Electronic Structure: from blackboard to source code

Week 1

Lecture 1-2: Introduction to Density Functional Theory. *The basic approximations: Born Oppenheimer adiabatic approximation and the effective potential concept. How does the effective potential look like (example: Hartree Fock)? DFT: Density as the basic quantity, Hohenberg-Kohn theorem and variational principle, Kohn-Sham auxiliary equations. Variational principle and the Hellmann-Feynman and stress theorems. The band structure interpretation and its shortcomings, band gap problem, Janak's theorem.*

Lecture 3: General description of a plane-wave pseudopotential code. *Self-consistent cycle vs global minimization and Car-Parrinello method. Block diagram of a SCF-type and a CP-type code. The basic modules: diagonalization/minimization (needs H*psi), building the density (needs BZ sampling), building the potential (needs Poisson's solver and exchange-correlation functionals). Initialization (the external potential) and termination (forces/stress and ionic evolution). The KS hamiltonian and wave functions in a PW basis set. Fast Fourier transform and the dual space formalism. How things scale with system dimensions ? Why do we need pseudopotentals ?*

Lecture 4-5: Pseudopotentials. *Empirical pseudopotentials. Transferability. First principles pseudopotential (unscreening of the reference atomic configuration). Norm Conserving Pseudopotentials: PP in the semilocal form, PP in the fully non-local Kleinman-Bylander form. Ghost States. Ultra Soft Pseudopotentials. Generalized eigenvalue problem and orthogonality. Projection Augmented Wave datasets. Total energy break up in grid and atomic contributions.*

Week 2

Lecture 6:Parallelization. *Parallelization tools and strategies: MPI and OpenMP; data and workload distribution; bandwidth and latency. Basic parallel operations (checkpoint, broadcast, collect, gather/scatter); communication intensive operations. Amdahl's law. Strong and weak scalability. Hierarchy of parallelization levels. Porting computational intensive modules to GPUs.*

Lecture 7: Solving the KS equation. *Iterative diagonalization drivers: Davidson diagonalization; Conjugate Gradient; DIIS. Hamiltonian preconditioning. Efficient evaluation of the KS hamiltonian and overlap matrix by dual space formalism and Kleinman-Bylander pseudopotential decomposition.*

Lecture 8: Symmetry. *How to use crystal symmetry to reduce the computational work load. Symmetrization of density, energy, forces and other tensorial quantities. Special points for BZ integration. Automatic generation of k-point grids. Gamma point special features.*

Lecture 9: Building the new charge density. *Brillouin zone sampling: periodic vs non periodic systems; metallic vs non metallic; magnetic vs non magnetic. US/PAW augmentation charges; real space vs reciprocal space approach. Charge density mixing: simple mixing; Broyden mixing. Error estimate, charge sloshing, preconditioning: Thomas Fermi and local TF mixing.*

Lecture 10: Building the new potential. *Hartree energy and potential and its corrections for isolated systems. Exchange-correlation functionals (no hybrids yet). Energy in LDA and GGA and how to take its derivative with respect to density.*

Week 3

Lecture 11: Advanced xc functionals. *Hybrids, implementation and challenges. Fock operator in a plane-wave approach; nested self-consistent loop; adaptively compressed exchange (ACE).*

Lecture 12: Treatment of van der Waals interactions. *vdW-DF functionals; Roman Perez-Soler interpolation scheme. Grimme's damped dispersion correction. Tatckenko-Scheffler vdW correction.*

Lecture 13: More about projectors and augmentation charges. *Real-space vs reciprocal-space implementation of beta and q functions. Are they equivalent ? If not what to do.*

Lecture 14: More about iterative diagonalization. *Functional derivatives are just derivative. Steeepest descent, conjugate gradient, preconditioned conjugate gradient. All we need is H_psi (and S_psi and g_psi).*

Lecture 15: Density Functional Perturbation Theory. *DFPT and lattice dynamical calculations. Block diagram of a linear response code. Consequences of symmetry. Definition and solution of the linear systems. Evaluation of the density response. Perturbed self-consistent potential. Computation of the dynamical matrix.*