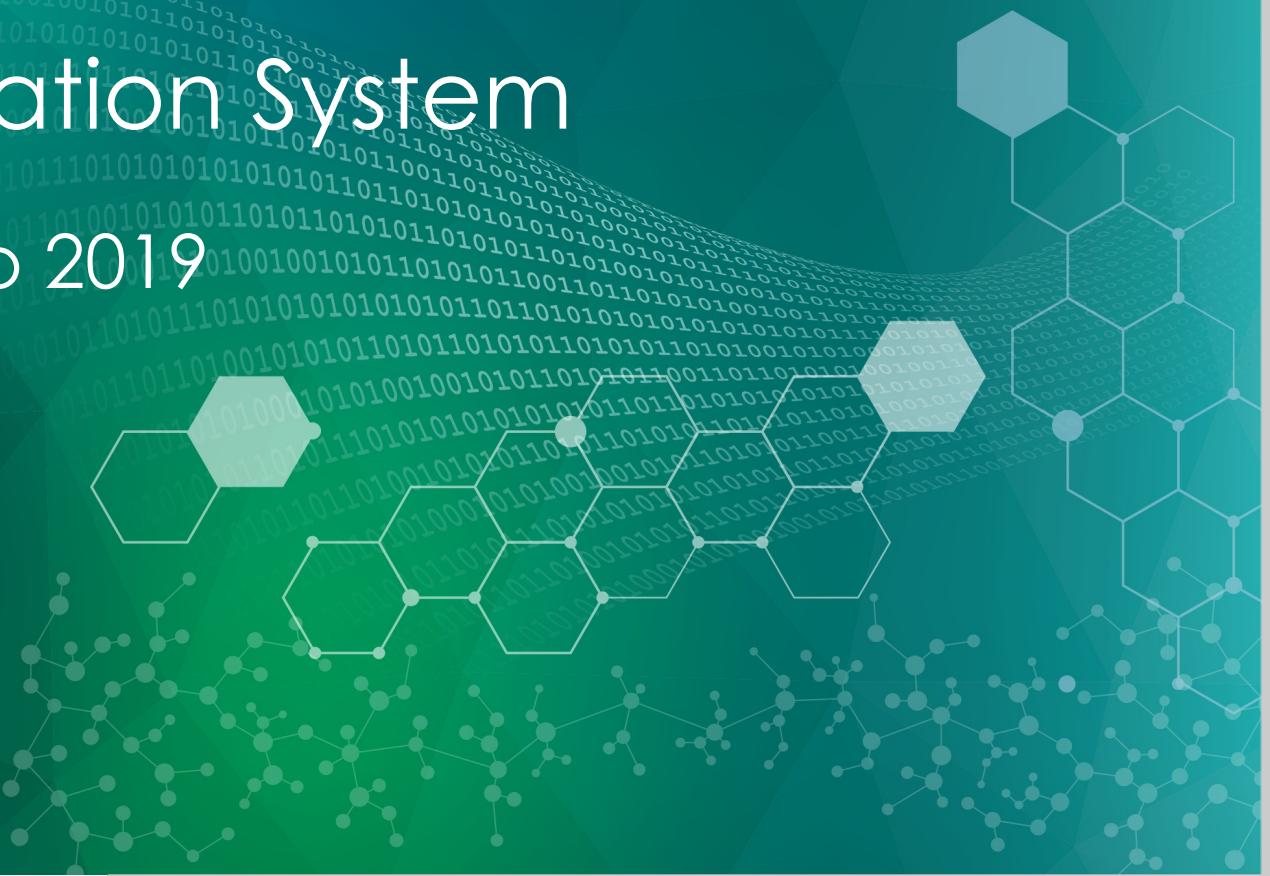


Nexus Workflow Automation System

QMCPACK Users Workshop 2019

Jaron T. Krogel

15 May 2019



ORNL is managed by UT-Battelle, LLC for the US Department of Energy



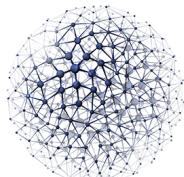
Overview

- Motivation for scientific workflow automation tools
- General information about Nexus, a workflow tool for QMCPACK
- Overview of working with Nexus from a user perspective
- Overview of workshop examples
- Additional Resources and Future directions

Motivation: Scientific Workflow Tools

Motivation: Scientific Workflow Automation

- Scientific workflow automation tools have grown in popularity
- Give the ability to perform high-throughput calculations (AFLOW, FireWorks) or simplify the calculation process for productivity (ASE)
- Growth in popularity indicates usefulness of the approach
- Existing tools primarily favor DFT codes, with an emphasis on VASP
- What about QMC?



Challenges for QMC: Control of Systematic Errors

- Production QMC results require many sub-calculations
 - Convergence of parameters: PW energy cutoffs, spline grid sizes, k-point grids, supercell sizes, wavefunction optimization, DMC timestep
 - Considering alternatives: trial wavefunction choice (DFT functional, level of QM-chemistry), pseudopotential choice, locality vs. T-moves
- This amounts to a great deal of work:
 - QMC often takes more time than DFT/QM chem. studies
 - High barrier to entry for newcomers

Challenges for QMC: Machine Hierarchies

Workstation



- DFT/HF
- QM Chem
- Data analysis

Institutional Cluster (CADES at ORNL)



- DFT/HF/QM Chem
- Selected-CI
- Wavefunction optimization

Leadership Computing (Summit at ORNL)



- Production Diffusion Monte Carlo

Working on multiple machines levels adds complexity, job monitoring adds time

General Information about Nexus

Nexus Workflow System Overview

- Developed QMC-centric workflow system to address these needs
- Nexus' Goals
 - Make QMC calculations more accessible (less steep learning curve for new users)
 - Automate time-consuming steps in QMC simulation process
 - Enable large scale job submission on a variety of supercomputing platforms
 - Make simulation workflows scriptable: e.g. scans over DFT functionals
 - Support every type of calculation possible with QMCPACK and provide documented examples (still aspirational, but support is broad)

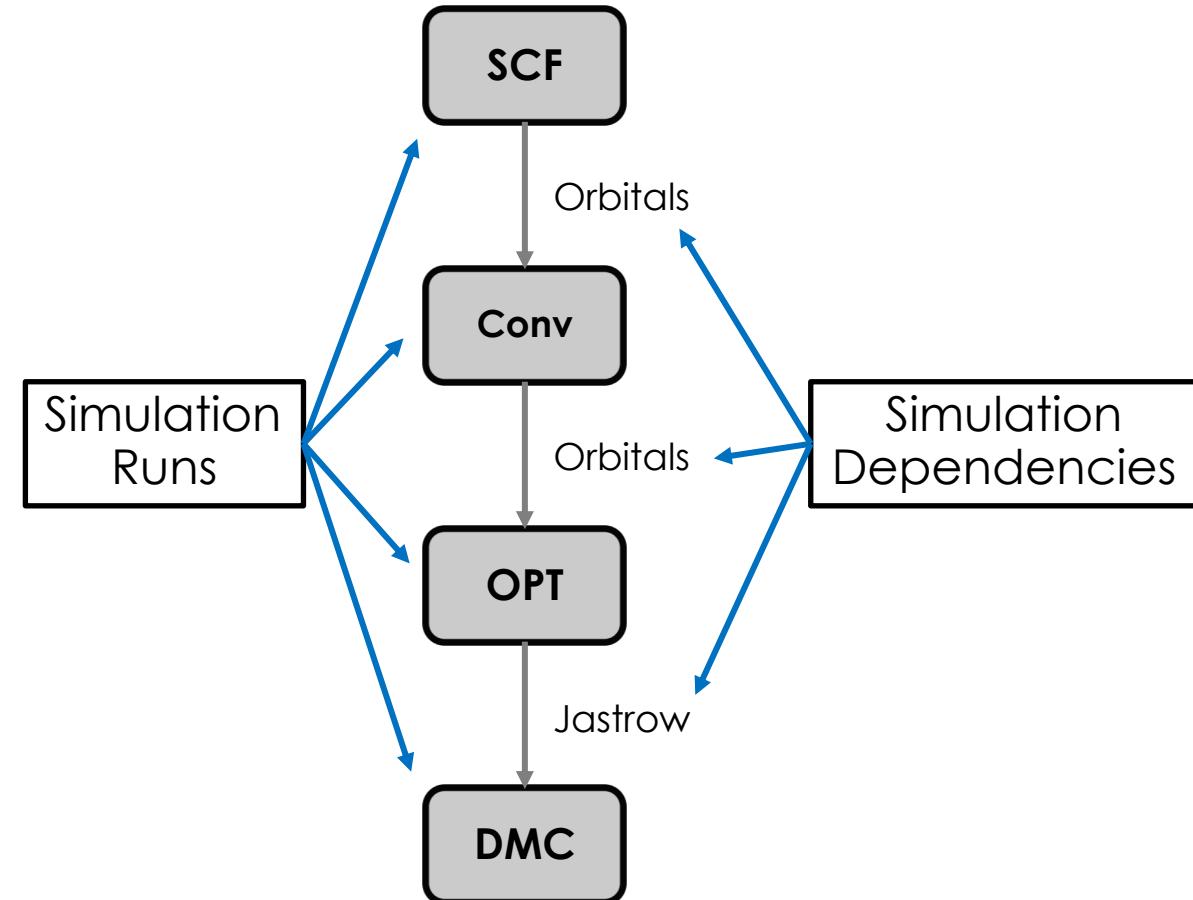
Nexus Core Features

- Simple Python interface for workflow composition
 - Meta input file for execution of all simulation codes
 - Brings all simulation programs together in single, coherent framework
- Input file generators
 - Automatic input file creation from minimal user inputs
- Monitoring
 - Automatic execution of simulation workflows and job monitoring
- Analysis
 - Automatic extraction of simulation results, accessible within user script

Nexus Workflow Execution/Monitoring

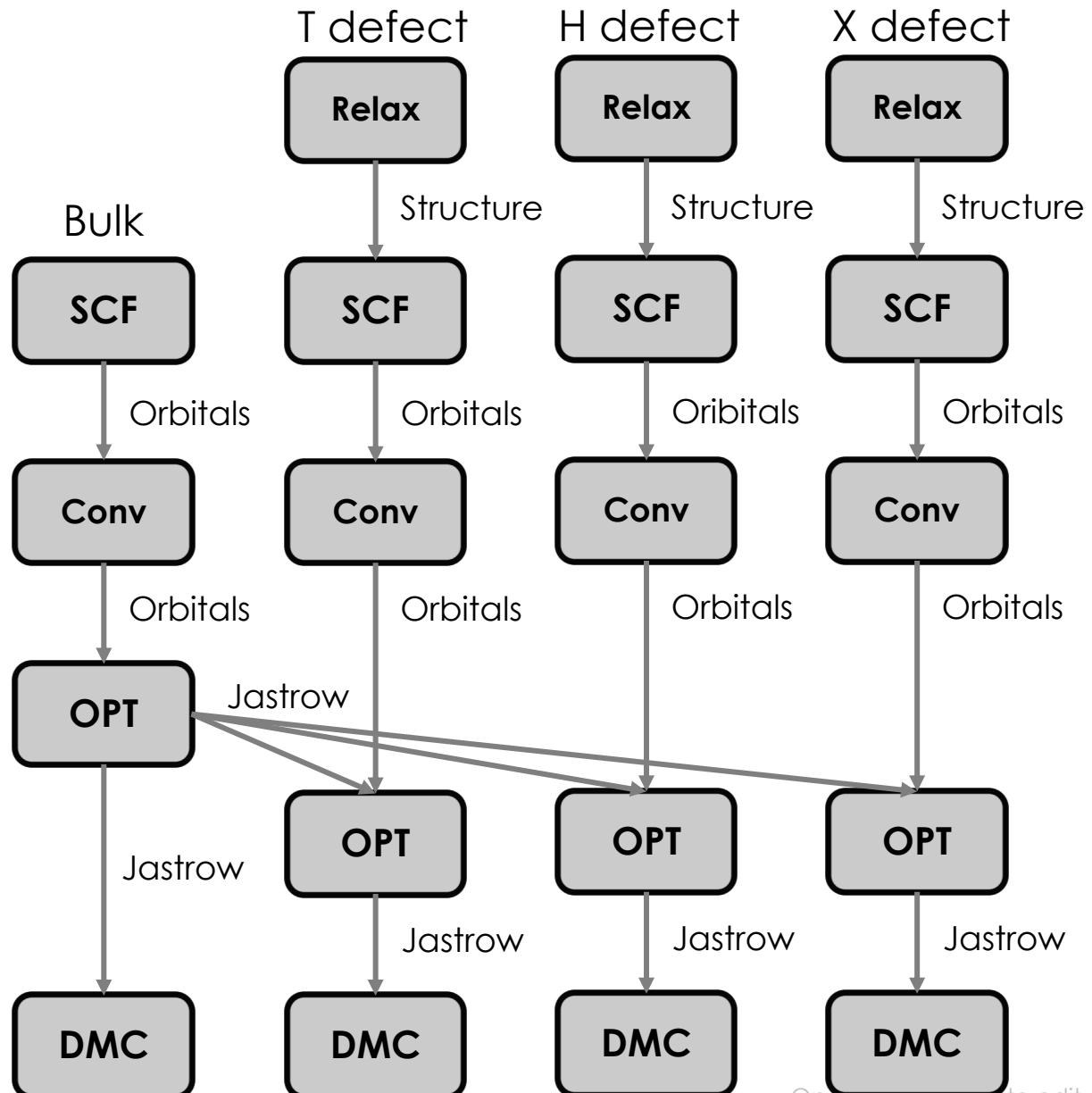
- Example Workflow
 - DMC calculation of bulk diamond
 - E.g. SCF with Quantum Espresso
 - Orbital conversion with pw2qmcpack
 - Jastrow optimization with QMCPACK
 - DMC with QMCPACK

