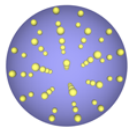# Tutorial 1: Basic GW calculations on silicon

David A. Strubbe
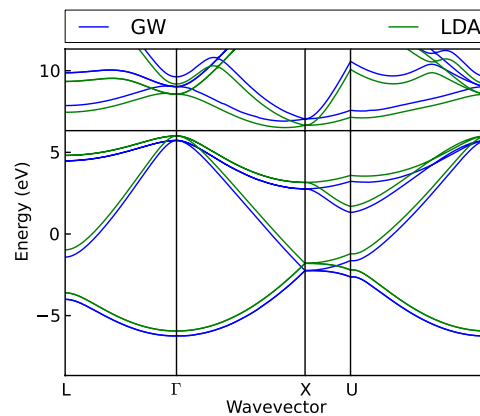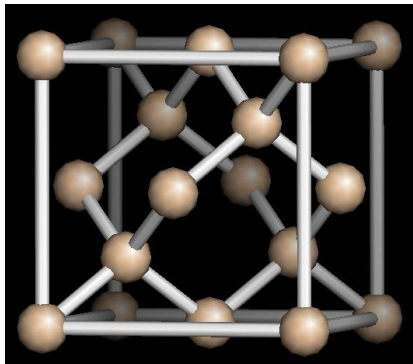
Department of Materials Science and Engineering,

