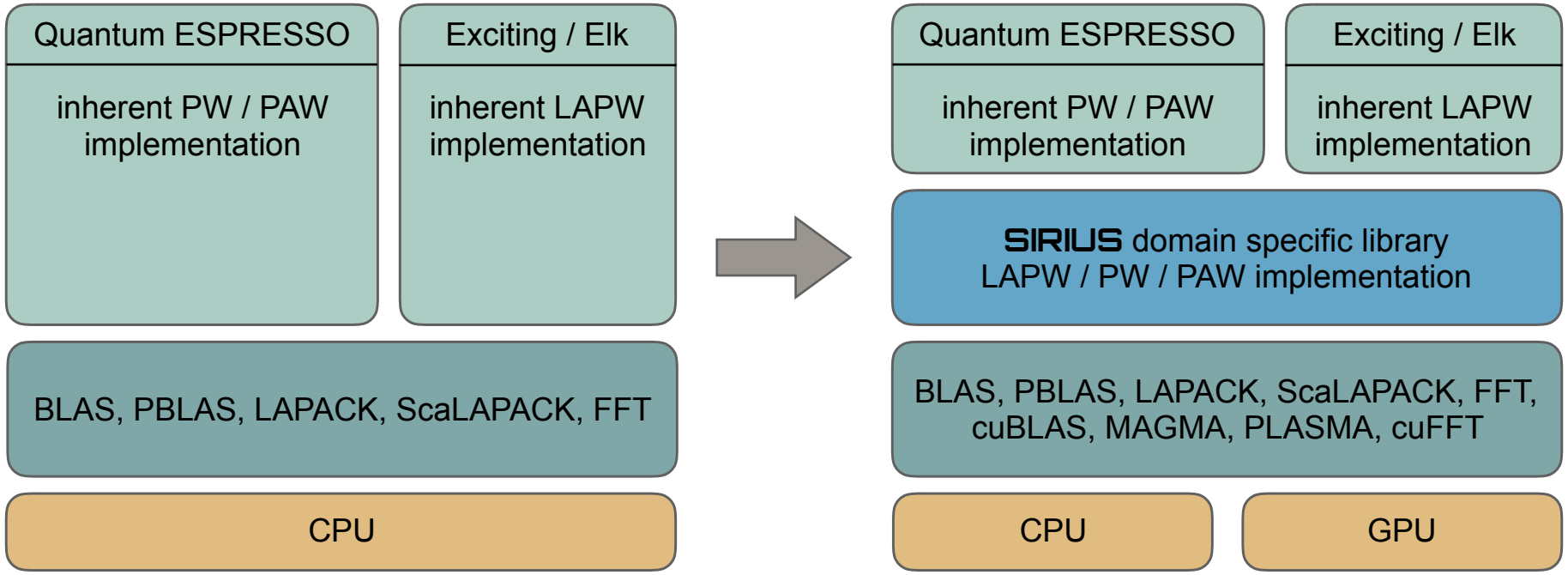
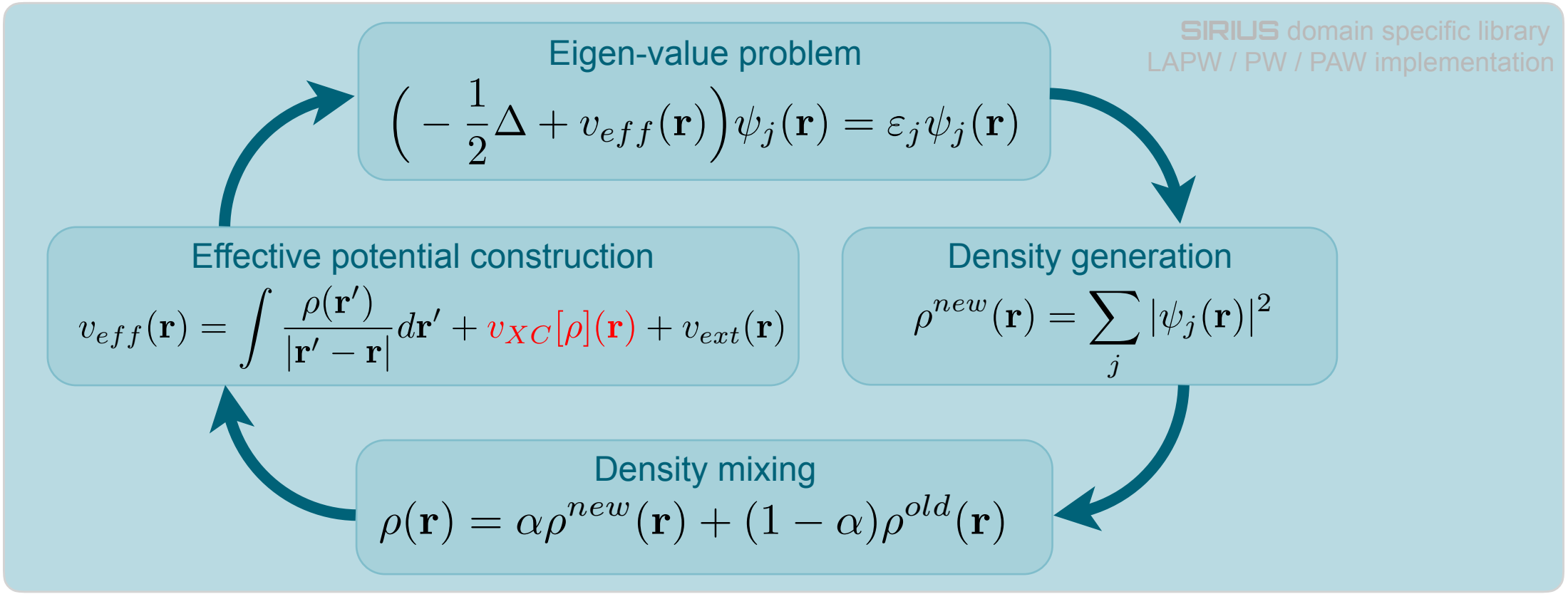


Where to draw the line?



Output:

wave-functions $\psi_j(\mathbf{r})$ and eigen energies ε_j

charge density $\rho(\mathbf{r})$ and magnetization $\mathbf{m}(\mathbf{r})$

total energy E_{tot}, atomic forces $\mathbf{F}_\alpha$ and stress tensor $\sigma_{\alpha\beta}$

SIRIUS library

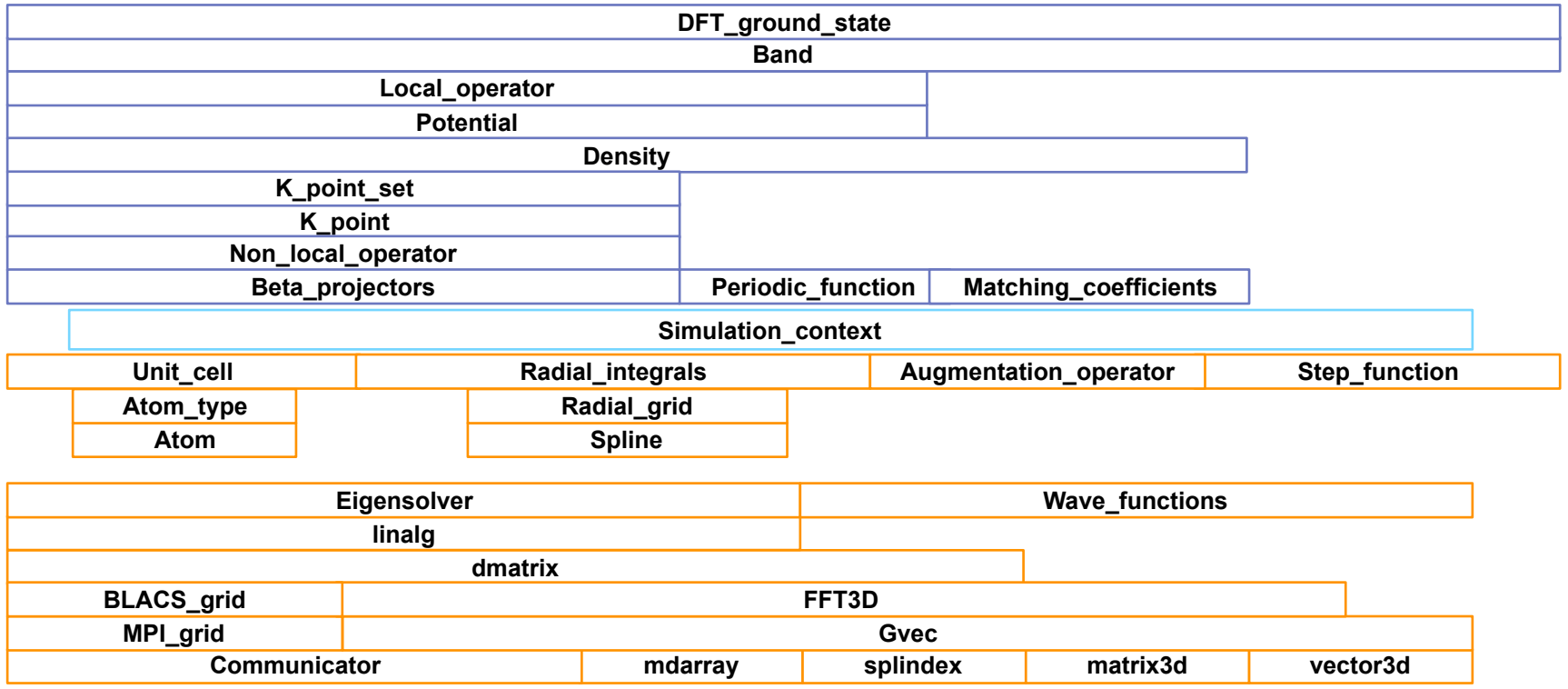
- full-potential (L)APW+lo
  - non-magnetic, collinear and non-collinear magnetic ground states
  - non-relativistic, ZORA and IORA valence solvers
  - Dirac solver for core states

- norm-conserving, ultrasoft and PAW pseudopotentials
  - non-magnetic, collinear and non-collinear magnetic ground states
  - spin-orbit correction
  - atomic forces
  - stress tensor
  - Gamma-point case

SIRIUS library

https://github.com/electronic-structure/SIRIUS

SIRIUS is a collection of classes that abstract away the different building blocks of PW and LAPW codes. The class composition hierarchy starts from the most primitive classes (**Communicator**, **mdarray**, etc.) and progresses towards several high-level classes (**DFT_ground_state**, **Band**, **Potential**, etc.). The code is written in C++11 with MPI, OpenMP and CUDA programming models.



