

Nexus Monthly User and Developer Meeting

Meeting 1: Nexus Overview

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Preliminary Agenda for Monthly Meetings

- User focused workflow demo
- Q&A about Nexus features, workflow how to's, etc.
- Feature demo/discussion
 - Feature(s) from user perspective (usage examples)
 - Feature(s) from developer perspective (code tour)

Agenda for this Meeting

- Workflow demos:
 - Command line settings: Mapping magnet./polar. landscape of BFO
 - Stepping through workflows: Simple diamond DFT to VMC
- Q&A about Nexus features, workflow how to's, etc. + Updates
- Overview of core Nexus classes
 - Class hierarchy and file layout
 - Core classes as viewed within user scripts

Overview of Nexus (background)

- Nexus
 - A scientific workflow automation tool
 - Object oriented Python
 - Started ~Oct. 2011 (7 years ago!)
 - Now ~60,000 lines of code, >300 significant classes
 - Documentation: https://docs.qmcpack.org/nexus_user_guide.pdf
 - Much more is needed!

Files located at: `nexus_training/monthly_meetings/01_181019_nexus_overview/`

Anatomy of a Nexus Script

01_nexus_script_elements/diamond.py

```
#! /usr/bin/env python

from nexus import settings, job, run_project
from nexus import generate_physical_system
from nexus import generate_pwscf
from nexus import generate_pw2qmcpack
from nexus import generate_qmcpack, vmc

settings(
    pseudo_dir      = './pseudopotentials',
    status_only     = 0,
    generate_only   = 0,
    sleep           = 3,
    machine          = 'ws16'
)

dia16 = generate_physical_system(
    units  = 'A',
    axes   = [[ 1.785,  1.785,  0. ],
              [ 0. ,  1.785,  1.785],
              [ 1.785,  0. ,  1.785]],
    elem   = ['C', 'C'],
    pos    = [[ 0. ,  0. ,  0. ],
              [ 0.8925, 0.8925, 0.8925]],
    tiling = (2,2,2),
    kgrid  = (1,1,1),
    kshift  = (0,0,0),
    C      = 4
)

scf = generate_pwscf(
    identifier      = 'scf',
    path            = 'diamond/scf',
    job             = job(cores=16, app='pw.x'),
    input_type      = 'generic',
    calculation    = 'scf',
    input_dft       = 'lda',
    ecutwfc        = 200,
    conv_thr        = 1e-8,
    nosym           = True,
    wf_collect      = True,
    system          = dia16,
    pseudos         = ['C.BFD.upf'],
)

conv = generate_pw2qmcpack(
    identifier      = 'conv',
    path            = 'diamond/scf',
    job             = job(cores=1, app='pw2qmcpack.x'),
    write_psir      = False,
    dependencies   = (scf, 'orbitals'),
)

qmc = generate_qmcpack(
    identifier      = 'vmc',
    path            = 'diamond/vmc',
    job             = job(cores=16, threads=4, app='qmcpack'),
    input_type      = 'basic',
    system          = dia16,
    pseudos         = ['C.BFD.xml'],
    jastrows        = [],
    calculations   = [
        vmc(
            walkers      = 1,
            warmupsteps = 20,
            blocks      = 200,
            steps       = 10,
            substeps    = 2,
            timestep    = .4
        )
    ],
    dependencies   = (conv, 'orbitals'),
)

run_project()
```

