QMCPACK Workshop 2023

Driving the "Batched" QMCPACK Code with Nexus

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https://github.com/QMCPACK/qmc_workshop_2023

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CPSFM Center for Predictive Simulation of Functional Materials

Sandia National Laboratories

Argonne NATIONAL LABORATORY

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Overview

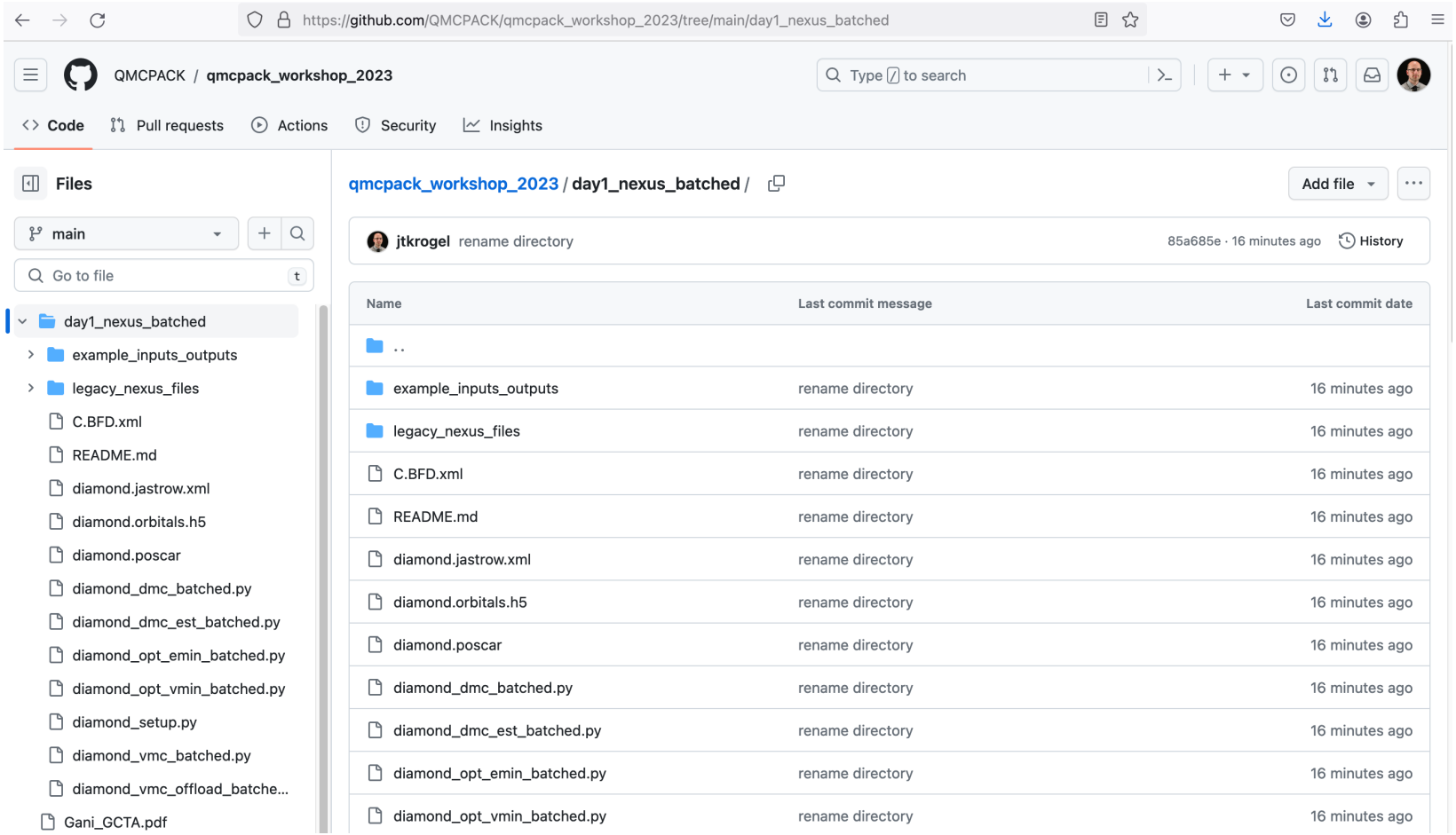
Example files on GitHub

Legacy vs Batched inputs in QMCPACK (XML) and Nexus (Python)