Doxygen documentation

https://electronic-structure.github.io/SIRIUS-doc/

dRlm_dr()

```
static void sirius::SHT::dRlm_dr ( int                          lmax__,
                                   vector3d< double > &         r__,
                                   mdarray< double, 2 > &       data__
                                 )
```

inline static

Compute the derivatives of real spherical harmonics over the components of cartesian vector.

The following derivative is computed:

$$\frac{\partial R_{\ell m}(\theta_r,\phi_r)}{\partial r_\mu} = \frac{\partial R_{\ell m}(\theta_r,\phi_r)}{\partial \theta_r}\frac{\partial \theta_r}{\partial r_\mu} + \frac{\partial R_{\ell m}(\theta_r,\phi_r)}{\partial \phi_r}\frac{\partial \phi_r}{\partial r_\mu}$$

The derivatives of angles are:

$$\frac{\partial \theta_r}{\partial r_x} = \frac{\cos(\phi_r)\cos(\theta_r)}{r}$$
$$\frac{\partial \theta_r}{\partial r_y} = \frac{\cos(\theta_r)\sin(\phi_r)}{r}$$
$$\frac{\partial \theta_r}{\partial r_z} = -\frac{\sin(\theta_r)}{r}$$

and

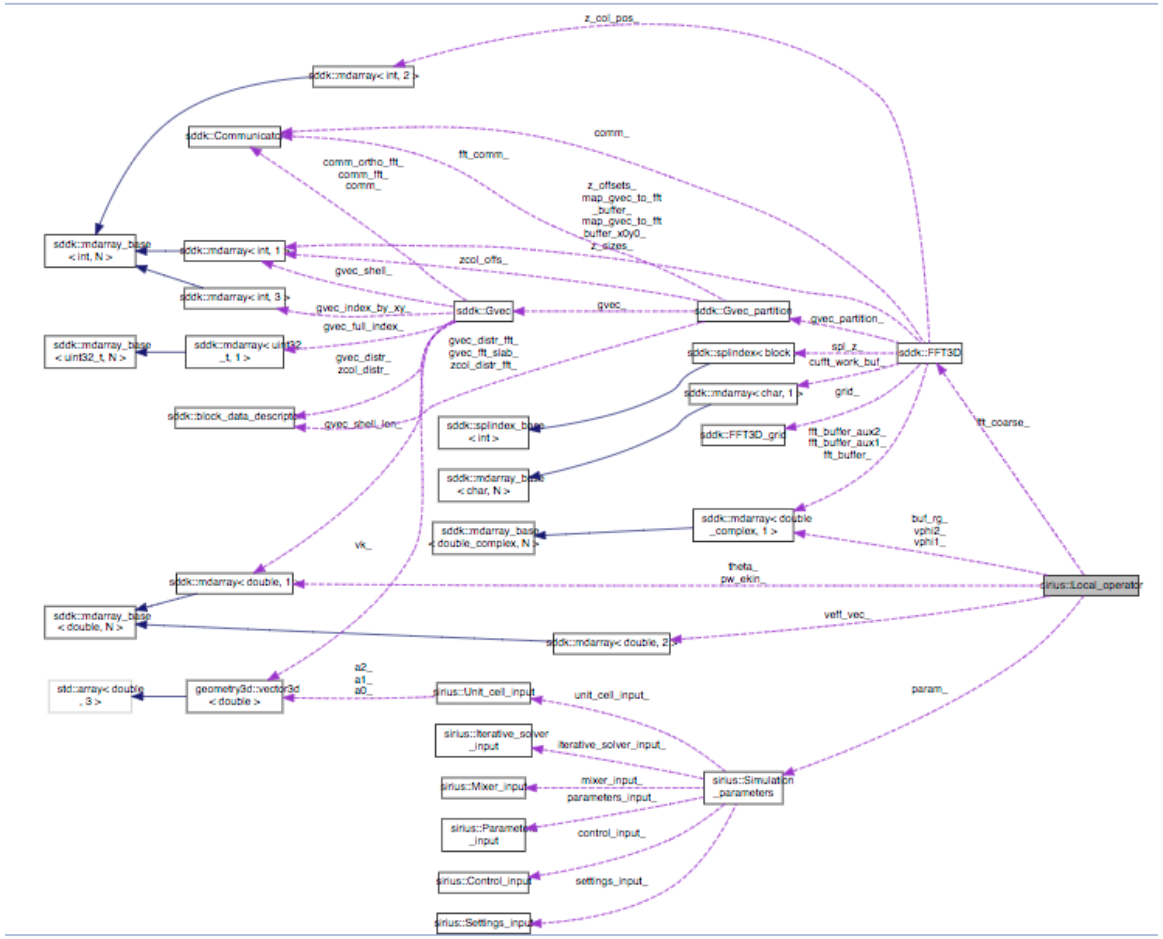
$$\frac{\partial \phi_r}{\partial r_x} = -\frac{\sin(\phi_r)}{\sin(\theta_r)r}$$
$$\frac{\partial \phi_r}{\partial r_y} = \frac{\cos(\phi_r)}{\sin(\theta_r)r}$$
$$\frac{\partial \phi_r}{\partial r_z} = 0$$

The derivative of ϕ has discontinuities at $\theta = 0, \theta = \pi$. This, however, is not a problem, because multiplication by the the derivative of $R_{\ell m}$ removes it.
The following functions have to be hardcoded:

$$\frac{\partial R_{\ell m}(\theta,\phi)}{\partial \theta}$$
$$\frac{\partial R_{\ell m}(\theta,\phi)}{\partial \phi}\frac{1}{\sin(\theta)}$$

Mathematica script for spherical harmonic derivatives:

```
Rlm[l_, m_, th_, ph_] :=
 If[m > 0, Sqrt[2]*ComplexExpand[Re[SphericalHarmonicY[l, m, th, ph]]],
   If[m < 0, Sqrt[2]*ComplexExpand[Im[SphericalHarmonicY[l, m, th, ph]]],
     If[m == 0, ComplexExpand[Re[SphericalHarmonicY[l, 0, th, ph]]]]
   ]
 ]
Do[Print[FullSimplify[D[Rlm[l, m, theta, phi], theta]]], {l, 0, 4}, {m, -l, l}]
Do[Print[FullSimplify[TrigExpand[D[Rlm[l, m, theta, phi], phi]/Sin[theta]]]], {l, 0, 4}, {m, -l, l}]
```



Potential class

- Generate LDA / GGA exchange-correlation potential from the density

$$v^{XC}(\mathbf{r}) = \frac{\delta E^{XC}[\rho(\mathbf{r}), \mathbf{m}(\mathbf{r})]}{\delta \rho(\mathbf{r})} \qquad \mathbf{B}^{XC}(\mathbf{r}) = \frac{\delta E^{XC}[\rho(\mathbf{r}), \mathbf{m}(\mathbf{r})]}{\delta \mathbf{m}(\mathbf{r})}$$

- Generate Hartree potential

$$v^{H}(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$$

- Generate local part of pseudo-potential

$$V_{loc}(\mathbf{G}) = \frac{1}{V} \sum_{\mathbf{T},\alpha} \int e^{-i\mathbf{G}\mathbf{r}} V_{loc}^{\alpha}(\mathbf{r} - \mathbf{T} - \tau_{\alpha}) d\mathbf{r}$$

- Generate D-operator matrix

$$D_{\xi\xi'}^{\alpha} = \int V(\mathbf{r}) Q_{\xi\xi'}^{\alpha}(\mathbf{r}) d\mathbf{r}$$

Density class

- Generate charge density and magnetization from the valence wave-functions

$$\boldsymbol{\rho}(\mathbf{r}) = \frac{1}{2}\Big(\mathbf{I}\rho(\mathbf{r}) + \boldsymbol{\sigma}\mathbf{m}(\mathbf{r})\Big) = \frac{1}{2}\begin{pmatrix} \rho(\mathbf{r}) + m_z(\mathbf{r}) & m_x(\mathbf{r}) - im_y(\mathbf{r}) \\ m_x(\mathbf{r}) + im_y(\mathbf{r}) & \rho(\mathbf{r}) - m_z(\mathbf{r}) \end{pmatrix} = \sum_j^{occ} \begin{pmatrix} \psi_j^{\uparrow *}(\mathbf{r})\psi_j^{\uparrow}(\mathbf{r}) & \psi_j^{\downarrow *}(\mathbf{r})\psi_j^{\uparrow}(\mathbf{r}) \\ \psi_j^{\uparrow *}(\mathbf{r})\psi_j^{\downarrow}(\mathbf{r}) & \psi_j^{\downarrow *}(\mathbf{r})\psi_j^{\downarrow}(\mathbf{r}) \end{pmatrix}$$