Invoke interpreter

Nexus imports

User settings

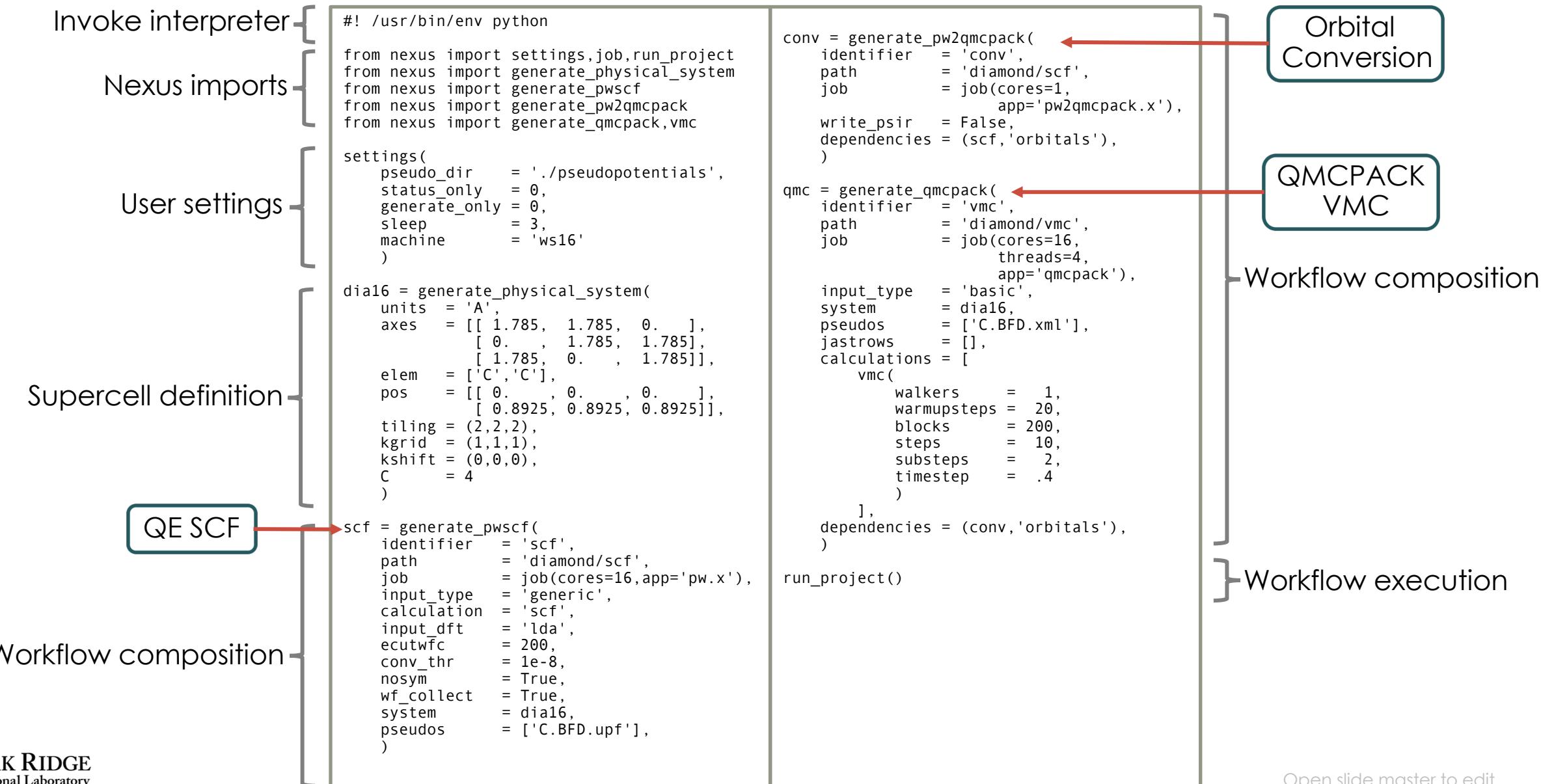
Supercell definition

Workflow composition

Workflow execution

Anatomy of a Nexus Script

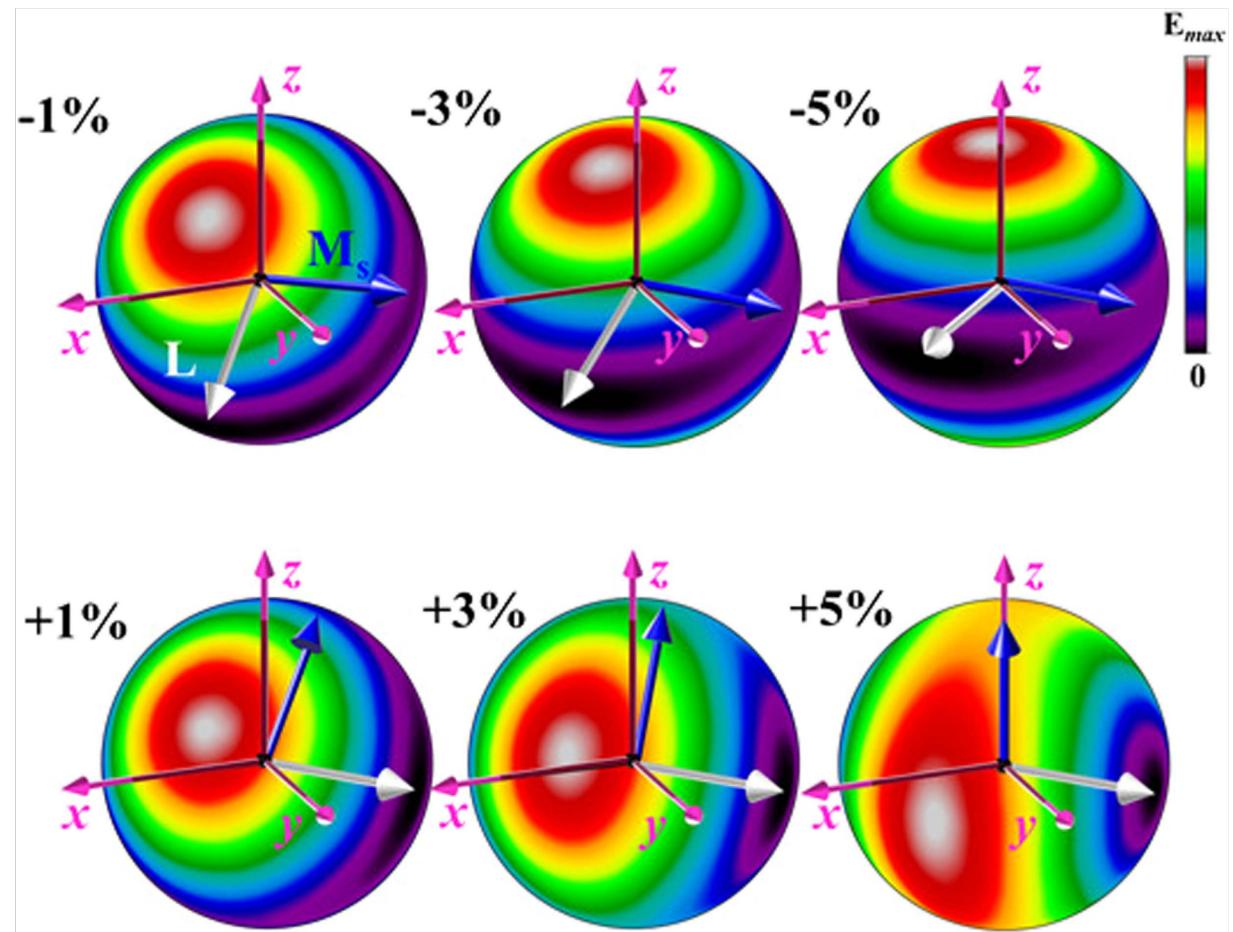
01_nexus_script_elements/diamond.py



Workflow Demo: Command Line Settings

BiFeO₃ Workflow

- Example modeled after high-throughput effort with Valentino Cooper and Hemant Dixit
- Interesting task to map magnetic energy landscape of strained BFO
- No strain: hard spin axis [111] direction, easy spin degenerate in (111) plane
- Compressive strain: hard spin [001], easy spin [110]
- Tensile strain: hard spin [100], easy spin [-110]
- 6048 VASP calculations



Magnetic energy landscape of BFO under compressive (-) and tensile (+) strain

Hemant Dixit, et al. Scientific reports 5 12969 (2015)

BiFeO₃ Workflow: Command Line Help

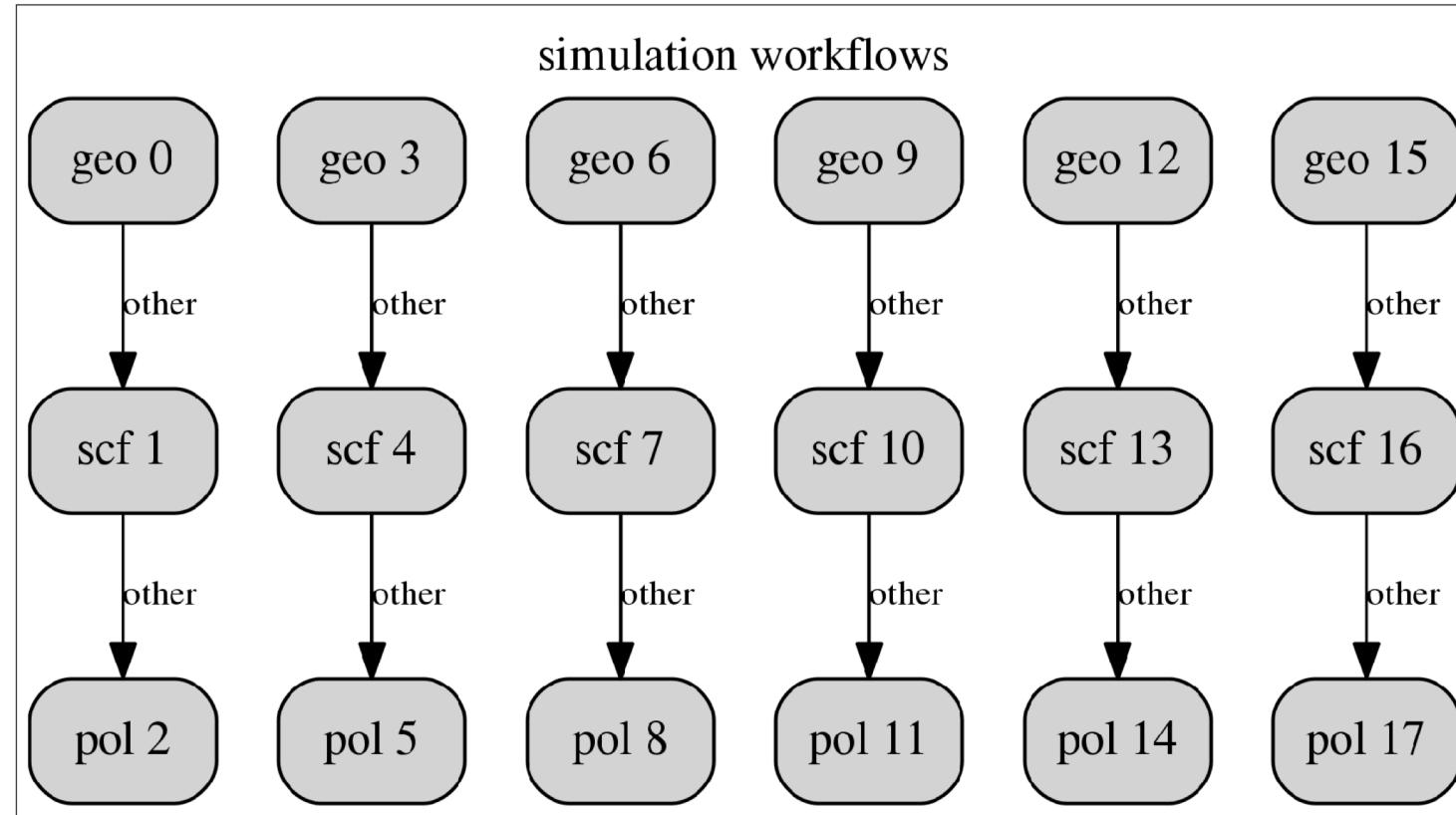
02_command_line_demo/bfo_strain_pol.py

```
>./bfo_strain_pol.py --help
```