Massachusetts Institute of Technology
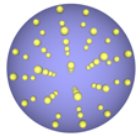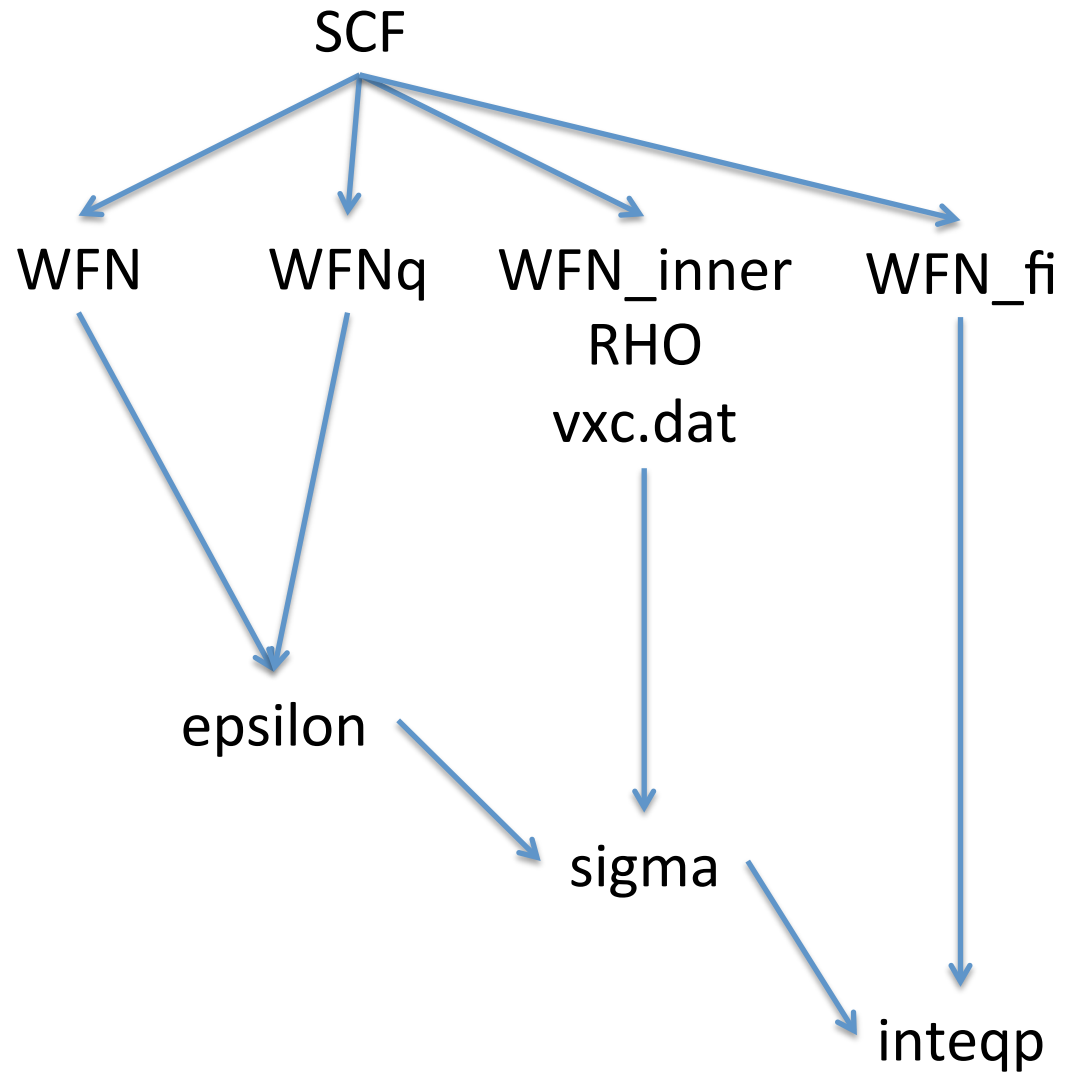
BerkeleyGW tutorial
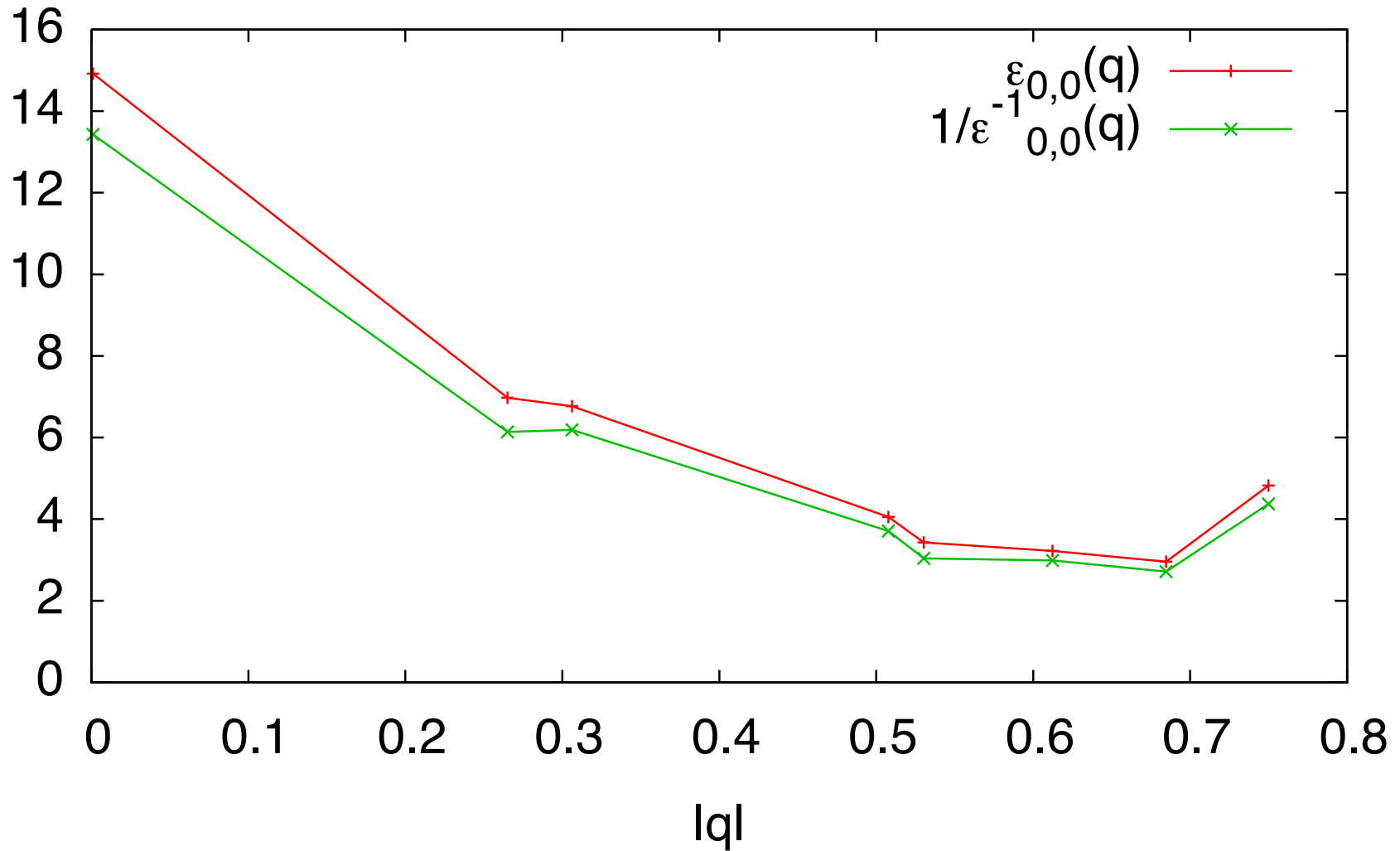22 November 2013