Bulk Workflow



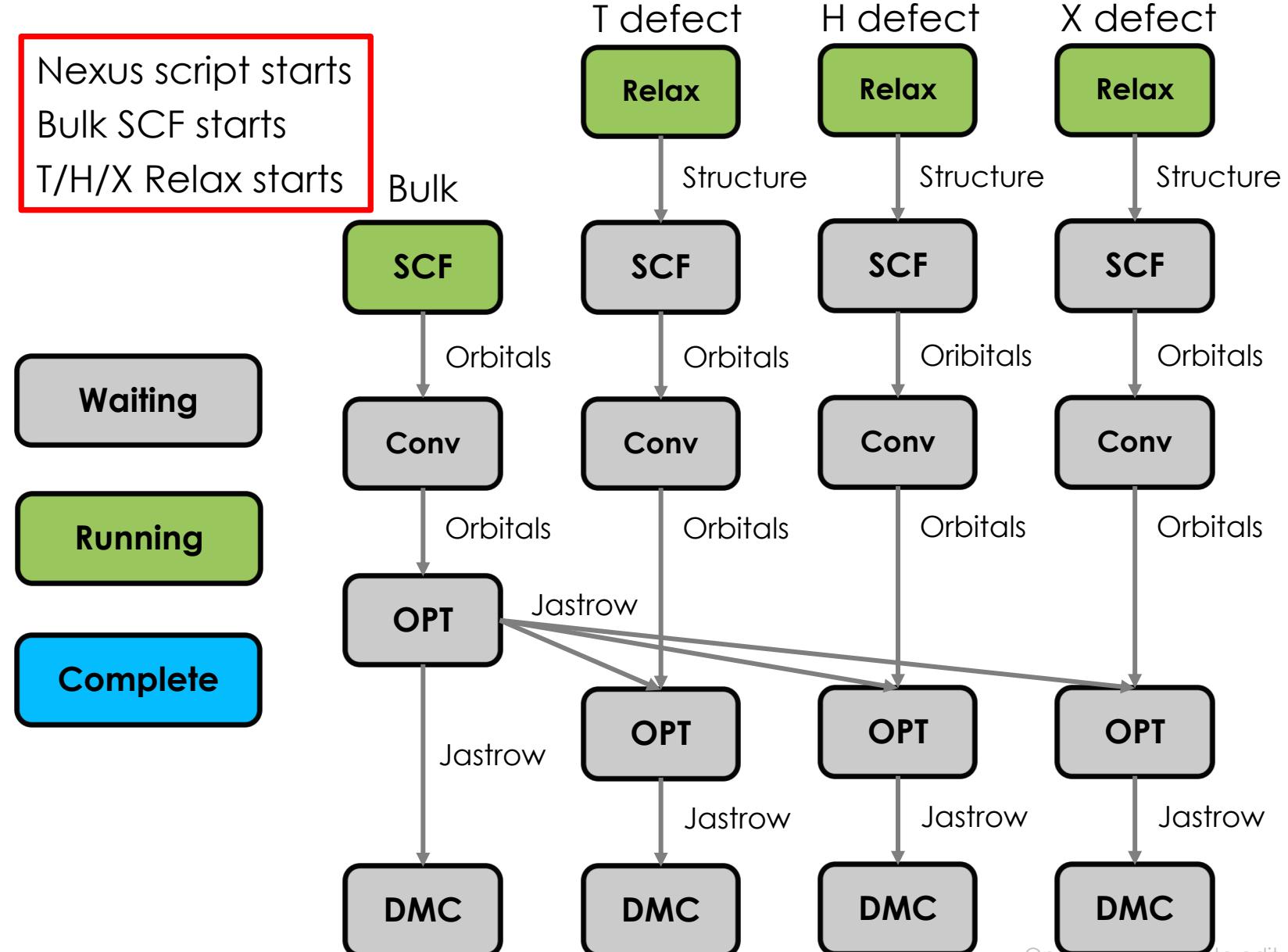
Nexus Workflow Execution/Monitoring

- Example Workflow
 - DMC calculation of bulk + T/H/X interstitials in diamond
- Parallel Execution
 - Independent jobs run separately
 - Dependencies processed automatically
 - All jobs monitored for completion



