QMCPACK USERS WORKSHOP 2019

Argonne NATIONAL LABORATORY

RUNNING QMCPACK EFFICIENTLY AT LARGE SCALE

QMCPACK

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OUTLINE

- New features
  - Size consistent T-moves
  - Hybrid orbital representation

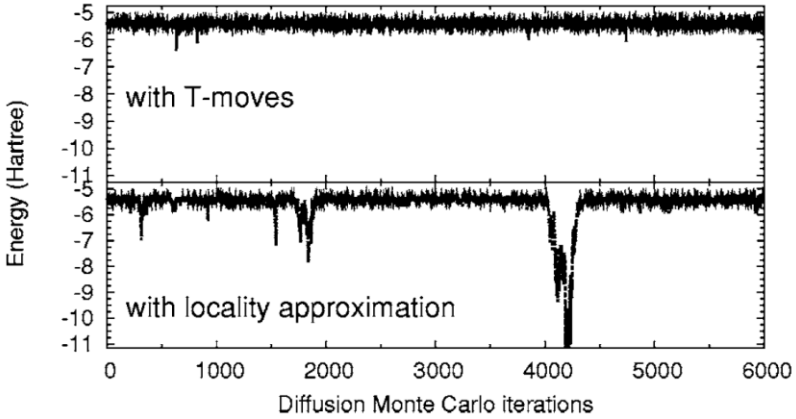
- Performance improvement
  - SoA transformation
  - Efficient walker data movement
  - Delayed update algorithm
  - Nested OpenMP threading
  - Thread affinity tool

NEW FEATURES

SIZE CONSISTENT T-MOVES

Needed for pseudopotential

- More stable DMC calculation
- Recover variational principle
- In DMC input section, nonlocalmoves=no, yes(v0), v1, v3
  - no, locality approximation
  - yes/v0 based on PRB 2006, not size consistent
  - v1, based on JCP 2010, size consistent. v2, not implemented
  - v3, an approximation v1, same accuracy with both light and heavy element.