- Variational Monte Carlo
- Optimization: Variance Minimization
- Optimization: Energy Minimization
- Diffusion Monte Carlo
- Physical Observables

A Nexus example of VMC on GPU's: working within memory limits

Example Files on GitHub



Example Files on GitHub

qmcpack_workshop_2023 / day1_nexus_batched / README.md

jtkrogel rename directory 85a685e · 19 minutes ago History

Preview Code Blame 31 lines (22 loc) · 1.23 KB Raw

Driving the Batched Code with Nexus

General details

- Diamond primitive cell (diamond.poscar)
- BFD pseudopotential (C.BFD.xml)
- DFT planewave/B-spline orbitals (diamond.orbitals.h5)
- Two body Jastrow (diamond.jastrow.xml)

Examples

- Variational Monte Carlo (diamond_vmc_batched.py)
- Optimization: Variance Minimization (diamond_opt_vmin_batched.py)
- Optimization: Energy Minimization (diamond_opt_emin_batched.py)
- Diffusion Monte Carlo (diamond_dmc_batched.py)
- DMC with Physical Observables (diamond_dmc_est_batched.py)
- VMC on GPU's with OpenMP Offload (diamond_vmc_offload_batched.py)

Other files

- Legacy versions of Nexus examples above (legacy_nexus_files)
- QMCPACK inputs and outputs for all examples (example_inputs_outputs)

Running the Examples

- Have working installs of QMCPACK and Nexus
- Update your path to QMCPACK (CPU real build) in diamond_setup.py
- (if necessary) update workstation/job core counts in diamond_setup.py
- Execute any desired example scripts (e.g. ./diamond_vmc_batched.py)
- Note: the GPU offload example (diamond_vmc_offload_batched.py) is intended to be run with the GPU/offload real build of QMCPACK. Build this version of the code (and have an available GPU) for representative results.

Example Files on GitHub

Main Workshop Site

https://github.com/QMCPACK/qmcpack_workshop_2023/day1_nexus_batched

Git Clone or Download

git clone https://github.com/QMCPACK/qmcpack_workshop_2023.git

wget https://github.com/QMCPACK/qmcpack_workshop_2023/archive/refs/heads/main.zip

Brief Instructions Available in README

TL;DR

```
git clone https://github.com/QMCPACK/qmcpack_workshop_2023.git
cd qmcpack_workshop_2023
emacs/vim diamond_setup.py  # set path to your qmcpack exe
./diamond_vmc_batched.py
# ./diamond_opt_vmin_batched.py , etc
```

Prior Material on Nexus

Nexus Manual & Paper

https://nexus-workflows.readthedocs.io/en/latest/

J. T. Krogel Comm. Phys. Commun. 198 154 (2016)
DOI: https://doi.org/10.1016/j.cpc.2015.08.012

2021 Workshop

https://github.com/QMCPACK/qmc_workshop_2021

(see week3_stats_and_nexus directory with README and pdf)

Reminder: Installing Nexus

git clone https://github.com/QMCPACK/qmcpack.git

export PYTHONPATH=/your/path/to/qmpack_repo/nexus/lib:$PYTHONPATH

export PATH=/your/path/to/qmcpack_repo/nexus/bin:$PATH

Variational Monte Carlo

VMC on CPU: Legacy vs Batched Inputs (QMCPACK)

