QMCPACK AND GPU

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Exascale Computing Project: application development

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PRE AND EXASCALE SYSTEMS IN 2022

Need to make the code work on all machines

NERSC Perlmutter

Oak Ridge Frontier

Argonne Polaris

Argonne Aurora

Make QMCPACK run well everywhere
ELECTRONIC STRUCTURE METHODS

QMC can be the new sweet spot

Time scale: picosecond = $10^{-12}$ seconds

Length scale: $10$ nm = $10^{-8}$ meters

accuracy (eV)

quantum chemistry

exact

0.001-0.01

0.05-0.1

0.5+

CI

superconductivity, magnetism

CC

QMC

DFT

TB

cohesion, barriers

chemical bonds

not ab initio

system size (electrons)

50

2,000

10,000

100,000

$N^7$

$N^{3-4}$

$N^{2-3}$

$N^3$
PETASCALE TO EXASCALE CHALLENGE
How large problem can we solve?

What is next?
1. Solve faster and more petascale problems
2. Solve much larger problems

Metal organic framework
153 atoms with 594 electrons, 10 meV total energy.

TiO2 polymorphs
216 atoms with 1536 electrons, 10 meV/f.u.

1k atoms
10k electrons
QMCPACK

- 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. 1\textsuperscript{st} level concurrency. Good for MPI and coarse level threads.

- Quantum: The computation in each walker can be heavy when solving many body systems (electrons). 2\textsuperscript{nd} level concurrency. Good for fine level threads and SIMD.

- Math libraries: BLAS/LAPACK, HDF5, FFTW
DIFFUSION MONTE CARLO SCHEMATICS

Old configurations  Random walking  Possible new configurations

Population

Walker

Load balancing communication

Possible new configurations

New configurations

w=0.8

w=1.6

w=2.4

w=0.3
PARALLELIZATION AND GPU PORTING
WALKER BASED PARALLELISM

Works extreme well on petascale supercomputers

▪ Weak scaling efficiency 99% on 2/3 Mira and 95% on almost full Titan.
▪ Weak scaling, fix work per node. Strong scaling, fix the total number of samples.
▪ Equilibration excluded.
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
  - Naturally, $N_e$ vector computation utilizing SIMD and SIMT. **CPU/GPU**
  - Kernels are $O(N_e^{2-3})$ per sample. Large $N_e$ **CPU**. Small $N_e$ **GPU**.

- Need a tailored approach for performance portability beyond programming models.

OPENMP OFFLOAD GPU IMPLEMENTATION

A bit more software technology to handle GPUs

▪ Use portable OpenMP target feature
  – Portable on NVIDIA, AMD, Intel GPUs. Fallback on CPU as well.
  – Multiple compilers. GNU, Clang, AOMP, NVHPC, OneAPI

▪ Multiple CPU threads to launch kernels to GPUs
  – Maximize GPU utilization. Overlapping compute and transfer by OpenMP.

▪ Specialized in CUDA/HIP to call NVIDIA/AMD/INTEL accelerated libraries.
  – cuBLAS/cuSolver, hipBLAS/hipSolver, MKL

▪ C++ templates to cover real/complex and full/mixed precision cases.
  – We use C++17 to keep our code concise.
Performance on Summit

- Porting starts in 2019.
- Steady performance improvements 3.10 to 3.14 (dev)
- Close or exceed CUDA performance
- There are still room to improve the performance.
- Passes tests, very usable in production
**V100 VS A100**

- GPU acceleration is significant
- The larger HBM helps throughput. Very similar to ML.
- A100 is almost 3X when running 256 atom problem.
- 16 GB is the bottleneck on V100
LESSONS LEARNED SO FAR

What is needed for a performance portable code

- Understand how to make CPU and GPU work efficiently
- Analyze the compute pattern and map the existing concurrency to proper parallelism given by the hardware
- OpenMP + vendor libraries strategy works
  - ~100 CUDA kernels down to ~10 CUDA kernels + ~10 offload regions
  - Very maintainable code with decent performance
MY OPINION ABOUT GPU PORTING
DATA MOVEMENT IS THE KEY OF PORTING

- Data locality is the top priority
  - Interconnect is slower than memory. We write performant MPI code
  - Memory is slower than cache. We implement cache friendly algorithms.
  - CPU-GPU bus is slower than GPU memory. We need to first worry about data transfer.

- Avoid any programming model which
  - Ignores the performance difference from host and GPU memory spaces.
  - Doesn’t provide explicit data movement control

- GPU 101 teaches kernel programming. It is not the key.

- Managing data movement requires understanding the whole algorithm and implementation. This needs domain expert knowledge.
MANAGE MORE LEVEL OF PARALLELISM

- At least two level of parallelism
  - CPU has core+SIMD
  - GPU has SM+SIMT lanes
  - In QMCPACK we have CPU threads + two level inside GPU kernel

- Reduction operation plays a key role in scientific computing
  - It is about locality and hierarchy
CUDA LANGUAGE IS NOT THE BEST CHOICE

For scientists

- Must be protected under macro. Macro means more test variants needed.
- Doesn’t run on hosts without GPUs.
  - Running and debugging on host are lot smoother and should catch most user errors
  - Host tooling are richer. Address and thread sanitizers, code coverage.
- Offload models are more appealing: OpenACC/OpenMP
- Restrict it to only serving library calls.
- Scientist needs to spend time on methods, algorithms. Leave the engineers to worry absolute performance.
OPENACC AND OPENMP

Competitors and siblings

- OpenMP has a richer feature set
- OpenACC is more developed for NVIDIA GPUs
- The needed developers’ knowledge is the same for GPU programming
- They are not necessarily interchangeable in syntax.
- Choose one based on your production environment and programming language.
- Keep in mind that compilers are never perfect. They have bugs but be kind to developers. Directive based programming model eases the burden of code developers and shifts that to compiler developers.
- CUDA doesn’t have a reduction!!!!
SUMMARY

- After a careful redesign of QMCPACK, we have new performance portable implementation, and it is the second time of GPU porting.
- OpenMP + vendor library strategy works well on NVIDIA GPUs and we are expanding the list of supported GPUs from different vendors.
- GPU porting is a chance to force designing and implementing better code. Don’t miss the opportunity.