Lecture Tue.3

Intro to the EPW code and recent developments

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Lecture Summary

- Brief introduction to EPW
- Computational flow
- Recent developments
- Future plans

Brief introduction to EPW [https://epw-code.org]

- Open-source Fortran code to calculate materials properties related to the electron-phonon interaction
  - Based on density-functional perturbation theory and maximally localized Wannier functions.
- One of core modules of Quantum ESPRESSO since 2016

Functionalities of EPW

- Interpolate electron-phonon matrix element on fine momentum grids
- Compute electron and phonon linewidths, scattering rates & lifetimes
- Electron and phonon spectral functions
- Electron-phonon coupling strength
- Superconducting properties
- Transport properties

Features of EPW

- Support LDA/GGA functionals
- MPI parallelization:
  - over **k** points and bands on coarse grids
  - over **k** points on fine grids
- Support spin-orbit coupling
- Support time-reversal symmetry
- Interpolate polar divergence correctly
- Integrated into QE and rely on Wannier90
- Have a test-farm for stability and portability of the code

Computational flow

epw.f90

```
  CALL epw_readin()
..
  IF (wannierize) CALL wann_run()
  CALL elphon_shuffle_wrap()
  >> CALL elphel2_shuffle
  > CALL ephwann_shuffle
..
```

➤ Read input keywords,
read wfns and misc. data from pw.x

Computational flow

epw.f90

```
  CALL epw_readin()
..
  IF (wannierize) CALL wann_run()
  CALL elphon_shuffle_wrap()
  >> CALL elphel2_shuffle
  > CALL ephwann_shuffle
..
```

➤ Generate inputs to W90 and Wannierization

Computational flow

epw.f90

```
  CALL epw_readin()
..
  IF (wannierize) CALL wann_run()
  CALL elphon_shuffle_wrap()
  >> CALL elphel2_shuffle
  > CALL ephwann_shuffle
..
```

➤ Calculated *e*-ph vertex on coarse grids

Computational flow

epw.f90

```
  CALL epw_readin()
..
  IF (wannierize) CALL wann_run()
  CALL elphon_shuffle_wrap()
  >> CALL elphel2_shuffle
  > CALL ephwann_shuffle
..
```

➤ Bloch to Wannier and Wannier to Bloch, + …

Computational flow:

Wannierization

- Call W90 as a library (run serially)
- Generate internally inputs (amn, mmn, etc.) to W90
- Generate directly real-space Wannier orbitals [.cube]
- Main input keywords of W90 ➤ inputs of EPW [Tue.4 Hands-on]
- Others can also be passed to W90 [Tue.4 Hands-on]

Computational flow:

e-ph evaluation

$$\boxed{g(\mathbf{k}_{\mathrm{c}},\mathbf{q}_{\mathrm{c}})} \blacktriangleright \boxed{g(\mathbf{R}_e,\mathbf{R}_p)} \blacktriangleright \boxed{g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})} \blacktriangleright \boxed{\sum\nolimits''_{n\mathbf{k}_{\mathrm{f}}}[g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})], \Pi''_{\nu\mathbf{q}_{\mathrm{f}}}[g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})], ...}$$

Computational flow:

e-ph evaluation

$$\boxed{\boxed{g(\mathbf{k}_\mathrm{c},\mathbf{q}_\mathrm{c})}} \rightarrow \boxed{g(\mathbf{R}_e,\mathbf{R}_p)} \rightarrow \boxed{g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})} \rightarrow \boxed{\sum\nolimits''_{n\mathbf{k}_\mathrm{f}}[g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})],\ \Pi''_{\nu\mathbf{q}_\mathrm{f}}[g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})],\ldots}$$

Wave functions from pw.x (NSCF)

$$g_{mn\nu}(\mathbf{k}_\mathrm{c},\mathbf{q}_\mathrm{c}) = \langle u_{m\mathbf{k}_\mathrm{c}+\mathbf{q}_\mathrm{c}} | \Delta_{\mathbf{q}_\mathrm{c}\nu} v^{\mathrm{KS}} | u_{n\mathbf{k}_\mathrm{c}} \rangle_{\mathrm{uc}}$$

Perturbing potentials
(In patterns basis)
from ph.x

$$\Delta_{\mathbf{q}_\mathrm{c}\nu} v^{\mathrm{KS}} = \sum_{\kappa\alpha} \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}_\mathrm{c}\nu}}}\, e_{\kappa\alpha,\nu}(\mathbf{q}_\mathrm{c})\, \partial_{\kappa\alpha,\mathbf{q}_\mathrm{c}} v^{\mathrm{KS}}$$

Caculated from
dynamical matrices from ph.x

, where $\partial_{\kappa\alpha,\mathbf{q}_\mathrm{c}} v^{\mathrm{KS}} = e^{-i\mathbf{q}_\mathrm{c}\cdot\mathbf{r}} \sum_p e^{i\mathbf{q}_\mathrm{c}\cdot\mathbf{R}_p} \frac{\partial V^{\mathbf{KS}}(\mathbf{r})}{\partial \tau_{\kappa\alpha p}}$

[Phys. Rev. B **76**, 165108 (2007), Rev. Mod. Phys. **89**, 1 (2017)]

Technicalities:

Difference from ph.x

ph.x explicitly calculates the states at **k** and **k**+**q** .

EPW folds the states at **k**+**q** by using the periodic gauge condition

$$u_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r}) = e^{-i\mathbf{G}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$$

Computational flow:

e-ph evaluation

$$\boxed{g(\mathbf{k}_{\mathrm{c}},\mathbf{q}_{\mathrm{c}})} \rightarrow \boxed{\boxed{g(\mathbf{R}_e,\mathbf{R}_p)}} \rightarrow \boxed{g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})} \rightarrow \boxed{\textstyle\sum''_{n\mathbf{k}_{\mathrm{f}}}[g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})], \Pi''_{\nu\mathbf{q}_{\mathrm{f}}}[g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})], \ldots}$$

$$g_{mn\kappa\alpha}(\mathbf{R}_p,\mathbf{R}_{p'}) = \langle \mathrm{w}_{m0}(\mathbf{R})|\frac{\partial V^{\mathrm{KS}}}{\partial \tau_{\kappa\alpha}}(\mathbf{r}-\mathbf{R}_{p'})|\mathrm{w}_{m0}(\mathbf{R}-\mathbf{R}_p)\rangle_{\mathrm{sc}}$$