Legacy

```
<simulation>
  <project id="vmc_legacy" series="0">
     <parameter name="driver_version">
        legacy
     </parameter>
  </project>
  <qmcsystem>
     <simulationcell> ... </simulationcell>
     <particleset name="e"> ... </particleset>
     <particleset name="ion0"> ... </particleset>
     <wavefunction name=”psi0”> ... </wavefunction>
     <hamiltonian name="h0"> ... </hamiltonian>
  </qmcsystem>
  <qmc method="vmc" move="pbyp" checkpoint="-1">
     <parameter name="warmupSteps"> 50   </parameter>
     <parameter name="blocks"     > 800  </parameter>
     <parameter name="steps"      > 10   </parameter>
     <parameter name="subSteps"   > 3    </parameter>
     <parameter name="timestep"   > 0.3  </parameter>
     <parameter name="useDrift"   > yes  </parameter>
     <parameter name="walkers"    > 1    </parameter>
   </qmc>
</simulation>
```

Batched

```
<simulation>
  <project id="vmc_legacy" series="0">
     <parameter name="driver_version">
        batched
     </parameter>
  </project>
  <qmcsystem>
     <simulationcell> ... </simulationcell>
     <particleset name="e"> ... </particleset>
     <particleset name="ion0"> ... </particleset>
     <wavefunction name=”psi0”> ... </wavefunction>
     <hamiltonian name="h0"> ... </hamiltonian>
  </qmcsystem>
  <qmc method="vmc" move="pbyp">
     <parameter name="warmupSteps"> 50   </parameter>
     <parameter name="blocks"     > 800  </parameter>
     <parameter name="steps"      > 10   </parameter>
     <parameter name="subSteps"   > 3    </parameter>
     <parameter name="timestep"   > 0.3  </parameter>
     <parameter name="useDrift"   > yes  </parameter>
   </qmc>
</simulation>
```

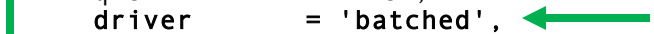
VMC on CPU: Legacy vs Batched Inputs (Nexus)

Legacy

```
qmc = generate_qmcpack(
    identifier   = 'vmc_legacy',
    path         = './',
    job          = qmc_job,
    input_type   = 'basic',
    system       = system,
    pseudos      = ['C.BFD.xml'],
    orbitals_h5  = './diamond.orbitals.h5',
    jastrows     = './diamond.jastrow.xml',
    corrections  = [],
    qmc          = 'vmc',
    warmupsteps  =  50,
    blocks       = 800,
    steps        =  10,
    substeps     =   3,
    timestep     = 0.3,
    usedrift     = True,
    )
```

Batched

```
qmc = generate_qmcpack(
    identifier   = 'vmc_batched',
    path         = './',
    job          = qmc_job,
    input_type   = 'basic',
    system       = system,
    pseudos      = ['C.BFD.xml'],
    orbitals_h5  = './diamond.orbitals.h5',
    jastrows     = './diamond.jastrow.xml',
    corrections  = [],
    qmc          = 'vmc',
    driver       = 'batched',
    warmupsteps  =  50,
    blocks       = 800,
    steps        =  10,
    substeps     =   3,
    timestep     = 0.3,
    usedrift     = True,
    )
```



Variance Optimization

OPT-VMIN on CPU: Legacy vs Batched (QMCPACK)

Legacy

```
<simulation>
  <project id="vmc_legacy" series="0">
    <parameter name="driver_version">
       legacy
    </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
  <loop max="6">
    <qmc method="linear" move="pbyp" checkpoint="-1">
      <cost name="energy"              > 0.0 </cost>
      <cost name="unreweightedvariance"> 1.0 </cost>
      <cost name="reweightedvariance"  > 0.0 </cost>
      <parameter name="warmupSteps"         > 300     </parameter>
      <parameter name="blocks"              > 100     </parameter>
      <parameter name="steps"               > 1       </parameter>
      <parameter name="subSteps"            > 10      </parameter>
      <parameter name="timestep"            > 0.3     </parameter>
      <parameter name="useDrift"            > no      </parameter>
      <parameter name="samples"             > 51200   </parameter>
      <parameter name="MinMethod"           > quartic </parameter>
      <parameter name="minwalkers"          > 0.3     </parameter>
      <parameter name="nonlocalpp"          > yes     </parameter>
      <parameter name="use_nonlocalpp_deriv"> yes     </parameter>
      <parameter name="useBuffer"           > yes     </parameter>
      <parameter name="alloweddifference"   > 0.0001  </parameter>
      <parameter name="exp0"                > -6      </parameter>
      <parameter name="bigchange"           > 10.0    </parameter>
      <parameter name="stepsize"            > 0.15    </parameter>
      <parameter name="nstabilizers"        > 1       </parameter>
    </qmc>
  </loop>
</simulation>
```

