Tutorial 1: Basic GW calculations on silicon

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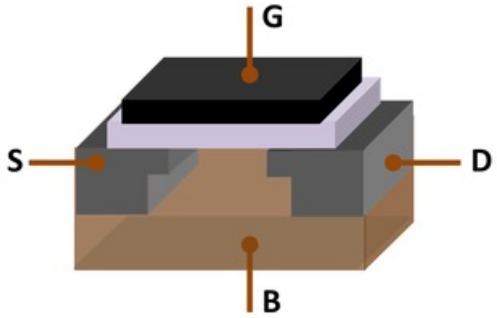
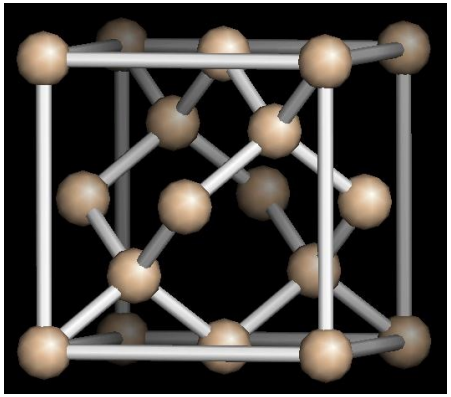
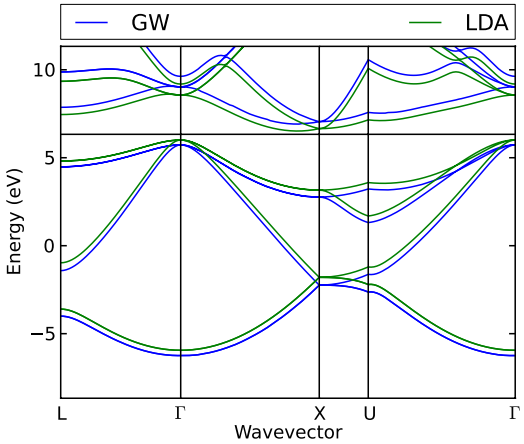






BerkeleyGW

BerkeleyGW
June 2022

For this tutorial we'll couple w/ QE, But Options Exist

We will use this option in the Tutorial today!

Pro: Most widely used interface for BerkeleyGW.

Con: Somewhat more complicated workflow.

Tutorial Goals

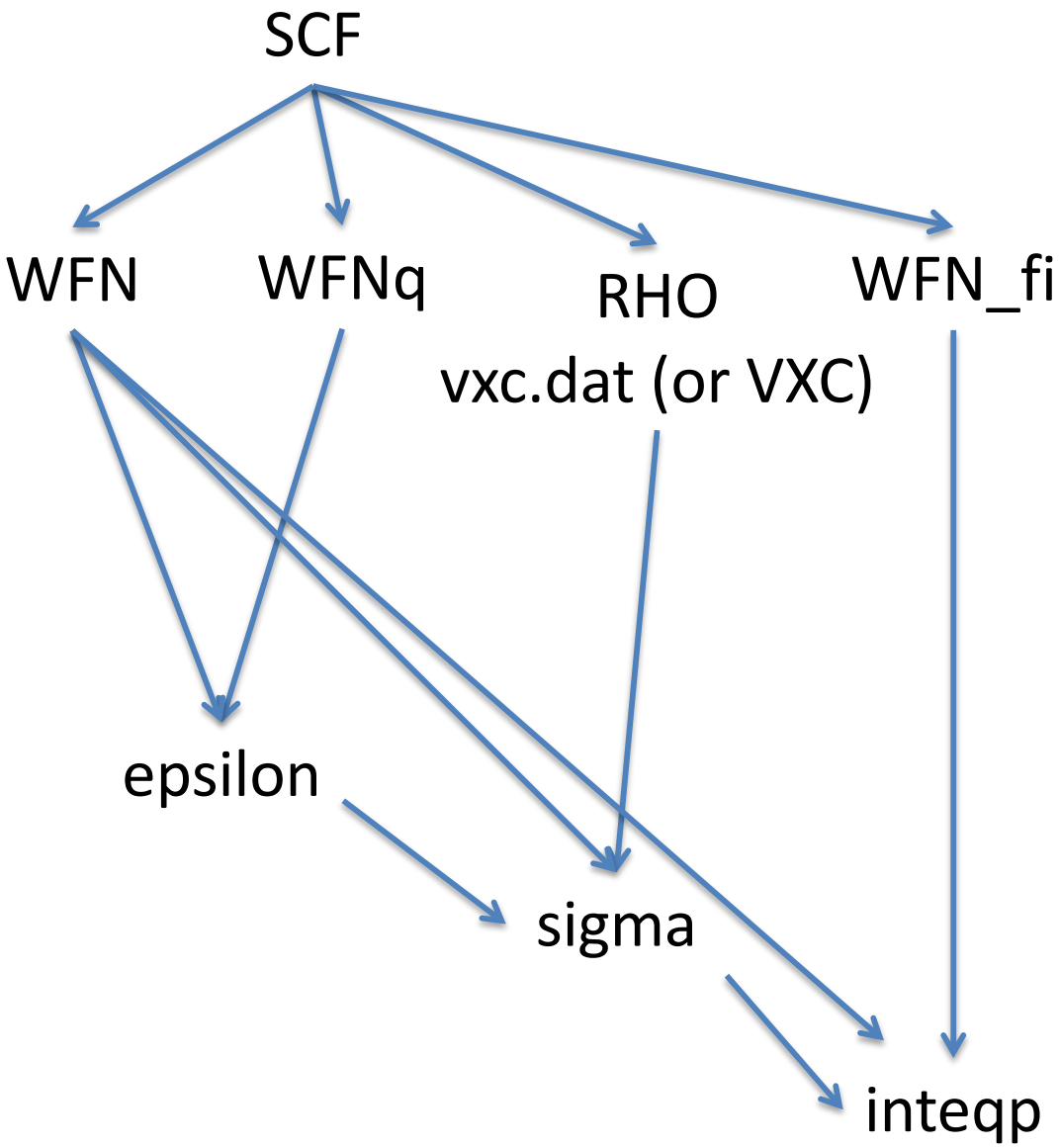
1. Understand the basic workflow of BerkeleyGW, and the relation between the grids, wavefunctions, and the Epsilon, Sigma, and Inteqp codes.
2. Run a basic GW calculation on silicon with the generalized plasmon pole (GPP) model.
3. Construct an interpolated bandstructure via scissors parameters and Inteqp.
4. Solve the Bethe-Salpeter equation for e-h excited states
5. Plot the absorption spectra with and without e-h interactions included