Options:	
--version	show program's version number and exit
-h, --help	show this help message and exit
--status_only	Report status of all simulations and then exit.
--status=STATUS	Controls displayed simulation status information. May be set to one of 'standard', 'active', 'failed', or 'ready'.
--generate_only	Write inputs to all simulations and then exit. Note that no dependencies are processed, e.g. if one simulation depends on another for an orbital file location or for a relaxed structure, this information will not be present in the generated input file for that simulation since no simulations are actually run with this option.
--graph_sims	Display a graph of simulation workflows, then exit.
--progress_tty	Print abbreviated polling messages.
--sleep=SLEEP	Number of seconds between polls. At each poll, simulations are actually run provided all simulations they depend on have successfully completed (default=3).
--machine=MACHINE	(Required) Name of the machine the simulations will be run on. Workstations with between 1 and 128 cores may be specified by 'ws1' to 'ws128' (works for any machine where only mpirun is used). For a complete listing of currently available machines (including those at HPC centers) please see the manual.
--account=ACCOUNT	Account name required to submit jobs at some HPC centers.
--runs=RUNS	Directory to perform all runs in. Simulation paths are appended to this directory (default=runs).
--results=RESULTS	Directory to copy out lightweight results data. If set to '', results will not be stored outside of the runs directory (default=results).
--local_directory=LOCAL_DIRECTORY	Base path where runs and results directories will be created (default=./).
--pseudo_dir=PSEUDO_DIR	Path to directory containing pseudopotential files (required if running with pseudopotentials).
--basis_dir=BASIS_DIR	Path to directory containing basis set files (useful if running gaussian based QMC workflows).
--ericfmt=ERICFMT	Path to the ericfmt file used with GAMESS (required if running GAMESS).
--mcppath=MCPPATH	Path to the mcpdata file used with GAMESS (optional for most workflows)
--vdw_table=VDW_TABLE	Path to the vdw_table file used with Quantum Espresso (required only if running Quantum Espresso with van der Waals functionals).
--qprc=QPRC	Path to the quantum_package.rc file used with Quantum Package.

BiFeO₃ Workflow: Graphing Simulation Workflows

```
>./bfo_strain_pol.py --graph_sims
```



Requires pydot and matplotlib

BiFeO₃ Workflow: Displaying Workflow Status

```
> ./bfo_strain_pol.py --status_only
```

```
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
    cascade 3 checking in
    cascade 6 checking in
    cascade 9 checking in
    cascade 12 checking in
    cascade 15 checking in
  checking cascade dependencies
    all simulation dependencies satisfied

  cascade status
    setup, sent_files, submitted, finished, got_output, analyzed, failed
    000000 0 ----- geo      ./runs/st_0.000_sh_1.120/
    000000 0 ----- scf      ./runs/st_0.000_sh_1.120/
    000000 0 ----- pol      ./runs/st_0.000_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.000_sh_1.125/
    000000 0 ----- scf      ./runs/st_0.000_sh_1.125/
    000000 0 ----- pol      ./runs/st_0.000_sh_1.125/
    000000 0 ----- geo      ./runs/st_0.000_sh_1.125/
    000000 0 ----- scf      ./runs/st_0.005_sh_1.120/
    000000 0 ----- pol      ./runs/st_0.005_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.005_sh_1.120/
    000000 0 ----- scf      ./runs/st_0.005_sh_1.120/
    000000 0 ----- pol      ./runs/st_0.005_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.005_sh_1.125/
    000000 0 ----- scf      ./runs/st_0.005_sh_1.125/
    000000 0 ----- pol      ./runs/st_0.005_sh_1.125/
    000000 0 ----- geo      ./runs/st_0.010_sh_1.120/
    000000 0 ----- scf      ./runs/st_0.010_sh_1.120/
    000000 0 ----- pol      ./runs/st_0.010_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.010_sh_1.125/
    000000 0 ----- scf      ./runs/st_0.010_sh_1.125/
    000000 0 ----- pol      ./runs/st_0.010_sh_1.125/
  setup, sent_files, submitted, finished, got_output, analyzed, failed
```

BiFeO₃ Workflow: Display Simulations to Run Next

```
> ./bfo_strain_pol.py --status_only --status=ready
```

```
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
    cascade 3 checking in
    cascade 6 checking in
    cascade 9 checking in
    cascade 12 checking in
    cascade 15 checking in
  checking cascade dependencies
    all simulation dependencies satisfied

  cascade status
    setup, sent_files, submitted, finished, got_output, analyzed, failed
    000000 0 ----- geo      ./runs/st_0.000_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.000_sh_1.125/
    000000 0 ----- geo      ./runs/st_0.005_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.005_sh_1.125/
    000000 0 ----- geo      ./runs/st_0.010_sh_1.120/
    000000 0 ----- geo      ./runs/st_0.010_sh_1.125/
  setup, sent_files, submitted, finished, got_output, analyzed, failed
```

BiFeO₃ Workflow: Execute the Workflow

```
> ./bfo_strain_pol.py
```

```
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
    cascade 3 checking in
    cascade 6 checking in
    cascade 9 checking in
    cascade 12 checking in
    cascade 15 checking in
  checking cascade dependencies
    all simulation dependencies satisfied

  starting runs:
~~~~~
elapsed time 0.0 s  memory 71.97 MB
  Entering ./runs/st_0.000_sh_1.120/ 0
    writing input files 0 geo
  Entering ./runs/st_0.000_sh_1.120/ 0
    sending required files 0 geo
    submitting job 0 geo
  Entering ./runs/st_0.000_sh_1.125/ 3
    writing input files 3 geo
  Entering ./runs/st_0.000_sh_1.125/ 3
    sending required files 3 geo
    submitting job 3 geo
  Entering ./runs/st_0.005_sh_1.120/ 6
    writing input files 6 geo
  Entering ./runs/st_0.005_sh_1.120/ 6
    sending required files 6 geo
    submitting job 6 geo
  Entering ./runs/st_0.005_sh_1.125/ 9
    writing input files 9 geo
```

