

# Lab 2: QMC Basics

QMC Training 2016

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# Lab Startup

- Login to Vesta
  - `ssh -Y username@vesta.alcf.anl.gov`
  - Click button on CRYPTOCARD
  - Password: PIN + CRYPTOCARD display
- Configure soft environment
  - `cp /projects/QMCPACK-Training/soft ~/.soft`
  - `resoft`
- Copy updated lab (manual) and slides
  - `/projects/QMCPACK-Training/username/qmcpack_manual.pdf`
  - `/projects/QMCPACK-Training/username/labs/lab2_qmc_basics/slides/lab_slides.pdf`
- Make sure qmca works for plotting
  - Find any scalar.dat file, type: `qmca -t -q e [your].scalar.dat`
  - relogin may be necessary

# Lab Objectives

- Learn to work with QMCPACK
  - Wavefunction optimization
  - Diffusion Monte Carlo: timestep extrapolation
- Test QMC pseudopotentials
  - Sources of pseudopotentials
  - Preliminary PP tests: ionization potentials, dimer properties
- Use QMCPACK automation tools
  - Increase productivity
  - Focus on project design rather than execution

# Lab Material

- Lab document: QMCPACK Manual Chapter 13
- Lab material located at:  
    `labs/lab2_qmc_basics`
  - `oxygen_atom`                      -Files for sections 13.4-8
  - `oxygen_dimer`                    -Files for section 13.9-10
  - `your_system`                    -Files for section 13.11
- `reference` sub-directories have completed results

# Outline of Lab Document

## 1. Overview

- Topics covered and lab outline (13.1-2)
- Full details about lab files and directories (13.3)

## 2. Testing PP atomic properties

- BFD pseudopotential database & PP conversion (13.4)
- Obtaining and converting DFT orbitals (neutral O) (13.5)
- Wavefunction optimization walkthrough (neutral O) (13.6)
- DMC timestep extrapolation (neutral & charged O) (13.7-8)
- Comparison of DMC ionization potential w/ experiment

# Outline of Lab Document

## 3. Testing PP dimer properties

- QMCPACK workflow automation w/ Nexus
- Example Nexus input (single VMC) (13.9)
- Automated oxygen dimer binding curve (DMC) (13.10)
- Comparison of DMC bind. energy & bond len. w/ exp.

## 4. (Optional) Running your system with QMCPACK

- Generate input files for (and run) PWSCF & QMCPACK (13.11)
- Diamond (8-atom conv. cell) provided as an example

# Lab Schedule

- 1:30pm – 3:00pm: Lab Sections 13.4-8
  - 1<sup>st</sup> test of BFD oxygen pseudopotential
  - Complete DMC calculation of oxygen atom ionization potential by hand
- 3:00pm – 4:00pm: Poster session
- 4:00pm – 5:00pm: Lab Section 13.9-10
  - 2<sup>nd</sup> test of BFD oxygen pseudopotential
  - Automated (Nexus) DMC calculations of oxygen dimer binding curve
- 5:00pm: Recap. and connections to later labs

# Lab Schedule

- Anytime: Lab Section 13.11
  - Running your system/application w/ QMCPACK
  - Feel free to discuss in depth with any instructor



# Let's Begin!

- All material located at:  
    `labs/lab2_qmc_basics`
- `reference` sub-directories have completed results
- Questions & exercises at the end of each section
  - Discuss answers & results w/ lab instructors, if desired

# Poster Session

(Return by 4:00pm)

# Lab Schedule

- 4:00pm – 5:00pm: Lab Sections 13.9-10
  - 2<sup>nd</sup> test of BFD oxygen pseudopotential
  - Automated (Nexus) DMC calculations of oxygen dimer binding curve.
- 5:00pm: Recap. and connections to later labs

# Brief Nexus Overview

# Components/Stages of QMC Projects

## Selecting atomic structure

- generating/manipulating structure
- DFT structural relaxation

## Selecting cell size/k-points

- VMC total energy vs cell size/k-points
- DMC total energy vs cell size

## Selecting wavefunction

- DFT orbital generation (scf/nscf)
- wavefunction conversion
- VMC Jastrow optimization

## Selecting QMC parameters

- meshfactor convergence (orbitals)
- timestep study

## Selecting pseudopotential

- DMC atomic ionization potential
- DMC dimer bonding

## Production DMC runs

- equation of state
- defect formation energy
- excitations
- surface adsorption

## For all of these

- write input files
- submit/monitor jobs
- analyze output data
- chain info between jobs