Batched

```
<simulation>
  <project id="vmc_batched" series="0">
     <parameter name="driver_version">
        batched
     </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
 <loop max="6">
    <qmc method="linear" move="pbyp" checkpoint="-1">
      <cost name="energy"              > 0.0 </cost>
      <cost name="unreweightedvariance"> 1.0 </cost>
      <cost name="reweightedvariance"  > 0.0 </cost>
      <parameter name="warmupSteps"         > 300     </parameter>
      <parameter name="blocks"              > 200     </parameter>
      <parameter name="steps"               > 22      </parameter>
      <parameter name="subSteps"            > 10      </parameter>
      <parameter name="timestep"            > 0.3     </parameter>
      <parameter name="useDrift"            > no      </parameter>
      <parameter name="MinMethod"           > quartic </parameter>
      <parameter name="minwalkers"          > 0.3     </parameter>
      <parameter name="nonlocalpp"          > yes     </parameter>
      <parameter name="use_nonlocalpp_deriv"> yes     </parameter>
      <parameter name="useBuffer"           > yes     </parameter>
      <parameter name="alloweddifference"   > 0.0001  </parameter>
      <parameter name="exp0"                > -6      </parameter>
      <parameter name="bigchange"           > 10.0    </parameter>
      <parameter name="stepsize"            > 0.15    </parameter>
      <parameter name="nstabilizers"        > 1       </parameter>
    </qmc>
  </loop>
</simulation>
```

samples = #mpi*#threads*blocks*steps

OPT-VMIN on CPU: Legacy vs Batched Inputs (Nexus)

Legacy

```
opt = generate_qmcpack(
    identifier   = 'opt_vmin_legacy',
    path         = './',
    job          = qmc_job,
    input_type   = 'basic',
    system       = system,
    pseudos      = ['C.BFD.xml'],
    orbitals_h5  = './diamond.orbitals.h5',
    corrections  = [],
    J2           = True,
    qmc          = 'opt',
    cycles       = 6,
    samples      = 51200,
    )
```

Batched

```
samples    = 51200
proc_elems = qmc_job.processes*qmc_job.threads
blocks     = 200
steps      = int(round(samples/(blocks*proc_elems)+.5))

opt = generate_qmcpack(
    identifier   = 'opt_vmin_batched',
    path         = './',
    job          = qmc_job,
    input_type   = 'basic',
    system       = system,
    pseudos      = ['C.BFD.xml'],
    orbitals_h5  = './diamond.orbitals.h5',
    J2           = True,
    corrections  = [],
    qmc          = 'opt',
    driver       = 'batched',
    cycles       = 6,
    blocks       = blocks,
    steps        = steps,
    )
```

Energy Optimization

OPT-EMIN on CPU: Legacy vs Batched (QMCPACK)

Legacy

```
<simulation>
  <project id="vmc_legacy" series="0">
    <parameter name="driver_version">
       legacy
    </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
  <loop max="3">
    <qmc method="linear" move="pbyp" checkpoint="-1">
      <parameter name="warmupSteps"          > 300          </parameter>
      <parameter name="blocks"               > 100          </parameter>
      <parameter name="steps"                > 1            </parameter>
      <parameter name="subSteps"             > 10           </parameter>
      <parameter name="timestep"             > 0.3          </parameter>
      <parameter name="useDrift"             > no           </parameter>
      <parameter name="samples"              > 51200        </parameter>
      <parameter name="MinMethod"            > OneShiftOnly </parameter>
      <parameter name="minwalkers"           > 0.0001       </parameter>
      <parameter name="nonlocalpp"           > yes          </parameter>
      <parameter name="use_nonlocalpp_deriv"> yes          </parameter>
    </qmc>
  </loop>
  <loop max="6">
    <qmc method="linear" move="pbyp" checkpoint="-1">
      <parameter name="warmupSteps"          > 300          </parameter>
      <parameter name="blocks"               > 100          </parameter>
      <parameter name="steps"                > 1            </parameter>
      <parameter name="subSteps"             > 10           </parameter>
      <parameter name="timestep"             > 0.3          </parameter>
      <parameter name="useDrift"             > no           </parameter>
      <parameter name="samples"              > 51200        </parameter>
      <parameter name="MinMethod"            > OneShiftOnly </parameter>
      <parameter name="minwalkers"           > 0.5          </parameter>
      <parameter name="nonlocalpp"           > yes          </parameter>
      <parameter name="use_nonlocalpp_deriv"> yes          </parameter>
    </qmc>
  </loop>
</simulation>
```