```
  Entering ./runs/st_0.005_sh_1.125/ 9
    sending required files 9 geo
    submitting job 9 geo
  Entering ./runs/st_0.010_sh_1.120/ 12
    writing input files 12 geo
  Entering ./runs/st_0.010_sh_1.120/ 12
    sending required files 12 geo
    submitting job 12 geo
  Entering ./runs/st_0.010_sh_1.125/ 15
    writing input files 15 geo
  Entering ./runs/st_0.010_sh_1.125/ 15
    sending required files 15 geo
    submitting job 15 geo
  Entering ./runs/st_0.000_sh_1.120/ 1
    Executing: qsub geo.qsub.in
      pid: 218367
  Entering ./runs/st_0.000_sh_1.125/ 4
    Executing: qsub geo.qsub.in
      pid: 218368
  Entering ./runs/st_0.005_sh_1.120/ 7
    Executing: qsub geo.qsub.in
      pid: 218369
  Entering ./runs/st_0.005_sh_1.125/ 10
    Executing: qsub geo.qsub.in
      pid: 218370
  Entering ./runs/st_0.010_sh_1.120/ 13
    Executing: qsub geo.qsub.in
      pid: 218371
  Entering ./runs/st_0.010_sh_1.125/ 16
    Executing: qsub geo.qsub.in
      pid: 218372
```

BiFeO₃ Workflow: Display Active Simulations

```
>./bfo_strain_pol.py --status_only --status=active
```

```
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
    cascade 3 checking in
    cascade 6 checking in
    cascade 9 checking in
    cascade 12 checking in
    cascade 15 checking in
  checking cascade dependencies
    all simulation dependencies satisfied

  cascade status
    setup, sent_files, submitted, finished, got_output, analyzed, failed
    111000 0 218367 geo ./runs/st_0.000_sh_1.120/
    111000 0 218368 geo ./runs/st_0.000_sh_1.125/
    111000 0 218369 geo ./runs/st_0.005_sh_1.120/
    111000 0 218370 geo ./runs/st_0.005_sh_1.125/
    111000 0 218371 geo ./runs/st_0.010_sh_1.120/
    111000 0 218372 geo ./runs/st_0.010_sh_1.125/
  setup, sent_files, submitted, finished, got_output, analyzed, failed
```

Workflow Demo: Stepping Through Workflows

Stepping through workflows: Pausing at Submission Step

03_skip_submit_demo/diamond.py

```
#!/usr/bin/env python

from nexus import settings, job, run_project
from nexus import generate_physical_system
from nexus import generate_pwscf
from nexus import generate_pw2qmcpack
from nexus import generate_qmcpack, vmc

settings(
    pseudo_dir      = './pseudopotentials',
    status_only     = 0,
    generate_only   = 0,
    sleep           = 3,
    machine          = 'ws16'
)

dia16 = generate_physical_system(
    units      = 'A',
    axes       = [[ 1.785,  1.785,  0. ],
                  [ 0. ,  1.785,  1.785],
                  [ 1.785,  0. ,  1.785]],
    elem        = ['C', 'C'],
    pos         = [[ 0. ,  0. ,  0. ],
                  [ 0.8925,  0.8925,  0.8925]],
    tiling      = (2,2,2),
    kgrid       = (1,1,1),
    kshift      = (0,0,0),
    C           = 4
)

scf = generate_pwscf(
    skip_submit = True,
    identifier  = 'scf',
    path        = 'diamond/scf',
    job         = job(cores=16, app='pw.x'),
    input_type   = 'generic',
    calculation = 'scf',
    input_dft   = 'lda',
    ecutwfc    = 200,
    conv_thr    = 1e-8,
    nosym       = True,
    wf_collect  = True,
    system      = dia16,
    pseudos     = ['C.BFD.upf'],
)

conv = generate_pw2qmcpack(
    skip_submit = True,
    identifier  = 'conv',
    path        = 'diamond/scf',
    job         = job(cores=1,
                      app='pw2qmcpack.x'),
    write_psir   = False,
    dependencies = (scf, 'orbitals')
)

qmc = generate_qmcpack(
    skip_submit = True,
    identifier  = 'vmc',
    path        = 'diamond/vmc',
    job         = job(cores=16,
                      threads=4,
                      app='qmcpack'),
    input_type   = 'basic',
    system      = dia16,
    pseudos     = ['C.BFD.xml'],
    jastrows    = [],
    calculations = [
        vmc(
            walkers      = 1,
            warmupsteps = 20,
            blocks      = 200,
            steps       = 10,
            substeps    = 2,
            timestep    = .4
        )
    ],
    dependencies = (conv, 'orbitals')
)

run_project()
```

Inputs will be written for
SCF step, but job will
not be submitted

Stepping through workflows: Pausing at Submission Step

skip_submit all True

```
>./diamond.py
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
  checking cascade dependencies
    all simulation dependencies satisfied
starting runs:
~~~~~
elapsed time 0.0 s  memory 64.15 MB
  Entering ./runs/diamond/scf 0
    writing input files 0 scf
  Entering ./runs/diamond/scf 0
    sending required files 0 scf
SCF Write
Project finished
>ls runs/diamond/scf/
C.BFD.upf      scf.in
pwscf_output   sim_scf
```

scf skip_submit False

```
>./diamond.py
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
  checking cascade dependencies
    all simulation dependencies satisfied
starting runs:
~~~~~
elapsed time 0.0 s  memory 64.14 MB
  submitting job 0 scf
  Entering ./runs/diamond/scf 0
    Executing:
      export OMP_NUM_THREADS=1
      mpirun -np 16 pw.x -input scf.in
SCF Run
elapsed time 3.0 s  memory 64.19 MB
  Entering ./runs/diamond/scf 0
    copying results 0 scf
  Entering ./runs/diamond/scf 0
    analyzing 0 scf
elapsed time 6.1 s  memory 64.26 MB
  Entering ./runs/diamond/scf 1
    writing input files 1 conv
  Entering ./runs/diamond/scf 1
    sending required files 1 conv
Conv Write
Project finished
>ls runs/diamond/scf/
C.BFD.upf      scf.err  sim_conv
conv.in        scf.in   sim_scf
pwscf_output   scf.out
```

conv skip_submit False

```
>./diamond.py
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
  checking cascade dependencies
    all simulation dependencies satisfied
starting runs:
~~~~~
elapsed time 0.0 s  memory 64.15 MB
  submitting job 1 conv
  Entering ./runs/diamond/scf 1
    Executing:
      export OMP_NUM_THREADS=1
      mpirun -np 1 pw2qmcpack.x<conv.in
Conv Run
elapsed time 3.0 s  memory 64.20 MB
  Entering ./runs/diamond/scf 1
    copying results 1 conv
  Entering ./runs/diamond/scf 1
    analyzing 1 conv
elapsed time 6.1 s  memory 64.21 MB
  Entering ./runs/diamond/vmc 2
    writing input files 2 vmc
  Entering ./runs/diamond/vmc 2
    sending required files 2 vmc
VMC Write
Project finished
>ls runs/diamond/vmc/
C.BFD.xml      vmc.info.xml  vmc.s000.qmc.xml
C.pp.dat       vmc.in.xml   vmc.s000.scalar.dat
sim_vmc        vmc.out      vmc.s000.stat.h5
vmc.err        vmc.s000.cont.xml
```