[Phys. Rev. B **76**, 165108 (2007), Rev. Mod. Phys. **89**, 1 (2017)]

Use of minimal-distance replica selection for Wannier interpolation

[J. Phys. Cond. Matt. 32, 165902 (2020), arXiv:2105.04192 (2021)]

Computational flow:

e-ph evaluation

$$\boxed{g(\mathbf{k}_\mathrm{c},\mathbf{q}_\mathrm{c})} \rightarrow \boxed{g(\mathbf{R}_e,\mathbf{R}_p)} \rightarrow \boxed{\boxed{g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})}} \rightarrow \boxed{\sum\nolimits''_{n\mathbf{k}_\mathrm{f}}[g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})], \Pi''_{\nu\mathbf{q}_\mathrm{f}}[g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})], \ldots}$$

$$g_{mn\nu}(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f}) = \sqrt{\frac{\hbar}{2M_\kappa\omega_{\mathbf{q}_\mathrm{f}\nu}}}\sum_{pp'} e^{i(\mathbf{k}_\mathrm{f}\cdot\mathbf{R}_p+\mathbf{q}_\mathrm{f}\cdot\mathbf{R}_{p'})}$$
$$\times\,[U_{\mathbf{k}_\mathrm{f}+\mathbf{q}_\mathrm{f}}\, g(\mathbf{R}_p,\mathbf{R}_{p'})\cdot e_{\kappa\alpha,\nu}(\mathbf{q}_\mathrm{f})\, U^\dagger_{\mathbf{k}_\mathrm{f}}]_{mn}$$

[Phys. Rev. B **76**, 165108 (2007), Rev. Mod. Phys. **89**, 1 (2017)]

Use of crystal symmetry (w.r.t **k**) and
Fermi window

Computational flow:

e-ph evaluation

$$\boxed{g(\mathbf{k}_\mathrm{c},\mathbf{q}_\mathrm{c})} \rightarrow \boxed{g(\mathbf{R}_e,\mathbf{R}_p)} \rightarrow \boxed{g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})} \rightarrow \boxed{\textstyle\sum''_{n\mathbf{k}_\mathrm{f}}[g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})],\ \Pi''_{\nu\mathbf{q}_\mathrm{f}}[g(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})],\ \ldots}$$

$$\begin{aligned}\Sigma''_{n\mathbf{k}_\mathrm{f}}(\omega,T) =& \pi\sum_{m\nu}\int_\mathrm{BZ}\frac{d\mathbf{q}_\mathrm{f}}{\Omega_\mathrm{BZ}}|g_{mn\nu}(\mathbf{k}_\mathrm{f},\mathbf{q}_\mathrm{f})|^2 \\ &\{[n_{\mathbf{q}_\mathrm{f}\nu}(T)+f_{m\mathbf{k}_\mathrm{f}+\mathbf{q}_\mathrm{f}}(T)]\delta(\omega-(\varepsilon_{m\mathbf{k}_\mathrm{f}+\mathbf{q}_\mathrm{f}}-\varepsilon_\mathrm{F})+\omega_{\mathbf{q}_\mathrm{f}\nu}) \\ &+[n_{\mathbf{q}_\mathrm{f}\nu}(T)+1-f_{m\mathbf{k}_\mathrm{f}+\mathbf{q}_\mathrm{f}}(T)]\delta(\omega-(\varepsilon_{m\mathbf{k}_\mathrm{f}+\mathbf{q}_\mathrm{f}}-\varepsilon_\mathrm{F})-\omega_{\mathbf{q}_\mathrm{f}\nu})\}\end{aligned}$$

[Comput. Phys. Commun. **209**, 116 (2016), Rev. Mod. Phys. **89**, 1 (2017)]

Technicalities:

e-ph evaluation on coarse grids

- Use of the periodic gauge condition for folding $u_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r}) = e^{-i\mathbf{G}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$

- Use of crystal symmetry

$$\begin{aligned} g_{mn\nu}(\mathbf{k}, S\mathbf{q}) &= \langle \psi_{m,\mathbf{k}+S\mathbf{q}}(\mathbf{r}) | \partial_{\nu,S\mathbf{q}} V(\mathbf{r}) | \psi_{n,\mathbf{k}}(\mathbf{r}) \rangle \\ &= \langle \psi_{m,\mathbf{k}+S\mathbf{q}}(\mathbf{r}) | \partial_{\nu\mathbf{q}} V(\{S|\mathbf{v}\}^{-1}\mathbf{r}) | \psi_{n,\mathbf{k}}(\mathbf{r}) \rangle \\ &= \langle \psi_{m,\mathbf{k}+S\mathbf{q}}(\{S|\mathbf{v}\}\mathbf{r}) | \partial_{\nu\mathbf{q}} V(\mathbf{r}) | \psi_{n,\mathbf{k}}(\{S|\mathbf{v}\}\mathbf{r}) \rangle \end{aligned}$$

- Use of time-reversal symmetry

(only when the small group of **q** doesn’t include **q** <> -**q** operation)

$$g_{mn\nu}(\mathbf{k}, -S\mathbf{q}) = \langle \psi_{m,\mathbf{k}-S\mathbf{q}}(\{S|\mathbf{v}\}\mathbf{r}) | \left(\partial_{\nu\mathbf{q}} V(\mathbf{r}) \right)^* | \psi_{n,\mathbf{k}}(\{S|\mathbf{v}\}\mathbf{r}) \rangle$$

[Phys. Rev. B **76**, 165108 (2007), Comput. Phys. Commun. **209**, 116 (2016)]

General design principles

- Improve the computational workflow
- Reduce the computational size
- Optimize the computation

Improvement on workflow

- Divide EPW into two separate codes
- Incorporate NSCF step into EPW
- Start from irreducible coarse grids.
- Other simplifications

Efficient calculation of *e*-ph vertex

- e-ph vertex is a main ingredient to calculate electron-phonon related quantities

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = \langle \psi_{m,\mathbf{k}+\mathbf{q}}(\mathbf{r}) | \partial_{\nu,\mathbf{q}} V(\mathbf{r}) | \psi_{n,\mathbf{k}}(\mathbf{r}) \rangle$$

- A large portion of time spent on its evaluation in EPW
- Calculated in plane-waves basis on coarse grids and in reduced basis on dense grids after Wannier interpolation
- Gauges of wave functions are arbitrary, but consistent ones should be used throughout all calculations
- On coarse grids, calculated for all pairs of states at ***k*** and ***k*+*q*** $N_b^2 \times N_k \times N_q \times N_\nu$(evaluations)