Workflow for the GW Bandstructure

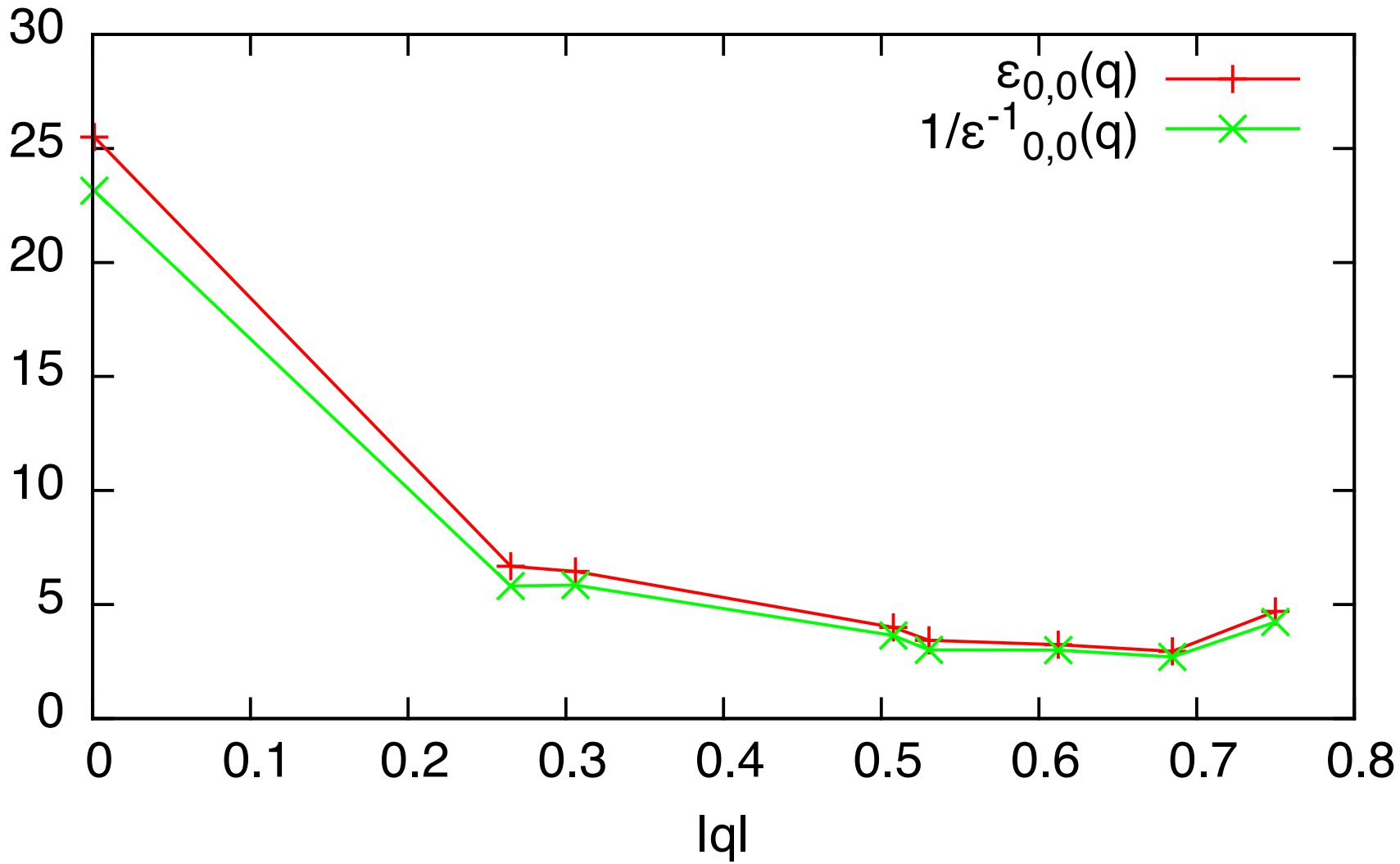
DFT: Quantum ESPRESSO

Utilities:
kgrid.x
wfn_rho_vxc_info.x

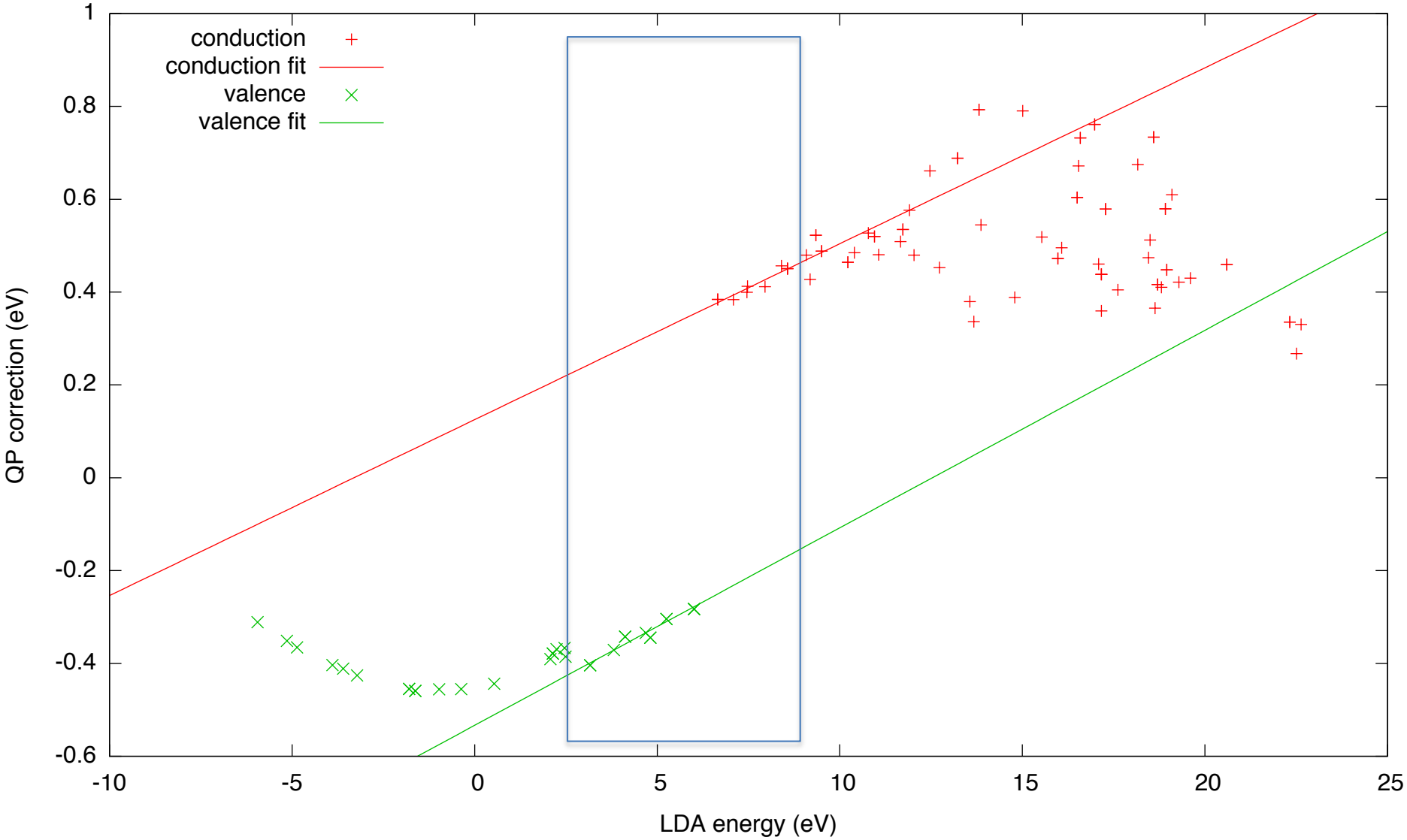
BerkeleyGW



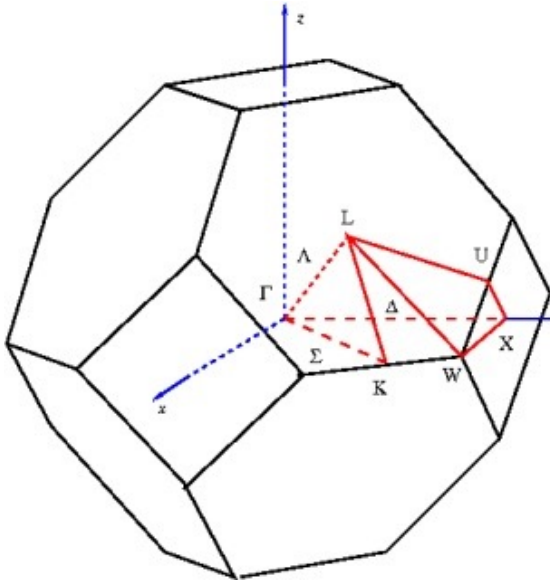
Epsilon: screening as a function of $|q|$

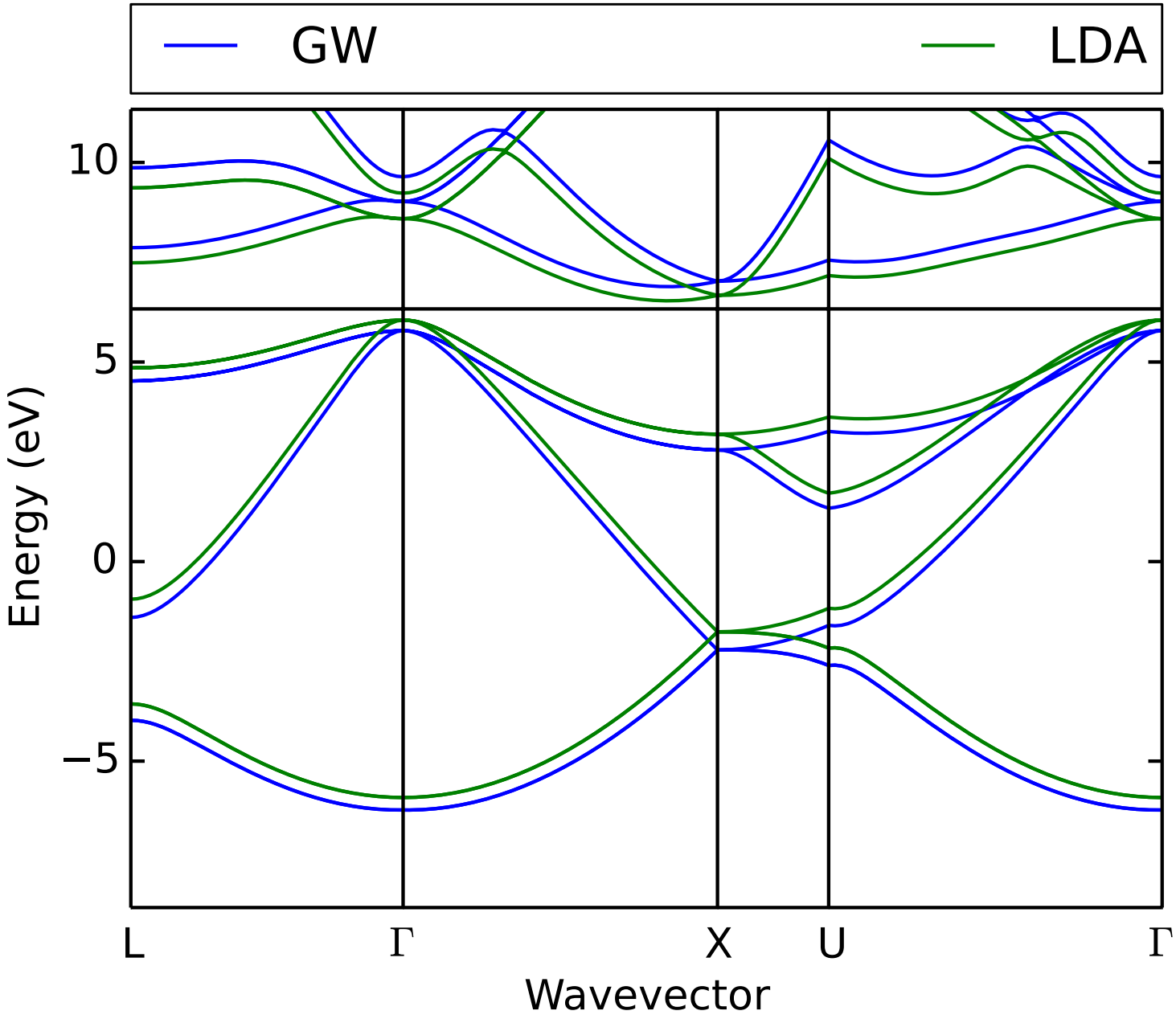


Sigma: QP corrections as a function of LDA energy, with linear fits



Inteqp: interpolated bandstructure





BSE in BerkeleyGW — What is the basis?

$$H^{\mathrm{BSE}}_{vc\boldsymbol{k},v'c'\boldsymbol{k}'} = (E_{c\boldsymbol{k}} - E_{v\boldsymbol{k}})\delta_{vv'}\delta_{cc'}\delta_{v\boldsymbol{k}\boldsymbol{k}} + K_{vc\boldsymbol{k},v'c'\boldsymbol{k}'}$$

diagonal dense

- Challenge: Quasiparticle corrections and Kernel matrix elements must be computed on a very fine k-point grid
  - E.g. Monolayer MoS_2 requires 300x300 k-grid to converge!
  - We already know how to **interpolate** the Quasiparticle corrections. Can we do something similar for the Kernel?

