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Localised Orbitals, Periodic Systems and Backflow using CASINO (180' lab)

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Getting started

1. Log on to tungsten.
2. Type "~train06/install_casino".
3. Type "source ~/.cshrc".
4. Type "rehash".

Directories called CASINO, Silicon_loc, Silicon222, Silicon333 and Neon should have appeared in your home directory. You can now start on the worksheets.

Note that you should use "runqmc nnodes 4 time 00:15" to submit a 15-minute, 4-processor CASINO job on tungsten. (NB, 15 minutes is appropriate for some of the optimisation examples in Worksheet 2; 5 minutes should be fine for the VMC calculations in Worksheet 1.)

Topics

- Worksheet 1: Using localised orbitals in CASINO (1 hour)
  - ° Brief introduction to CASINO's input files
  - ° VMC calculations using CASINO
  - ° Plane-wave and blip representations
  - ° Localised orbitals
- Worksheet 2: QMC calculations for periodic systems: dealing with finite-size effects (1 hour)
  - ° Wave-function optimisation
  - ° Single-particle finite-size effects
  - ° MPC interaction
- Worksheet 3: QMC calculations using backflow (1 hour)
  - ° Optimising backflow parameters
  - ° DMC calculations using CASINO
  - ° Plotting the backflow transformation