(number of bands N_b, $\mathbf{k}$ vector N_k, $\mathbf{q}$ vector N_q, and modes N_ν)

Efficient calculation of e-ph vertex:

Coarse grids: reduction of computational size

- Exploit the crystal symmetry to reduce the number of evaluations for e-ph vertex

$$\begin{aligned} g_{mn\nu}(\mathbf{k}, S\mathbf{q}) &= \langle \psi_{m,\mathbf{k}+S\mathbf{q}}(\mathbf{r}) | \partial_{\nu,S\mathbf{q}} V(\mathbf{r}) | \psi_{n,\mathbf{k}}(\mathbf{r}) \rangle \\ &= \langle \psi_{m,\mathbf{k}+S\mathbf{q}}(\mathbf{r}) | \partial_{\nu\mathbf{q}} V(\{S|\mathbf{v}\}^{-1}\mathbf{r}) | \psi_{n,\mathbf{k}}(\mathbf{r}) \rangle \\ &= \langle \psi_{m,\mathbf{k}+S\mathbf{q}}(\{S|\mathbf{v}\}\mathbf{r}) | \partial_{\nu\mathbf{q}} V(\mathbf{r}) | \psi_{n,\mathbf{k}}(\{S|\mathbf{v}\}\mathbf{r}) \rangle \end{aligned}$$

[Phys. Rev. B **76**, 165108 (2007)]

- If the following relations hold throughout all wave functions,

$$\begin{aligned} \psi_{m,S^{-1}\mathbf{k}+\mathbf{q}}(\mathbf{r}) &= \psi_{m,\mathbf{k}+S\mathbf{q}}(\{S|\mathbf{v}\}\mathbf{r}) \\ \psi_{n,S^{-1}\mathbf{k}}(\mathbf{r}) &= \psi_{n,\mathbf{k}}(\{S|\mathbf{v}\}\mathbf{r}) \end{aligned}$$

- Can we use the symmetry relation between e-ph vertices?

$$g_{mn\nu}(\mathbf{k}, S\mathbf{q}) = g_{mn\nu}(S^{-1}\mathbf{k}, \mathbf{q})$$

Efficient calculation of e-ph vertex:

Coarse grids: reduction of computational size

- We can’t use the equation below to reduce the number of evaluations:

$$g_{mn\nu}(\mathbf{k}, S\mathbf{q}) = g_{mn\nu}(S^{-1}\mathbf{k}, \mathbf{q})$$

  - Ex) For the inversion operation in the little group of the wavevector ***k***, and its odd-parity state *n*,

$$\psi_{n\mathbf{k}}(\{S|\mathbf{v}\}\mathbf{r}) = \{S|\mathbf{v}\}^{-1}\psi_{n\mathbf{k}}(\mathbf{r}) = -\psi_{n\mathbf{k}}(\mathbf{r}) \neq \psi_{n,S^{-1}\mathbf{k}}(\mathbf{r})$$

$[S^{-1} = S \text{ for inversion operation}]$

- We need to multiply the additional factors (the same for states at ***k***+***q***):

$$\boxed{g_{mn\nu}(\mathbf{k}, S\mathbf{q}) = \sum_{m'n'} \langle \psi_{m',S^{-1}\mathbf{k}+\mathbf{q}}(\mathbf{r}) | \psi_{m,\mathbf{k}+S\mathbf{q}}(\{S|\mathbf{v}\}\mathbf{r}) \rangle^{*} g_{m'n'\nu}(S^{-1}\mathbf{k}, \mathbf{q}) \langle \psi_{n',S^{-1}\mathbf{k}}(\mathbf{r}) | \psi_{n\mathbf{k}}(\{S|\mathbf{v}\}\mathbf{r}) \rangle}$$

Efficient calculation of *e*-ph vertex:

Coarse grids: reduction of computational size

- We can reduce the number of evaluations:
  - For each $\boldsymbol{q}_{\mathrm{irr}}$, explicitly evaluate the e-ph vertex
  - For the star of $\boldsymbol{q}_{\mathrm{irr}}$, skip the explicit evaluation by using the symmetry relation of e-ph vertex
- Speedup by a factor of $N_{\boldsymbol{q}}/N_{\boldsymbol{q}\mathrm{irr}}$ (-α)
  - For GaN with 6x6x6 ***k*** and ***q*** points ($N_{\boldsymbol{q}}/N_{\boldsymbol{q}\mathrm{irr}}$=7.7) , speedup by 4

Efficient calculation of *e*-ph vertex:

Fine grids: optimize the computation

- Symmetry broken during Wannierization

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = \sum_{pp'} e^{i(\mathbf{k}\cdot\mathbf{R}_p + \mathbf{q}\cdot\mathbf{R}_{p'})} \sum_{m'n'\kappa\alpha} U_{mm'\mathbf{k}+\mathbf{q}} g_{m'n'\kappa\alpha}(\mathbf{R}_p, \mathbf{R}_{p'}) U^{\dagger}_{n'n\mathbf{k}} u_{\kappa\alpha,\mathbf{q}\nu}\,.$$

, where Wigner-Seitz vector $\mathbf{R}_{p(p')}$, rotation matrix U, eigenmode u, band index $m(m'), n(n')$, mode index ν, and Cartesian directions α

