Qbox hands-on exercises

Files are available on midway.rcc.uchicago.edu at /project2/miccom-school/qbox

Read the file /project2/miccom-school/qbox/README

Methane molecule
- Ground state calculation
- Relaxation
- Molecular dynamics
- visualization of energy, temperature, distances, using Qbox tools
- Examples of bad choices of parameters leading to incorrect simulations

Water molecule
- Ground state calculation
- Relaxation
- Molecular dynamics
- Analysis of trajectories, vibrational spectrum calculation

Water molecule in an external electric field
- Oscillations of the molecule in the field during MD simulation

C60
- Ground state calculation
- Relaxation
- HOMO-LUMO gap calculation
- Calculation of Maximally Localized Wannier Functions (MLWFs)

Liquid water H2O32
- Ground state calculation
- Molecular dynamics
- mean-square displacement of oxygen and hydrogen atoms

Silicon FCC cell
- Ground state of FCC crystal, primitive cell
- Calculation of the stress tensor
- Cell relaxation
- Compression under 10 GPa

Liquid silicon 64-atom cubic cell
- Ground state calculation
- Molecular dynamics with thermostat
- Simulation of a metallic system
- Melting
- Calculation of mean-square displacement