- Generate core charge density (full-potential case)
- Generate density matrix

$$d^{\alpha}_{\xi\xi'} = \langle \beta^{\alpha}_{\xi} | \hat{N} | \beta^{\alpha}_{\xi'} \rangle = \sum_{j\mathbf{k}} \langle \beta^{\alpha}_{\xi} | \Psi_{j\mathbf{k}} \rangle n_{j\mathbf{k}} \langle \Psi_{j\mathbf{k}} | \beta^{\alpha}_{\xi'} \rangle$$

- Augment charge density $\tilde{\rho}(\mathbf{G}) = \sum_{\alpha} \sum_{\xi\xi'} d^{\alpha}_{\xi\xi'} Q^{\alpha}_{\xi'\xi}(\mathbf{G})$

- Symmetrize density and magnetization
- Mix density and magnetization

Band class

- Setup and solves the Kohn-Sham eigen-value problem

$$\hat{\mathbf{H}}|\Psi\rangle = \varepsilon|\Psi\rangle$$

  - Full-potential LAPW case: $\mathbf{H}x=\varepsilon\mathbf{S}x$, direct diagonalization of dense matrix

  - Pseudopotential PW case: $\mathbf{H}x=\varepsilon x$ (norm-conserving pseudo) or $\mathbf{H}x=\varepsilon\mathbf{S}x$ (ultrasoft pseudo), iterative diagonalization of dense matrix
    - Conjugate gradient
    - LOBPCG
    - RMM-DIIS
    - Chebyshev filtering method
    - Davidson algorithm

Band class

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All solvers were tried, Davidson method works the best

Davidson iterative solver

- We want to solve eigen-value problem $\mathbf{H}\tilde{\psi}_j = \varepsilon_j \tilde{\psi}_j$

Davidson iterative solver

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Key idea of the Davidson iterative solver: start with a subspace spanned by a guess to ψ_j and expand it with preconditioned residuals.

Davidson iterative solver: application of the Hamiltonian

- Application of the Laplace operator (kinetic energy)

$$-\frac{1}{2}\Delta\psi_j(\mathbf{r}) = \sum_{\mathbf{G}}\Big(-\frac{1}{2}\Delta e^{i\mathbf{G}\mathbf{r}}\Big)\tilde{\psi}_j(\mathbf{G}) = \sum_{\mathbf{G}} e^{i\mathbf{G}\mathbf{r}}\frac{G^2}{2}\tilde{\psi}_j(\mathbf{G})$$

- Application of the local part of potential

$$\tilde{\psi}_j(\mathbf{G}) \xrightarrow{FFT^{-1}} \psi_j(\mathbf{r}) \rightarrow v_{eff}(\mathbf{r})\psi_j(\mathbf{r}) \xrightarrow{FFT} \tilde{h}_{\psi_j}(\mathbf{G})$$

- Application of the non-local local part of potential

$$\sum_{\alpha\xi}\beta^{\alpha}_{\xi}(\mathbf{G})\sum_{\xi'}D^{\alpha}_{\xi\xi'}\sum_{\mathbf{G}'}\beta^{\alpha*}_{\xi'}(\mathbf{G}')\tilde{\psi}_j(\mathbf{G}') \rightarrow \tilde{h}_{\psi_j}(\mathbf{G})$$

zgemm#1

zgemm#2

zgemm#3

Davidson iterative solver: algorithm

- Initialize the trial basis set: $\tilde{\phi}_j^0 \Leftarrow \tilde{\psi}_j$

Davidson iterative solver: algorithm

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Davidson iterative solver: algorithm