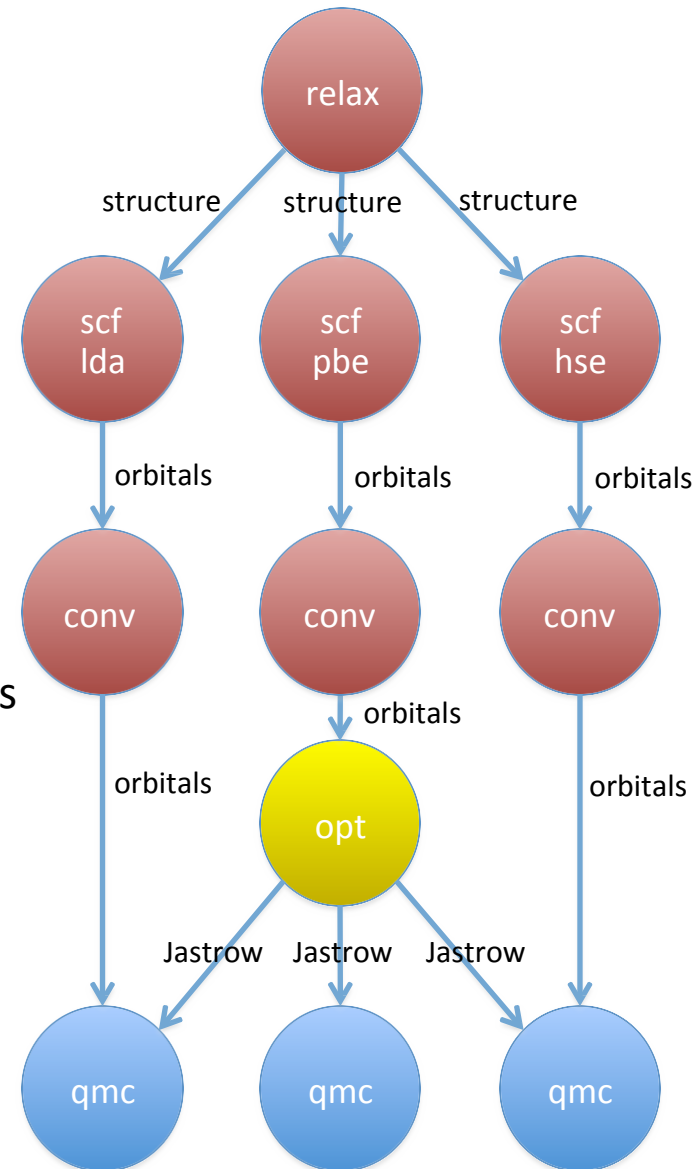
# Simplifying Project Management

## Nexus

- main idea: make each project component easier
- high-level scripting env. for arbitrary workflows
- automated input file generation & job submission
- data flow bet. chained jobs handled automatically
- memory of finished jobs: no resubmissions

## Advantages

- allows focus on project design and interpreting results
- removes opportunities for error propagation
- automatic record of work, easy to reproduce
- greater productivity overall



# Working with Nexus

## User Interface

- basic use through input file like Python script
- more advanced workflows w/ loops & logic

## Typical stages

- specify settings: PP directory, job monitoring, ...
- generate structure or read from file
- create simulation objects w/ minimal inputs
- specify data dependencies among simulations
  - structure, charge density, orbitals, jastrow, ...
- write input files & run jobs

```
qmc = generate_qmcpack(  
    identifier    = 'dmc',  
    path          = 'diamond/dmc',  
    job           = job(cores=16),  
    system        = diamond,  
    input_type    = 'basic',  
    pseudos       = ['C.BFD.xml'],  
    calculations  = [  
        vmc(warmupsteps = 20,  
            blocks      = 200,  
            steps       = 10,  
            substeps    = 3,  
            timestep    = 0.3,  
            samples     = 2048  
        ),  
        dmc(warmupsteps = 24,  
            blocks      = 200,  
            steps       = 10,  
            timestep    = 0.01  
        )  
    ]  
)
```





# Summary

- Topics covered
  - pseudopotential conversion w/ ppconvert
  - performing optimization & DMC by hand with QMCPACK
  - use of Nexus automation tools
  - pseudopotential testing: IP's & dimer properties
  - (optional) orbital generation/conversion with PWSCF/  
pw2qmcpack, optimization & DMC with QMCPACK for solid  
diamond (or your own system) via Nexus

# Connections with Labs 3 & 4

- Wednesday Lab: Norm Tubman
  - More extensive calculations of molecules (GAMESS)
  - Advanced wavefunctions: multideterminants
- Thursday Lab: Luke Shulenburger
  - More extensive calculations of solids (PWSCF)
  - Tiling, twist averaging, quasi-2D
  - More examples of workflow automation (Nexus)

