IAP 2016: Electronic-structure software tutorials

Instructor: Dr. David Strubbe
Sign-up by Jan 8 by emailing dstrubbe@mit.edu
2-5 pm, 8-119, Jan 12, 14, 19, 21
http://web.mit.edu/~dstrubbe/www/iap_tutorials.html

octopus

BerkeleyGW

www.tddft.org/programs/octopus  www.berkeleygw.org
DFT and TDDFT  GW approximation and Bethe-Salpeter equation

Pre-requisites:
• Basic knowledge of command-line usage of Linux/BSD/MacOS.
• Basic knowledge of simulation techniques in electronic structure
  for solid-state physics or quantum chemistry (i.e. what is DFT).
Goals

Learn the basics of how to use the Octopus and BerkeleyGW codes (why these two...?)

Learn about time-dependent density-functional theory (TDDFT) and many-body perturbation theory (GW approximation and Bethe-Salpeter equation)

See how these calculation techniques work in practice

Learn when these methods and codes will be useful for your work

Learn about parallel computing, some molecular/solid-state phenomenology, visualization/plotting
Schedule

2-5 pm, Room 8-119

**Jan 12:** introduction to Octopus, TDDFT theory, and NERSC ground-state DFT tutorials in Octopus

**Jan 14:** more discussion of TDDFT
time-dependent and more specialized tutorials in Octopus

**Jan 19:** introduction to BerkeleyGW and GW approximation
band structure of Si tutorial in BerkeleyGW

**Jan 21:** introduction to Bethe-Salpeter equation
optical spectrum of Si tutorial in BerkeleyGW

*lots more tutorials available if you have more time and interest...*
Instructors

Overall: Dr. David Strubbe, postdoctoral associate in Jeffrey Grossman’s group, Dept. of Materials Science and Engineering, MIT

Octopus: Jacob Sanders, PhD student in Alán Aspuru-Guzik’s group, Department of Chemistry and Chemical Biology, Harvard University

BerkeleyGW: Dr. Huashan Li, postdoctoral associate in Jeffrey Grossman’s group, Dept. of Materials Science and Engineering, MIT
The codes

Both free and open-source *ab initio* simulation packages
Widely used in academic community (albeit not as much as Gaussian, VASP, ...)
Developers around the world, open to collaboration

**Octopus**: real-space pseudopotential DFT and TDDFT.
Primarily for molecules or low-dimensional systems (dot, wire, sheet)
Time propagation, model systems, exotic levels of theory, massively parallel calculations. Optical properties. DFT, TDDFT are limited by XC approximations

**BerkeleyGW**: plane-wave many-body perturbation theory (begins with DFT)
Bulk crystals, low-dimensional nanostructures, molecules
Quasiparticle band structure (GW approximation),
optical properties and excitons (Bethe-Salpeter equation)
Rigorous diagrammatic theory unlike DFT, *ab initio* even to chemists
Massively parallel calculations (need lots of memory and cores)
Where to run

Octopus: your laptop, your group’s local cluster, or NERSC. small calculations may be simpler to run on local machine. (don’t take up your time installing now though)

BerkeleyGW: all on NERSC. bigger calculations, more complicated scripts

• Training accounts from National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory
• Need to sign User Agreement
• Will expire Jan 31
• Definitely use for BerkeleyGW part even if you have a NERSC account already
Cori (phase 1): Intel, Cray hardware/software

System configuration: 1,630 nodes, each with 128 GB memory, two 16-core Intel Haswell CPUs 2.3 GHz

To log in, run ssh trainX@cori.nersc.gov in your terminal, substituting the actual name of your training account.

Run your jobs from directories on the scratch disk, which has better I/O performance. cd $SCRATCH to get there.

Be aware that since this machine is far away, running X-Windows programs may be quite slow; better to do it locally.
You submit jobs to the SLURM scheduler by the sbatch command, e.g. `sbatch job.scr`, which will put them in the queue for execution when there is free space. Be sure you do this from the directory where your input files are located. The job script (see example below) specifies parameters about how many cores to use, what commands to run, etc.

You can see what jobs you currently have in the queue by executing `squeue -u $USER`, so you can see when your job finishes. A status code will be shown in the ST column: PD = pending, i.e. waiting in the queue, R = running, CG = completing. Example:

```
JOBID   USER   ACCOUNT  NAME       PARTITION  QOS   NODES  TIME_LIMIT  TIME  ST  START_TIME
921487  dstrubbe  mp149  test_pulpo  regular  normal  1   4:00:00     0:00  PD   N/A
```

If you make a mistake, you can cancel a job by `scancel JOBID`, where JOBID is the number written by `squeue`.

After the run, you will have a file in the directory from which you submitted the job, called `slurm-JOBID.out`. If the job failed for some reason unrelated to the code, the error message will be there.

```bash
#!/bin/bash
#SBATCH -J methane
#SBATCH -n 1
#SBATCH -p debug
#SBATCH -t 00:30:00
#SBATCH --export=ALL

cd $SLURM_SUBMIT_DIR
srun -n 4 /project/projectdirs/mp149/IAP2015/octopus-5.0.1/bin/octopus_mpi &> output
```
Octopus Developers

Current developers:
- Joseba Alberdi
- Xavier Andrade
- Alberto Castro
- Tilman Dannert
- Umberto De Giovannini
- Alain Delgado Gran
- Nicole Helbig
- Hannes Huebener
- Rene Jestaedt
- Joaquim Jornet-Somoza
- Ask Horth Larsen
- Irina Lebedeva
- Miguel A.L. Marques (hyllios)
- Fernando Nogueira
- Micael Oliveira
- Carlo Andrea Rozzi
- Angel Rubio
- Ravindra Shinde
- José R. F. Sousa
- David Strubbe
- Iris Theophilou
- Alejandro Varas
- Matthieu Verstraete
- Philipp Wopperer

Former developers:
- Heiko Appel
- Fulvio Berardi
- Johanna Fuks
- David Kammerlander
- Kevin Krieger
- Florian Lorenzen
- Danilo Nitsche
- Roberto Olivares-Amaya
- Arto Sakko
- Axel Thimm
- Jessica Walkenhorst
- Jan Werschnik
The actual octopus tutorials


Today

The ground state
- Hydrogen atom - getting started
- Nitrogen atom - basic input variables
- Methane molecule - converging a ground-state calculation
- Centering geometry - using the utility oct-center-geom
- Benzene molecule - making 3D plots

NERSC has XCrySDen, VisIt installed if you don’t. 
module load xcrysden (or visit)

Thursday

Optical-response calculations
- Time-dependent run
- Optical spectra from time-propagation - how to obtain the absorption spectrum through the explicit solution of the time-dependent Kohn-Sham equations
- Optical spectra from Casida’s equation - how to solve Casida’s equation to get an optical spectrum

Extra ones

Model systems
- Harmonic oscillator
- Helium atom
- Particle in an octopus

Others
- Large systems: the Fullerene molecule
- Periodic systems
- Geometry optimization

Get to work!