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```
=== QE output ===
Dynamical RAM for wfc: 2.50 MB
Dynamical RAM for <psi|beta>: 2.81 MB
Dynamical RAM for psi: 10.02 MB
Dynamical RAM for hpsi: 10.02 MB
Dynamical RAM for spsi: 10.02 MB
============================
```

and psi is $\tilde{\phi}_j$ here

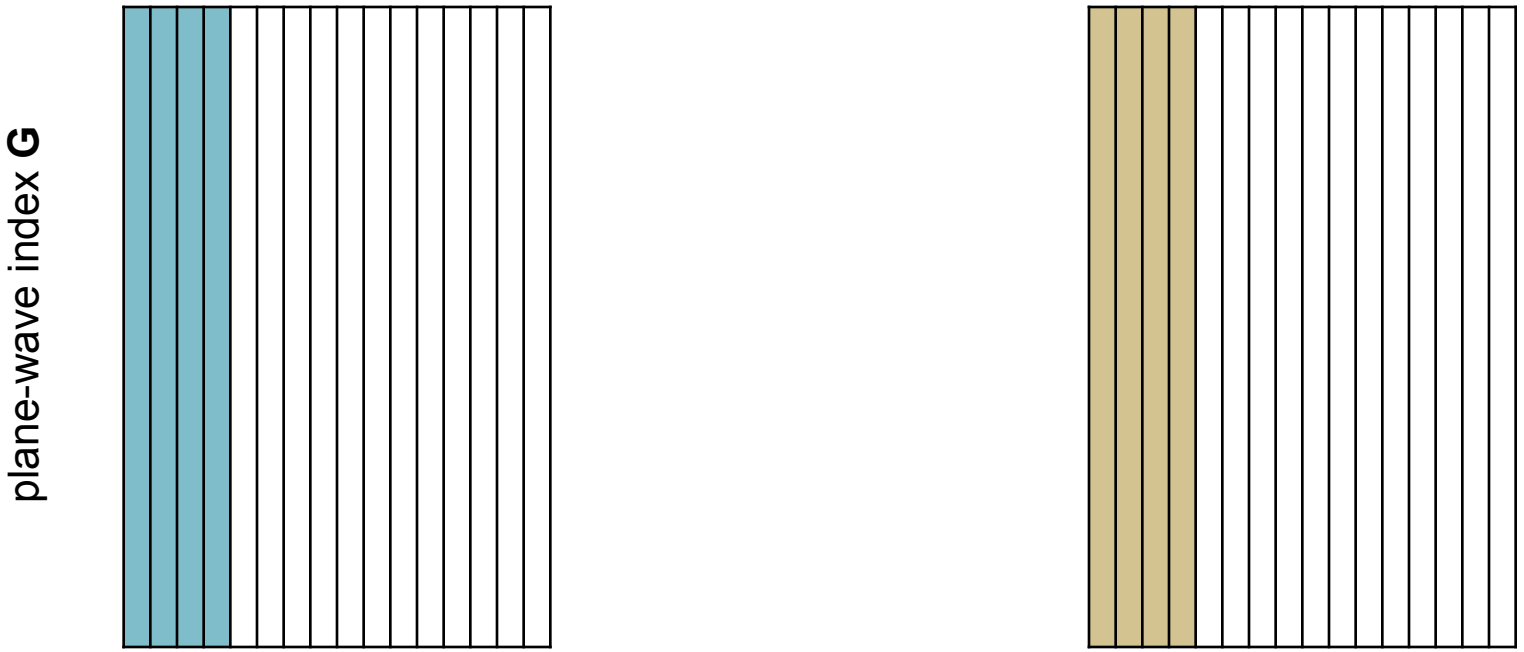
diago_david_ndim	INTEGER
Default:	4
diago_thr_init	REAL
diago_full_acc	LOGICAL

Davidson iterative solver

- Initialize subspace basis functions and apply Hamiltonian

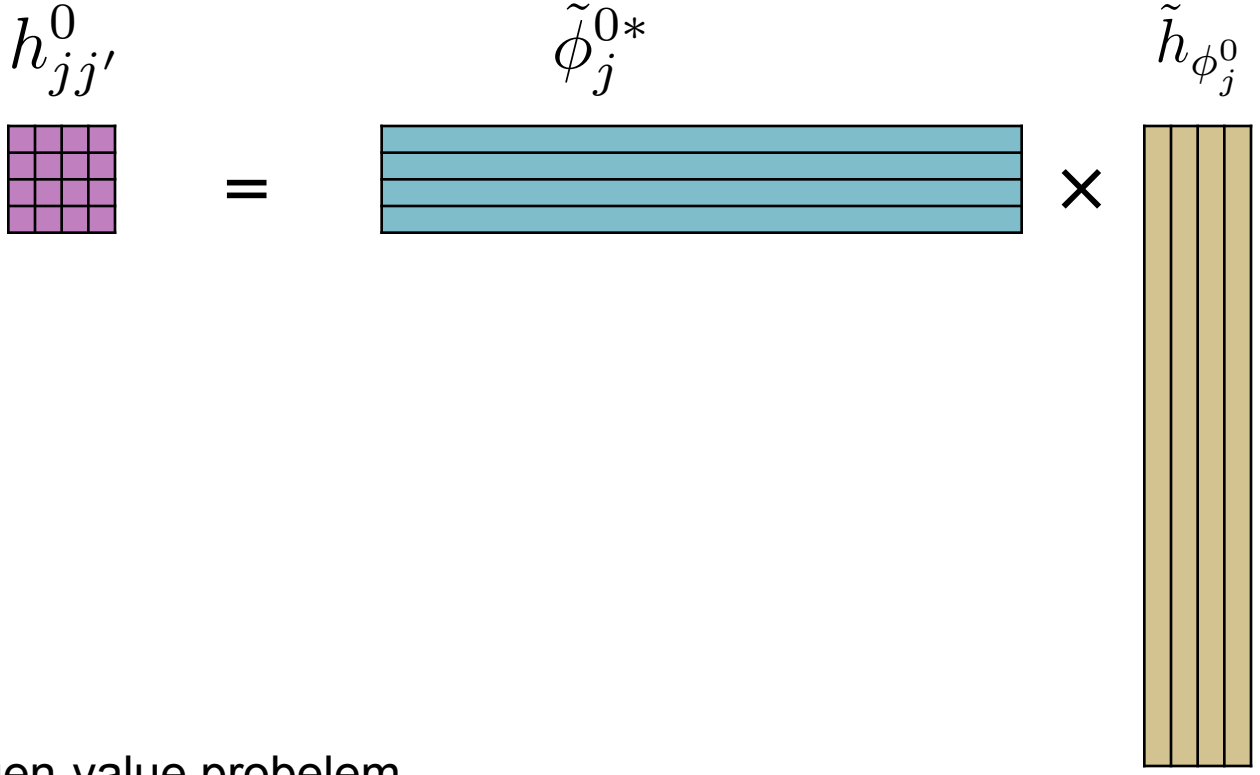
$\tilde{\phi}_j^0$

$\tilde{h}_{\phi_j^0} = \mathbf{H}\tilde{\phi}_j^0$

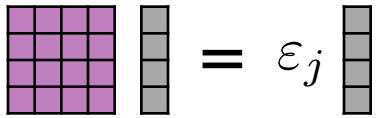


Davidson iterative solver

- Compute reduced Hamiltonian matrix

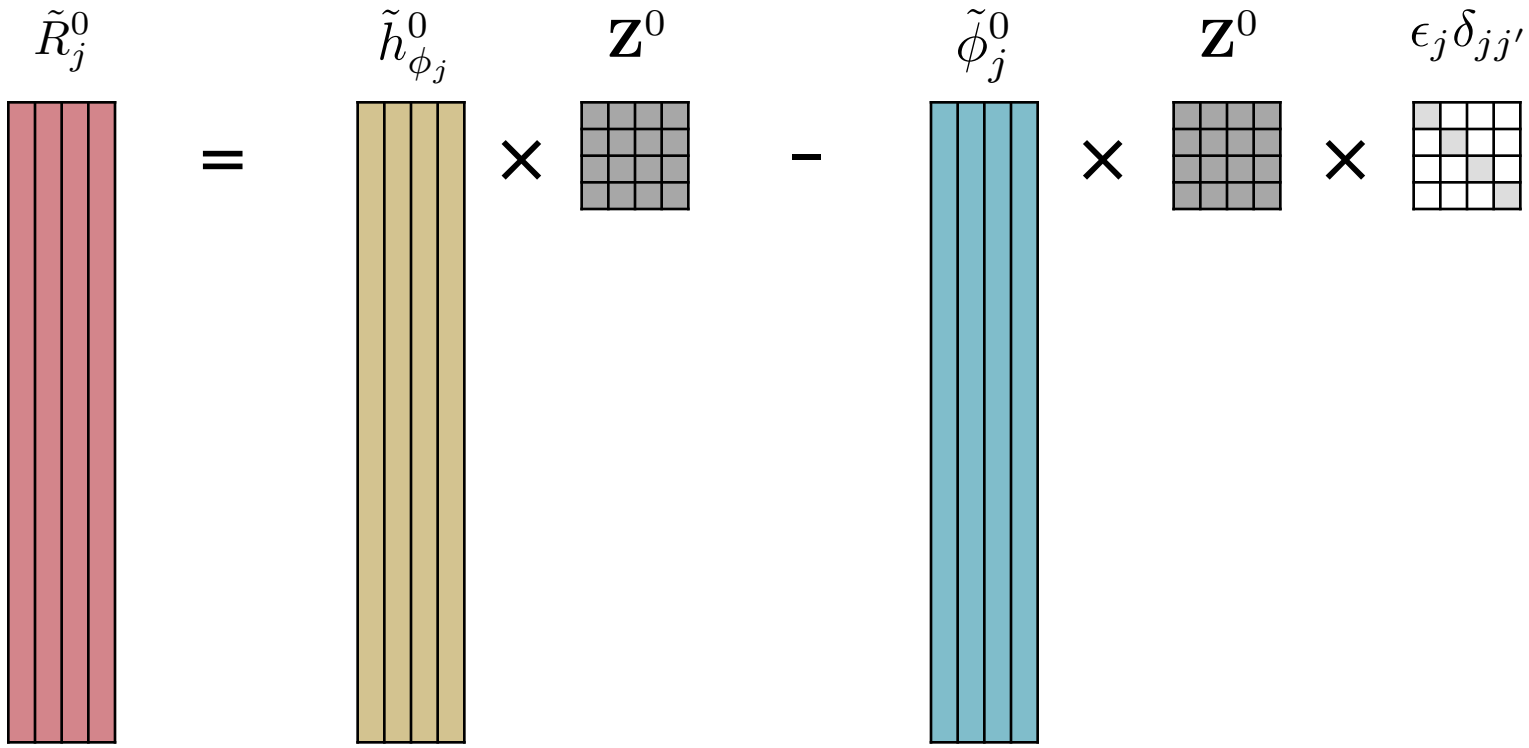