BSE in BerkeleyGW — Interpolation

- Computing the Kernel matrix elements is expensive

$$\langle vc\mathbf{k}_{\mathrm{fi}}|K|v'c'\mathbf{k}'_{\mathrm{fi}}\rangle$$

"fine (fi)" grid refers to the dense k-grid needed to converge the solution of the BSE

- We want to compute the kernel on a "coarse" grid and interpolate the "fine" grid

$$\langle vc\mathbf{k}_{\mathrm{co}}|K|v'c'\mathbf{k}'_{\mathrm{co}}\rangle \longrightarrow \langle vc\mathbf{k}_{\mathrm{fi}}|K|v'c'\mathbf{k}'_{\mathrm{fi}}\rangle$$

- Linear interpolation? Wannier interpolations? K.p interpolation?

No complex phases Hard to operate/unstable Unreliable

- BerkeleyGW: Projection interpolation
  - Explicitly generate coarse- and fine-grid WFNs
  - Expand of fine-grid WFNs in term of coarse-grid WFNs.
  - Captures band crossing, etc.

BSE in BerkeleyGW — Interpolation Scheme

- Step 0: Obtain WFNs on coarse grid and fine grid

- Step 1: Expand fine WFNs in terms of coarse WFNs

$$u_{n\mathbf{k}_{\rm fi}} = \sum_{n'} C^{\mathbf{k}_{\rm co}}_{n,n'} u_{n'\mathbf{k}_{\rm co}} \qquad C^{\mathbf{k}_{\rm co}}_{n,n'} = \int d\mathbf{r}\, u_{n\mathbf{k}_{\rm fi}}(\mathbf{r}) u^*_{n'\mathbf{k}_{\rm co}}(\mathbf{r})$$

- Step 2: Interpolate QP energies (assume Σ is diagonal in $(n\mathbf{k})$):

$$E^{\rm QP}_n(\mathbf{k}_{\rm fi}) = \quad E^{\rm MF}_n(\mathbf{k}_{\rm fi}) + \left\langle \sum_{n'} \left| C^{\mathbf{k}_{\rm co}}_{n,n'} \right|^2 \left(E^{\rm QP}_{n'}(\mathbf{k}_{\rm co}) - E^{\rm MF}_{n'}(\mathbf{k}_{\rm co}) \right) \right\rangle_{\mathbf{k}_{\rm co}}$$

- Step 3: Interpolate BSE Kernel matrix elements (head+wings+body):

$$\langle vc\mathbf{k}_{\rm fi}|K|v'c'\mathbf{k}'_{\rm fi}\rangle = \sum_{n_1,n_2,n_3,n_4} C^{\mathbf{k}_{\rm co}}_{c,n_1} C^{*\mathbf{k}_{\rm co}}_{v,n_2} C^{*\mathbf{k}'_{\rm co}}_{c',n_3} C^{\mathbf{k}'_{\rm co}}_{v',n_4} \langle n_2 n_1 \mathbf{k}_{\rm co}|K|n_4 n_3 \mathbf{k}'_{\rm co}\rangle$$

BSE in BerkeleyGW — Interpolation Scheme

- Note: a direct interpolation of K is not very accurate
  - Explicit dependence on $\mathbf{q}_{\mathrm{fi}} = \mathbf{k}_{\mathrm{fi}} - \mathbf{k}'_{\mathrm{fi}} \neq \mathbf{q}_{\mathrm{co}} = \mathbf{k}_{\mathrm{co}} - \mathbf{k}'_{\mathrm{co}}$
- We decompose the kernel matrix elements into components having different analytical behavior wrt $\mathbf{k}$–$\mathbf{k}'$:

$$\langle vc\mathbf{k}|K|v'c'\mathbf{k}'\rangle = \frac{a_{vc\mathbf{k},v'c'\mathbf{k}'}}{A(\mathbf{k}'-\mathbf{k})} + \frac{b_{vc\mathbf{k},v'c'\mathbf{k}'}}{B(\mathbf{k}'-\mathbf{k})} + \frac{c_{vc\mathbf{k},v'c'\mathbf{k}'}}{C(\mathbf{k}'-\mathbf{k})}$$

- We interpolate each component individually.
  - Ex: for 3D semiconductor:

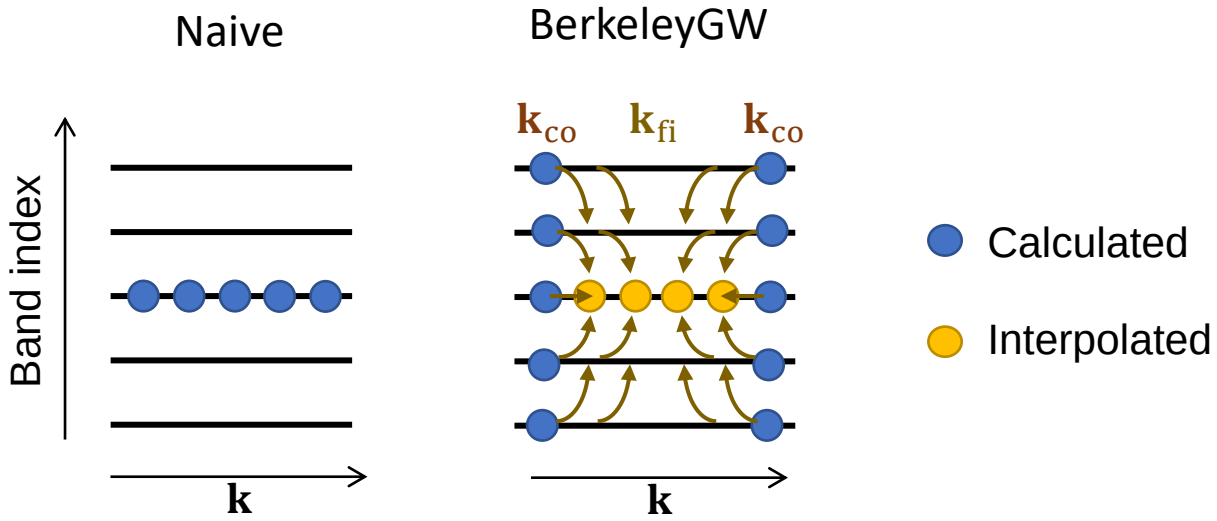
$$A(\mathbf{q}) = q^2, \qquad B(\mathbf{q}) = q, \qquad C(\mathbf{q}) = 1$$

- Important flags: `screening_*` and `*truncation`

BSE in BerkeleyGW — Interpolation Scheme

- In practice: trading bands for k-points

$$\langle vc\mathbf{k}_{\mathrm{fi}}|K|v'c'\mathbf{k}'_{\mathrm{fi}}\rangle = \sum_{n_1,n_2,n_3,n_4} C^{\mathbf{k}_{\mathrm{co}}}_{c,n_1} C^{*\mathbf{k}_{\mathrm{co}}}_{v,n_2} C^{*\mathbf{k}'_{\mathrm{co}}}_{c',n_3} C^{\mathbf{k}'_{\mathrm{co}}}_{v',n_4} \langle n_2 n_1 \mathbf{k}_{\mathrm{co}}|K|n_4 n_3 \mathbf{k}'_{\mathrm{co}}\rangle$$

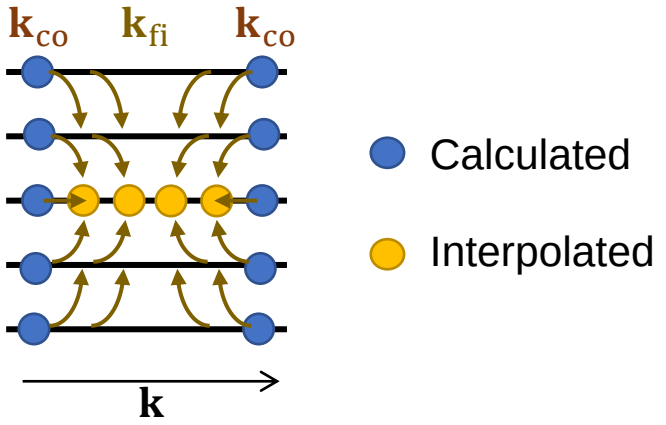


- How to get a good interpolation?
  - Include a large number of bands from the coarse grid and start from a coarse grid that is not too coarse.