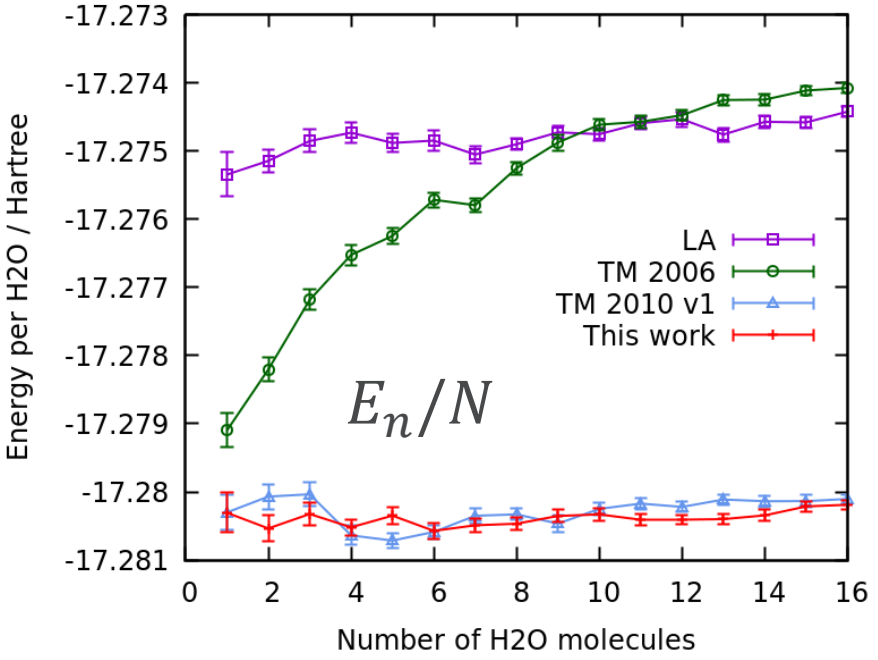


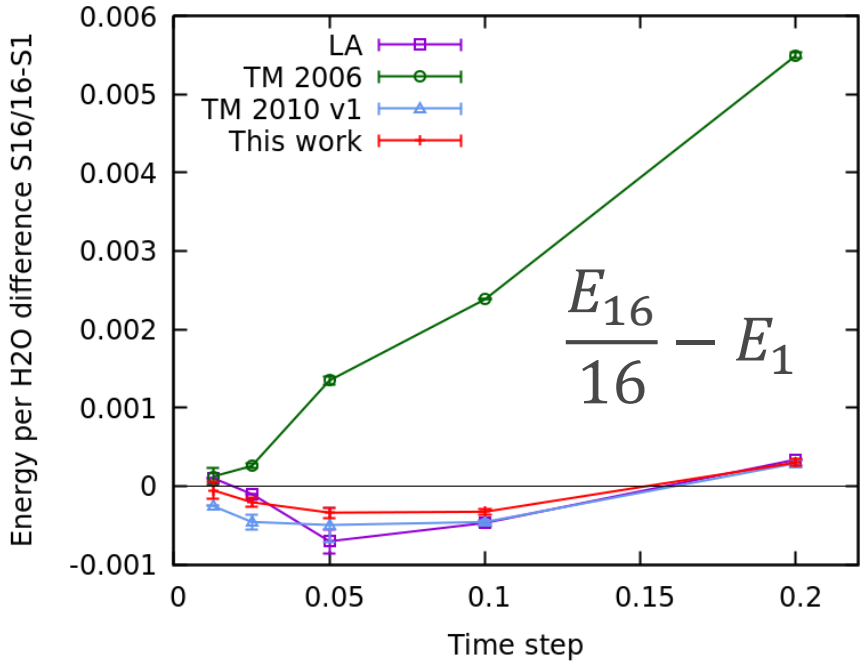
M. Casula, Phys.Rev.B 74, 161102(R) 2006
M. Casula et al, J.Chem.Phys. 132, 154113 (2010)

Computational cost no <= v0 < v3 << v1

SIZE CONSISTENT T-MOVES

Consistent energy per H2O molecule as the number increases

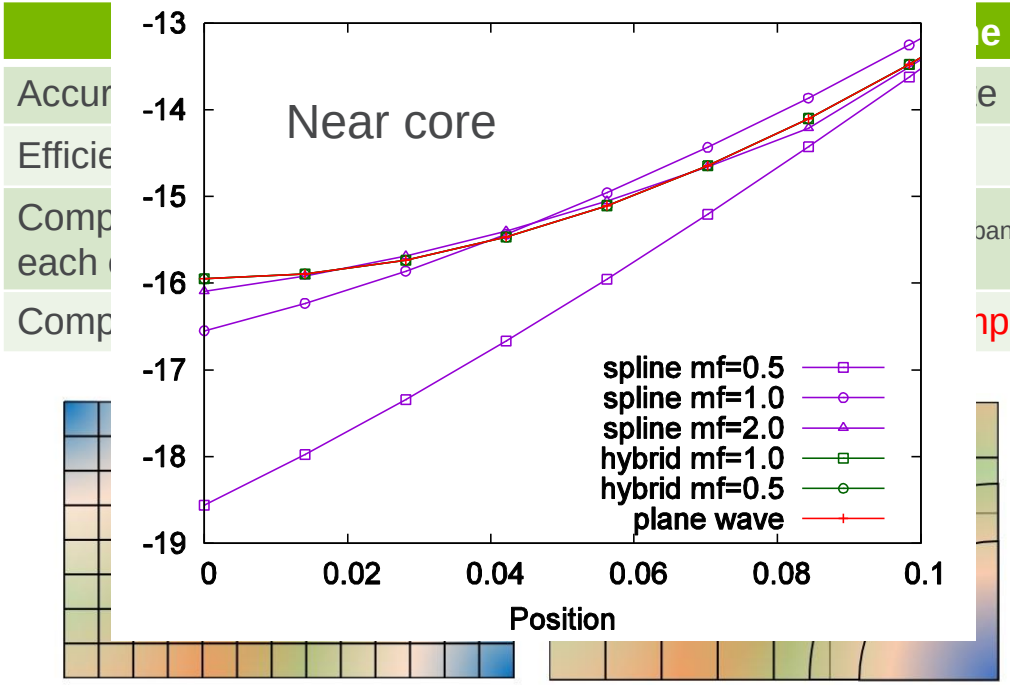




HYBRID ORBITAL REPRESENTATION

Retain high accuracy with much less memory

- Regular 3d cubic spline orbitals compute fast at the cost of large memory footprint.
- High bandwidth memory has limited capacity on modern architectures
- Atomic orbital in A, regular spline in C. Buffer region in B.
- The new way gives high accuracy with much less memory needed