- Compute eigen-value probelem



Davidson iterative solver

- Compute residuals



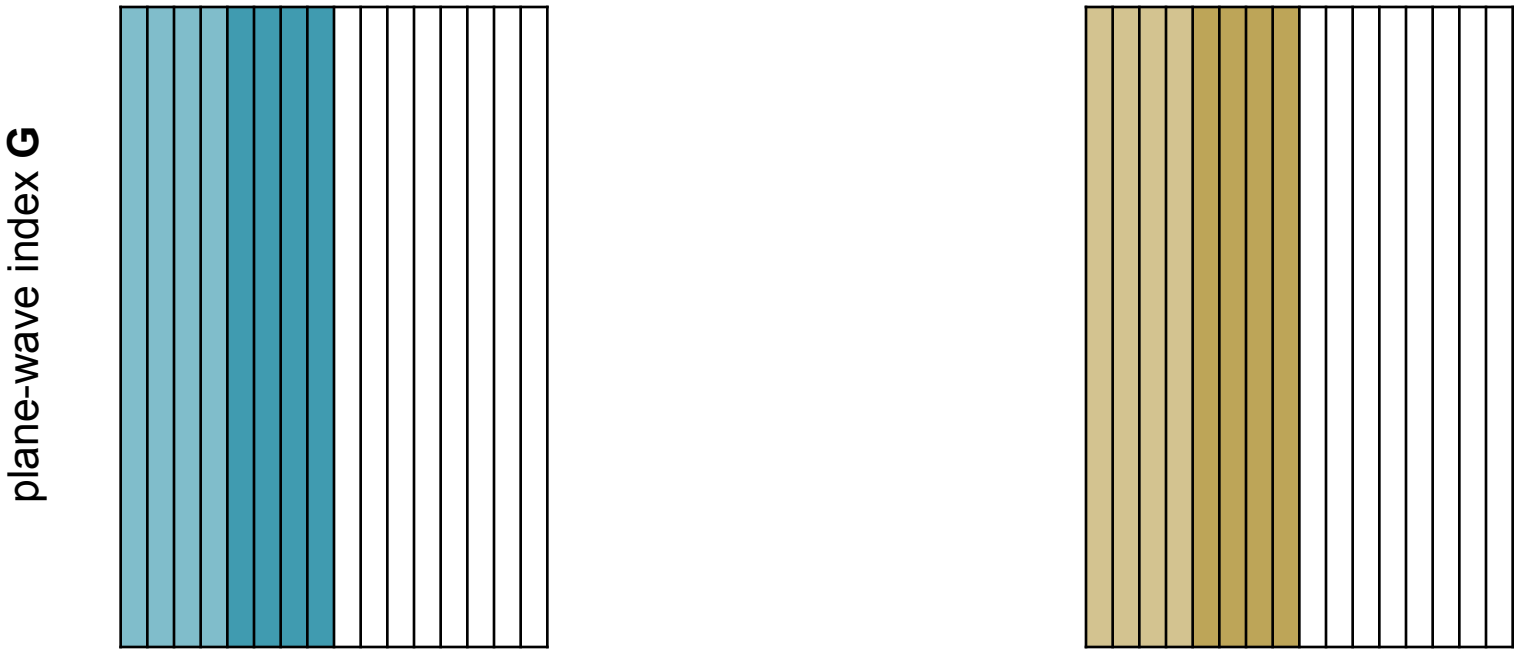
- Apply preconditioner: $P\tilde{R}^0_j(\mathbf{G}) = (H_{\mathbf{GG}} - \varepsilon_j)^{-1}\tilde{R}^0_j(\mathbf{G})$

Davidson iterative solver

- Expand variational space and apply Hamiltonian to new basis functions

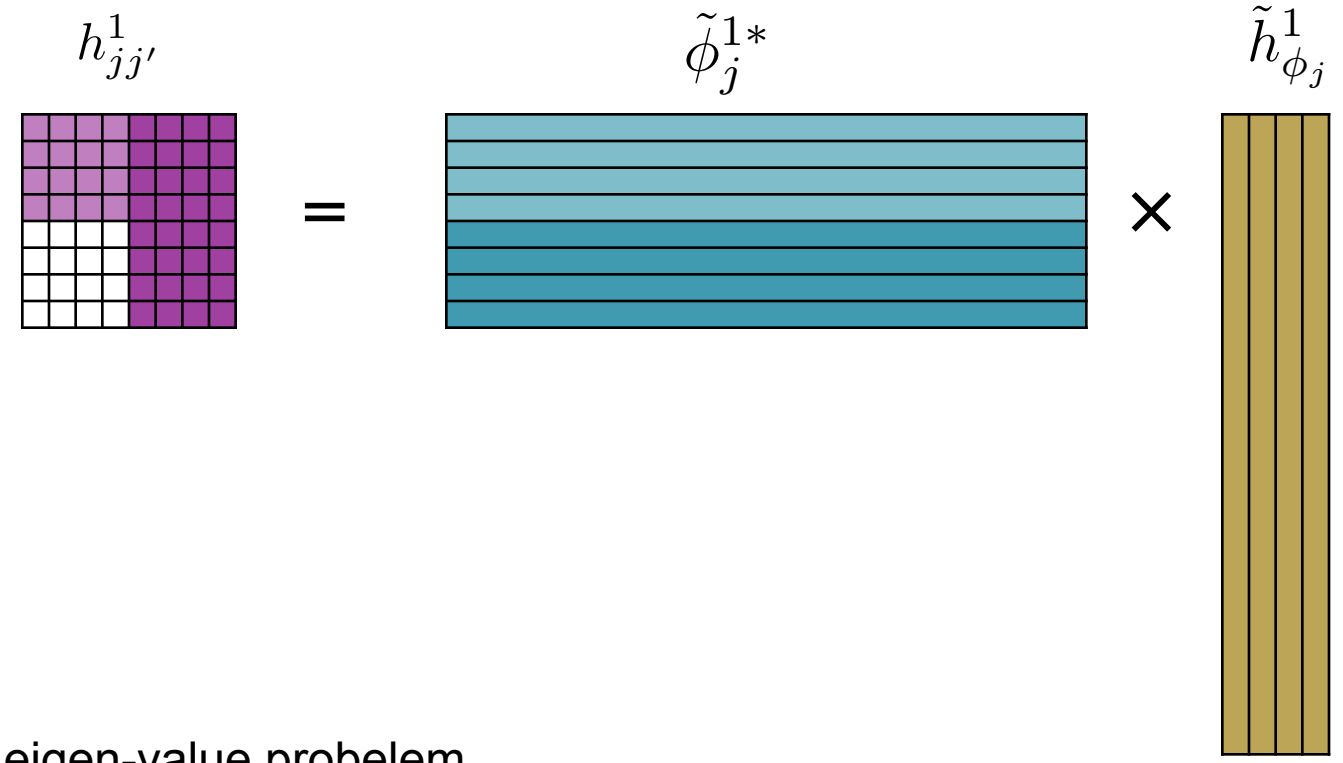
$$\tilde{\phi}_j^1 = \tilde{\phi}_j^0 \bigoplus P\tilde{R}_j^0$$

$$\tilde{h}_{\phi_j^1} = \mathbf{H}\tilde{\phi}_j^1$$



Davidson iterative solver

- Compute reduced Hamiltonian matrix



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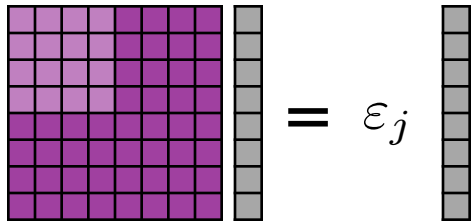
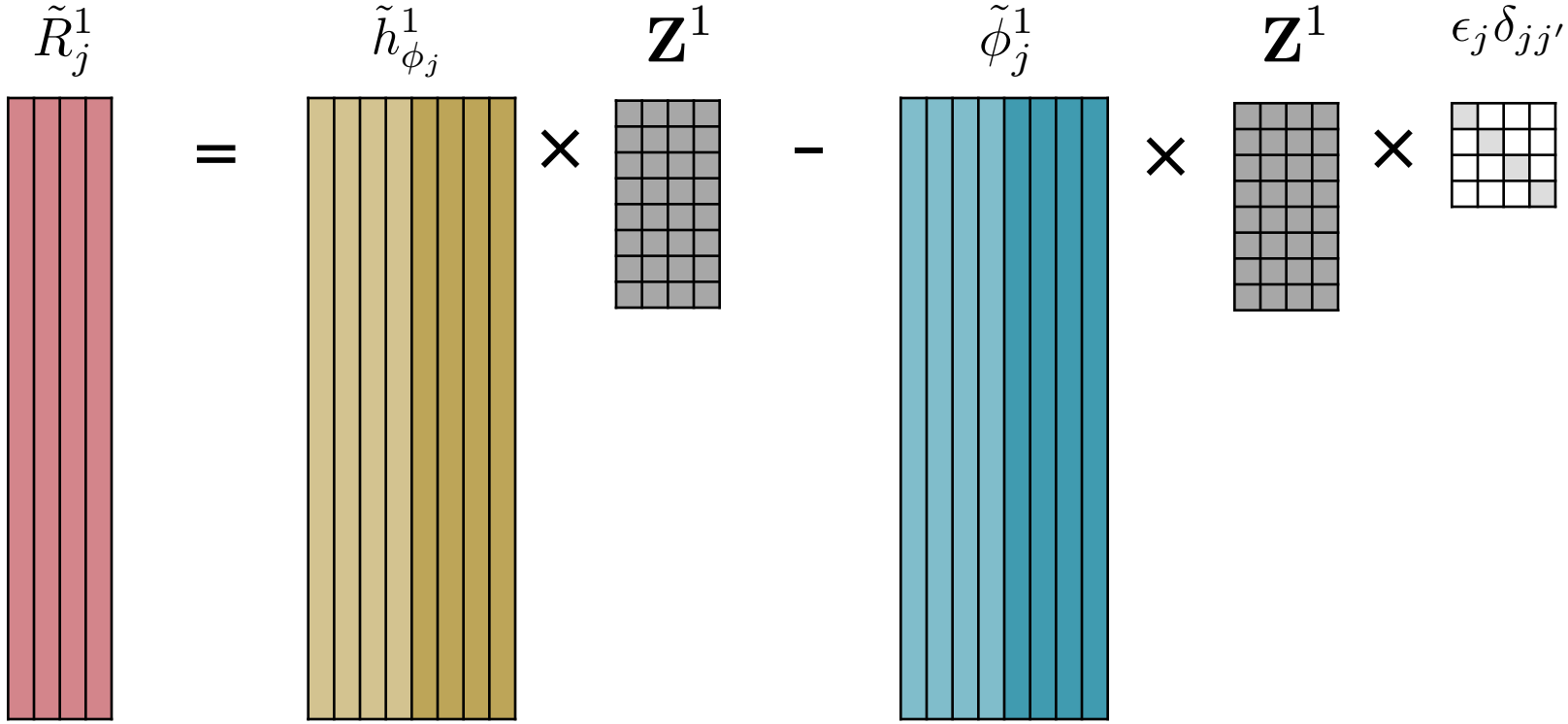


Davidson iterative solver