vmc skip_submit False

```
>./diamond.py
Project starting
  checking for file collisions
  loading cascade images
    cascade 0 checking in
  checking cascade dependencies
    all simulation dependencies satisfied
starting runs:
~~~~~
elapsed time 0.0 s  memory 64.14 MB
  submitting job 2 vmc
  Entering ./runs/diamond/vmc 2
    Executing:
      export OMP_NUM_THREADS=4
      mpirun -np 4 qmcpack vmc.in.xml
VMC Run
elapsed time 3.0 s  memory 2415.31 MB
elapsed time 6.0 s  memory 286.72 MB
elapsed time 9.1 s  memory 286.72 MB
elapsed time 12.1 s  memory 286.72 MB
elapsed time 15.1 s  memory 286.74 MB
elapsed time 18.1 s  memory 286.75 MB
elapsed time 21.2 s  memory 286.76 MB
elapsed time 24.2 s  memory 286.76 MB
elapsed time 27.2 s  memory 286.76 MB
elapsed time 30.2 s  memory 286.77 MB
elapsed time 33.3 s  memory 64.19 MB
  Entering ./runs/diamond/vmc 2
    copying results 2 vmc
  Entering ./runs/diamond/vmc 2
    analyzing 2 vmc
Project finished
>ls runs/diamond/vmc/
C.BFD.xml      vmc.info.xml  vmc.s000.qmc.xml
C.pp.dat       vmc.in.xml   vmc.s000.scalar.dat
sim_vmc        vmc.out      vmc.s000.stat.h5
vmc.err        vmc.s000.cont.xml
```

Stepping through workflows: generate inputs + DIY submit

04_generate_only_demo/diamond.py

```
#!/usr/bin/env python

from nexus import settings, job, run_project
from nexus import generate_physical_system
from nexus import generate_pwscf
from nexus import generate_pw2qmcpack
from nexus import generate_qmcpack, vmc

settings(
    pseudo_dir      = './pseudopotentials',
    status_only     = 0,
    generate_only = 1,
    sleep           = .3,
    machine         = 'oic5'
)

< skipping job details that go here... >

dia16 = generate_physical_system(
    units      = 'A',
    axes       = [[ 1.785,  1.785,  0. ],
                  [ 0. ,  1.785,  1.785],
                  [ 1.785,  0. ,  1.785]],
    elem       = ['C', 'C'],
    pos        = [[ 0. ,  0. ,  0. ],
                  [ 0.8925,  0.8925,  0.8925]],
    tiling     = (2,2,2),
    kgrid      = (1,1,1),
    kshift     = (0,0,0),
    C          = 4
)

scf = generate_pwscf(
    identifier   = 'scf',
    path         = 'diamond/scf',
    job          = scf_job,
    input_type   = 'generic',
    calculation  = 'scf',
    input_dft    = 'lda',
    ecutwfc     = 200,
    conv_thr    = 1e-8,
    nosym       = True,
    wf_collect  = True,
    system      = dia16,
    pseudos     = ['C.BFD.upf'],
)
```

```
conv = generate_pw2qmcpack(
    identifier   = 'conv',
    path         = 'diamond/scf',
    job          = conv_job,
    write_psir   = False,
    dependencies = (scf, 'other'),
)

qmc = generate_qmcpack(
    identifier   = 'vmc',
    path         = 'diamond/vmc',
    job          = qmc_job,
    input_type   = 'basic',
    system      = dia16,
    pseudos     = ['C.BFD.xml'],
    orbitals_h5 = '../scf/pwscf_output/pwscf.pwscf.h5',
    jastrows    = [],
    calculations = [
        vmc(
            walkers      = 1,
            warmupsteps = 20,
            blocks      = 200,
            steps       = 10,
            substeps    = 2,
            timestep    = .4
        )
    ],
    dependencies = (conv, 'other'),
)

run_project()
```

Stepping through workflows: generate inputs + DIY submit

```
>./diamond.py
```

```
elapsed time 0.0 s memory 62.30 MB
Entering ./runs/diamond/scf 0
    writing input files 0 scf
Entering ./runs/diamond/scf 0
    sending required files 0 scf
    submitting job 0 scf
Entering ./runs/diamond/scf 1
    Would have executed: qsub scf.qsub.in

elapsed time 0.7 s memory 62.39 MB
Entering ./runs/diamond/scf 0
    copying results 0 scf
Entering ./runs/diamond/scf 0
    analyzing 0 scf

elapsed time 1.3 s memory 62.42 MB
Entering ./runs/diamond/scf 1
    writing input files 1 conv
Entering ./runs/diamond/scf 1
    sending required files 1 conv
    submitting job 1 conv
Entering ./runs/diamond/scf 2
    Would have executed: qsub conv.qsub.in

elapsed time 1.9 s memory 62.43 MB
Entering ./runs/diamond/scf 1
    copying results 1 conv
Entering ./runs/diamond/scf 1
    analyzing 1 conv

elapsed time 2.5 s memory 62.43 MB
Entering ./runs/diamond/vmc 2
    writing input files 2 vmc
Entering ./runs/diamond/vmc 2
    sending required files 2 vmc
    submitting job 2 vmc
Entering ./runs/diamond/vmc 3
    Would have executed: qsub vmc.qsub.in

elapsed time 3.2 s memory 62.52 MB
Entering ./runs/diamond/vmc 2
    copying results 2 vmc
Entering ./runs/diamond/vmc 2
    analyzing 2 vmc
```

Project finished

```
>ls runs/diamond/scf/
C.BFD.upf  conv.qsub.in  scf.in      sim_conv
conv.in     pwscf_output  scf.qsub.in sim_scf

>ls runs/diamond/vmc
C.BFD.xml  vmc.in.xml
sim_vmc    vmc.qsub.in
```

```
# submit scf manually
>cd runs/diamond/scf/
>qsub scf.qsub.in
218394.b21l01.oic.ornl.gov
>grep '!' scf.out
!    total energy = -22.52257768 Ry