BSE in BerkeleyGW — Interpolation Scheme

- How do I know if I included enough bands?

$$\mathrm{Error}(\mathrm{n}, \mathbf{k}_{\mathrm{fi}}) = 1 - \sum_{n'} \left| C_{n,n'}^{\mathbf{k}_{\mathrm{fi}}} \right|^2$$



- Detail of “completion relation”:
  `dvmat_norm.dat`
  `dcmat_norm.dat`

`absorption.out / inteqp.out`

BerkeleyGW Workflow

Step 0: Calculate QP–corrected band structure on a coarse grid

`epsmat.h5`, $\{E_c\}_{\text{co}}$, $\{E_v\}_{\text{co}}$

`kernel.x`

Step 1: Calculate BSE kernel on the same coarse grid

$[K]_{\text{co}}$

`absorption.x`

Step 2: Interpolate to a fine k-grid and build BSE Hamiltonian…

$$[H]_{\text{co}} \Rightarrow [H]_{\text{fi}}$$

… and diagonalize BSE Hamiltonian

$$\text{evals}\ [H]_{\text{fi}} \Rightarrow \varepsilon_2$$

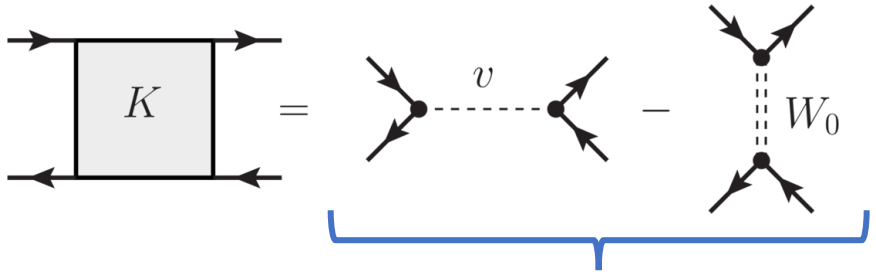
1. Kernel

kernel.x

Step 1: Calculate BSE kernel on the same coarse grid

$$[K]_{\mathrm{co}}$$

- Time consuming: Computes $(n_v n_c n_k)^2$ matrix elements
- Input: epsmat.h5, eps0mat.h5, WFN_co
- Output:



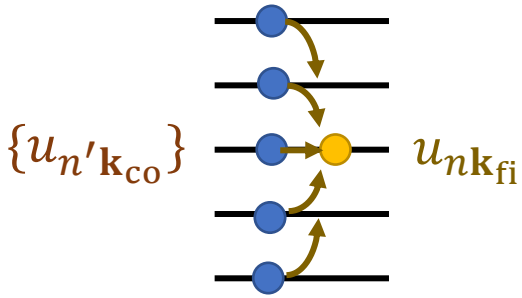
bsemat.h5

- Recommended: Use same WFN_co as WFN_inner in Sigma

1. Kernel

Sample **kernel.inp**

```
number_val_bands <?>
number_cond_bands <?>

<?>_symmetries_coarse_grid
screening_<?>
```



You'll typically want to use symmetries here, so put:
use_symmetries_coarse_grid

Bands counted wrt FE:

- vbm, vbm-1, …
- cbm, cbm+1, …

Remember to calculate Kernel on more bands because of the interpolation!

(# of bands in Sigma can't be less than this number!)

2. Absorption

absorption.x

Step 2: Interpolate to a fine k-grid and build BSE Hamiltonian…

$$[H]_{\text{co}} \Rightarrow [H]_{\text{fi}}$$

… and diagonalize BSE Hamiltonian

$$\text{evals } [H]_{\text{fi}} \Rightarrow \varepsilon_2$$

- Absorption needs same coarse WFN_co from Kernel
- Two fine WFN files are needed

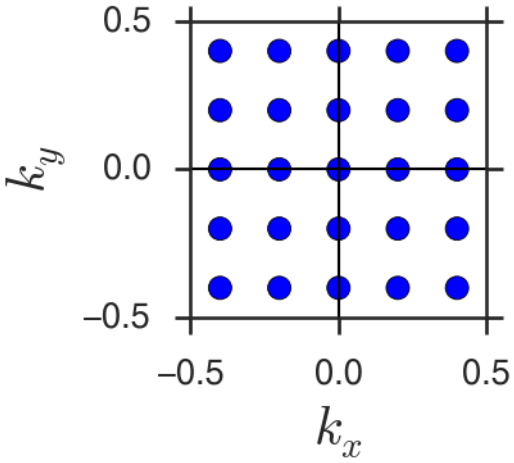
$$\varepsilon_2(-\mathbf{q},\omega) \propto \sum_S |\langle 0|\hat{v}|S\rangle|^2 \delta[\omega - \Omega_S] \qquad \langle 0|\hat{v}|S\rangle = \frac{\Omega_S}{q} \sum_{vc\mathbf{k}} A^S_{vc\mathbf{k}} \langle v\mathbf{k}+\mathbf{q}|e^{-i\mathbf{q}\cdot\mathbf{r}}|c\mathbf{k}\rangle$$