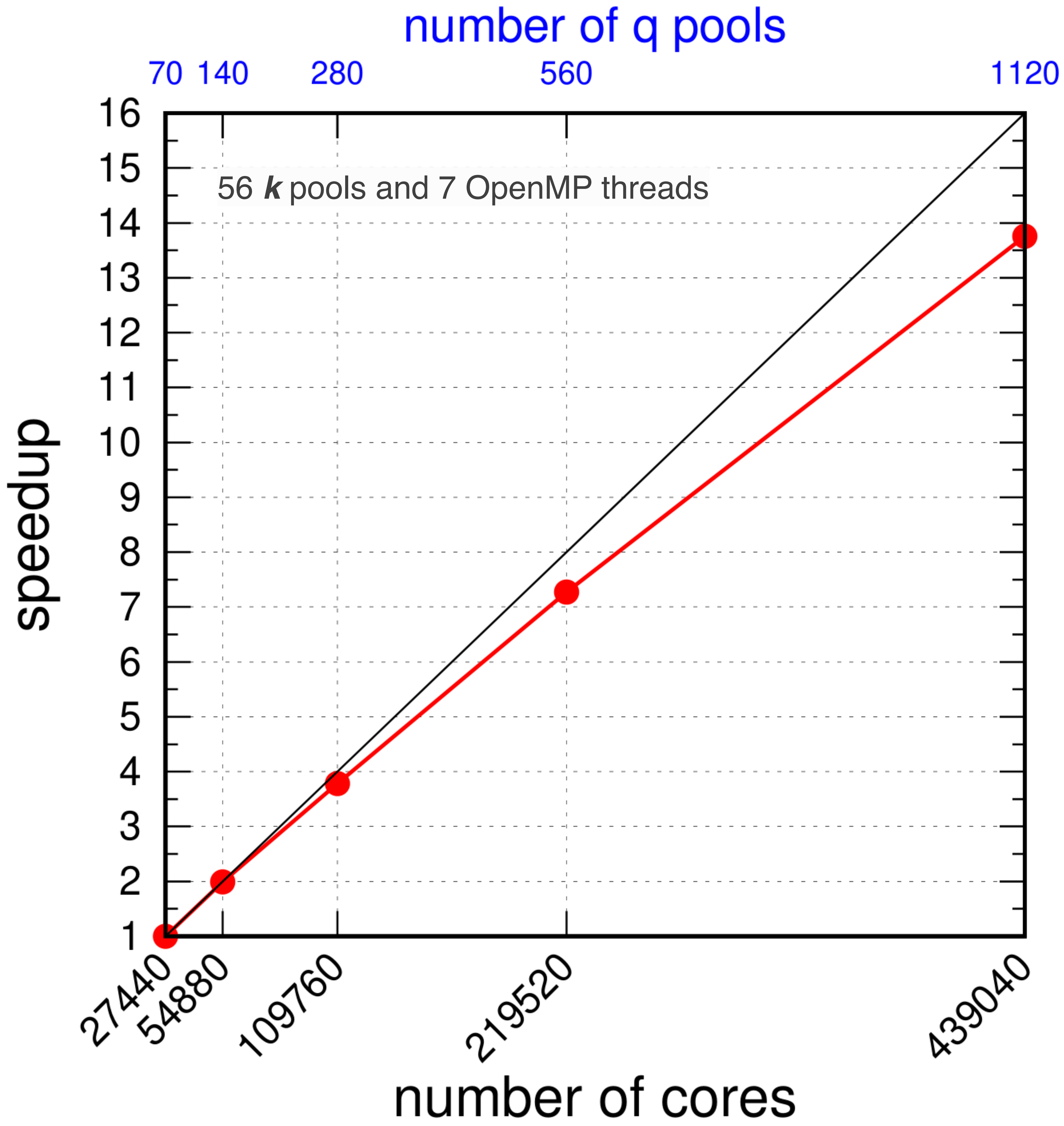
[Phys. Rev. B **76**, 165108 (2007), Rev. Mod. Phys. **89**, 1 (2017)]

- Instead, hybrid parallelization scheme enables highly-scalable evaluations
  - ***q*** point parallelization using MPI
  - ***k*** point parallelization using MPI and OpenMP

Efficient calculation of e-ph vertex:

Fine grids: optimize the computation

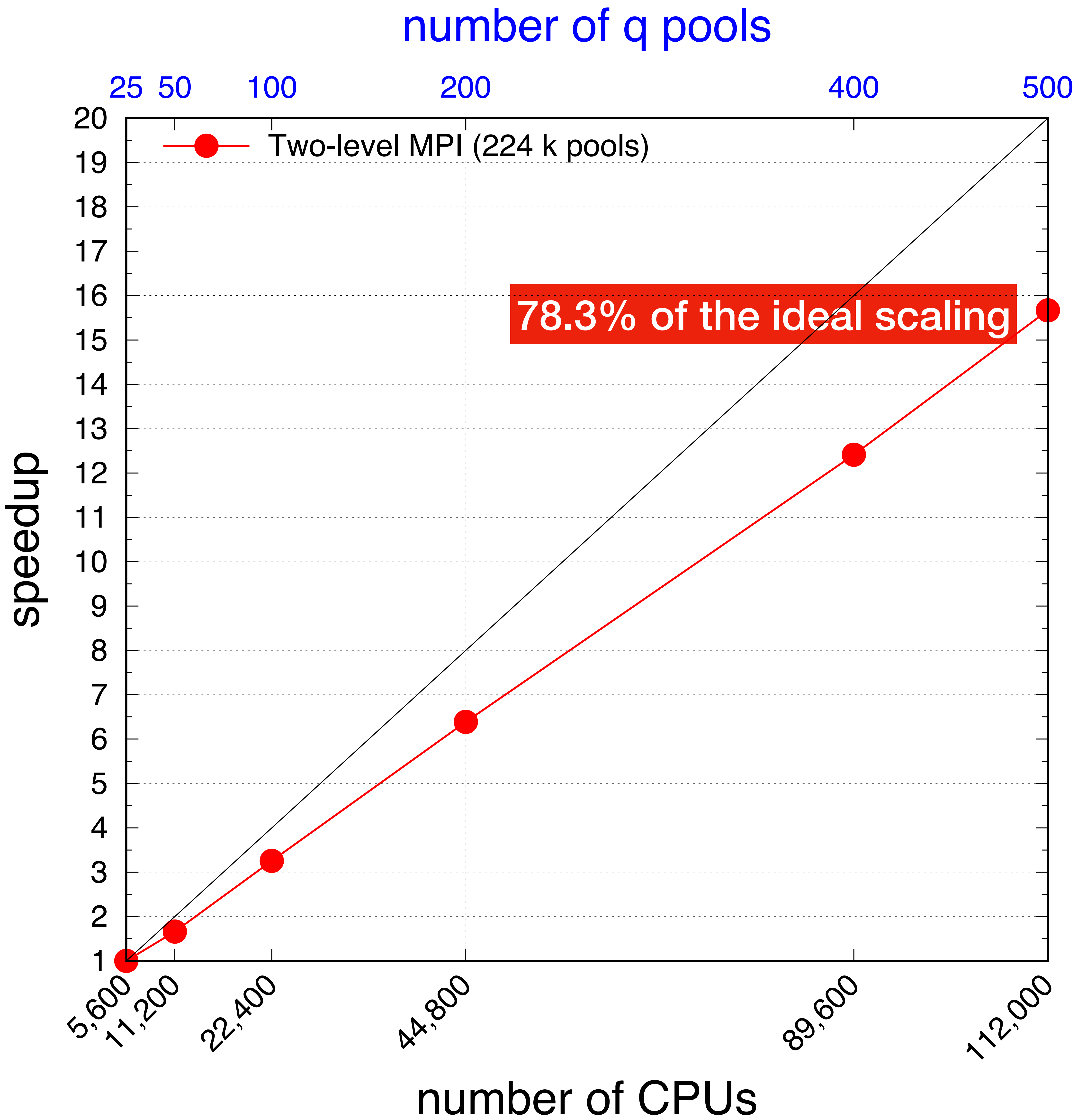
- Hybrid two-level MPI and OpenMP
- 86% speedup of the ideal one on half-million cores
  [done on Frontera during Texascale Days in Dec. 2020]
- Time-to-solution of 21 min. for the interpolation of e-ph vertex on 10^6 full ***k*** and ***q*** points with 3 bands for MgB_2 ($8.1\text{x}10^{13}$ elements)