HYBRID ORBITAL REPRESENTATION

Easy to use design

- AO conversion is parallelized inside QMCPACK
- A few input control needed
- Use nexus for parameter scan

```
<determinantset type="bspline" source="i"
   href="pwscf.h5"
   tilematrix="1 1 3 1 2 -1 -2 1 0"
   twistnum="-1" gpu="yes"
   meshfactor="0.8" twist="0 0 0"
   precision="single" hybridrep="yes"
   smoothing_scheme="Consistent"
   smoothing_function="LEKS2018">
   ...
</determinantset>
```

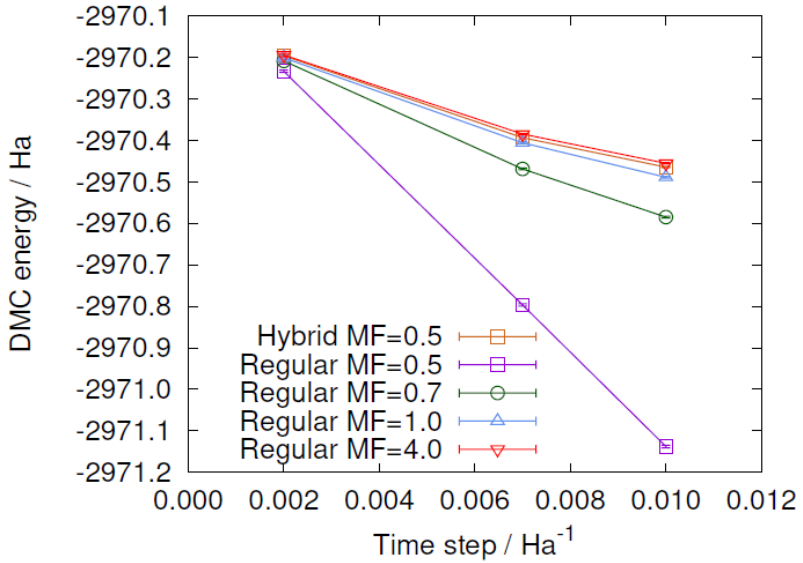
Per specie

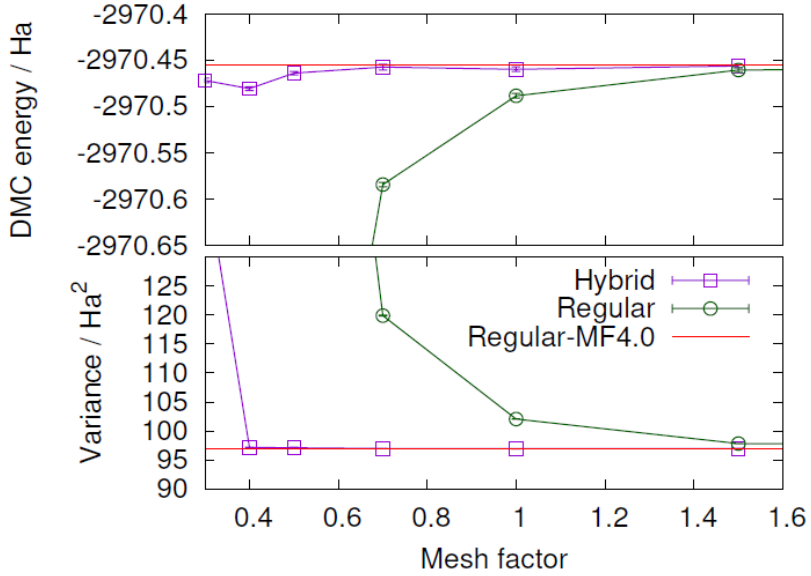
```
<group name="Ni">
   <parameter name="charge">         18 </parameter>
   <parameter name="valence">        18 </parameter>
   <parameter name="atomicnumber" > 28
</parameter>
   <parameter name="cutoff_radius" > 1.6
</parameter>
   <parameter name="inner_cutoff" >  1.3 </parameter>
   <parameter name="lmax" >          5 </parameter>
   <parameter name="spline_radius" > 1.8
</parameter>
   <parameter name="spline_npoints">  91
</parameter>
</group>
```