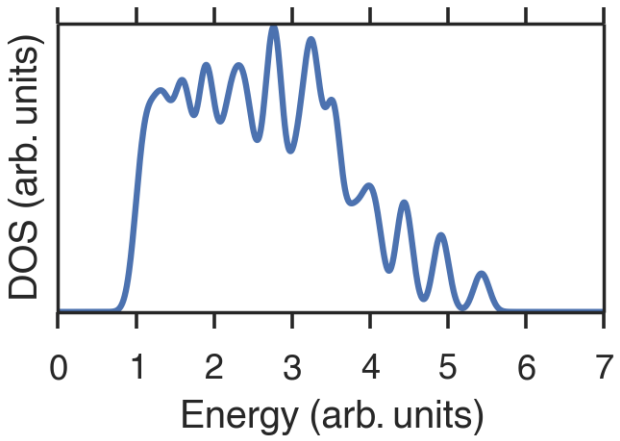
- Typically q is 10^{-3}
- Fine WFN files:
  - WFN_fi: for conduction states $|c\mathbf{k}\rangle$
  - WFNq_fi: for q-shifted valence states $|v\mathbf{k}+\mathbf{q}\rangle$

Direction of q = polarization of light= difference between $\{\mathbf{k}\}$ in WFNq and $\{\mathbf{k}\}$ in WFN

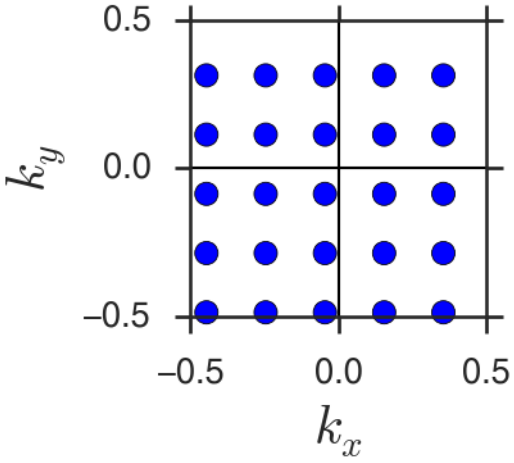
2. Absorption — Randomly Shifted k-grids

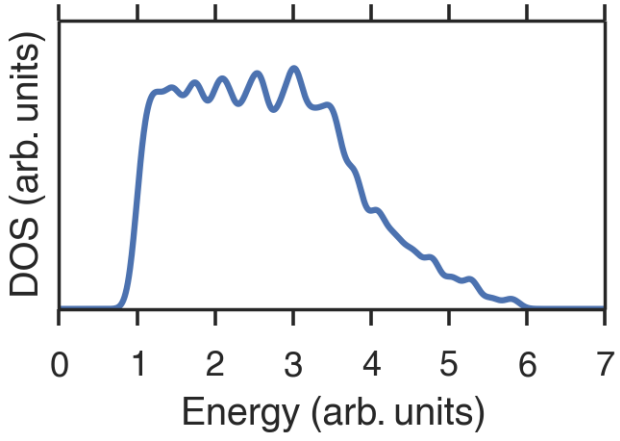
WFN_fi, no k-shift





WFN_fi, random k-shift





2. Absorption — Randomly Shifted k-grids

Sample **absorption.inp**

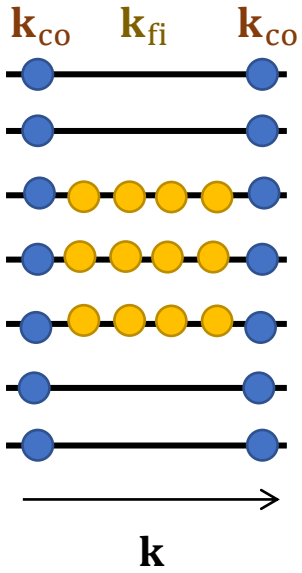
```
diagonalization

number_val_bands_coarse <?>
number_cond_bands_coarse <?>
number_val_bands_fine <?>
number_cond_bands_fine <?>

use_symmetries_coarse_grid
no_symmetries_fine_grid
no_symmetries_shifted_grid

screening_semiconductor

use_velocity

gaussian_broadening
energy_resolution 0.15

eqp_co_corrections
```

Unshifted grid (WFN_co)

Both randomly shifted grids (WFN_fi and WFNq_fi)

Broaden each delta function.

Interpolate eqp_co.dat



2. **k**-, **q**-grids and bands

For reference: simplified approach for tutorial

	k-grid	# bands	Comments
SCF	uniform, no shift	occupied	
WFN	uniform, no shift	many	
WFNq	WFN + **q**-shift	occupied	
epsilon.inp **q**-points	WFN but $\mathbf{q}_0$ instead of 0	many	bands to sum over
WFN_inner	WFN	many	bands to sum over
sigma.inp **k**-points	subset of WFN_inner	few	can choose to calculate Sigma just for bands of interest
WFN_co	WFN_inner	few	
WFN_fi (absorption)	uniform, random shift	few	
WFNq_fi	WFN_fi + **q**-shift	occupied	
WFN_fi (inteqp)	anything	few	whatever is of interest

Getting Started

Proceed according to the instructions:

```
$ cd $SCRATCH

$ mkdir EP-SCHOOL_BGW ; cd EP-SCHOOL_BGW

$ cp /work2/06868/giustino/EP-SCHOOL/Fri.7.DelBen.tar .

$ tar -xvf Fri.7.DelBen.tar
```

Follow instructions in each README file