Extension of Hybrid Parallelization Sheme:

Superconducting module

- Done on Frontera up to 112,000 cores
- MgB_2
  - 36x36x36 *k* and *q* fine grids (2,413 irreducible **k** points and 46,656 full **q** points)
  - No Fermi window (five bands considered)
  - Maximum number (40) of iterations set for benchmark purpose
- Use of low I/O mode



Other additions

- Symmetric *e*-ph vertex in USPP and PAW
- OpenMP parallelization for *G* operations
- Parallel I/O using parallel HDF5
    - Reduce the time for I/O
        - Average time of 15.3 sec for file I/O of 3.3 TB using 5,040 cores [done on Summit with GPFS file system]
    - Reduce the number of files to minimum
    - Increased portability and flexibility
- Optimized linear tetrahedron method [Phys. Rev. B **89**, 094515 (2014)]

Symmetric *e*-ph vertex in USPP and PAW

- Only a few correction terms needed to add to ultrasoft pseudopotential (USPP) case [Phys. Rev. B **81**, 075123 (2010)]

$$\boxed{\sum_{\sigma}\sum_{I,mn}\Delta D^{1,\sigma,\mu}_{I,mn} b^{\sigma,\lambda}_{I,mn}}$$

$$\text{where } \Delta D^{1,\sigma,\mu}_{I,mn} = \left(\frac{dD^{1,\sigma}_{I,mn}}{d\mu} - \frac{d\tilde{D}^{1,\sigma}_{I,mn}}{d\mu}\right),\ \frac{dD^{1,\sigma}_{I,mn}}{d\mu} = \sum_{\sigma_1}\int_{\Omega_I} d^3r\,\Phi^{I,\mathrm{AE}}_m(\mathbf{r})\Phi^{I,\mathrm{AE}}_n(\mathbf{r})\frac{dV^{I,\sigma}_{\mathrm{eff}}}{d\rho^{1,I}_{\sigma_1}}\frac{d\rho^{1,I}_{\sigma_1}}{d\mu}$$

$$,\ \text{and } b^{\sigma,\mu}_{I,mn} = \sum_i \langle\tilde{\psi}_{i,\sigma}|\frac{\partial(|\beta^I_m\rangle\langle\beta^I_n|)}{\partial\mu}|\tilde{\psi}_{i,\sigma}\rangle - \sum_i \langle\tilde{\psi}_{i,\sigma}|\beta^I_m\rangle\langle\beta^I_n|\delta^\mu\tilde{\psi}_{i,\sigma}\rangle$$

- Calculation of terms common in both PAW and USPP parallelized over ***G***

Symmetric *e*-ph vertex in USPP and PAW

- Use of symmetric expression of e-ph vertex
  [Phys. Rev. B **100**, 174304 (2019), Phys. Rev. B **101**, 184302 (2020)]

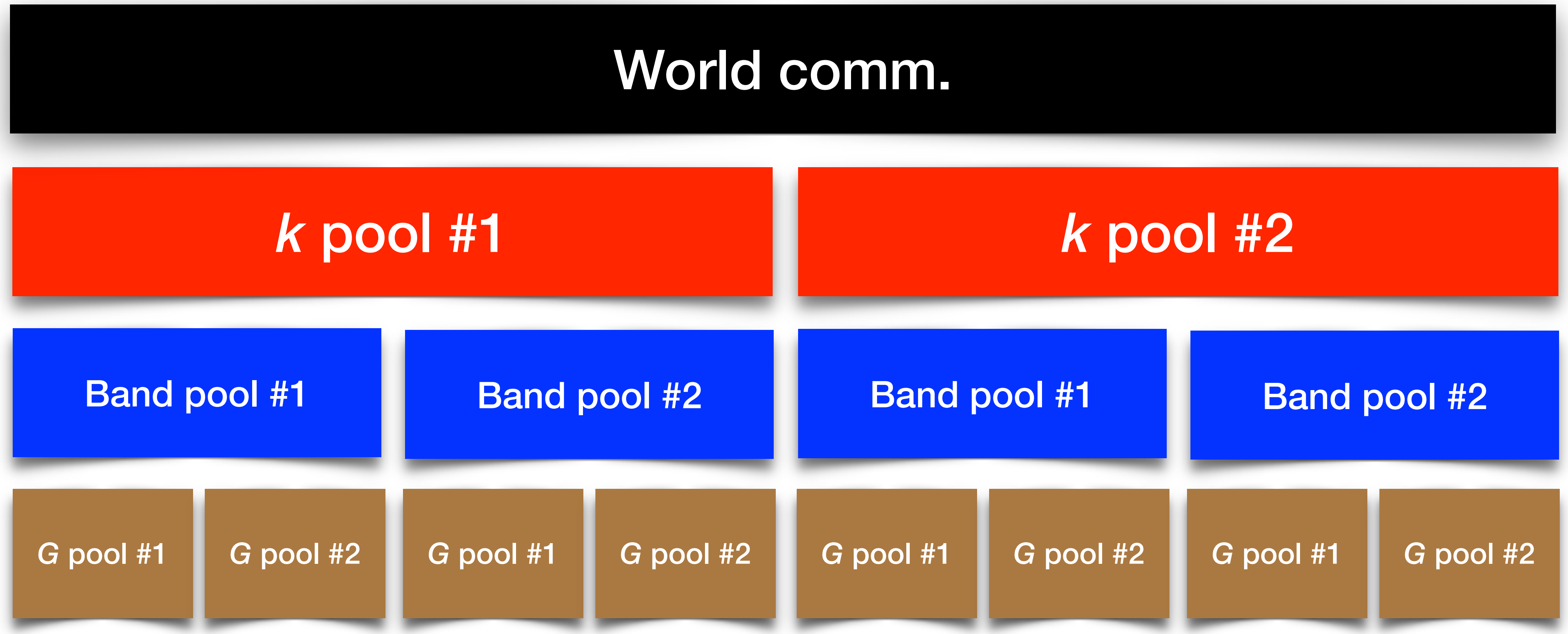
$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = \underbrace{\langle \tilde{\Psi}_{m,\mathbf{k}+\mathbf{q}} | \partial_{\nu\mathbf{q}} \tilde{H} - \epsilon_{n\mathbf{k}} \partial_{\nu\mathbf{q}} \tilde{S} | \tilde{\Psi}_{n\mathbf{k}} \rangle}_{g^{\mathrm{QE}}_{mn\nu}(\mathbf{k},\mathbf{q})} + (\epsilon_{n\mathbf{k}} - \epsilon_{m,\mathbf{k}+\mathbf{q}}) \langle \tilde{\Psi}_{m,\mathbf{k}+\mathbf{q}} | \hat{T}^{\dagger} \partial_{\nu\mathbf{q}} \hat{T} | \tilde{\Psi}_{n\mathbf{k}} \rangle$$