Red required, Blue optional

HYBRID ORBITAL REPRESENTATION

High accuracy NiO calculation with MF=0.5





8X memory saving

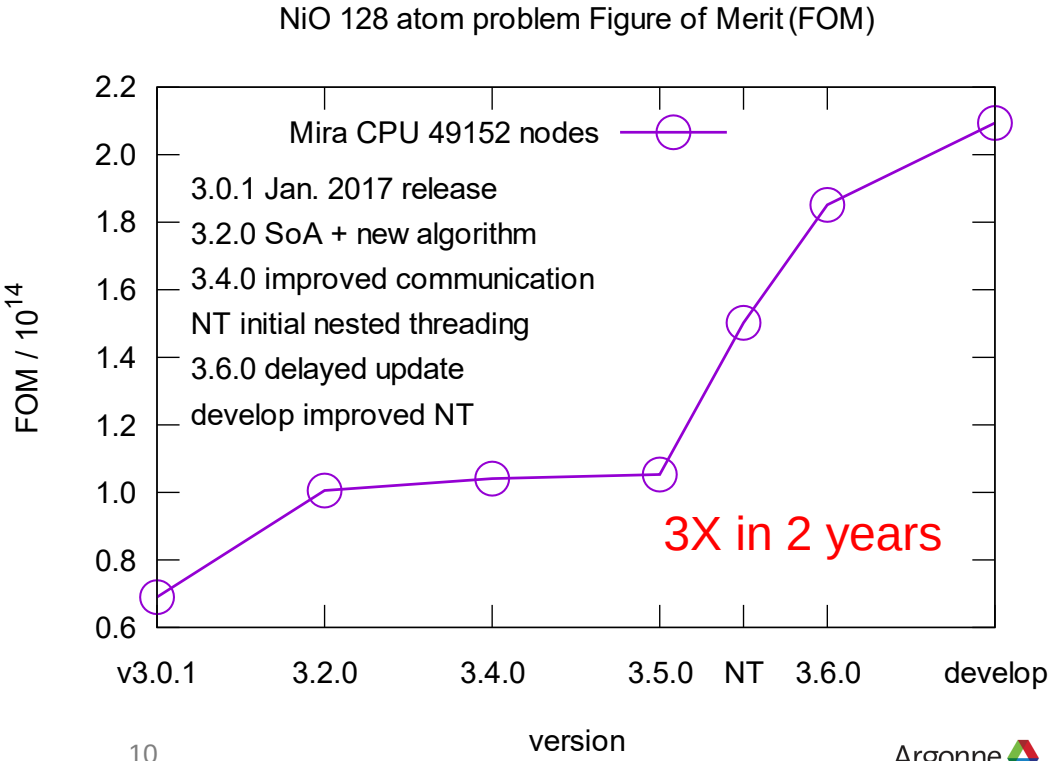
YL et al, J.Chem.Phys. 149, 034108 (2018)

PERFORMANCE IMPROVEMENTS

DRAMATIC IMPROVEMENT ON THE CPU

New parallelization and new algorithms

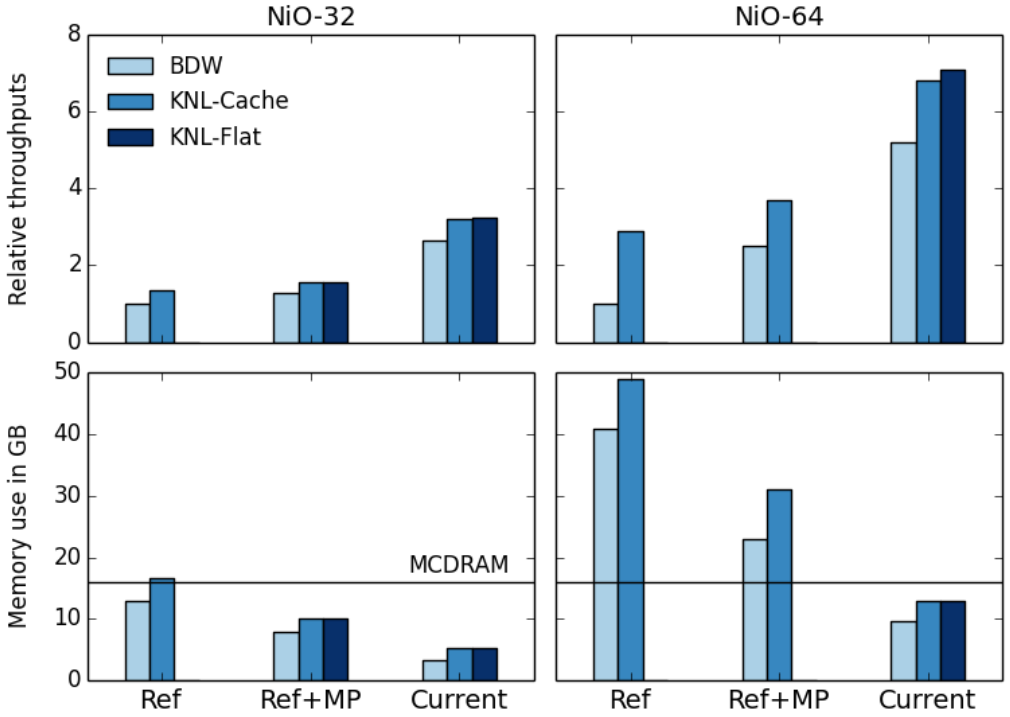
- Mixed precision support on CPU
- All the changes we did are portable to all the CPU architectures. Intel, AMD, IBM, ARM
- Xeon and Xeon Phi has much higher speed-up than 3x