Batched

```
<simulation>
  <project id="vmc_batched" series="0">
     <parameter name="driver_version">
        batched
     </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
  <loop max="3">
    <qmc method="linear" move="pbyp" checkpoint="-1">
      <parameter name="warmupSteps"          > 300          </parameter>
      <parameter name="blocks"               > 200          </parameter>
      <parameter name="steps"                > 22           </parameter>
      <parameter name="subSteps"             > 10           </parameter>
      <parameter name="timestep"             > 0.3          </parameter>
      <parameter name="useDrift"             > no           </parameter>
      <parameter name="MinMethod"            > OneShiftOnly </parameter>
      <parameter name="minwalkers"           > 0.0001       </parameter>
      <parameter name="nonlocalpp"           > yes          </parameter>
      <parameter name="use_nonlocalpp_deriv"> yes          </parameter>
    </qmc>
  </loop>
  <loop max="6">
    <qmc method="linear" move="pbyp" checkpoint="-1">
      <parameter name="warmupSteps"          > 300          </parameter>
      <parameter name="blocks"               > 200          </parameter>
      <parameter name="steps"                > 22           </parameter>
      <parameter name="subSteps"             > 10           </parameter>
      <parameter name="timestep"             > 0.3          </parameter>
      <parameter name="useDrift"             > no           </parameter>
      <parameter name="MinMethod"            > OneShiftOnly </parameter>
      <parameter name="minwalkers"           > 0.5          </parameter>
      <parameter name="nonlocalpp"           > yes          </parameter>
      <parameter name="use_nonlocalpp_deriv"> yes          </parameter>
    </qmc>
  </loop>
</simulation>
```

OPT-EMIN on CPU: Legacy vs Batched Inputs (Nexus)

Legacy

```
opt = generate_qmcpack(
    identifier   = 'opt_emin_legacy',
    path         = './',
    job          = qmc_job,
    input_type   = 'basic',
    system       = system,
    pseudos      = ['C.BFD.xml'],
    orbitals_h5  = './diamond.orbitals.h5',
    J2           = True,
    corrections  = [],
    qmc          = 'opt',
    minmethod    = 'oneshift',
    var_cycles   = 3,
    cycles       = 6,
    samples      = 51200,
    )
```

Batched

```
samples    = 51200
proc_elems = qmc_job.processes*qmc_job.threads
blocks     = 200
steps      = int(round(samples/(blocks*proc_elems)+.5))

opt = generate_qmcpack(
    identifier   = 'opt_emin_batched',
    path         = './',
    job          = qmc_job,
    input_type   = 'basic',
    system       = system,
    pseudos      = ['C.BFD.xml'],
    orbitals_h5  = './diamond.orbitals.h5',
    J2           = True,
    corrections  = [],
    qmc          = 'opt',
    driver       = 'batched',
    minmethod    = 'oneshift',
    var_cycles   = 3,
    cycles       = 6,
    blocks       = blocks,
    steps        = steps,
    )
```

Diffusion Monte Carlo

DMC on CPU: Legacy vs Batched Inputs (QMCPACK)