$$\Rightarrow \boxed{|g_{mn\nu}(\mathbf{k},\mathbf{q})| = |g^{*}_{nm\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q})|}$$

- For use with USPP as well, ignore the negligible term with derivatives of on-site partial waves

New Parallel Structure

$$\boxed{g(\mathbf{k}_{\mathrm{c}},\mathbf{q}_{\mathrm{c}})} \rightarrow \boxed{g(\mathbf{R}_e,\mathbf{R}_p)} \quad \rightarrow \quad \boxed{g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})} \rightarrow \boxed{\begin{array}{l}\sum''_{n\mathbf{k}_{\mathrm{f}}}[g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})],\\ \Pi''_{\nu\mathbf{q}_{\mathrm{f}}}[g(\mathbf{k}_{\mathrm{f}},\mathbf{q}_{\mathrm{f}})],\ldots\end{array}}$$

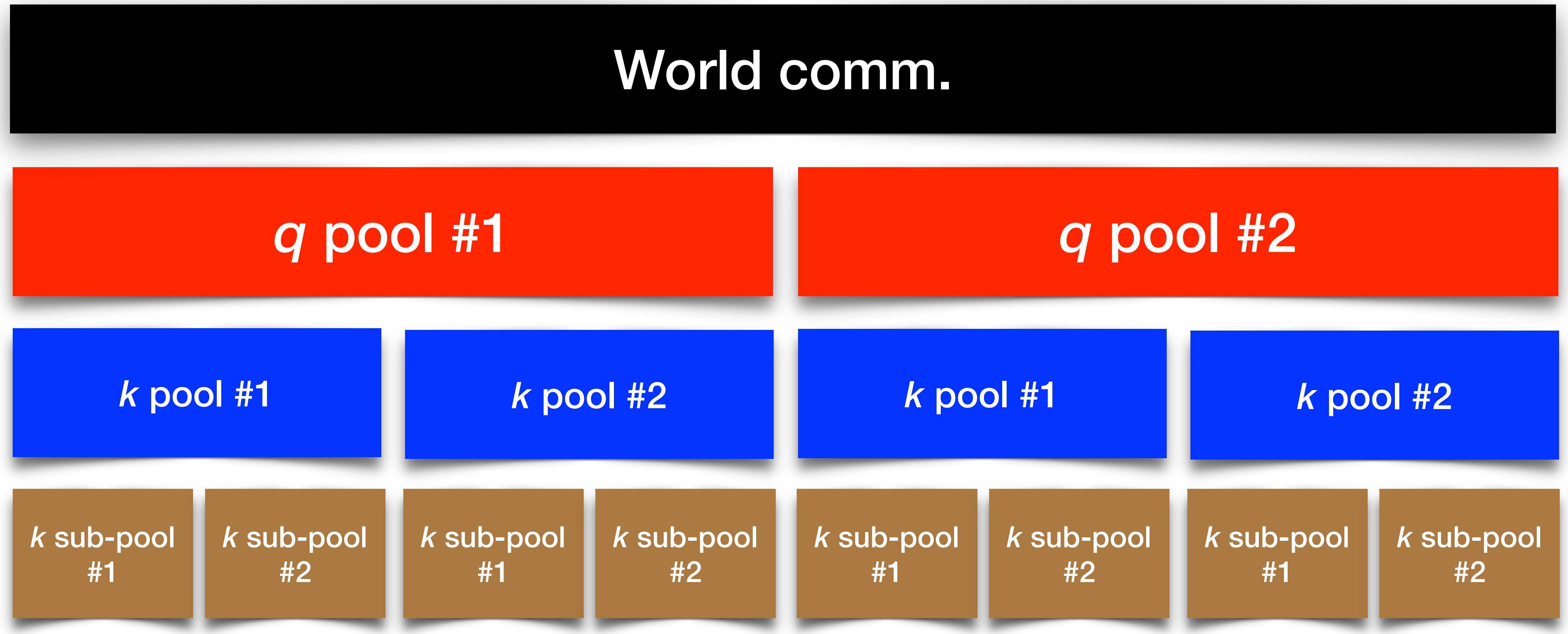


World comm.

k pool #1 | *k* pool #2

Band pool #1 | Band pool #2 | Band pool #1 | Band pool #2

G pool #1 | *G* pool #2 | *G* pool #1 | *G* pool #2 | *G* pool #1 | *G* pool #2 | *G* pool #1 | *G* pool #2



World comm.

q pool #1 | *q* pool #2

k pool #1 | *k* pool #2 | *k* pool #1 | *k* pool #2

k sub-pool #1 | *k* sub-pool #2 | *k* sub-pool #1 | *k* sub-pool #2 | *k* sub-pool #1 | *k* sub-pool #2 | *k* sub-pool #1 | *k* sub-pool #2