Structure of Array (SoA) transformation

Compile time selection

- Introduced in v3.2 and turned on by default in v3.7
- Leverage CPU SIMD hardware using OpenMP 4.0 SIMD
- Jastrow e-e N^2 memory, Jastrow e-e-I N^3 memory down to N memory
- Jastrow computational cost reduces to a very small fraction



A. Mathuriya, YL et al. pp 38 SC17

EFFICIENT WALKER DATA MOVEMENT

Turn on by default since v3.4

- Keep a memory pool for each walker for the wavefunction data
- Wavefunction objects reference the pools without copying data

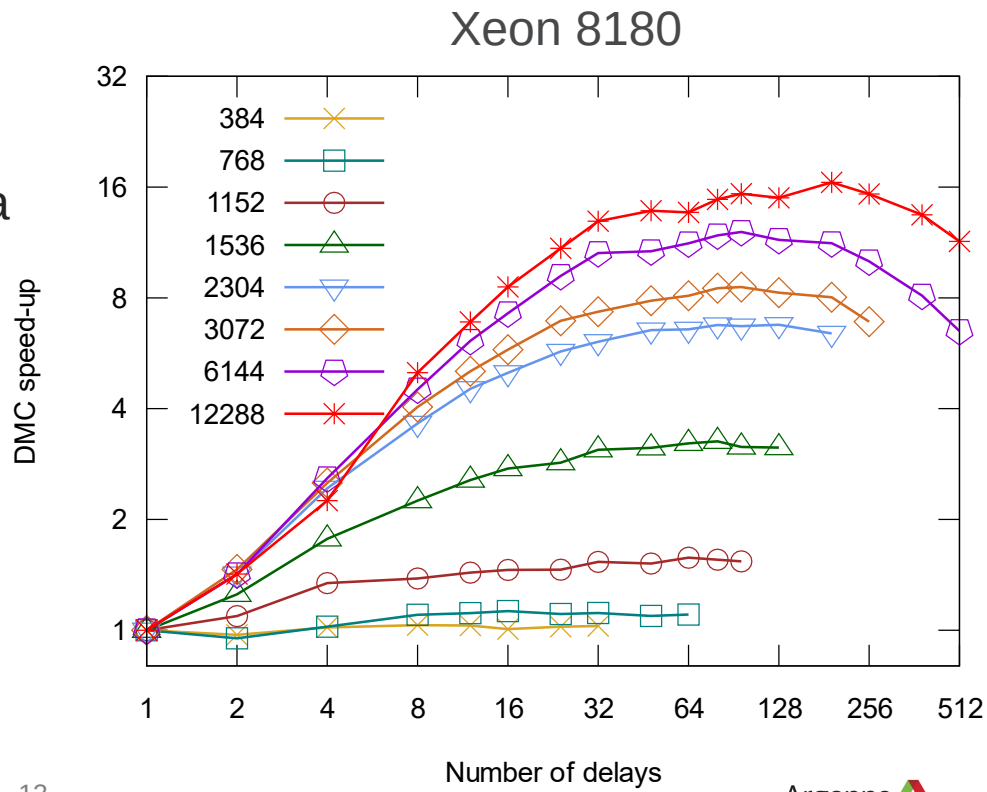
- Walker exchanging within a MPI rank copies memory directly
- Walker exchanging between MPI ranks uses non blocking send/recv pools without packing and unpacking

- 2x speed up on full machine runs on OLCF Titan.