# submit conv manually
>qsub conv.qsub.in
218395.b21l01.oic.ornl.gov
>grep 'JOB DONE' conv.out
JOB DONE.

# submit vmc manually
>cd ..\vmc
>qsub vmc.qsub.in
218396.b21l01.oic.ornl.gov
>qmca -q e *scalar*
vmc series 0 LocalEnergy = -87.835842 +/- 0.020231
```

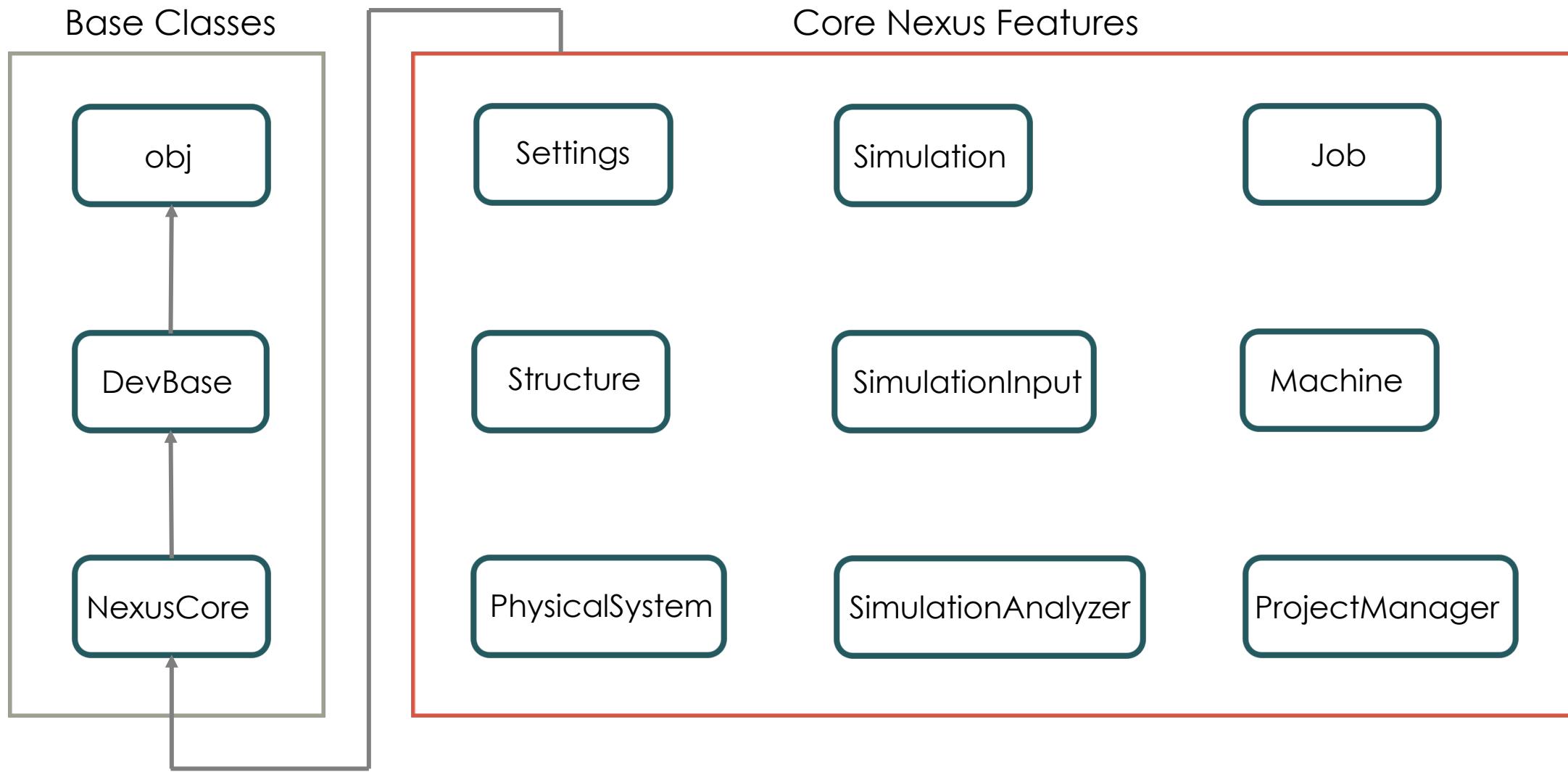
Question & Answer + Updates

Question & Answer + Updates

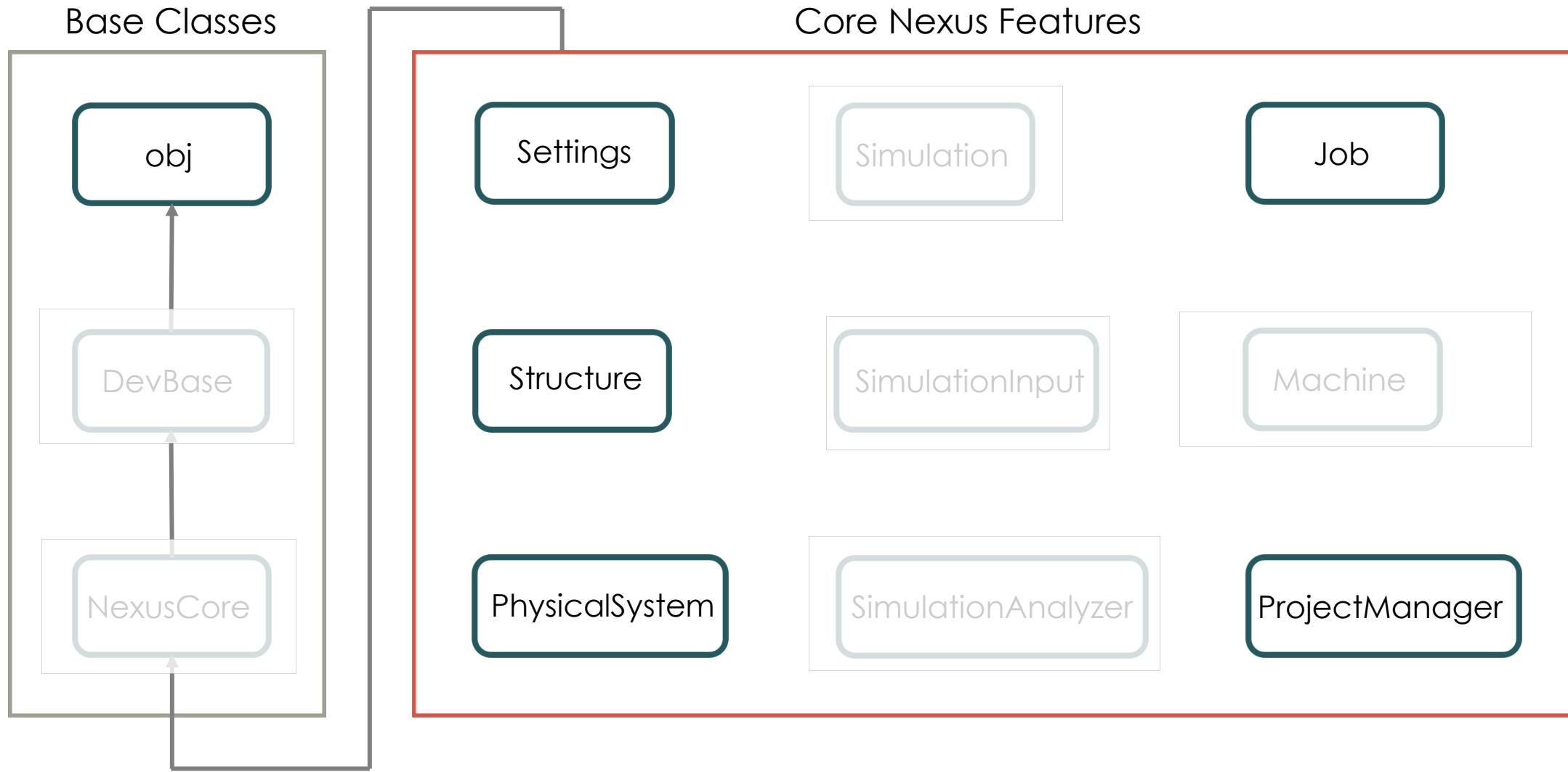
- Q&A for Nexus features, workflow how to's, code details, etc
- Updates on current development
- Order
 - ANL, NCSU, ORNL, SNL, UIUC

Overview of Core Nexus Classes

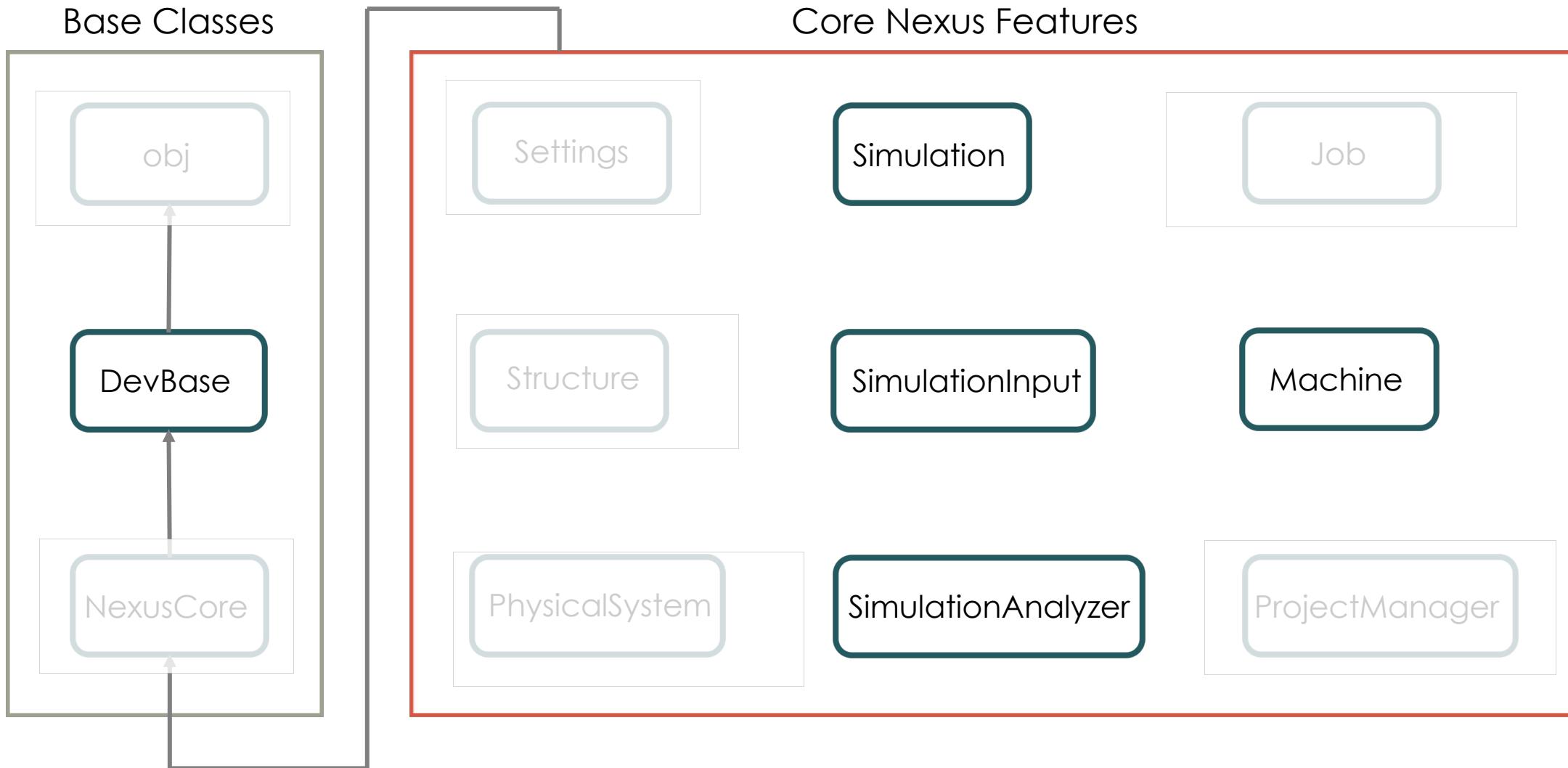
Core Nexus Classes: Hierarchy



Core Nexus Classes: Intended for Direct Instantiation/Use



Core Nexus Classes: Intended as Base for Development



Core Nexus Classes: Description/Use

Base Classes

obj

Generic container abilities

DevBase

Base class for Nexus and related tools (e.g. qmca)

NexusCore

Base class marking central Nexus classes

Core Nexus Features

Settings

Applies user settings, sets global Nexus information

Simulation

Handles simulation execution and simulation dependencies