- Compute residuals



- Apply preconditioner: $P\tilde{R}^1_j(\mathbf{G}) = (H_{\mathbf{GG}} - \varepsilon_j)^{-1}\tilde{R}^1_j(\mathbf{G})$

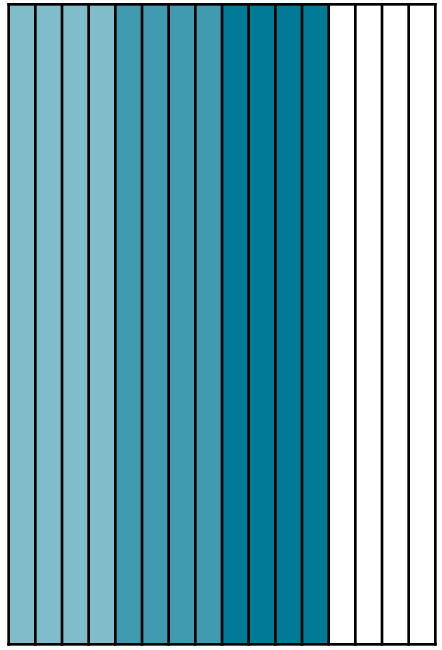
Davidson iterative solver

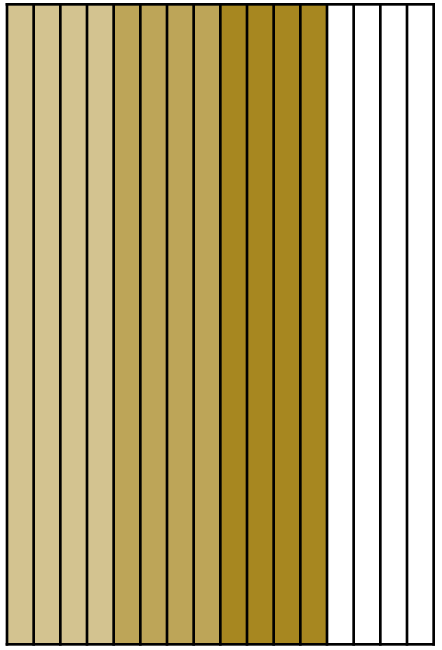
- Continue to expand variational space

$$\tilde{\phi}_j^2 = \tilde{\phi}_j^1 \bigoplus P\tilde{R}_j^1$$

$$\tilde{h}_{\phi_j^2} = \mathbf{H}\tilde{\phi}_j^2$$

plane-wave index **G**





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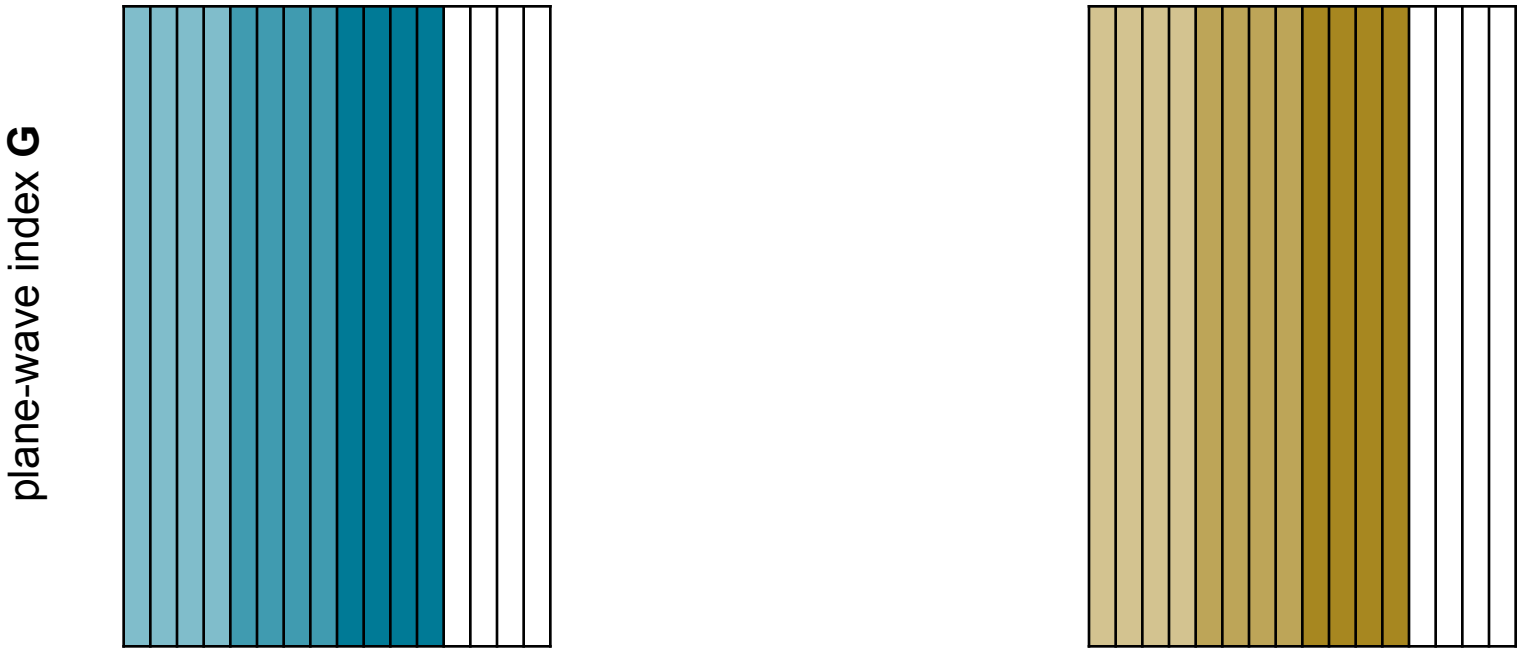
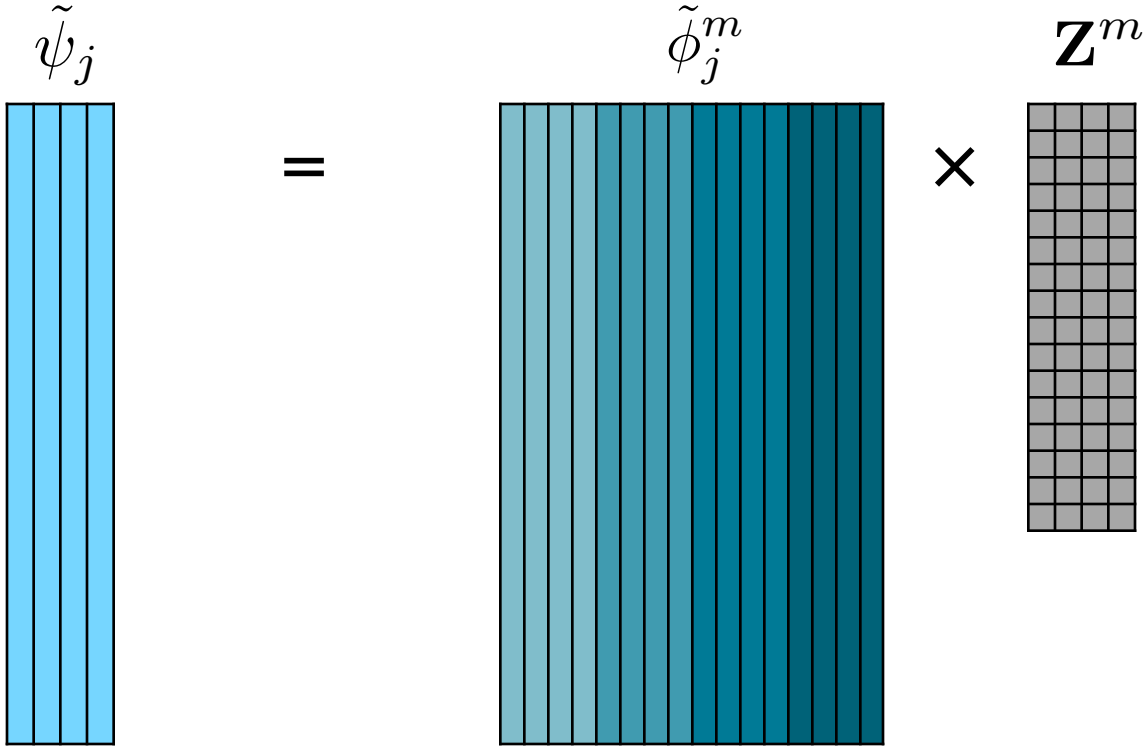


Iterate until the convergence (all residuals are zero) is reached

Davidson iterative solver

- Recompute the wave-functions



- Take ε_j from the last subspace diagonalization