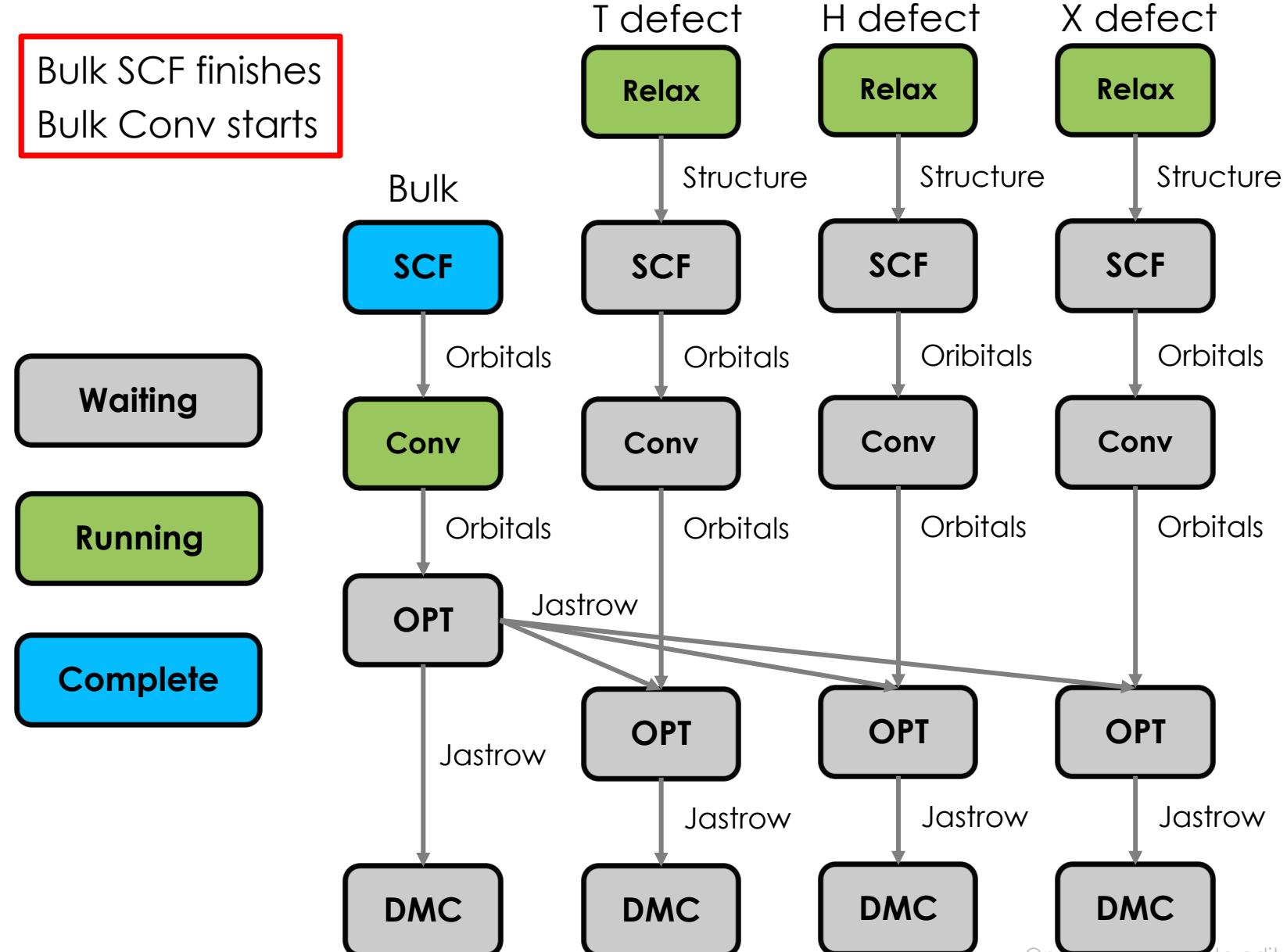
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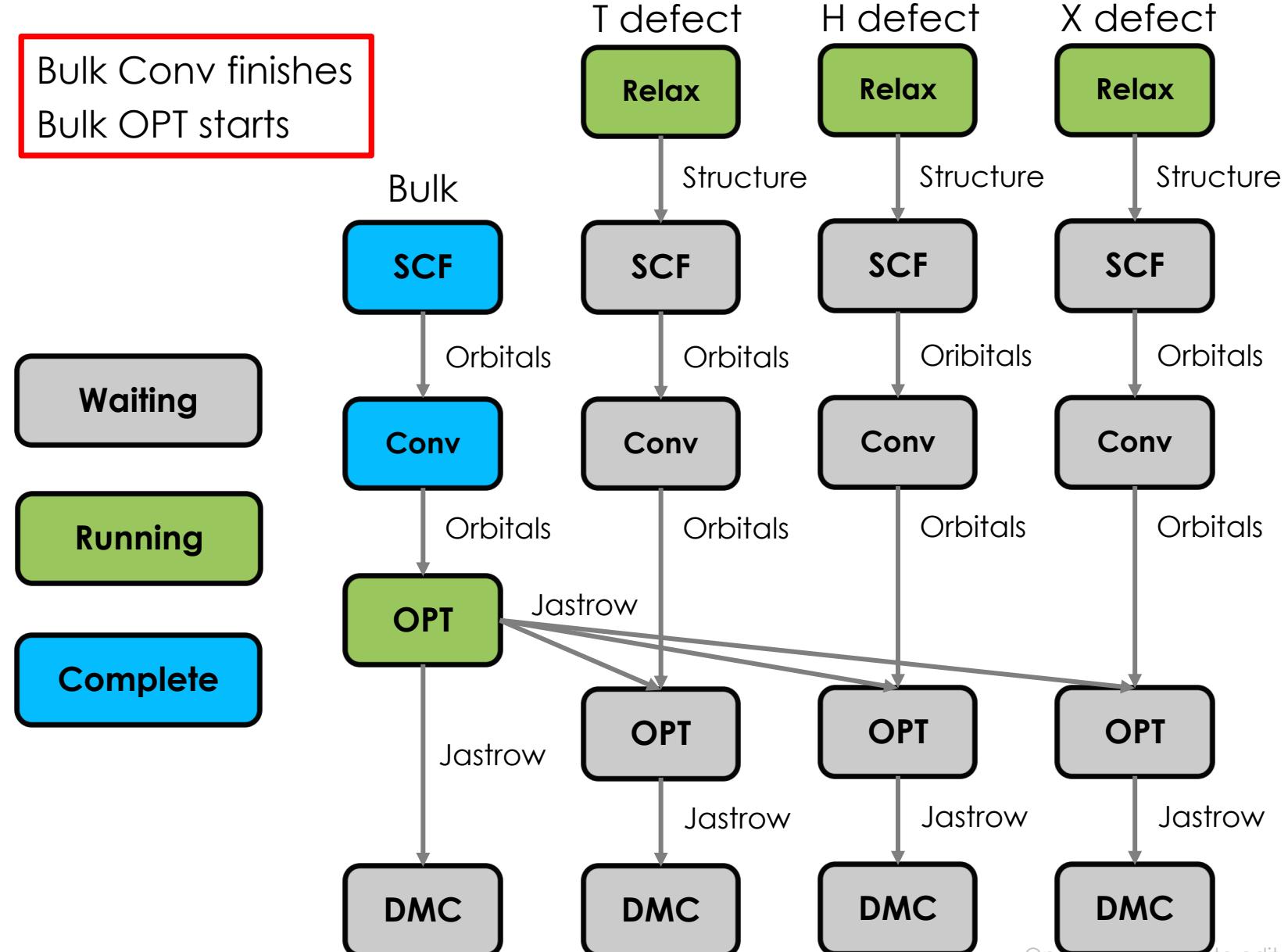
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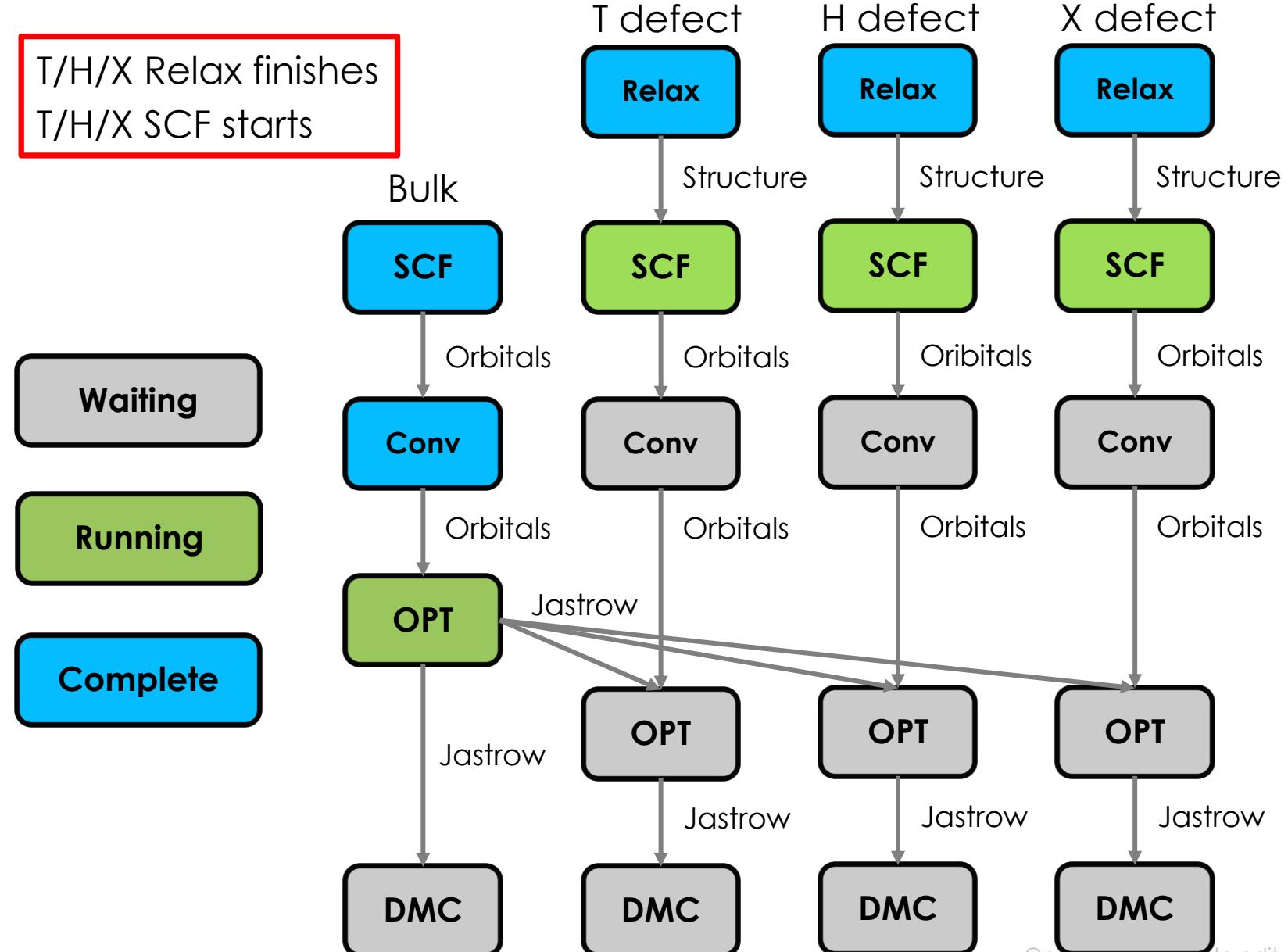
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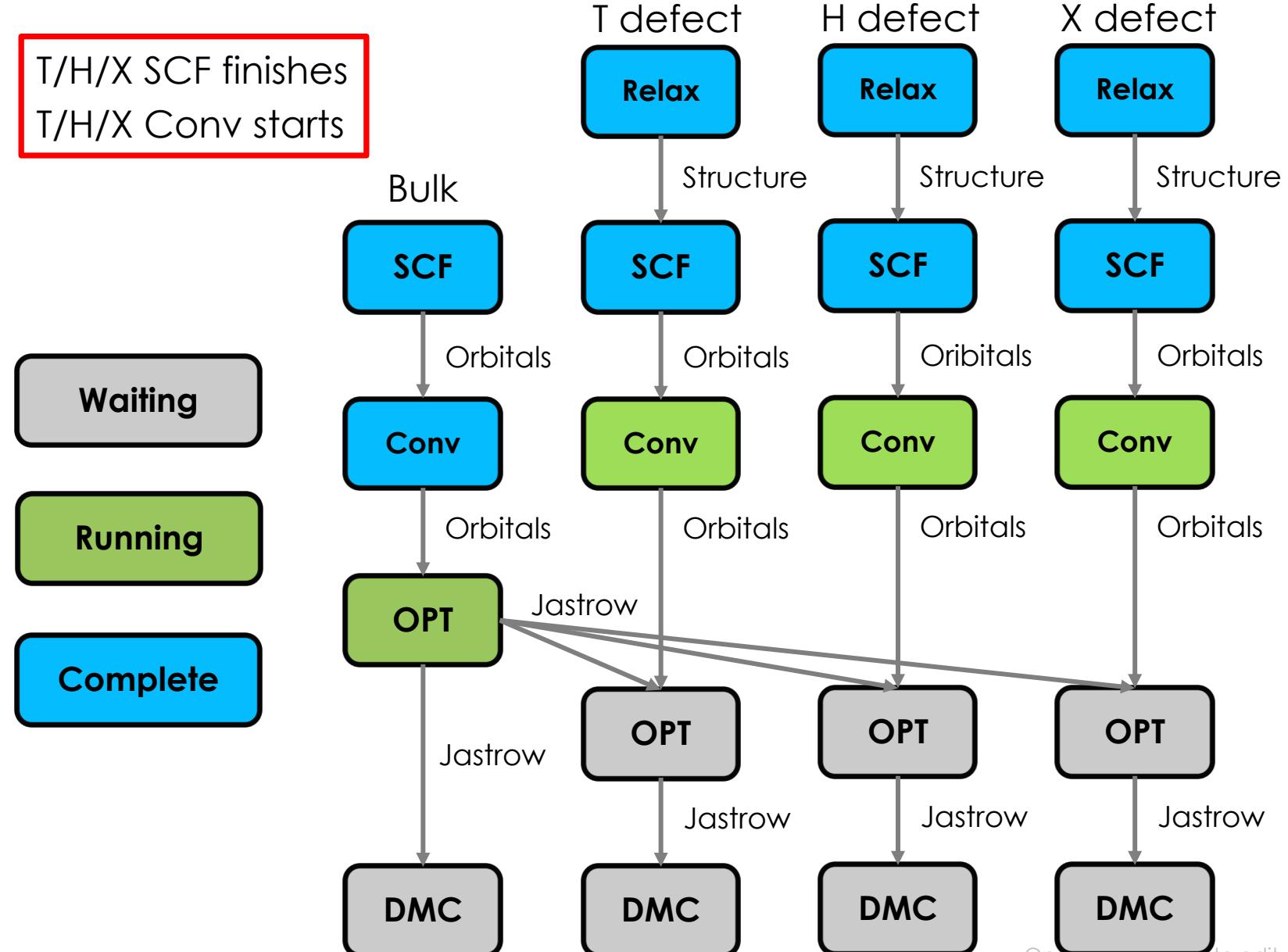
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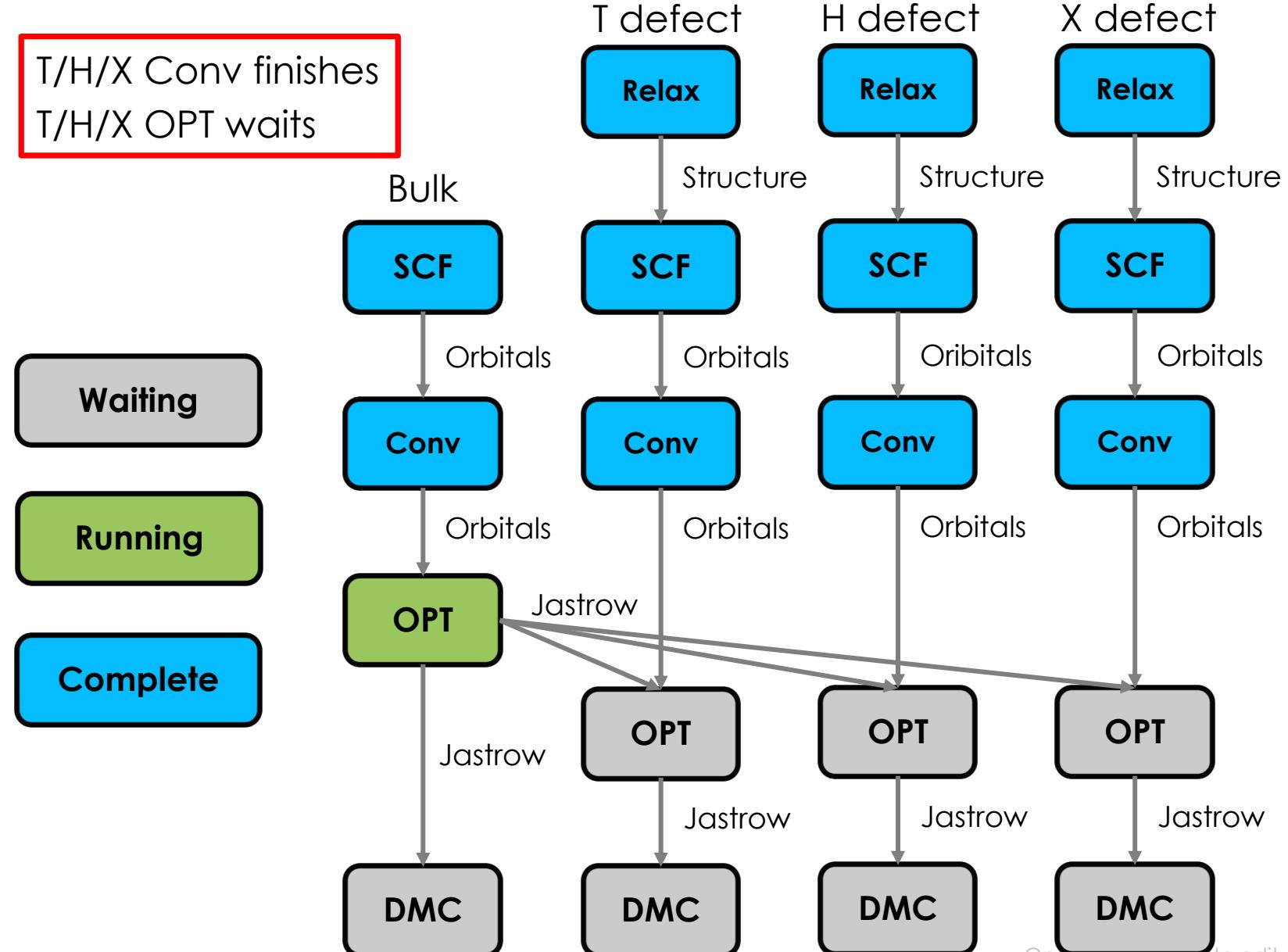