Job

Contains job execution details (# nodes, # hours, queue, etc)

Structure

Represents atomic structure and simulation cell

SimulationInput

Handles input file read/write

Machine

Manages internal/external job queue and job submission

PhysicalSystem

Adds electron/particle info on top of atomic structure

SimulationAnalyzer

Handles output data read and further data analysis

ProjectManager

Manages workflow identification, execution, and monitoring

Core Nexus Classes: File Locations

Base Classes

obj

generic.py

DevBase

developer.py

NexusCore

nexus_base.py

Core Nexus Features

Settings

nexus.py

Simulation

simulation.py

Job

machines.py

Structure

structure.py

SimulationInput

simulation.py

Machine

machines.py

PhysicalSystem

physical_system.py

SimulationAnalyzer

simulation.py

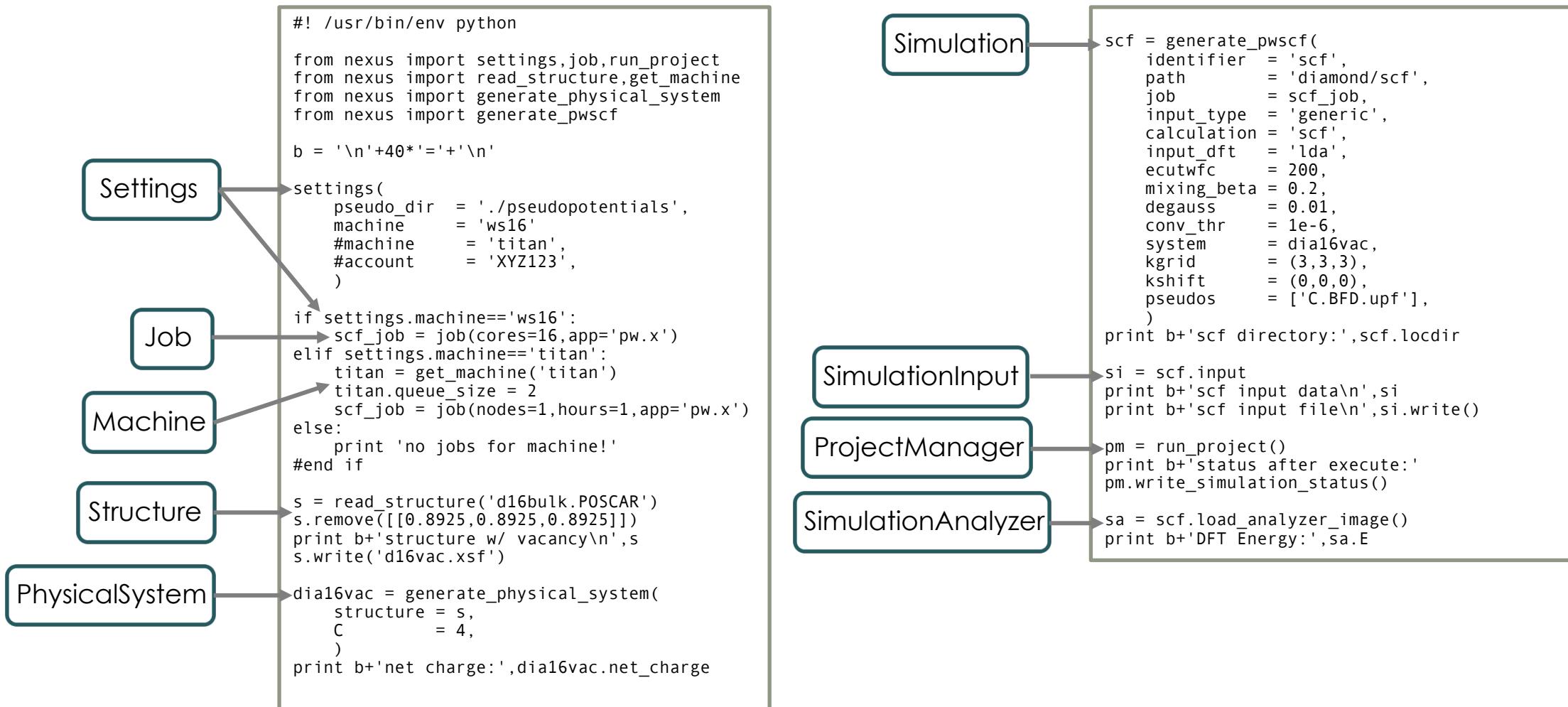
ProjectManager

project_manager.py

Files listed above are located at `nexus/library/`

Core Classes as Viewed Inside User Scripts

05_core_classes_demo/diamond.py



Core Classes as Viewed Inside User Scripts

