

# QMCPACK Workshop 2023

## Driving the “Batched” QMCPACK Code with Nexus

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[https://github.com/QMCPACK/qmc\\_workshop\\_2023](https://github.com/QMCPACK/qmc_workshop_2023)

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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

QMCPACK / qmcpack\_workshop\_2023

Q Type to search

>

+

<> Code Pull requests Actions Security Insights

Files

main

Go to file

day1\_nexus\_batched

example\_inputs\_outputs

legacy\_nexus\_files

C.BFD.xml

README.md

diamond.jastrow.xml

diamond.orbitals.h5

diamond.poscar

diamond\_dmc\_batched.py

diamond\_dmc\_est\_batched.py

diamond\_opt\_emin\_batched.py

diamond\_opt\_vmin\_batched.py

diamond\_setup.py

diamond\_vmc\_batched.py

diamond\_vmc\_offload\_batche...

Gani\_GCTA.pdf

qmcpack\_workshop\_2023 / day1\_nexus\_batched /

Add file

jtkrogel rename directory 85a685e · 16 minutes ago History

Name	Last commit message	Last commit date
..		
example_inputs_outputs	rename directory	16 minutes ago
legacy_nexus_files	rename directory	16 minutes ago
C.BFD.xml	rename directory	16 minutes ago
README.md	rename directory	16 minutes ago
diamond.jastrow.xml	rename directory	16 minutes ago
diamond.orbitals.h5	rename directory	16 minutes ago
diamond.poscar	rename directory	16 minutes ago
diamond_dmc_batched.py	rename directory	16 minutes ago
diamond_dmc_est_batched.py	rename directory	16 minutes ago
diamond_opt_emin_batched.py	rename directory	16 minutes ago
diamond_opt_vmin_batched.py	rename directory	16 minutes ago

# Example Files on GitHub

qmcpack\_workshop\_2023 / day1\_nexus\_batched / README.md



jtkroger 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](https://github.com/QMCPACK/qmcpack_workshop_2023/day1_nexus_batched)

## Git Clone or Download

git clone [https://github.com/QMCPACK/qmcpack\\_workshop\\_2023.git](https://github.com/QMCPACK/qmcpack_workshop_2023.git)

wget [https://github.com/QMCPACK/qmcpack\\_workshop\\_2023/archive/refs/heads/main.zip](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](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/qmcpack_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="aloweddifference" > 0.0001 </parameter>
      <parameter name="exp0" > -6 </parameter>
      <parameter name="bigchange" > 10.0 </parameter>
      <parameter name="stepsize" > 0.15 </parameter>
      <parameter name="nstablizers" > 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="allowedifference" > 0.0001 </parameter>
      <parameter name="exp0" > -6 </parameter>
      <parameter name="bigchange" > 10.0 </parameter>
      <parameter name="stepsize" > 0.15 </parameter>
      <parameter name="nstablizers" > 1 </parameter>
    </qmc>
  </loop>
</simulation>
```

$$\text{samples} = \text{\#mpi} * \text{\#threads} * \text{blocks} * \text{steps}$$

# 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>
  </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>
  </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>
  </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>
  </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="pby" 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="pby" 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="pby" 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="pby">
    <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="pby">
    <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="pby">
    <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>
  <qmc system> ... </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?**