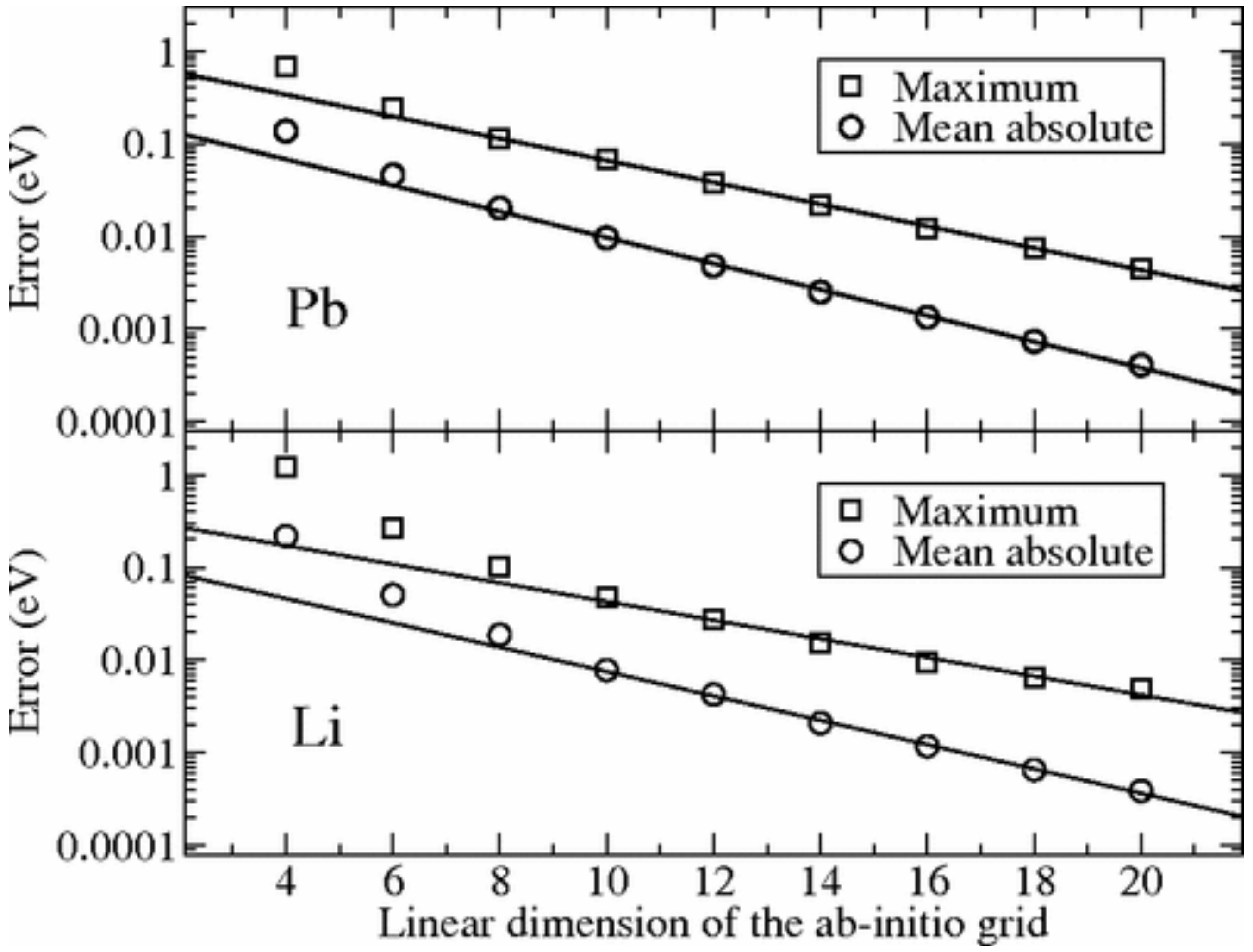
Short-term plans

- Easy construction of (symmetric) localized basis
- Non-collinear magnetism

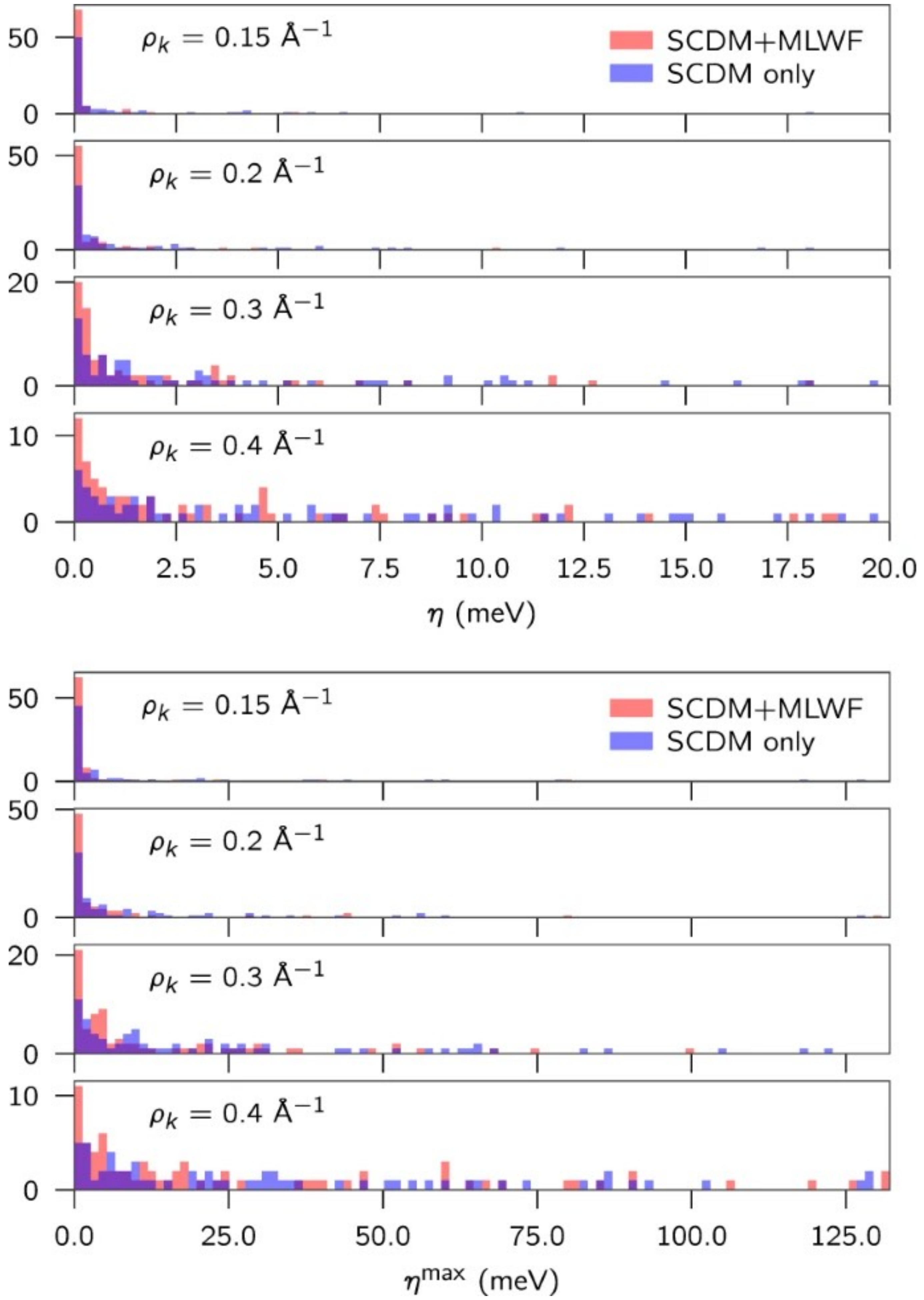
Short-term plans

Easy construction of (symmetric) localized basis

- Importance of high grid density



[Phys. Rev. B 75, 195121 (2007)]



[npj Comput Mater 6, 66 (2020)]

Short-term plans

Easy construction of (symmetric) localized basis

- Projectability [Phys. Rev. B **88**, 165127 (2013)]
- Optimal choice of SCDM-k parameters [npj Comput Mater **6**, 66 (2020)]
- Energy window optimization [Phys. Rev. Materials **2**, 103805 (2018)]

Mid-term plans

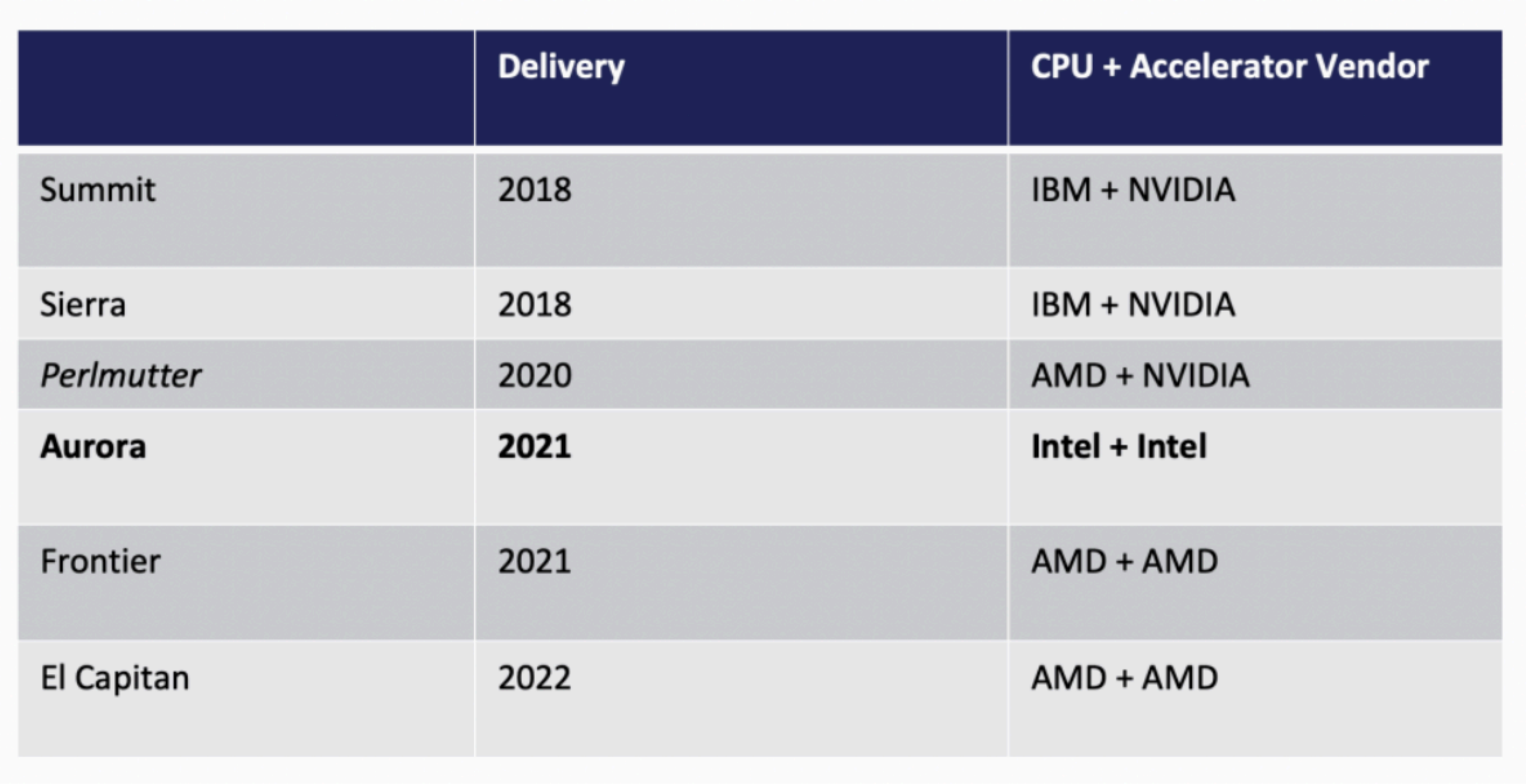
- Port EPW to the heterogeneous architecture (GPU)
- Interface EPW to other DFT codes

Mid-term plans

Porting EPW to GPU

- Importance of OpenMP
- Choice of programming models

An Overview of Some DOE Systems



	Delivery	CPU + Accelerator Vendor
Summit	2018	IBM + NVIDIA
Sierra	2018	IBM + NVIDIA
Perlmutter	2020	AMD + NVIDIA
Aurora	**2021**	**Intel + Intel**
Frontier	2021	AMD + AMD
El Capitan	2022	AMD + AMD

https://alcf.anl.gov/support-center/aurora/porting-aurora

References

- F. Giustino et al., Phys. Rev. B 76, 165108 (2007) [link]
- C. Verdi et al., Phys. Rev. Lett. 115, 176401 (2015) [link]
- S. Ponc´e et al., Comput. Phys. Commun. 209, 116 (2016) [link]
- F. Giustino, Rev. Mod. Phys. 89, 1 (2017) [link]

More Info

- https://epw-code.org
- https://forum.epw-code.org
- https://gitlab.com/QEF/q-e