```

structure w/ vacancy
axes          = [[ 3.57 3.57 0. ]
                  [ 0.   3.57 3.57]
                  [ 3.57 0.   3.57]]
background_charge = 0
bconds        = ['p' 'p' 'p']
center         = [ 3.57 3.57 3.57]
dim            = 3
elem           = ['C' 'C' 'C' 'C' 'C'
                  'C' 'C' 'C' 'C' 'C'
                  'C' 'C' 'C' 'C' 'C']
folded_structure = None
frozen         = None
kaxes          = [
    [ 0.87999794 0.87999794 -0.87999794]
    [-0.87999794 0.87999794 0.87999794]
    [ 0.87999794 -0.87999794 0.87999794]]
kpoints        = []
kweights       = []
mag            = []
pos            = [
    [ 0.     0.     0.    ]
    [ 1.785 1.785 0.    ]
    [ 2.6775 2.6775 0.8925]
    [ 0.     1.785 1.785 ]
    [ 0.8925 2.6775 2.6775]
    [ 1.785 3.57 1.785 ]
    [ 2.6775 4.4625 2.6775]
    [ 1.785 0.     1.785 ]
    [ 2.6775 0.8925 2.6775]
    [ 3.57 1.785 1.785 ]
    [ 4.4625 2.6775 2.6775]
    [ 1.785 1.785 3.57 ]
    [ 2.6775 2.6775 4.4625]
    [ 3.57 3.57 3.57 ]
    [ 4.4625 4.4625 4.4625]]
scale          = 1.0
units          = A
=====
net charge: 0
=====
scf directory: ./runs/diamond/scf

```

```

scf input data
atomic_positions
atoms          = [...]
positions      = [...]
specifier      = alat
end atomic_positions
atomic_species
atoms          = ['C']
masses          = 12.011
end masses
pseudopotentials
C              = C.BFD.upf
end pseudopotentials
end atomic_species
cell_parameters
specifier      = cubic
vectors        = [...]
end cell_parameters
control
calculation   = scf
outdir         = pwscf_output
prefix         = pwscf
pseudo_dir    = './'
end control
electrons
conv_thr      = 1e-06
electron_maxstep = 1000
mixing_beta   = 0.2
end electrons
k_points
grid          = (3, 3, 3)
shift          = (0, 0, 0)
specifier      = automatic
end k_points
system
celldm(1)     = 1.0
degauss        = 0.01
ecutwfc       = 200
hubbard_u     = None
ibrav          = 0
input_dft     = lda
nat            = 15
nspin          = 1
ntyp           = 1
tot_charge    = 0
end system

```

```

scf input file
&CONTROL
calculation   = 'scf'
outdir         = 'pwscf_output'
prefix         = 'pwscf'
pseudo_dir    = './'
/
&SYSTEM
celldm(1)     = 1.0
degauss        = 0.01
ecutwfc       = 200
ibrav          = 0
input_dft     = 'lda'
nat            = 15
nspin          = 1
ntyp           = 1
tot_charge    = 0
/
&ELECTRONS
conv_thr      = 1e-06
electron_maxstep = 1000
mixing_beta   = 0.2
/
ATOMIC_SPECIES
C 12.011 C.BFD.upf
ATOMIC_POSITIONS alat
C 0.00000000 0.00000000 0.00000000
C 3.37316115 3.37316115 0.00000000
C 5.05974172 5.05974172 1.68658057
C 0.00000000 3.37316115 3.37316115
C 1.68658057 5.05974172 5.05974172
C 3.37316115 6.74632229 3.37316115
C 5.05974172 8.43290286 5.05974172
C 3.37316115 0.00000000 3.37316115
C 5.05974172 1.68658057 5.05974172
C 6.74632229 3.37316115 3.37316115
C 8.43290286 5.05974172 5.05974172
C 3.37316115 3.37316115 6.74632229
C 5.05974172 5.05974172 8.43290286
C 6.74632229 6.74632229 6.74632229
C 8.43290286 8.43290286 8.43290286
K_POINTS automatic
3 3 3 0 0 0
CELL_PARAMETERS cubic
6.74632229 6.74632229 0.00000000
0.00000000 6.74632229 6.74632229
6.74632229 0.00000000 6.74632229

```

```

Project starting
  checking for file collisions
  loading cascade images
  cascade 0 checking in
  checking cascade dependencies
  all simulation dependencies ...
starting runs:
=====
elapsed time 0.0 s memory 64.01 MB
  Entering ./runs/diamond/scf 0
    writing input files 0 scf
  Entering ./runs/diamond/scf 0
    sending required files 0 scf
  submitting job 0 scf
  Entering ./runs/diamond/scf 0
    Executing:
      export OMP_NUM_THREADS=1
      mpirun -np 16 pw.x -input scf.in
=====
elapsed time 3.0 s memory 783.43 MB
elapsed time 6.1 s memory 943.62 MB
elapsed time 9.1 s memory 970.92 MB
elapsed time 12.1 s memory 987.89 MB
elapsed time 15.1 s memory 1008.28 MB
elapsed time 18.2 s memory 1027.84 MB
elapsed time 21.2 s memory 64.11 MB
  Entering ./runs/diamond/scf 0
    copying results 0 scf
  Entering ./runs/diamond/scf 0
    analyzing 0 scf
Project finished
=====
status after execute:
=====
cascade status
setup,sent_files,submitted,finished,...
  111111 0 28418 scf
./runs/diamond/scf
=====
setup,sent_files,submitted,finished,...
=====
DFT Energy: -170.26013064

```

Open slide master to edit

Next Monthly Meeting

- Date/Time: Friday Nov. 16th 1-2pm EST
- BlueJeans link: <https://bluejeans.com/190169126>
- Tentative topic: Nexus development environment
- Feature demo and/or topic requests welcome!