Legacy

```
<simulation>
  <project id="dmc_legacy" series="0">
     <parameter name="driver_version">
        legacy
     </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
  <qmc method="vmc" move="pbyp" checkpoint="-1">
     <parameter name="walkers"      > 1    </parameter>
     <parameter name="warmupSteps"  > 50   </parameter>
     <parameter name="blocks"       > 100  </parameter>
     <parameter name="steps"        > 5    </parameter>
     <parameter name="subSteps"     > 3    </parameter>
     <parameter name="timestep"     > 0.3  </parameter>
     <parameter name="useDrift"     > yes  </parameter>
     <parameter name="samples"      > 1024 </parameter>
  </qmc>
  <qmc method="dmc" move="pbyp" checkpoint="-1">
     <parameter name="warmupSteps"  > 20   </parameter>
     <parameter name="blocks"       > 20   </parameter>
     <parameter name="steps"        > 5    </parameter>
     <parameter name="timestep"     > 0.02 </parameter>
     <parameter name="nonlocalmoves"> yes  </parameter>
  </qmc>
  <qmc method="dmc" move="pbyp" checkpoint="-1">
     <parameter name="warmupSteps"  > 20   </parameter>
     <parameter name="blocks"       > 200  </parameter>
     <parameter name="steps"        > 10   </parameter>
     <parameter name="timestep"     > 0.01 </parameter>
     <parameter name="nonlocalmoves"> yes  </parameter>
  </qmc>
</simulation>
```

Batched

```
<simulation>
  <project id="dmc_batched" series="0">
     <parameter name="driver_version">
        batched
     </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
  <qmc method="vmc" move="pbyp">
     <parameter name="total_walkers"> 1024 </parameter>
     <parameter name="warmupSteps"  > 50   </parameter>
     <parameter name="blocks"       > 100  </parameter>
     <parameter name="steps"        > 5    </parameter>
     <parameter name="subSteps"     > 3    </parameter>
     <parameter name="timestep"     > 0.3  </parameter>
     <parameter name="useDrift"     > yes  </parameter>
  </qmc>
  <qmc method="dmc" move="pbyp">
     <parameter name="total_walkers"> 1024 </parameter>
     <parameter name="warmupSteps"  > 20   </parameter>
     <parameter name="blocks"       > 20   </parameter>
     <parameter name="steps"        > 5    </parameter>
     <parameter name="timestep"     > 0.02 </parameter>
     <parameter name="nonlocalmoves"> yes  </parameter>
  </qmc>
  <qmc method="dmc" move="pbyp">
     <parameter name="total_walkers"> 1024 </parameter>
     <parameter name="warmupSteps"  > 20   </parameter>
     <parameter name="blocks"       > 200  </parameter>
     <parameter name="steps"        > 10   </parameter>
     <parameter name="timestep"     > 0.01 </parameter>
     <parameter name="nonlocalmoves"> yes  </parameter>
  </qmc>
</simulation>
```

DMC on CPU: Legacy vs Batched Inputs (Nexus)

Legacy

```
qmc = generate_qmcpack(
    identifier        = 'dmc_legacy',
    path              = './',
    job               = qmc_job,
    input_type        = 'basic',
    system            = system,
    pseudos           = ['C.BFD.xml'],
    orbitals_h5       = './diamond.orbitals.h5',
    jastrows          = './diamond.jastrow.xml',
    corrections       = [],
    qmc               = 'dmc',
    # vmc
    vmc_warmupsteps   =  50,
    vmc_blocks        = 100,
    vmc_steps         =   5,
    vmc_substeps      =   3,
    vmc_timestep      = 0.3,
    vmc_usedrift      = True,
    vmc_samples       = 1024,
    # dmc equilibration
    eq_dmc            = True,
    eq_warmupsteps    = 20,
    eq_blocks         = 20,
    eq_steps          =  5,
    eq_timestep       = 0.02,
    # main dmc
    warmupsteps       = 20,
    blocks            = 200,
    steps             =  10,
    timestep          = 0.01,
    nonlocalmoves     = True,
    )
```