Workflow for the tutorial

paratecSGL

kgrid.x
wfn_rho_vxc_info.x

BerkeleyGW

SCF

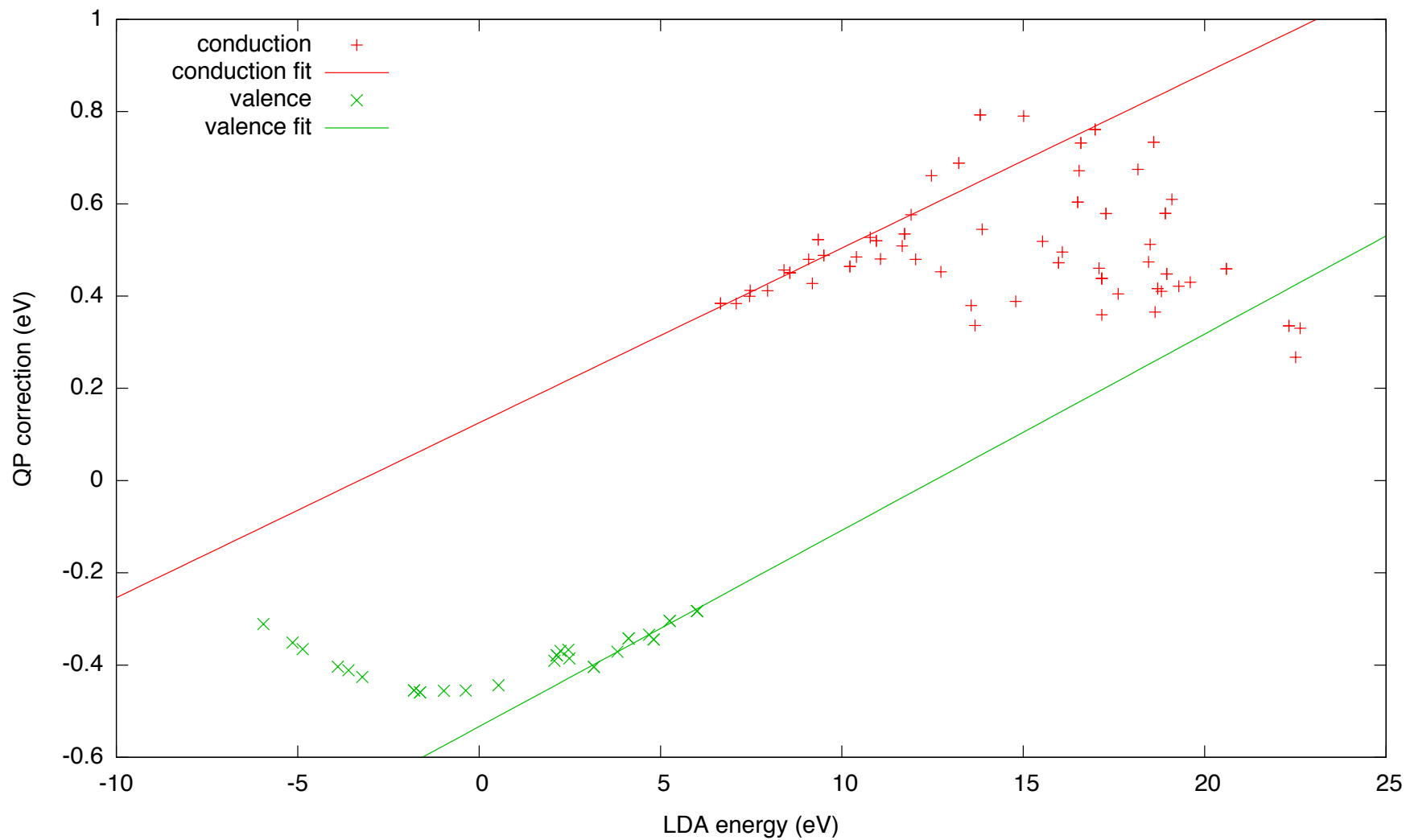WFN   WFNq   WFN_inner   WFN_fi
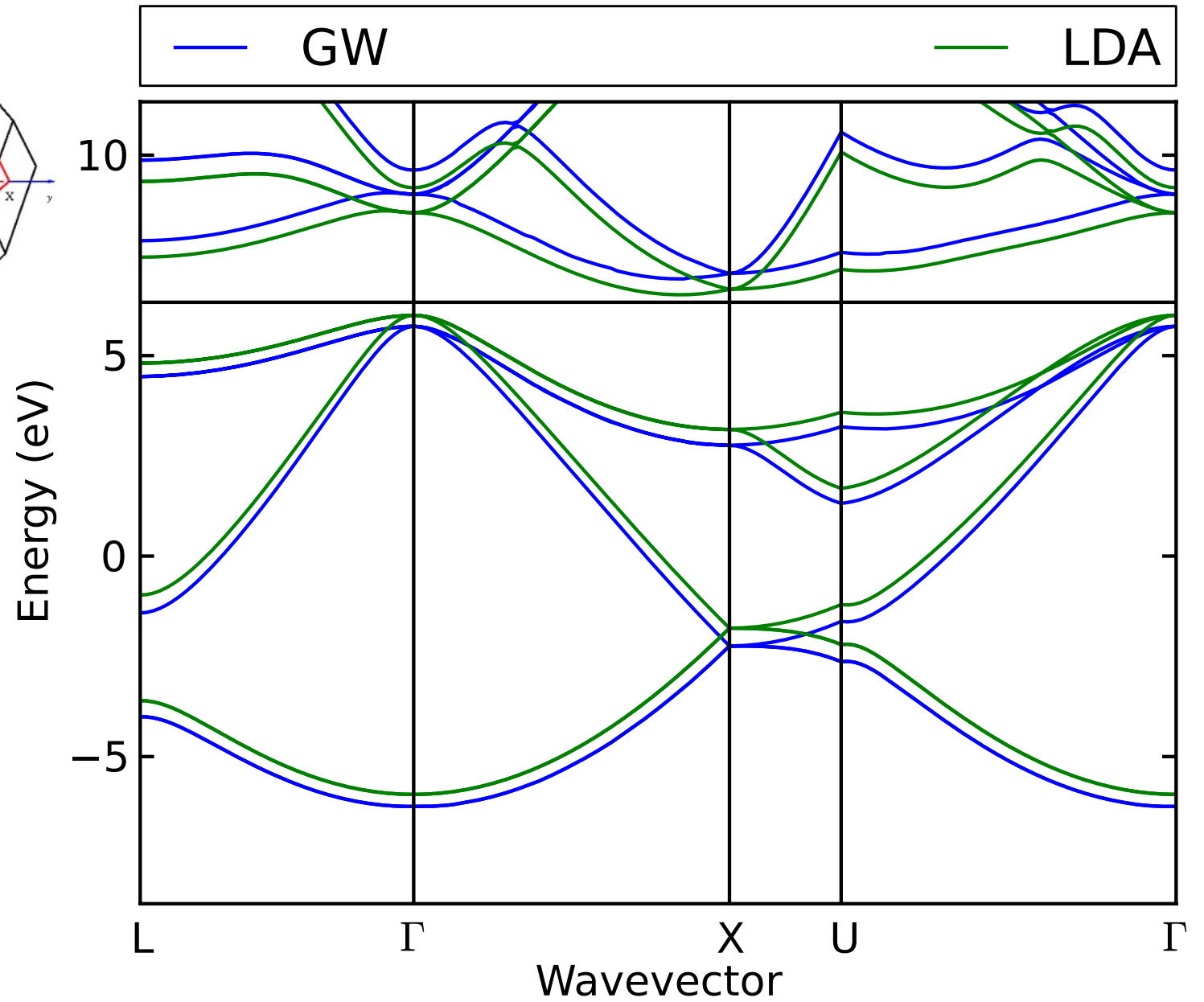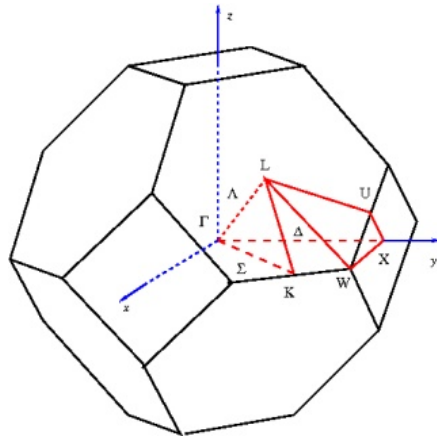
RHO

vxc.dat

epsilon

sigma

inteqp

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

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

Inteqp: interpolated bandstructure

http://www.berkeleygw.org/releases/manual_v1.0.6.html

BerkeleyGW manual (version 1.0.6)

Contents

Goals

Basic goals:
1. Understand the basic workflow of BerkeleyGW, and the relation between the k-grids, wavefunctions, Epsilon, Sigma, and Inteqp.
2. Run a basic GW calculation on silicon.
3. Construct an interpolated bandstructure via scissors parameters and Inteqp.

Stretch goals:
1. Compare your Sigma GW results with Hartree-Fock and/or static COHSEX. What inputs are no longer necessary? How do the results compare?
2. Modify the example for GaAs and repeat each step of the calculation.

```
module load paratec/6.0.0
module load espresso/5.0.3
module load berkeleygw/1.0.6

cd $SCRATCH
cp -r /project/projectdirs/m1694/BGW-2013/1.1-silicon .

http://www.berkeleygw.org/releases/manual_v1.0.6.html
```