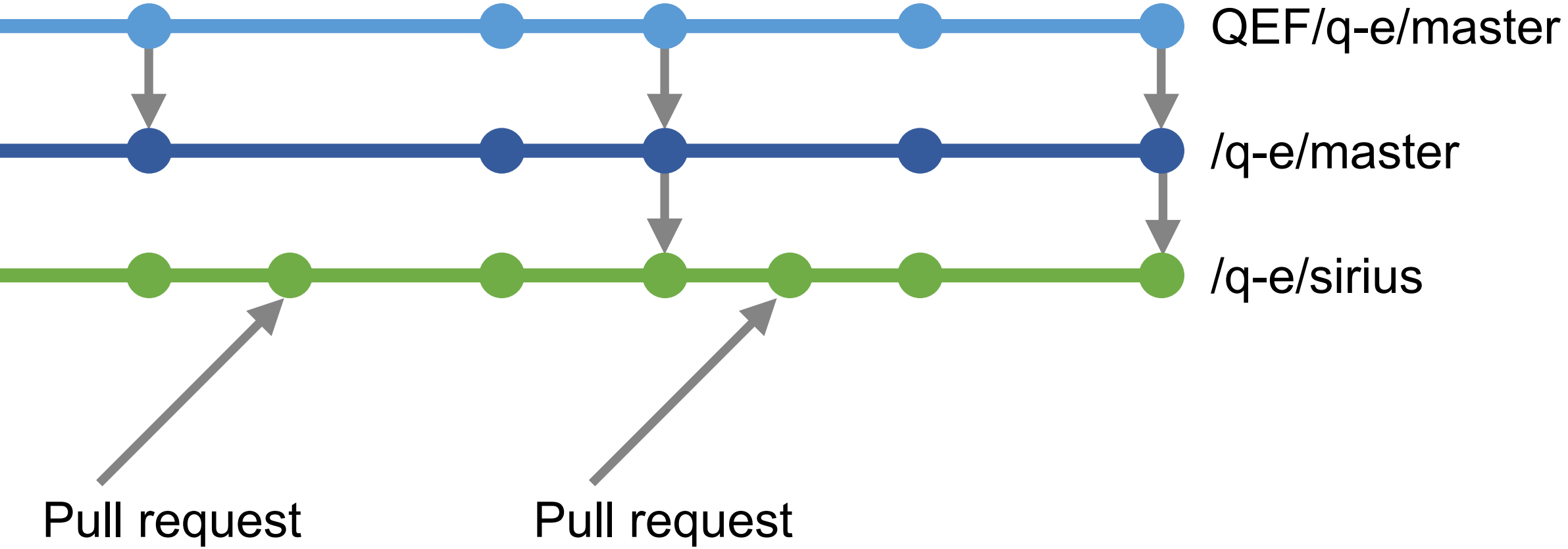
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

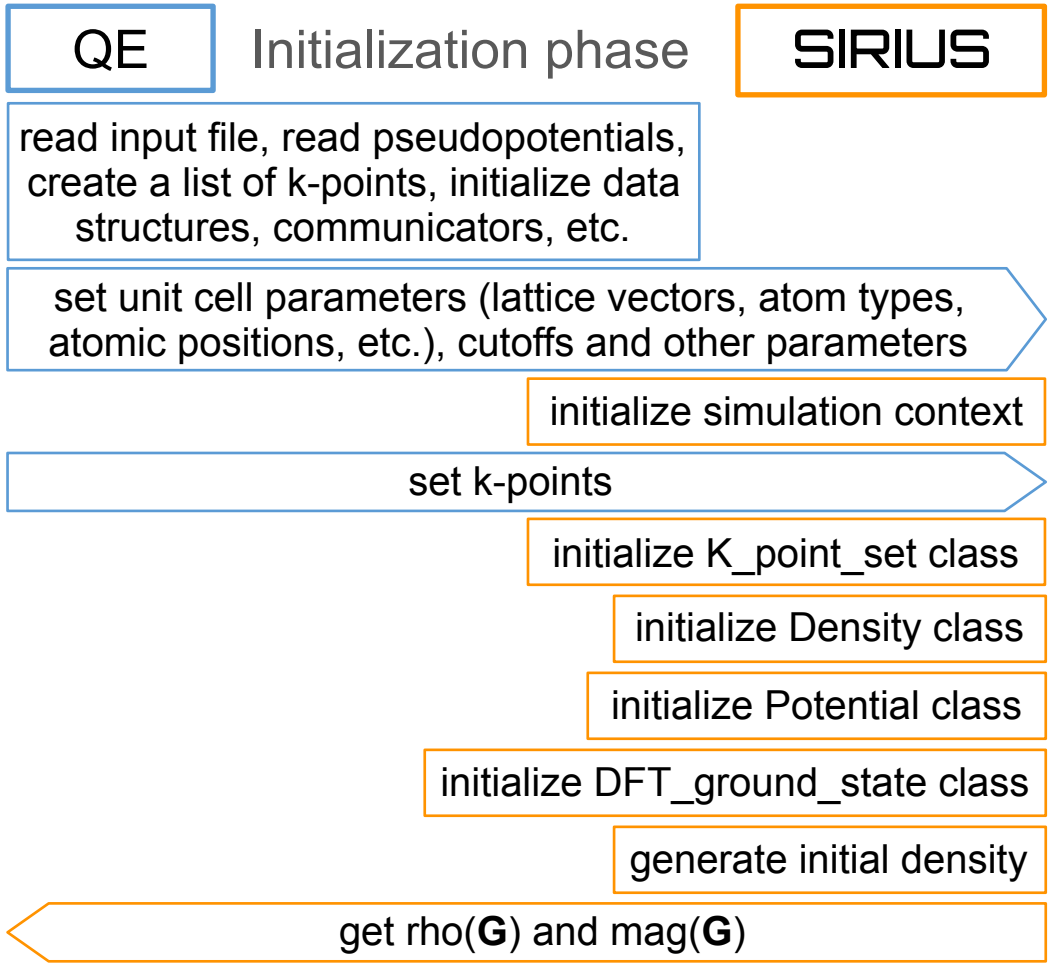
SIRIUS-enabled Quantum ESPRESSO

Development cycle

https://github.com/electronic-structure/q-e



Example of QE/SIRIUS interoperability



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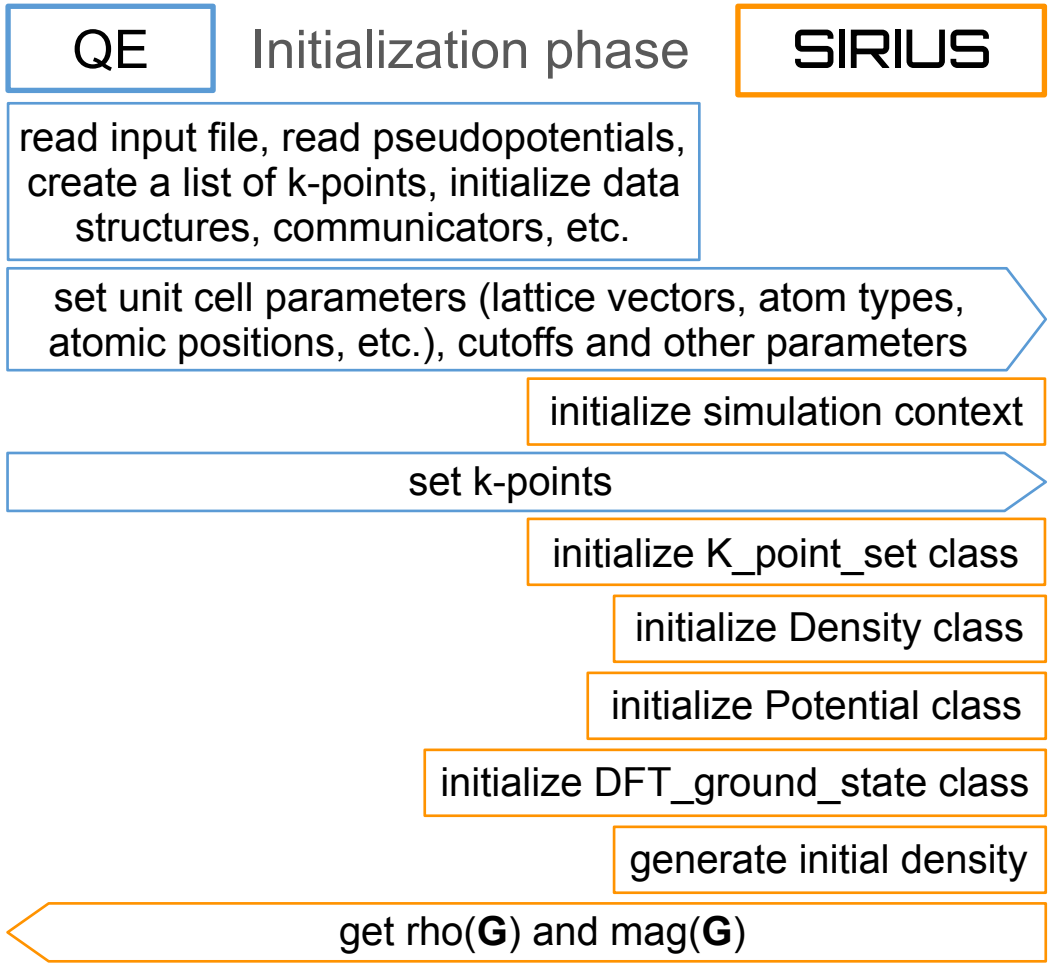
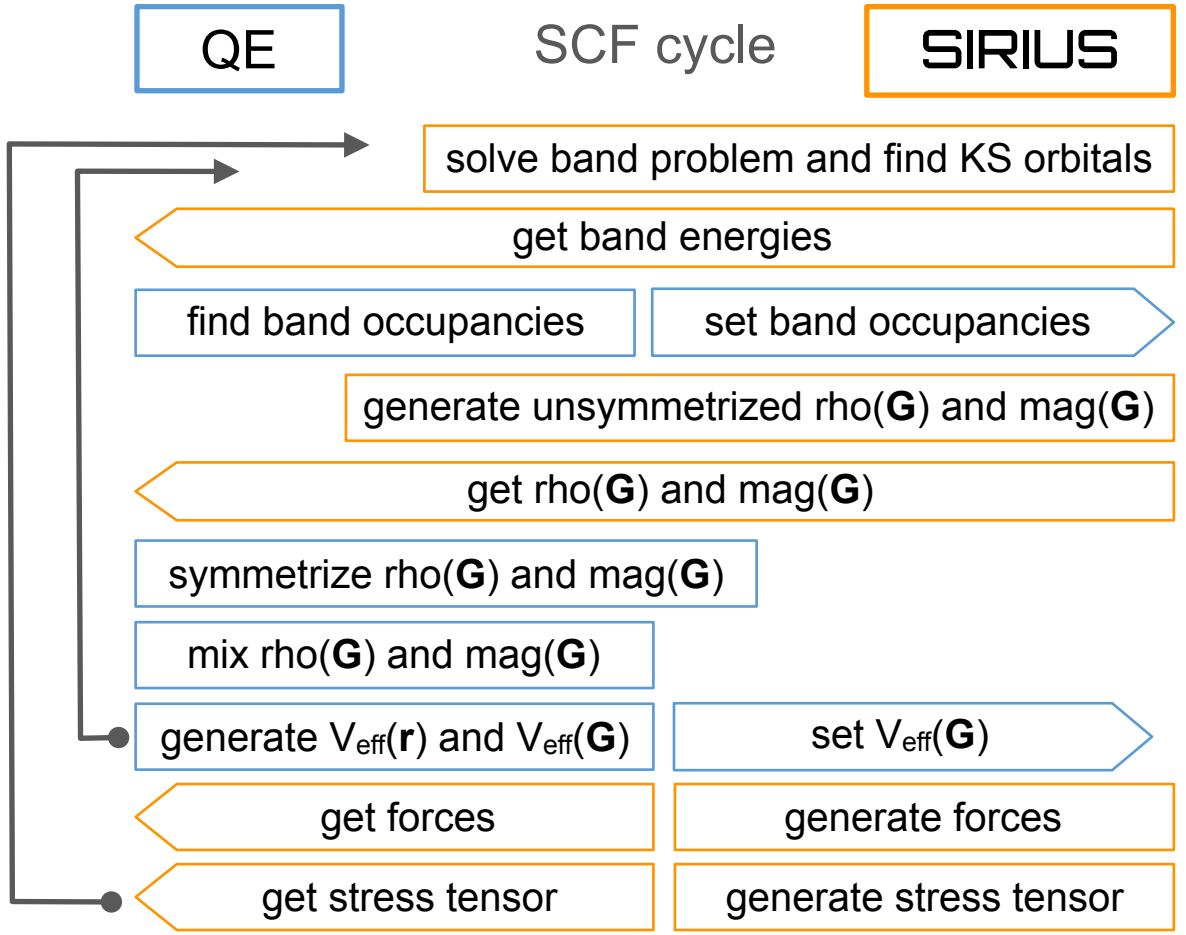
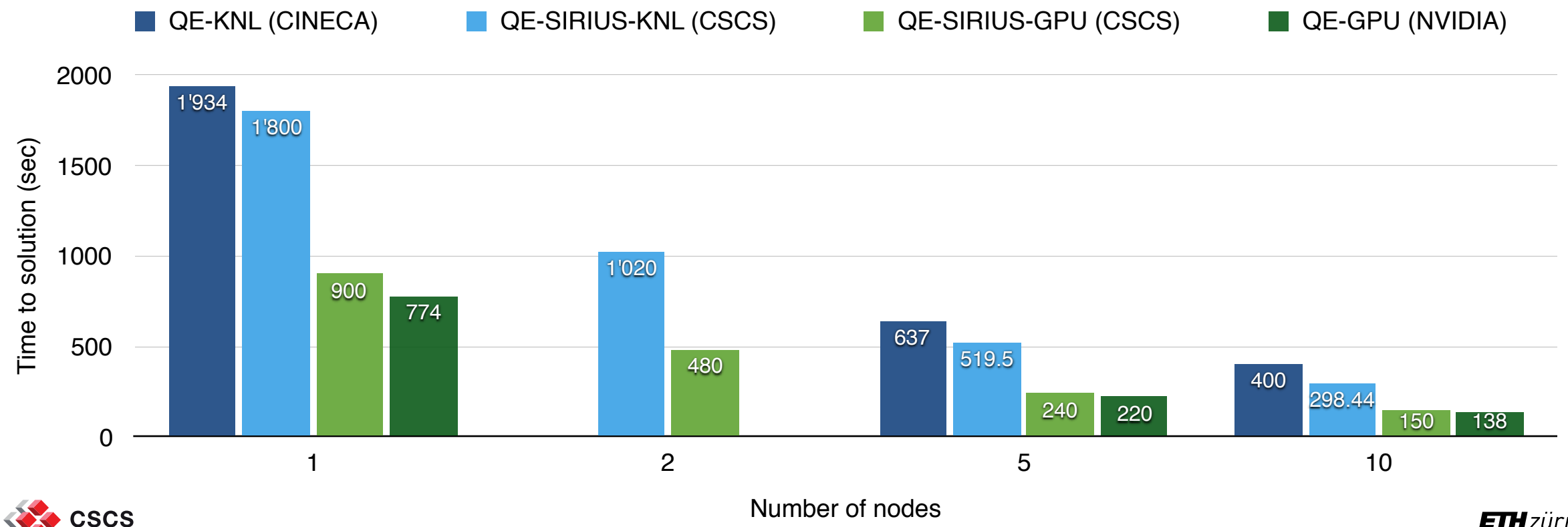




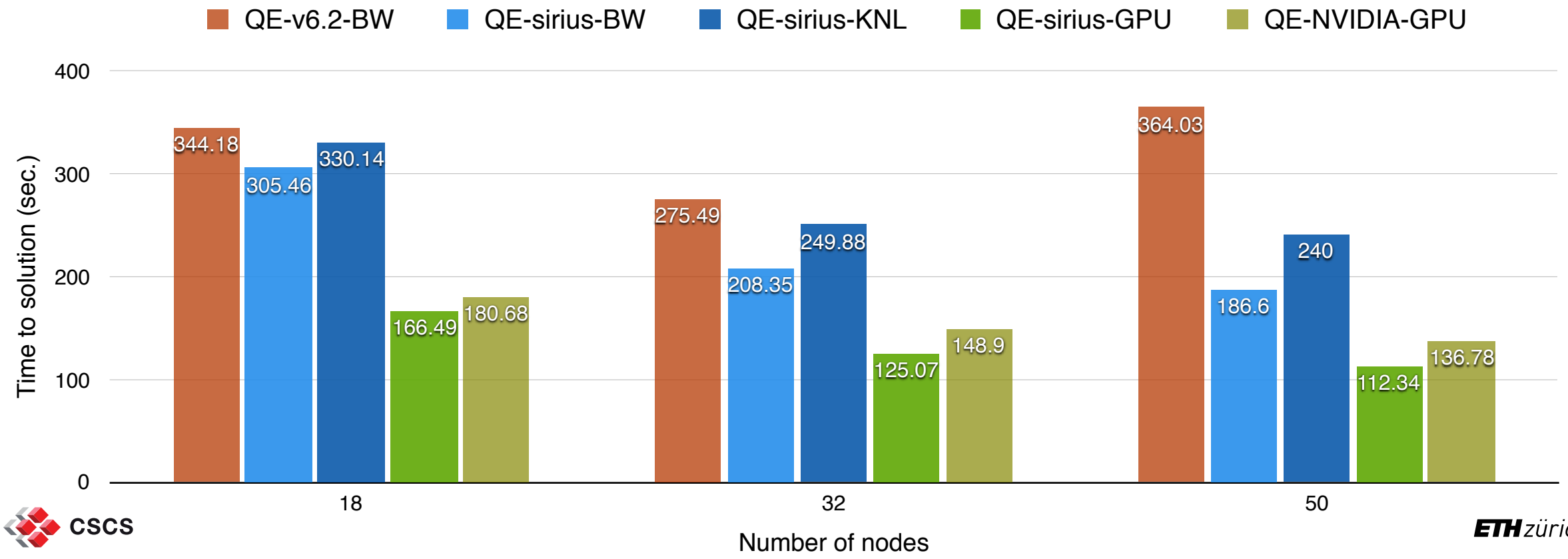
Variable cell relaxation of $Si_{63}Ge$

Performance benchmark of the QE, Cuda Fortran version of QE and SIRIUS-enabled QE codes for the 64-atom unit cell of $Si_{1-x}Ge_x$ The runs we performed on on hybrid nodes with 12-core Intel Haswell @2.5GHz + NVIDIA Tesla P100 card (QE-GPU, QE-SIRIUS-GPU) and on nodes with 68-core Intel Xeon Phi processor @1.4 GHz (QE-KNL). Time for the full 'vc-relax' calculation is reported.



Ground state of Pt-cluster in water

Performance benchmark of the QE and SIRIUS-enabled QE codes for the 288-atom unit cell of Pt cluster embedded in the water. The runs we performed on dual socket 18-core Intel Broadwell @2.1GHz nodes (BW), on hybrid nodes with 12-core Intel Haswell @2.5GHz + NVIDIA Tesla P100 card (GPU) and on nodes with 64-core Intel Xeon Phi processor @1.3 GHz (KNL). ELPA eigen-value solver was used for CPU runs. Time for the SCF ground state calculation is reported.



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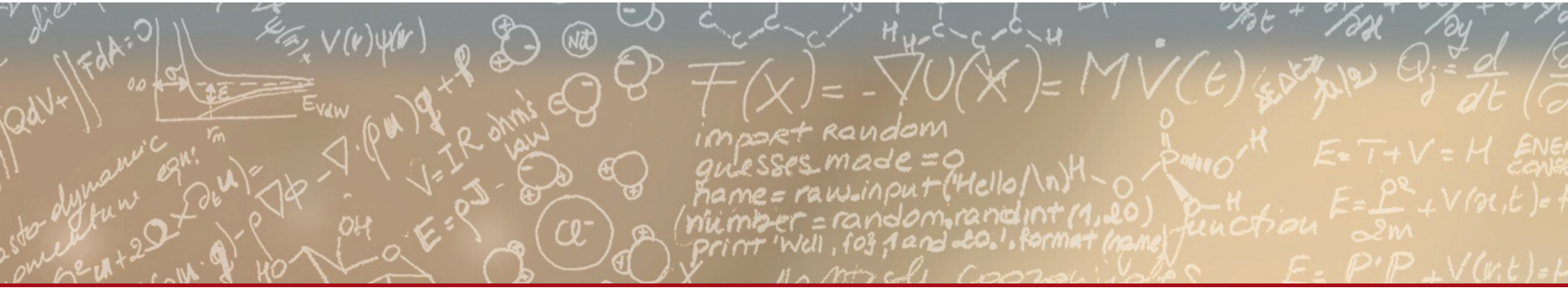

Thank you for your attention.