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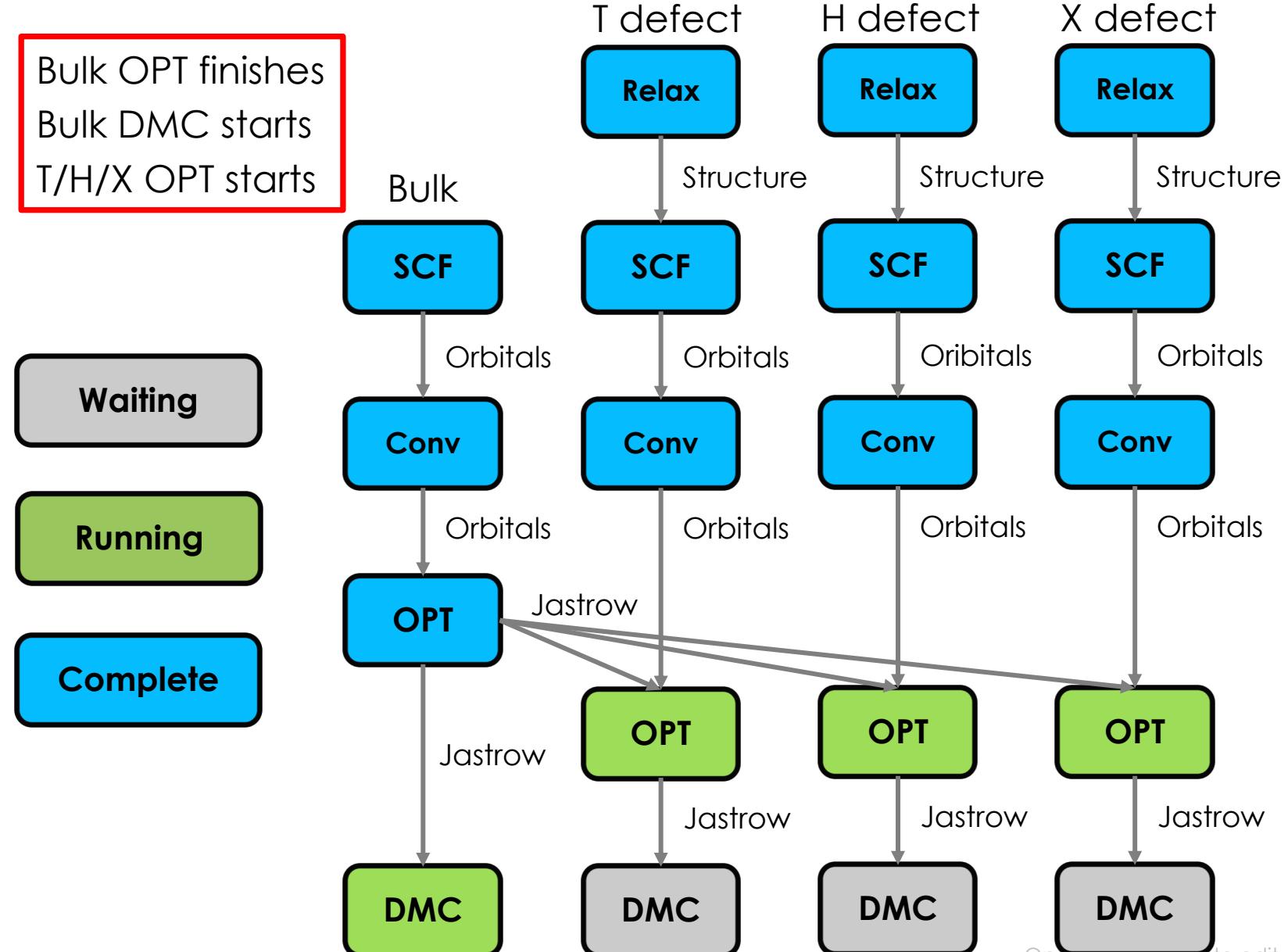
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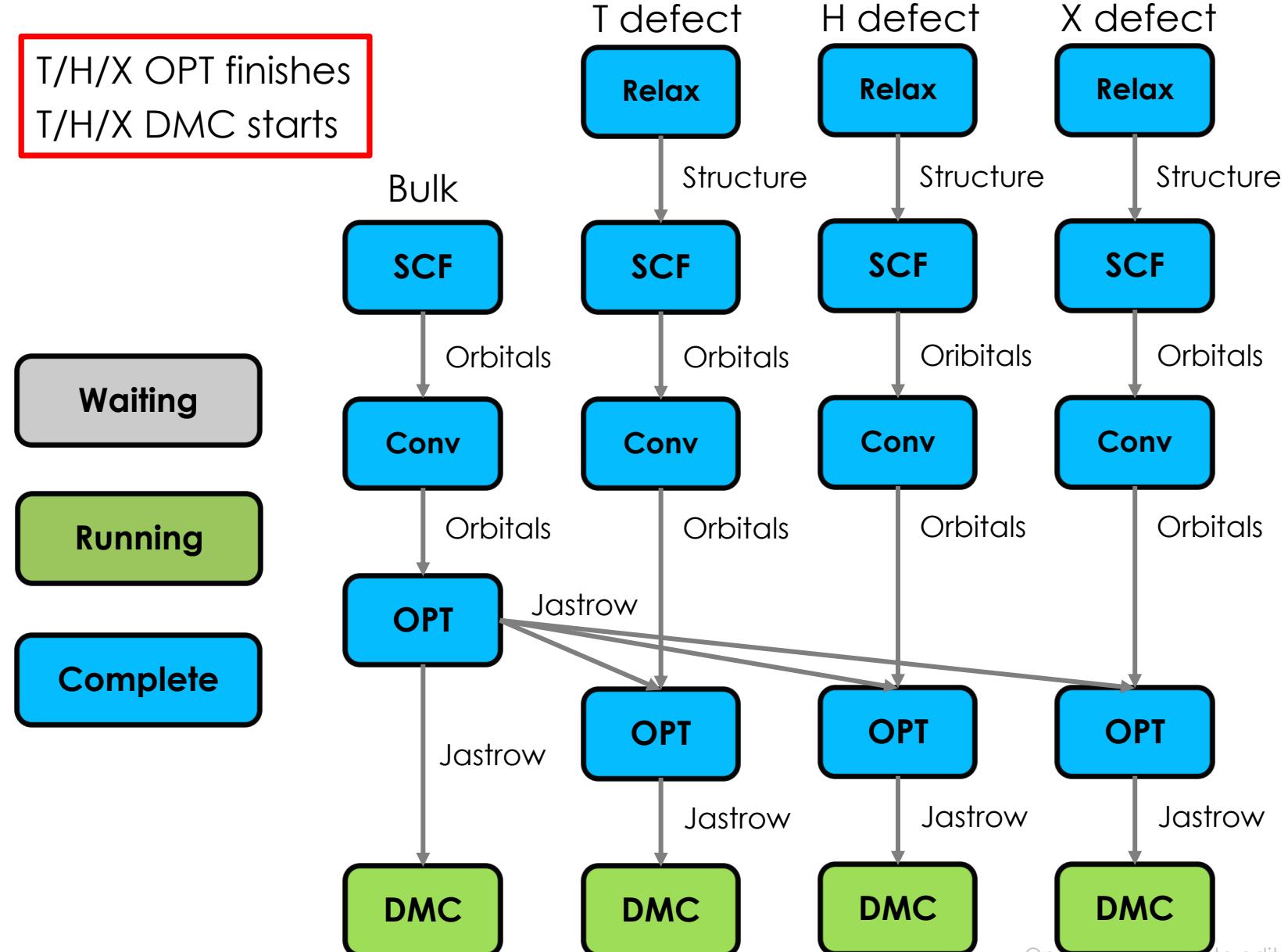
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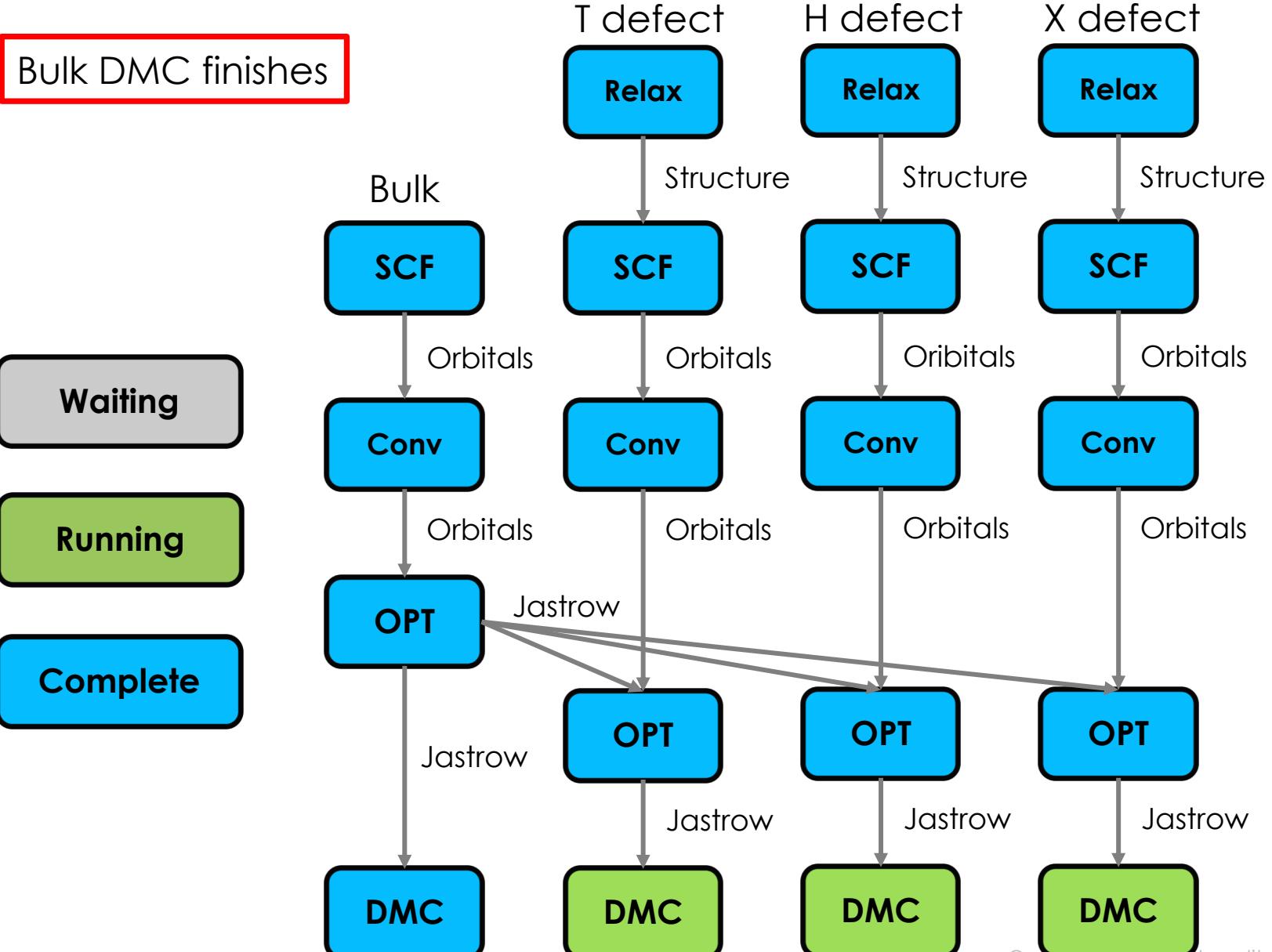
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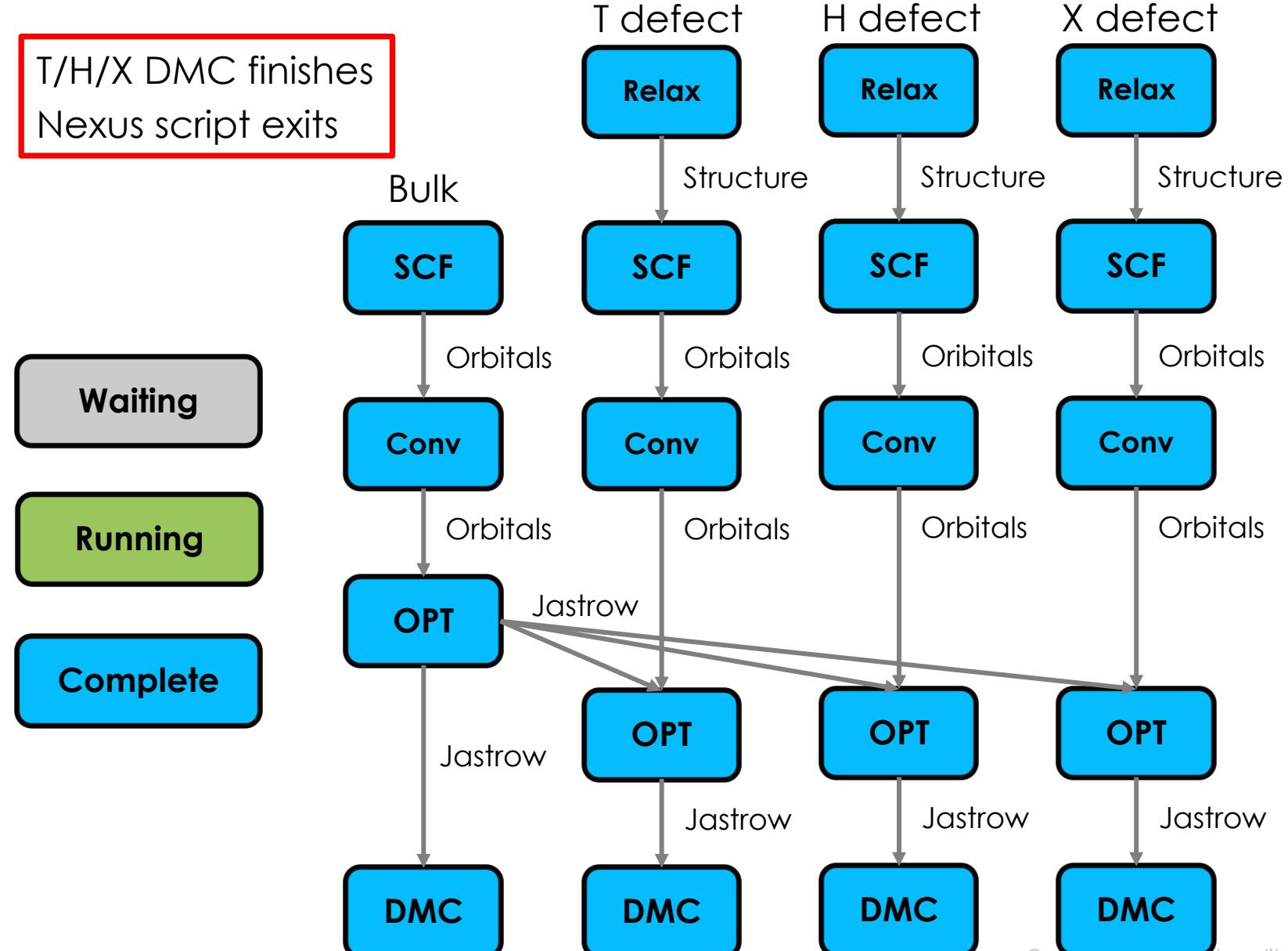
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Nexus Workflow Execution/Monitoring