Batched

```
qmc = generate_qmcpack(
    identifier        = 'dmc_batched',
    path              = './',
    job               = qmc_job,
    input_type        = 'basic',
    system            = system,
    pseudos           = ['C.BFD.xml'],
    orbitals_h5       = './diamond.orbitals.h5',
    jastrows          = './diamond.jastrow.xml',
    corrections       = [],
    qmc               = 'dmc',
    driver            = 'batched',
    # vmc
    vmc_warmupsteps   =  50,
    vmc_blocks        = 100,
    vmc_steps         =   5,
    vmc_substeps      =   3,
    vmc_timestep      = 0.3,
    vmc_usedrift      = True,
    # dmc equilibration
    eq_dmc            = True,
    eq_warmupsteps    = 20,
    eq_blocks         = 20,
    eq_steps          =  5,
    eq_timestep       = 0.02,
    # main dmc
    total_walkers     = 1024,
    warmupsteps       = 20,
    blocks            = 200,
    steps             =  10,
    timestep          = 0.01,
    nonlocalmoves     = True,
    )
```

Physical Observables

DMC+Obs. on CPU: Legacy vs Batched (QMCPACK)

Legacy

```
<simulation>
  <project id="dmc_est_legacy" series="0">
     <parameter name="driver_version">
        legacy
     </parameter>
  </project>
  <qmcsystem>
    <simulationcell> ... </simulationcell>
    <particleset name="e"> ... </particleset>
    <particleset name="ion0"> ... </particleset>
    <wavefunction name="psi0"> ... </wavefunction>
    <hamiltonian name="h0" type="generic" target="e">
      <pairpot type="coulomb" name="ElecElec" .../>
      <pairpot type="coulomb" name="IonIon" .../>
      <pairpot type="pseudo" name="PseudoPot" ...>
        <pseudo elementType="C" href="C.BFD.xml"/>
      </pairpot>
      <pairpot type="MPC" name="MPC" ecut="60.0" physical="no" .../>
      <estimator name="KEcorr" type="chiesa" .../>
      <estimator type="spindensity" name="SpinDensity">
        <parameter name="dr"> 0.3 0.3 0.3 </parameter>
      </estimator>
      <estimator type="momentum" samples="20" kmax="4"/>
      <estimator type="dm1b" name="DensityMatrices">
        <parameter name="energy_matrix"> no           </parameter>
        <parameter name="integrator"   > uniform_grid </parameter>
        <parameter name="points"       > 4            </parameter>
        <parameter name="basis"        > spo_ud spo_dm </parameter>
        <parameter name="evaluator"    > matrix       </parameter>
        <parameter name="center"       > 0 0 0        </parameter>
      </estimator>
    </hamiltonian>
  </qmcsystem>
  <qmc method="vmc" move="pbyp"> ... </qmc>
  <qmc method="dmc" move="pbyp"> ... </qmc>
  <qmc method="dmc" move="pbyp"> ... </qmc>
</simulation>
```

Batched

```
<simulation>
  <project id="dmc_est_batched" series="0">
     <parameter name="driver_version">
        batched
     </parameter>
  </project>
  <qmcsystem>
    <simulationcell> ... </simulationcell>
    <particleset name="e"> ... </particleset>
    <particleset name="ion0"> ... </particleset>
    <wavefunction name="psi0"> ... </wavefunction>
    <hamiltonian name="h0" type="generic" target="e">
      <pairpot type="coulomb" name="ElecElec" .../>
      <pairpot type="coulomb" name="IonIon" .../>
      <pairpot type="pseudo" name="PseudoPot" ...>
        <pseudo elementType="C" href="C.BFD.xml"/>
      </pairpot>
      <pairpot type="MPC" name="MPC" ecut="60.0" physical="no" .../>
    </hamiltonian>
    <estimators>
      <estimator type="spindensity" name="SpinDensity">
        <parameter name="dr"> 0.3 0.3 0.3 </parameter>
      </estimator>
      <estimator type="MomentumDistribution" samples="20" kmax="4"/>
      <estimator type="OneBodyDensityMatrices" name="DensityMatrices">
        <parameter name="energy_matrix"> no           </parameter>
        <parameter name="integrator"   > uniform_grid </parameter>
        <parameter name="points"       > 4            </parameter>
        <parameter name="basis"        > spo_ud spo_dm </parameter>
        <parameter name="evaluator"    > matrix       </parameter>
        <parameter name="center"       > 0 0 0        </parameter>
      </estimator>
    </estimators>
  </qmcsystem>
  <qmc method="vmc" move="pbyp"> ... </qmc>
  <qmc method="dmc" move="pbyp"> ... </qmc>
  <qmc method="dmc" move="pbyp"> ... </qmc>
</simulation>
```

