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PERFORMANCE PORTABLE DESIGN
QMCPACK

In a nutshell

- QMCPACK, is a modern high-performance open-source Quantum Monte Carlo (QMC) simulation code for electronic structure calculations of molecular, quasi-2D and solid-state systems.
- The code is C/C++ and adopts MPI+X(OpenMP/CUDA)
- Monte Carlo: massive Markov chains (walkers) evolving in parallel. 1st level concurrency.
- Quantum: The computation in each walker can be heavy when solving many body systems (electrons). 2nd level concurrency.
MAPPING CONCURRENCY TO PARALLELISM

Monte Carlo can be a challenge for parallelism

- Walkers $N_w$ are not data parallel but task parallel
  - Workload per electron move depends on accept/reject. GPU
  - Workload per step moving all the electrons is roughly equal. CPU

- Electrons are data parallel
  - Kernels are $O(N_e^{2-3})$ per sample. Large $N_e$ CPU. Small $N_e$ GPU.
  - Naturally, $N_e$ vector computation utilizing SIMD and SIMT. CPU/GPU

- Simulations need $N_e$ from 10 to 10000 depending on the scientific questions
  - Use $N_w$ and $N_e$ to balance compute node efficiency and time-to-solution.
  - Need a tailored approach for performance portability beyond programming models.
MAPPING CONCURRENCY TO PARALLELISM

Need a flexible scheme at high level for all sizes of Nw and Ne

- Our CPU/GPU portability experience since 2010
  - Walker batching saves GPU kernel overhead in small problems.
  - Lock-step algorithm has performance penalty with large problem sizes.
  - Incompatible internal APIs and diverged code paths without fallback for missing features.
    - CPU QMC drivers have no walker batching
    - Legacy CUDA QMC drivers are very bad with large problem sizes

- Requirement for performance portable code
  - Feature complete
  - Computationally intensive pieces accelerated and selected at run time
  - Single source is desired but architectural specialization is possible and only allowed at the bottom level.
  - Not restricted to a particular programming model at high abstraction level
MAPPING CONCURRENCY TO PARALLELISM

Design unified QMC driver design for flexible dispatching

- The walker population with a node is subdivided into crowds.
  - Legacy CPU drivers have crowd size 1.
  - Legacy CUDA drivers have 1 crowd.

- Walkers within a crowd evolve in lock step at every single electron move. Data parallelism.

- Walkers between crowds are not synchronized until all the single electron moves are completed within a step. Task parallelism.

- Lower levels have both batched and non-batched APIs. Fallback is by default and can be specialized.
PERFORMANCE PORTABLE IMPLEMENTATION
MAPPING CONCURRENCY TO PARALLELISM

Threads and streams

- Crowds are mapped to CPU threads.  
  - No idle. Nested threads are optional.
- Crowds leverage GPU streams/queues explicitly or implicitly.
- Desynchronized crowds keep the computing device busy.

Time evolution

Crowd 0

Crowd 1

Unified batched QMC driver execution on an accelerator

MiniQMC concurrent crowds
IBM XL OpenMP runtime
IMPLEMENTATION STRATEGY

The current status

- Spline single particle orbital evaluations are implemented using OpenMP target offload
- Slater determinant updates are implemented using cuBLAS/cuSolver.
- Both batched and non-batched code path are specialized for maximal performance.
- Non-local pseudopotential evaluation supports additional batching for quadrature points evaluation.
- Jastrow factors and distance tables remains on the CPU for the moment.
PERFORMANCE PORTABILITY WITH OPENMP

A touch journey in 2019

- 2019 PPP meeting, IBM XL C/C++ compiler is the only working compiler for QMCPACK

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Cray 9.1 inherits Clang 9 math function issues.
PERFORMANCE PORTABILITY WITH OPENMP

A lot of exciting improvements in 2020


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Workaround in cmake
INTERACT WITH COMPILER DEVELOPERS

QMCPACK OpenMP offload works cross platforms

- LLVM and SOLLVE fixed 17/20 bug reports. 4 requested optimization added.
- AOMP fixed 9/14.
- Contribute tests to vendor compiler team via early hardware access program.
- Having our own testing. [https://cdash.qmcpack.org](https://cdash.qmcpack.org)

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PERFORMANCE ON SUMMIT

NiO benchmark at various sizes

- Clang becomes better than XL in overall performance.
- Clang has a more efficient runtime but slower kernels.
- At 512 atom size. New GPU code is way more efficient.
- With optimized code paths, the new GPU implementation reaches at least 50% performance of legacy CUDA code which offloads more to GPU and use async computation.
IMPROVEMENTS NEEDED IN QMCPACK

Keep effort in making the code better

- QMCPACK developers put a large effort on refactoring the existing code and adding a better design. The progress is not easily visible to the outside but fundamentally important to make all things happen. Will keep doing this non-stop.

- Need to further reduce data movement and synchronization. This requires making more computation go asynchronously.

- Use algorithmic innovation to fundamentally solve problems.
IMPROVEMENTS NEEDED OUTSIDE QMCPACK

Software stack missing pieces

- In OpenMP, we need
  - target nowait async support with task dependency.
  - More GPU related 5.0 features implemented.
  - Interoperability with vendor programming models.
  - Vendor compilers more reliable and capable.

- Libraries
  - Need batched BLAS1/2, see online manual and cublas_missing_functions

- Tools
  - OpenMP friendly debugger and profiler.