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Electronic Structure Codes Supported by Nexus

QMCPACK



QUANTUMESPRESSO



pyscf



Electronic Structure Codes Supported by Nexus

- **QMCPACK**: wavefunction optimization, VMC, DMC, RMC
- **Quantum Espresso**: DFT SCF/NSCF, structural optimization, post-processing tools, orbital conversion
- **VASP**: DFT SCF, structural optimization, nudged elastic band
- **GAMESS**: HF, DFT, CASSCF, CISD, etc, wavefunction conversion
- **PySCF**: HF, DFT, CCSD, etc, wavefunction conversion
- **Quantum Package**: HF, Selected-CI (CIPSI), wavefunction conversion

Machine Environments Supported by Nexus

- **OLCF:** Eos, Titan, Summit
- **ALCF:** Vesta, Cetus, Mira, Theta
- **SNL:** Sky Bridge, Chama, Serrano, Solo
- **NERSC:** Edison, Cori
- **NCSA:** BlueWaters
- **TACC:** Lonestar, Stampede2



Fairly straightforward to extend to new machines

QMC Projects Supported by Nexus

1. Krogel et al., Phys. Rev. B 88 035137 (2013) QMC energy density
2. Krogel et al., Phys. Rev. B 90 035125 (2014) QMC energy density matrix
3. Foyevtsoa et al., Phys. Rev. X 4 031003 (2014) Ca_2CuO_3 spin gap
4. Santana et al., J. Chem. Phys. 142 164705 (2015) ZnO cohesive energy, band gap, H impurities
5. Mitra et al., J. Chem. Phys. 143 164710 (2015) NiO Cohesive energy, band gap, oxygen vacancy
6. Krogel et al., Phys. Rev. B 93 075143 (2016) Pseudopotentials for Sc-Zn
7. Santana et al., J. Chem. Phys. 144 174707 (2016) $\text{CaO}, \text{SrO}, \text{BaO}, \text{Sc}_2\text{O}_3, \text{Y}_2\text{O}_3, \text{La}_2\text{O}_3$ cohesive energy and EOS
8. Krogel et al., J. Chem. Phys. 146 244101 (2017) Locality errors in DMC
9. Dzubak et al., J. Chem. Phys. 147 024102 (2017) Locality errors of OPT/BFD pseudopotentials
10. Dzubak et al., J. Chem. Phys. 147 174703 (2017) MnNiO_3 EOS and band gap
11. Santana et al., J. Chem. Phys. 147 034701 (2017) $\text{SrFeO}_3, \text{LaFeO}_3$ EOS, oxygen vacancy
12. Kylänpää et al., Phys. Rev. Mater. 1 065408 (2017) VO_2 electron density
13. Santana et al., J. Chem. Theo. Comp. 13 5604 (2017) $(\text{LaFeO}_3)_2/(\text{SrFeO}_3)$ superlattice, oxygen vacancy
14. Krogel et al., J. Chem. Phys. 148 044110 (2018) Smoothed multiscale B-spline orbitals
15. Sharma et al., ACS Nano 12 7159 (2018) VO_2 oxygen vacancy
16. Saritas et al., Phys. Rev. Mater. 2 085801 (2018) $\text{MnO}, \text{MnO}_2, \text{LaMnO}_3$ EOS and cohesive energy
17. Saritas et al., Phys. Rev. B 98 155130 (2018) CoO polymorphs, cohesive energy, band gap
18. Kadioglu et al., J. Chem. Phys. 148 214706 (2018) Bilayer Arsenene binding energy
19. Archibald et al., J. Chem. Phys. 164 116 (2018) Benzene struct. opt. via Gaussian process
20. Saritas et al., J. Phys. Chem. Lett. 10 67 (2019) $\text{Al}_2\text{O}_3, \text{MgO}, \text{Y}_2\text{O}_3, \text{K}_2\text{SiF}_6$ band gaps
21. Kylänpää et al., Phys. Rev. B 99 075154 (2019) VO_2 Compton profile

User's Perspective: Working with Nexus

Working with Nexus: Installation

Download

```
>mkdir /your/path/to  
>cd /your/path/to  
>git clone https://github.com/QMCPACK/qmcpack  
>cd /your/path/to/qmcpack/nexus
```

Installation

```
export PYTHONPATH=/your/path/to/qmcpack/nexus/lib:$PYTHONPATH  
export PATH=/your/path/to/qmcpack/nexus/bin:$PATH
```

Testing

```
>nxs-test
```

1/16 generic_logging.....	Passed	0.00 sec
2/16 generic_intrinsics.....	Passed	0.00 sec
3/16 generic_extensions.....	Passed	0.00 sec
4/16 nexus_imports.....	Passed	0.32 sec
5/16 settings.....	Passed	0.00 sec
6/16 machines.....	Passed	2.30 sec
7/16 structure.....	Passed	0.54 sec
8/16 pwscf_input.....	Passed	0.02 sec
9/16 example_gamess_H2O.....	Passed	1.60 sec
10/16 example_qmcpack_oxygen_dimer.....	Passed	0.73 sec
11/16 example_qmcpack_H2O.....	Passed	0.74 sec
12/16 example_qmcpack_LiH.....	Passed	0.84 sec
13/16 example_qmcpack_diamond.....	Passed	1.22 sec
14/16 example_pwscf_relax_Ge_T.....	Passed	0.71 sec
15/16 example_qmcpack_c20.....	Passed	0.74 sec
16/16 example_qmcpack_graphene.....	Passed	0.84 sec

100% tests passed, 0 tests failed out of 16

Total test time = 10.61 sec

Working with Nexus: User Script Composition

Invoke interpreter

Nexus imports

User settings

System definition

Workflow composition

```
#! /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()
```

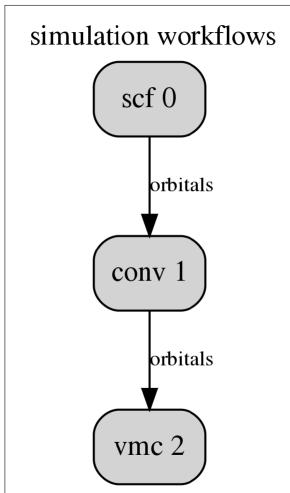
Workflow composition

Workflow execution

Working with Nexus: User Script Execution

Graph simulation workflows

```
>./diamond.py --graph_sims
```



Check initial run status

```
>./diamond.py --status_only
```

```
...
```

```
cascade status
setup, sent_files, submitted, finished, ...
000000 0 ----- scf      ./runs/diamond/scf
000000 0 ----- conv     ./runs/diamond/scf
000000 0 ----- vmc     ./runs/diamond/vmc
setup, sent_files, submitted, finished, ...
```

Execute workflows (monitored via polling)

```
>./diamond.py
...
starting runs:
~~~~~
elapsed time 0.0 s   memory 102.16 MB
...
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 102.29 MB
elapsed time 6.1 s   memory 102.32 MB
...
Entering ./runs/diamond/scf 1
Executing:
  export OMP_NUM_THREADS=1
  mpirun -np 1 pw2qmcpack.x<conv.in
elapsed time 9.1 s   memory 102.32 MB
elapsed time 12.2 s   memory 102.32 MB
...
Entering ./runs/diamond/vmc 2
Executing:
  export OMP_NUM_THREADS=4
  mpirun -np 4 qmcpack vmc.in.xml
elapsed time 15.2 s   memory 418.06 MB
...
elapsed time 45.6 s   memory 102.41 MB
Project finished
```

Check final run status

```
>./diamond.py --status_only
```

```
...
```

```
cascade status
setup, sent_files, submitted, finished, ...
111111 0 10641    scf      ./runs/diamond/scf
111111 0 10723    conv     ./runs/diamond/scf
111111 0 10742    vmc     ./runs/diamond/vmc
setup, sent_files, submitted, finished, ...
```

Process results