DMC+Obs. on CPU: Legacy vs Batched Inputs (Nexus)

Legacy

```
estimators = [
    spindensity(
        dr          = (0.3,0.3,0.3)
        ),
    momentum(
        kmax        = 4,
        samples     = 20,
        ),
    dm1b(
        basis       = sposet(type='bspline',size=8),
        reuse       = True,
        integrator  = 'uniform_grid',
        points      = 4,
        center      = (0,0,0),
        ),
    ]

qmc = generate_qmcpack(
    identifier        = 'dmc_est_legacy',
    ...
    corrections       = ['mpc','chiesa'],
    estimators        = estimators,
    qmc               = 'dmc',
    # vmc
    ...
    # dmc equilibration
    ...
    # main dmc
    ...
    )
```

Batched

```
estimators = [
    spindensity(
        dr          = (0.3,0.3,0.3)
        ),
    momentumdistribution(
        kmax        = 4,
        samples     = 20,
        ),
    onebodydensitymatrices(
        basis       = sposet(type='bspline',size=8),
        reuse       = True,
        integrator  = 'uniform_grid',
        points      = 4,
        center      = (0,0,0),
        ),
    ]

qmc = generate_qmcpack(
    identifier        = 'dmc_est_batched',
    ...
    corrections       = ['mpc'],
    estimators        = estimators,
    qmc               = 'dmc',
    driver            = 'batched',
    # vmc
    ...
    # dmc equilibration
    ...
    # main dmc
    ...
    )
```

GPU Offload: Memory Limits

VMC on GPU's (Offload): Working within Memory Limits

```
walkers_scan = [   1,   2,   4,   8,  16,  32,
                  64,  96, 128, 180, 256, 300,
                 360, 436, 512, 600, 720, 864,
                1024,1216,1440]

qmc = generate_qmcpack(
    identifier       = 'vmc_offload_scan',
    path             = './',
    job              = qmc_job,
    input_type       = 'basic',
    system           = system,
    pseudos          = ['C.BFD.xml'],
    orbitals_h5      = './diamond.orbitals.h5',
    jastrows         = './diamond.jastrow.xml',
    corrections      = [],
    driver           = 'batched',
    delay_rank       = 4,
    det_batch        = True,
    calculations     = [
        vmc(walkers_per_rank = walkers_per_rank,
            warmupsteps      = 3,
            blocks           = 3,
            steps            = 3,
            substeps         = 3,
            timestep         = 0.3,
            usedrift         = True,
            #crowds           = , # integer, optional
            ) for walkers_per_rank in walkers_scan
        ]
    )

# next do vmc/dmc in production w/ selected walkers
```

```
<simulation>
  <project id="vmc_legacy" series="0">
     <parameter name="driver_version">
        batched
     </parameter>
  </project>
  <qmcsystem> ... </qmcsystem>
  <qmc method="vmc" move="pbyp">
     <parameter name="walkers_per_rank"> 1   </parameter>
     ...
  </qmc>
  <qmc method="vmc" move="pbyp">
     <parameter name="walkers_per_rank"> 2   </parameter>
     ...
  </qmc>
  <qmc method="vmc" move="pbyp">
     <parameter name="walkers_per_rank"> 4   </parameter>
     ...
  </qmc>
  <qmc method="vmc" move="pbyp">
     <parameter name="walkers_per_rank"> 8   </parameter>
     ...
  </qmc>
  <qmc method="vmc" move="pbyp">
     <parameter name="walkers_per_rank"> 16  </parameter>
     ...
  </qmc>
  ...
</simulation>
```

Questions?