DELAYED UPDATE ALGORITHM

Added since v3.6

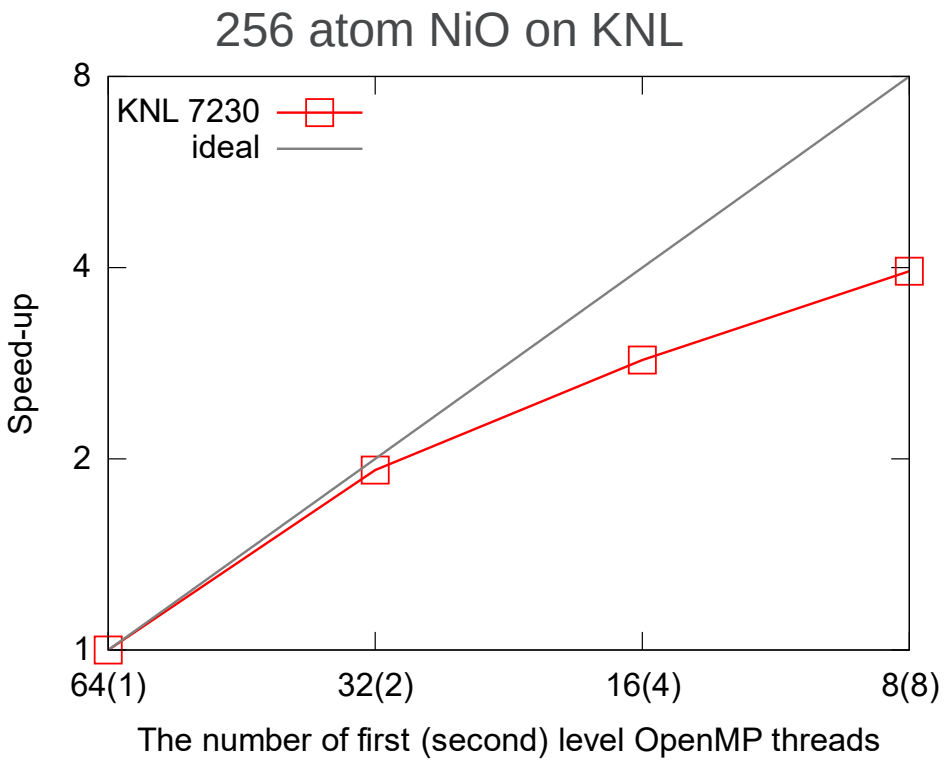
- Change Sherman-Morrison rank-1 update to delayed update using Sherman-Morrison-Woodbury formula
- Matters more on large problem sizes
- <slaterdeterminant delay_rank="32">
- Try starting from 32, the best choice depends on the system and QMC methods.



NESTED OPENMP THREADING

Go beyond 1 core per walker

- The computation of a walker is further accelerated by putting more than 1 core.
- Using two level OpenMP threading
- The speed-up of walkers evolving in one step, $1/t$



THREAD AFFINITY IS IMPORTANT

We provide a tool

- Use qmc-check-affinity to check if the threads are bind to the right cores
- Core ID order is vendor specific. Always check this on a new machine
- Nested OpenMP needs more nobs to control. It is similar to other MPI+OpenMP programs.
- Use one MPI rank per NUMA(socket) if memory allows.

OMP_NESTED=true OMP_PLACES=threads
OMP_PROC_BIND=spread,close OMP_NUM_THREADS=4,4
mpirun -np 1 ./bin/qmc-check-affinity
OpenMP enables 4 1st level threads, and 4 2nd level threads.

MPI rank 0 L1 tid 0 L2 tid 0 is placed on Core ID 0
MPI rank 0 L1 tid 0 L2 tid 1 is placed on Core ID 1
MPI rank 0 L1 tid 0 L2 tid 2 is placed on Core ID 2
MPI rank 0 L1 tid 0 L2 tid 3 is placed on Core ID 3
…
MPI rank 0 L1 tid 3 L2 tid 0 is placed on Core ID 12
MPI rank 0 L1 tid 3 L2 tid 1 is placed on Core ID 13
MPI rank 0 L1 tid 3 L2 tid 2 is placed on Core ID 14
MPI rank 0 L1 tid 3 L2 tid 3 is placed on Core ID 15

BATCHED NLPP EVALUATION

- Target batched nonlocal pseudo potential evaluation for hardware efficiency.
- Input example
  - <pairpot name="PseudoPot" type="pseudo" source="i" wavefunction="psi0" format="xml" algorithm="batched">
- Useful for hybrid orbital representation, nest threading.

MISC

- New QE releases with pw2qmcpack
  - https://github.com/ye-luo/q-e/releases

FUTURE DEVELOPMENT

- One code path with complete features for CPU and GPU.
  - New scheme has been prototyped.
  - Algorithm changes on QMCPACK facilitate this
  - Goal: efficient execution for small, medium and large problems.
- More observables.

Q&A