```
grep '!  ' runs/diamond/scf/scf.out
!      total energy          =      -22.52257768 Ry
>qmca -e 20 -q e runs/diamond/vmc/*scalar*
runs/diamond/vmc series 0 LocalEnergy = -87.789516
                                         +/- 0.032402
```

Working with Nexus: Changing Machine Environments

Workstation

```
settings(  
    ...  
    machine = 'ws16'  
)  
  
qmc = generate_qmcpack(  
    ...  
    job = job(cores = 16,  
              threads = 4),  
)
```

```
export OMP_NUM_THREADS=4  
mpirun -np 4 qmcpack qmc.in.xml
```

Institutional Cluster (CADES at ORNL)

```
settings(  
    ...  
    machine = 'cades',  
    account = 'qmc',  
)  
  
qmc = generate_qmcpack(  
    ...  
    job = job(nodes = 4,  
              threads = 4,  
              hours = 8),  
)
```

```
#!/bin/bash  
#PBS -A qmc  
#PBS -W group_list=cades-qmc  
#PBS -q skylake  
#PBS -N vmc  
#PBS -o vmc.out  
#PBS -e vmc.err  
#PBS -l qos=std  
#PBS -l walltime=08:00:00  
#PBS -l nodes=4:ppn=36  
  
echo $PBS_O_WORKDIR  
cd $PBS_O_WORKDIR  
  
export OMP_NUM_THREADS=4  
mpirun -np 36 --npersocket 4 \  
qmcpack qmc.in.xml
```

Leadership Computing (Theta at ALCF)

```
settings(  
    ...  
    machine = 'theta',  
    account = 'QMCACC',  
)  
  
qmc = generate_qmcpack(  
    ...  
    job = job(nodes = 1024,  
              threads = 64,  
              hours = 5),  
)
```

```
#!/bin/bash  
#COBALT -q default  
#COBALT -A QMCACC  
#COBALT -n 1024  
#COBALT -t 300  
#COBALT -O vmc  
#COBALT --attrs mcdram=cache:numa=quad  
  
export OMP_NUM_THREADS=64  
aprun -n 1024 -e OMP_NUM_THREADS=64 -d 64 \  
-cc depth -j 1 -N 1 qmcpack qmc.in.xml
```

Working with Nexus: Job Bundling

```
...  
from nexus import bundle  
  
settings(  
    ...  
    machine = 'theta',  
    account = 'QMCACC',  
)  
  
sims = []  
  
for scale in [0.90,0.95,1.00,1.05,1.10]:  
    diamond_scaled = diamond.copy()  
    diamond_scaled.structure.rescale(scale)  
    ...  
    qmc = generate_qmcpack()  
    ...  
    system = diamond_scaled,  
    job    = job(nodes      = 512,  
                  threads   = 64,  
                  hours     = 5),  
    )  
    sims.append(qmc)  
#end for  
  
bundle(sims)  
  
run_project()
```

```
#!/bin/bash  
#COBALT -q default  
#COBALT -A QMCACC  
#COBALT -n 2560  
#COBALT -t 300  
#COBALT -O bundle  
#COBALT --attrs mcdram=cache:numa=quad  
  
export OMP_NUM_THREADS=64  
  
cd /projects/QMCACC/diamond/scale_0.9/qmc  
aprun -n 512 -e OMP_NUM_THREADS=64 -d 64 \  
-cc depth -j 1 -N 1 qmcpack qmc.in.xml >qmc.output 2>qmc.error&  
  
cd /projects/QMCACC/diamond/scale_0.95/qmc  
aprun -n 512 -e OMP_NUM_THREADS=64 -d 64 \  
-cc depth -j 1 -N 1 qmcpack qmc.in.xml >qmc.output 2>qmc.error&  
  
cd /projects/QMCACC/diamond/scale_1.0/qmc  
aprun -n 512 -e OMP_NUM_THREADS=64 -d 64 \  
-cc depth -j 1 -N 1 qmcpack qmc.in.xml >qmc.output 2>qmc.error&  
  
cd /projects/QMCACC/diamond/scale_1.05/qmc  
aprun -n 512 -e OMP_NUM_THREADS=64 -d 64 \  
-cc depth -j 1 -N 1 qmcpack qmc.in.xml >qmc.output 2>qmc.error&  
  
cd /projects/QMCACC/diamond/scale_1.1/qmc  
aprun -n 512 -e OMP_NUM_THREADS=64 -d 64 \  
-cc depth -j 1 -N 1 qmcpack qmc.in.xml >qmc.output 2>qmc.error&  
  
wait
```

Overview of Workshop Examples

Workshop Examples

Navigate to link below and view README file:

https://github.com/QMCPACK/qmcpack_workshop_2019/tree/master/day2_nexus

Enter Nexus examples directory:

```
>cd /home/ubuntu/qmcpack_workshop_2019/day2_nexus/
```

VMC/DMC workflows for QMCPACK starting from:

- Quantum Espresso
- PySCF
- Quantum Package

Examples fairly stand-alone, jump in at point of interest

- If new to Nexus, consider trying QE examples 1 and 2 first

Workshop Examples: Quantum Espresso + QMCPACK

day2_nexus/quantum_espresso

1. Diamond primitive cell: single DFT calculation with QE
2. Matrix-tiled diamond supercell: SCF, NSCF, Jastrow opt, VMC
3. Matrix-tiled diamond supercell: twist-averaged VMC
4. Matrix-tiled diamond supercell: DMC

Workshop Examples: PySCF + QMCPACK

day2_nexus/pyscf

1. Water molecule: single RHF calculation with PySCF
2. Diamond primitive cell: single RHF calculation with PySCF
3. Water molecule: RHF, cusp correction, J2/J3 opt, VMC, DMC
4. Diamond 2x1x1 supercell: RHF, Jastrow opt, VMC, DMC

Workshop Examples: Quantum Package + QMCPACK

day2_nexus/quantum_package

1. Water molecule: single RHF calculation with QP
2. Oxygen dimer: RHF, CIPSI, natural orbitals, final CIPSI
3. Water molecule: RHF, cusp correction, J2/J3 opt, VMC, DMC
4. Oxygen dimer: RHF, CIPSI, natural orbitals, final CIPSI, cusp correction, J2/J3 opt, VMC, DMC

Additional Resources & Future Directions

Additional Resources

- Reference paper (please cite!)
 - <https://doi.org/10.1016/j.cpc.2015.08.012>
- Nexus manual
 - https://docs.qmcpack.org/nexus_user_guide.pdf
- QMCPACK manual, labs 2, 4, & 5
 - https://docs.qmcpack.org/qmcpack_manual.pdf
- Slides and demo's from User's Meetings
 - https://github.com/QMCPACK/nexus_training

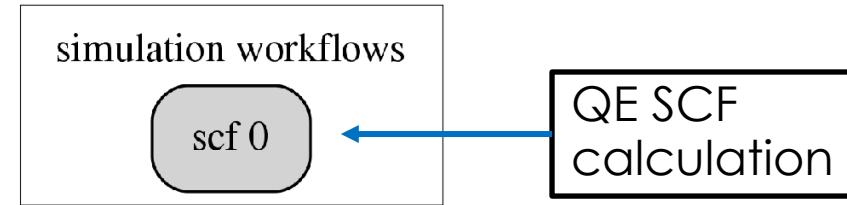
Future Directions

- Expanded feature support
 - Orbital and targeted excited state workflows
 - AFQMC workflows
- Expanded example set & function level documentation
- Move to Python 3
 - Nexus is currently Python 2
 - Many major libraries to sunset Python 2 support starting in 2020

Detailed View of Workshop Examples

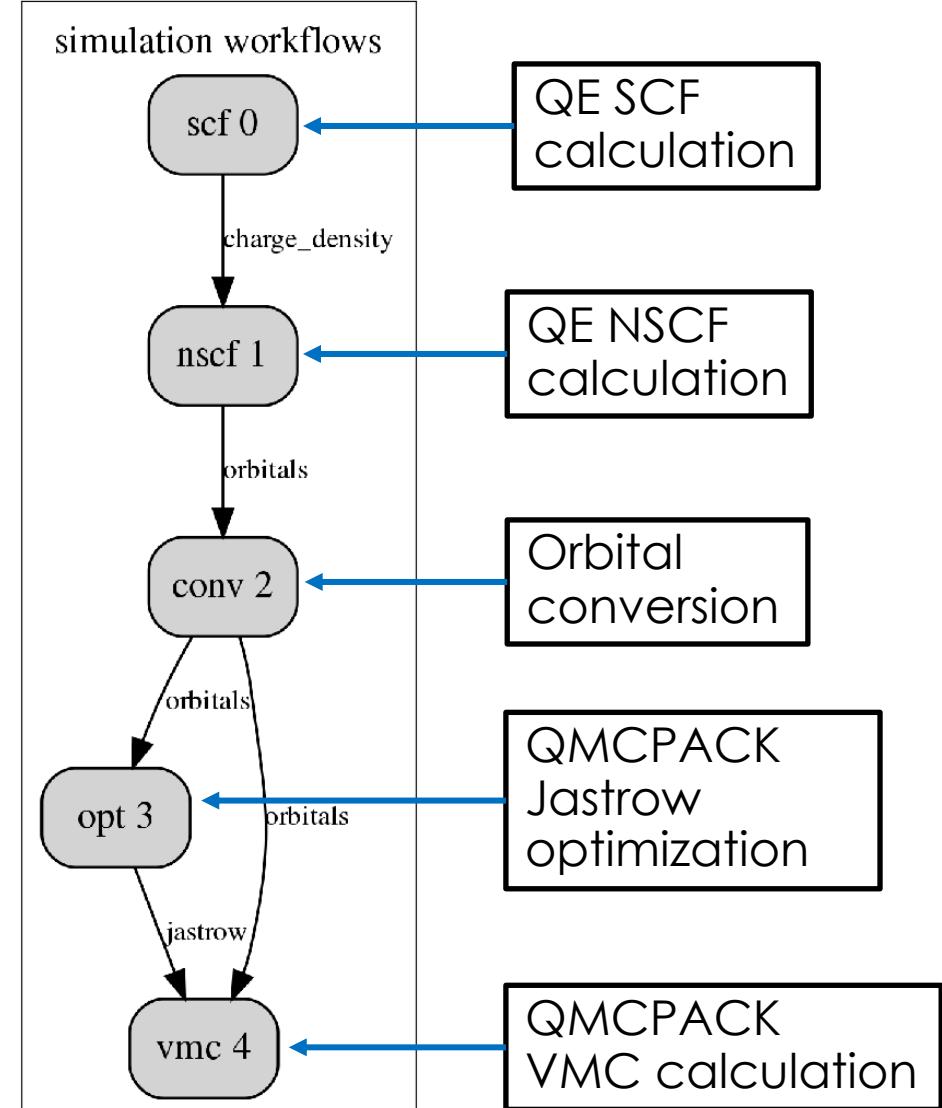
Workshop Examples: Quantum Espresso + QMCPACK

- Example 1
 - Diamond primitive cell
 - LDA calculation
 - BFD pseudopotentials



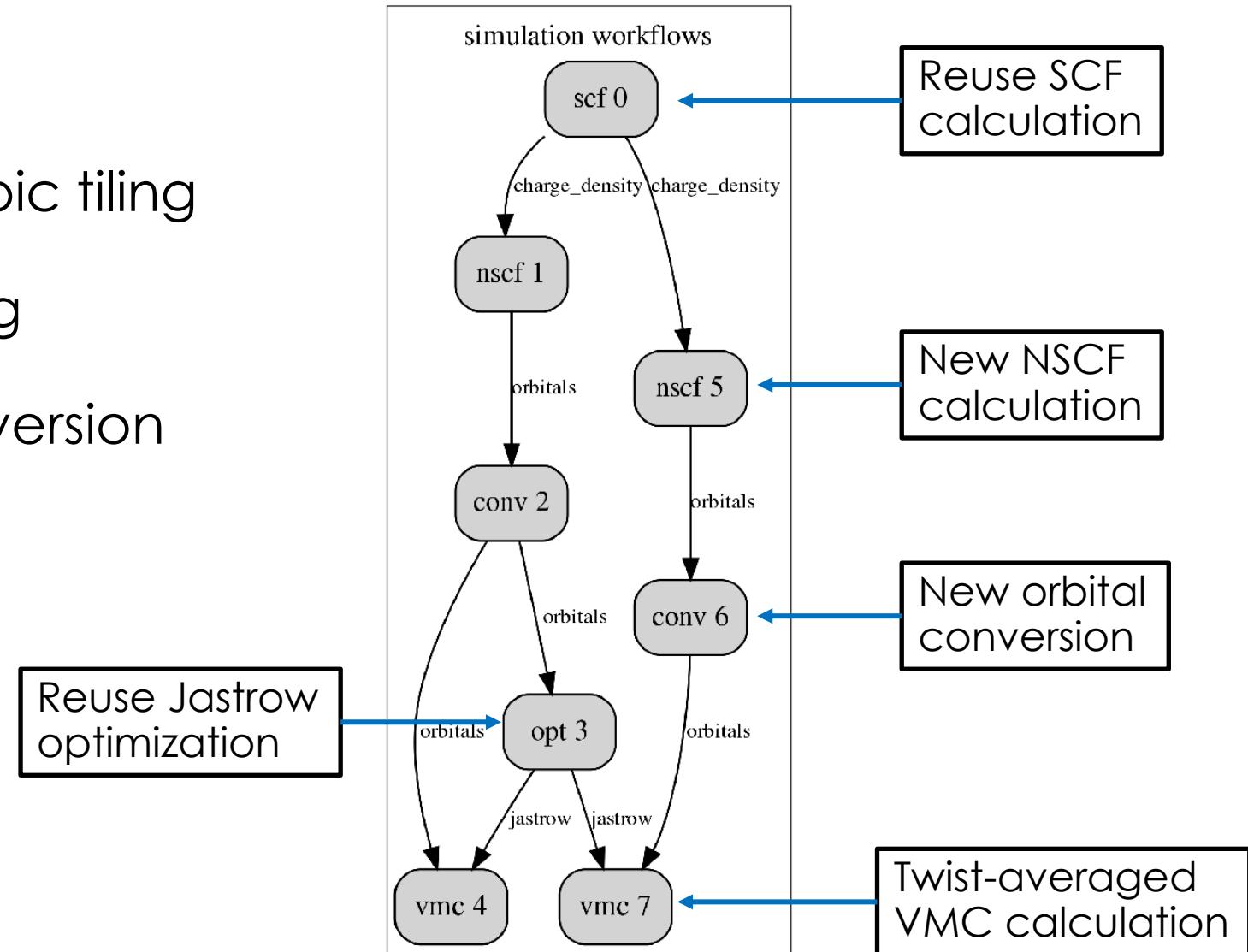
Workshop Examples: Quantum Espresso + QMCPACK

- Example 2
 - Diamond: fcc to cubic tiling
 - Gamma point
 - SCF, NSCF, orb. conversion
 - Jastrow optimization
 - VMC



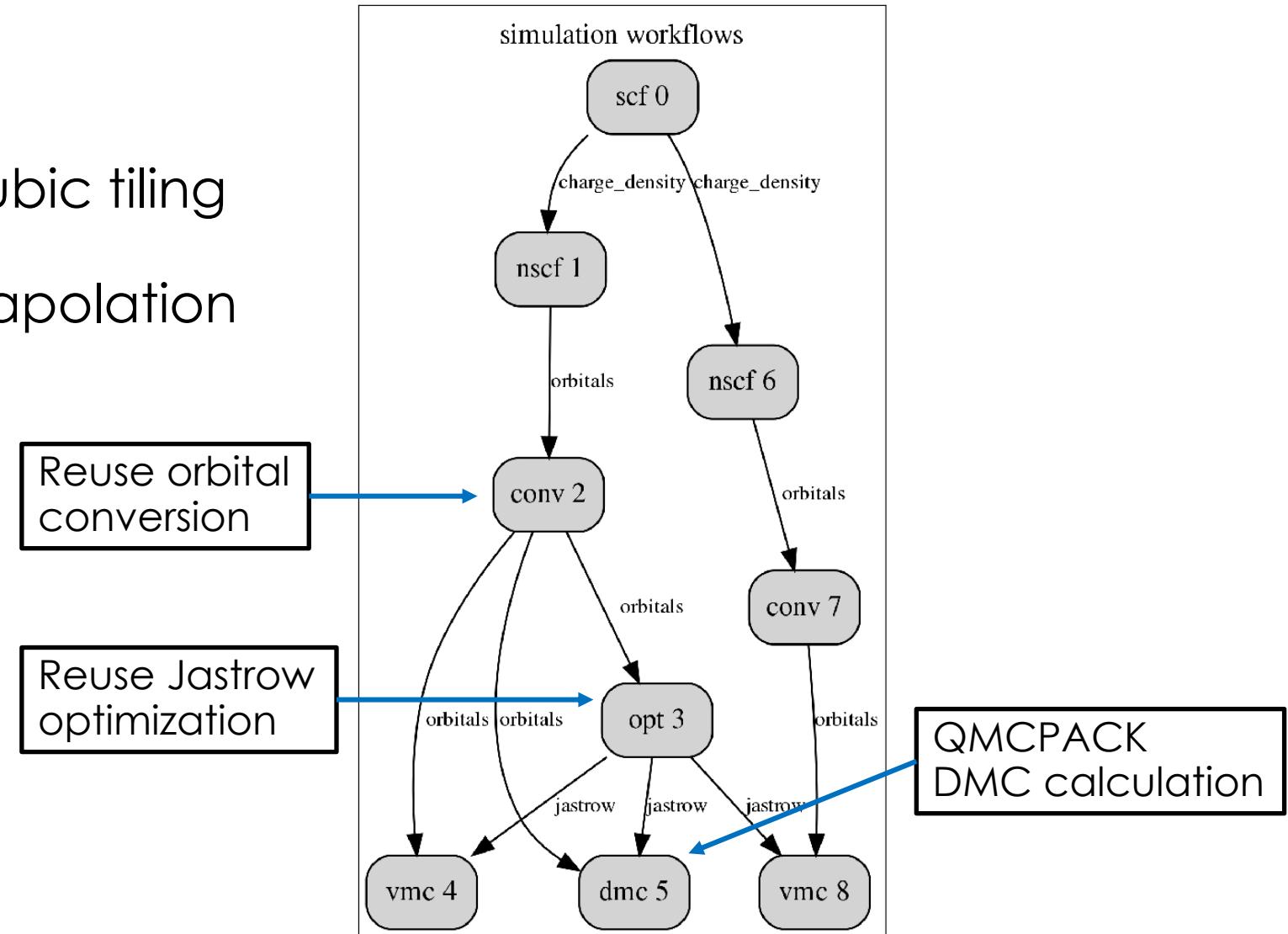
Workshop Examples: Quantum Espresso + QMCPACK

- Example 3
 - Diamond: fcc to cubic tiling
 - 2x2x2 twist averaging
 - SCF, NSCF, orb. conversion
 - Jastrow optimization
 - VMC



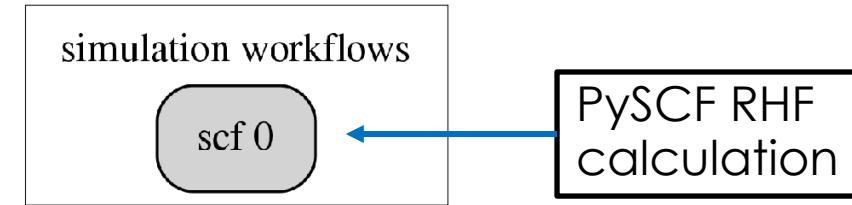
Workshop Examples: Quantum Espresso + QMCPACK

- Example 4
 - Diamond: fcc to cubic tiling
 - DMC timestep extrapolation



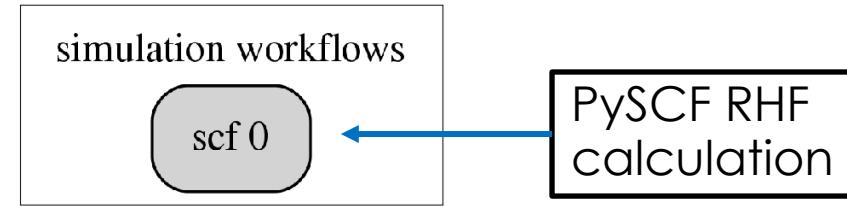
Workshop Examples: PySCF + QMCPACK

- Example 1
 - Water molecule
 - Restricted Hartree-Fock
 - Triple-zeta Gaussian basis
 - All electron



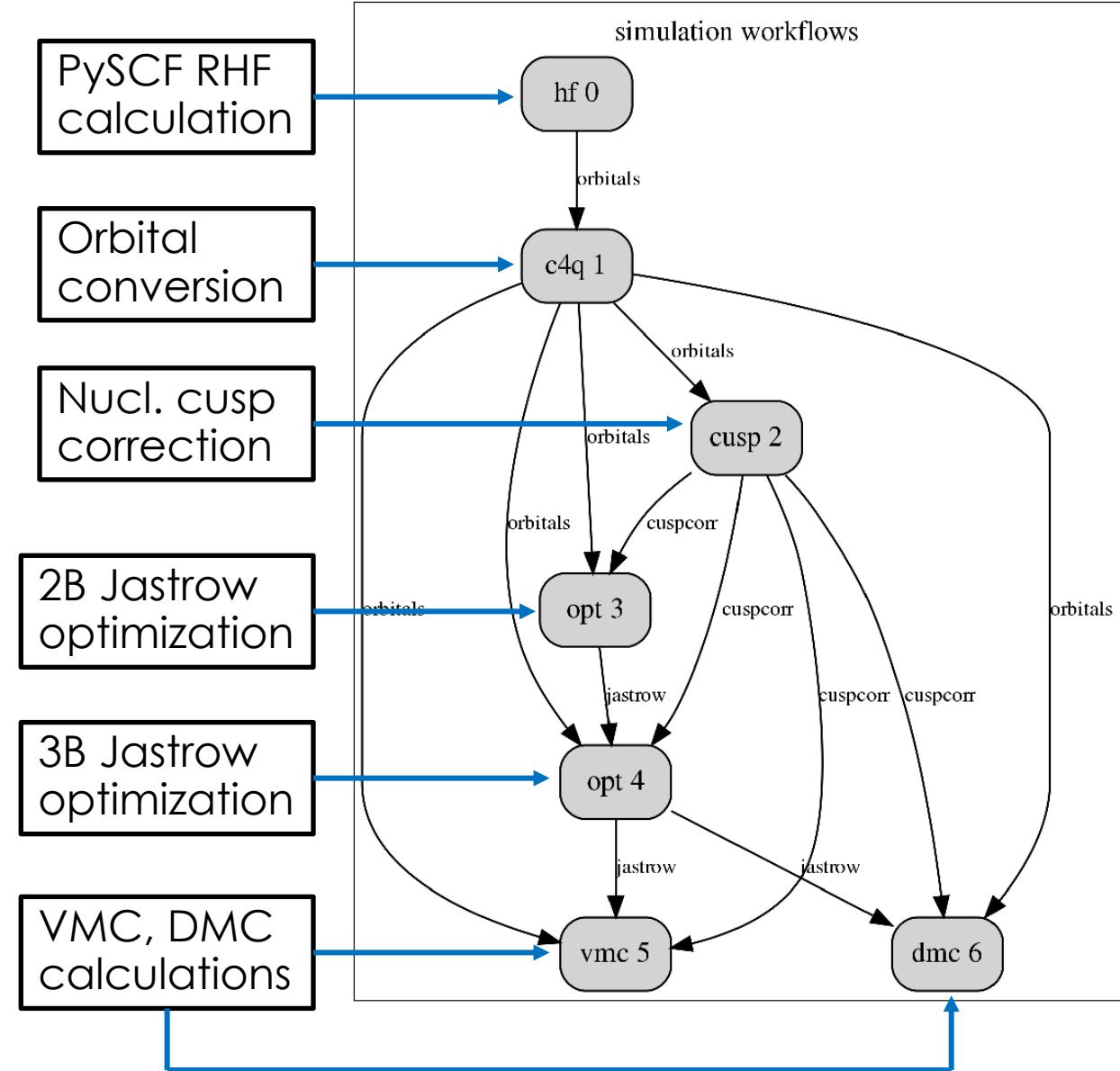
Workshop Examples: PySCF + QMCPACK

- Example 2
 - Diamond primitive cell
 - Gamma point
 - Restricted Hartree-Fock
 - Triple-zeta Gaussian basis
 - BFD ECP's



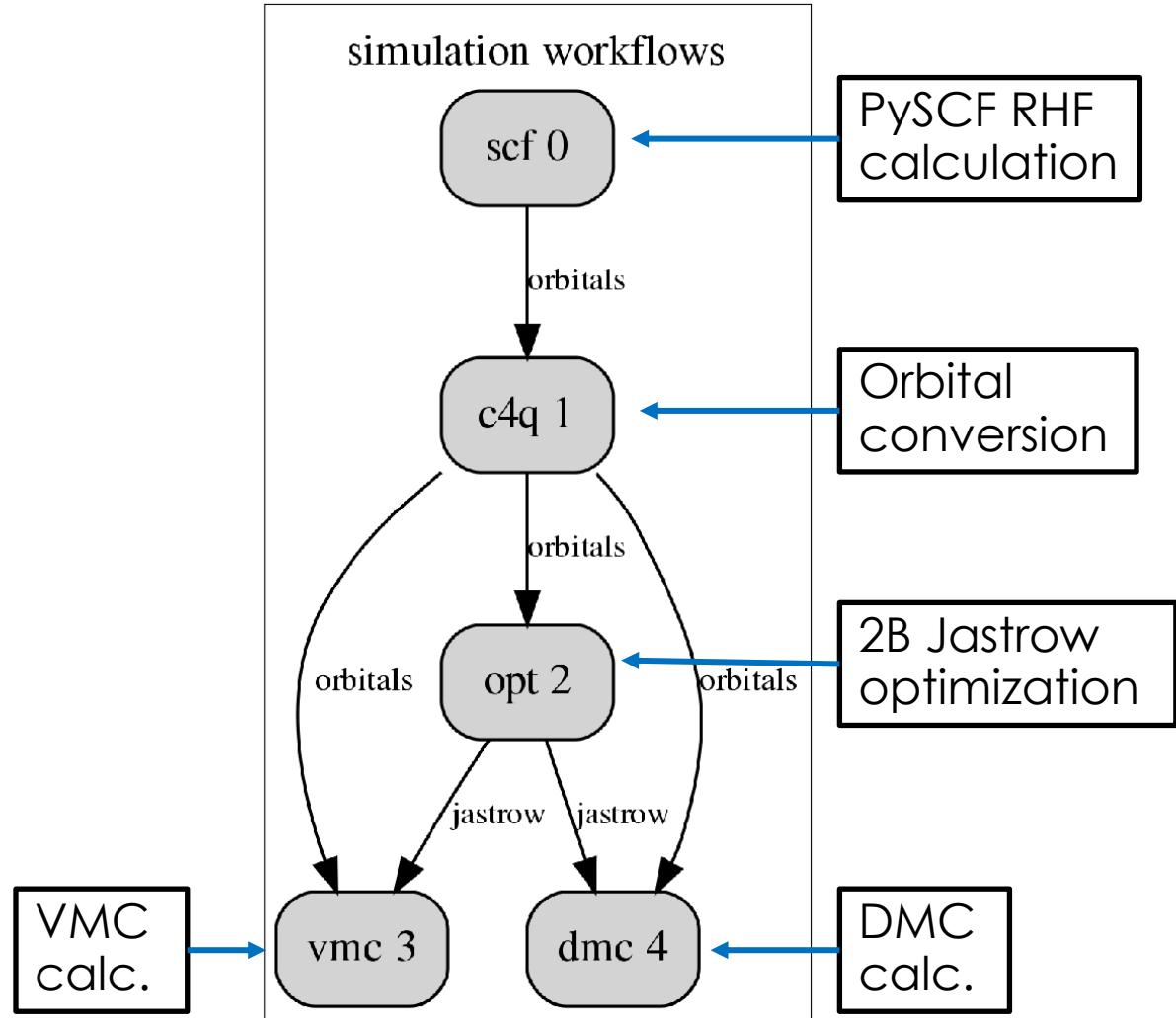
Workshop Examples: PySCF + QMCPACK

- Example 3
 - Water molecule
 - RHF, orbital conversion
 - Nuclear cusp correction
 - Two-body Jastrow opt
 - Three-body Jastrow opt
 - VMC and DMC



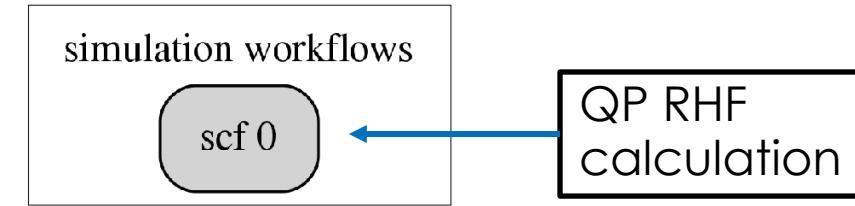
Workshop Examples: PySCF + QMCPACK

- Example 4
 - Diamond 2x1x1 cell
 - Gamma point
 - RHF, orbital conversion
 - Jastrow optimization
 - VMC and DMC



Workshop Examples: Quantum Package + QMCPACK

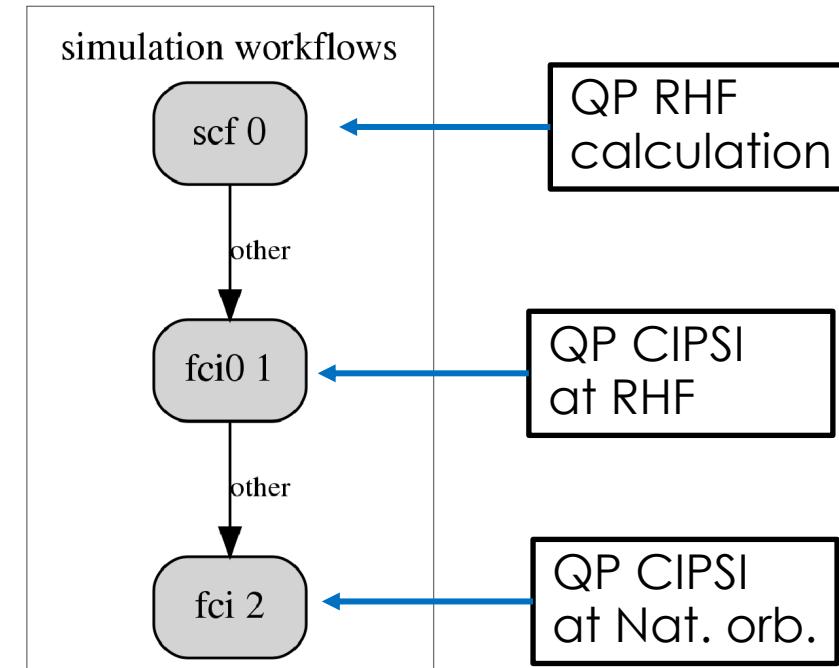
- Example 1
 - Water molecule
 - Restricted Hartree-Fock
 - Triple-zeta Gaussian basis
 - All electron



Workshop Examples: Quantum Package + QMCPACK

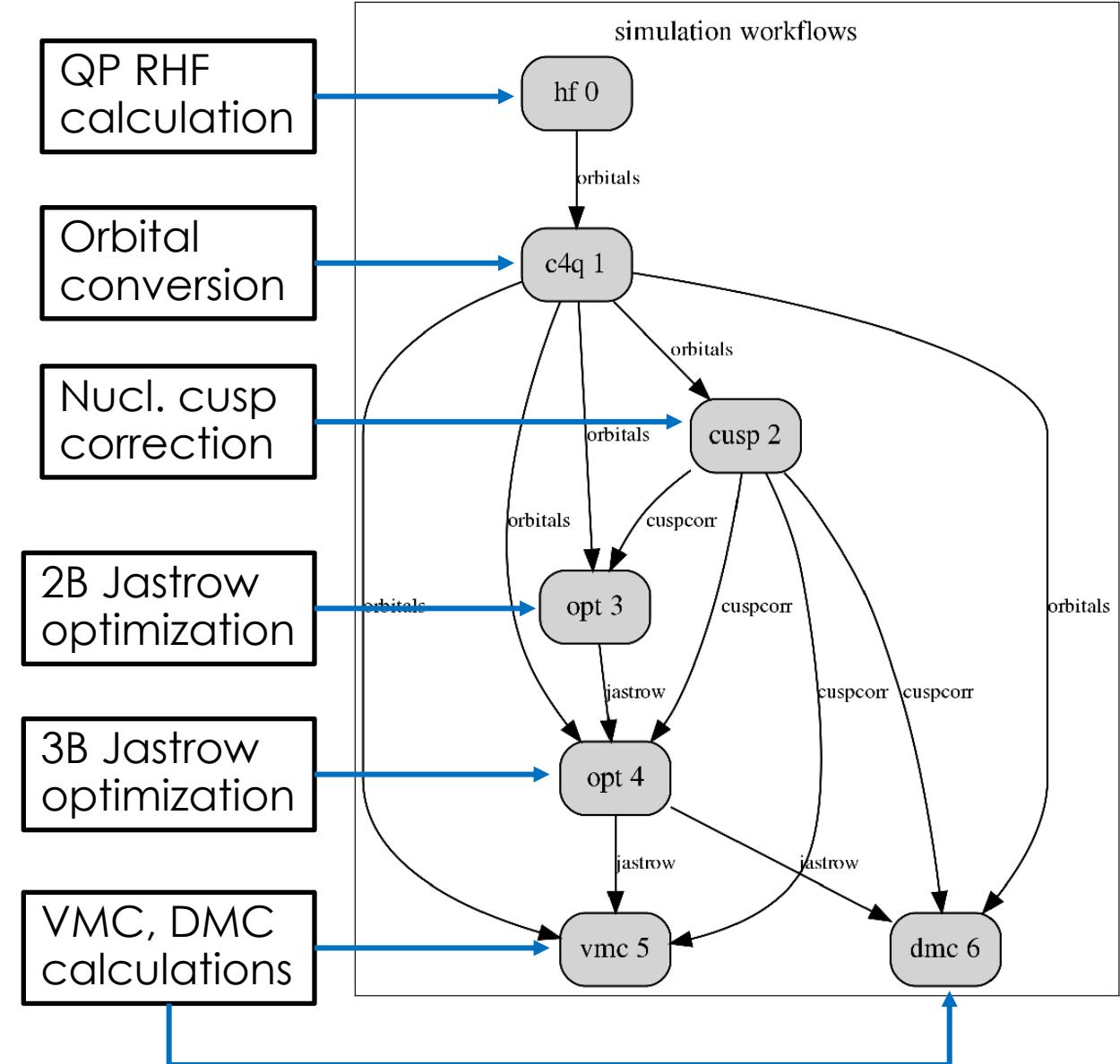
- Example 2

- Oxygen dimer
- All electron
- Restricted Hartree-Fock
- Selected CI (start at RHF)
- Natural orbitals from selected CI
- Selected CI (start from nat. orbs)



Workshop Examples: Quantum Package + QMCPACK

- Example 3
 - Water molecule
 - RHF, orbital conversion
 - Nuclear cusp correction
 - Two-body Jastrow opt
 - Three-body Jastrow opt
 - VMC and DMC



Workshop Examples: Quantum Package + QMCPACK

- Example 4
 - Oxygen dimer
 - RHF, CIPSI-RHF, CIPSI-NO
 - Wavefunction conversion
 - Nuclear cusp correction
 - Two-body Jastrow opt
 - Three-body Jastrow opt
 - VMC and DMC

