Experiences in Porting XGc to Summit

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presenting for the XGC Team
6/5D Simulations of Plasmas in “Toroidal” Tokamak Geometry

Torus, not a straight cylinder: physics and math become more complicated through spatial inhomogeneity and toroidal mode coupling.

- Simplified geometry approaches have limited applicability.
- Requires ~billion-trillion particles to describe important physics
- Extreme scale simulation

ITER

XGC1 Simulation

Poloidal magnetic flux label
\[ \psi(r) = 1 \text{ at } r/a=1, \ 0 \text{ at } r/a=0 \]
**XGC1 Particle-in-cell Code**

- Gyrokinetic approximation reduces 6D problem to 5D
- XGC1: Gyrokinetic particle-in-cell (PIC) code for modeling plasma in tokamak, especially in edge region and near separatrix
- Unstructured triangular grid aligned to flux surfaces to resolve edge geometry and separatrix, $O(10^6)$ triangles per plane for ITER
- NERSC Exascale Science Applications Program (NESAP) for Cori Phase II (Intel Xeon Phi) and Oak Ridge Center for Accelerated Application Readiness (CAAR) for Summit (Nvidia GPU)
- Performance portability achieved with OpenACC and OpenMP
XGC

- Center for High Fidelity Boundary Plasma Simulation
  https://hbps.pppl.gov/computing/xgc-1

- Mostly F90, Petsc, NTCC Splines, LAPACK, ADIOS for parallel I/O
- Key Kernels: electron push and multi-species collision
- Cuda Fortran in electron push to take advantage of texture cache
- OpenACC version of electron push and multi-species collision
- Separate versions of push kernel for vectorization on Intel KNL
Nonlinear multi-species collision


- Fokker-Planck-Landau collision operator

\[
\frac{\partial f_\alpha}{\partial t} = \sum_\beta C_{\alpha\beta} (f_\alpha, f'_\beta) \quad \text{where} \quad \mathbf{u} = \frac{\mathbf{v} - \mathbf{v}' - \mathbf{u}}{\mathbf{u}^3} \quad \text{and} \quad I = \text{identity tensor}
\]

\[
\frac{\partial}{\partial t} \int f_\alpha \phi d^3v = \sum_\beta \frac{e_\alpha^2 e_\beta^2 \ln \Lambda_{\alpha\beta}}{8\pi\varepsilon_0^2 m_\alpha} \int d^3\phi' \nabla \cdot \mathbf{U} \cdot \left( \frac{f_\alpha}{m_\beta} \nabla f'_\beta - \frac{f'_\beta}{m_\alpha} \nabla f_\alpha \right)
\]

\[
\left\langle \left\langle M_{\text{self/multi}} \right\rangle \right\rangle \equiv \int_0^{2\pi} \int_0^{2\pi} M_{\text{self/multi}} d\theta d\theta' \quad \text{where} \quad M_{\text{self/multi}} = \nabla \phi \cdot \mathbf{U} \cdot \left( \frac{\nabla'}{\nabla} \right) \quad \phi: \text{test function (1:density, v: momentum, v': energy)}
\]
Nonlinear Multi-species Collision Algorithm

- Density functions $f_{a/b}$, M x N velocity grid
- Backward Euler for time integration
- Implicit Picard fixed-point iteration to solve nonlinear equation.
- Finite difference/volume discretization
- Computation matrix coefficients E and D
  $O(M x N)$ complexity for each velocity grid point: $O(M^2 x N^2)$ - very expensive
- Spectral methods and FMM investigated

\[
\frac{f_{a}^{n+1} - f_{a}^{n}}{\Delta t} = \sum_{b} C_{ab}(f_{a}^{n+1}, f_{b}^{n+1})
\]

\[
\frac{f_{a}^{(k+1)} - f_{a}^{n}}{\Delta t} = \sum_{b} C_{ab}(f_{a}^{(k+1)}, f_{b}^{(k)})
\]
Collision Kernel

- Generate distribution from discrete particle data in Voronoi polygon of vertex (may need to merge subdomains to obtain sufficient number of particles)

- Solve non-linear equations by Picard fixed-point iteration in 2D velocity phase-space \((M \times N)\)

- **Independent system** on each mesh vertex, 5-point stencil on rectangular grid leads to banded matrix, and solved by LAPACK band solver (on CPU)

- New development in conservative resampling in mapping distribution back to particles may require solving least squares optimization problem with algebraic constraints
Collision Kernel (2)

- High cost in matrix construction:
  - high memory usage ($O(M^2 N^2)$) may limit number of concurrent kernels
  - large arrays preallocated (for each thread)
  - vectorized evaluation of elliptic functions to fill large arrays
  - efficient AVX vectorization on KNL and OpenACC on GPU
  - nested OpenMP parallelization on CPU
- Sparse matrix transferred and solved by LAPACK band solver (CPU)
- OpenMP threads launch OpenACC kernels
  - concerns about race conditions on Summit
  - disable OpenMP, run single kernel on GPU
- Future needs in multi-species collision can significantly increase the computation cost
OpenACC Memory Pool

- OpenACC memory pool as optimization feature
  acc_malloc(), acc_free()
- Less memory available for CUDA library or CUDA memory allocation
- PGI_ACC_POOL_ALLOC=0 to turn off this feature
- Other environment variables such as
  PGI_ACC_POOL_SIZE, PGI_ACC_POOL_THRESHOLD
- call acc_clear_freelists() to release memory to CUDA
Electron Push Kernel

• Electron **sub-cycling** requires about 50 time steps per ion time step, particles can travel cross many planes on torus

• Expensive operations (MPI communication, data movement, allocate device memory) to replicate field information to all GPUs

• **Push performed on GPU without further communication**

• **GPU kernel is limited by memory access, not FLOPS**

• Solve initial value ODE by Runge-Kutta method
• Heuristics to balance work load and device memory
Electron Push Kernel (2)

- **Deep call graph** of Fortran module routines and data structures:
  - push one particle to completion
  - essentially embarrassingly parallel
  - interpolation from cubic splines
  - locate particle in unstructured triangle mesh (heuristic to check same triangle)
  - CUDA Fortran to use texture cache
  - OpenACC version

- On Titan, push particles on both GPU (>=70%) and CPU (<=30%)
Optimization for GPU

- Array of Structure (AoS) on CPU, Structure of Array (SoA) on GPU, so data **transpose** required
- Tuning parameter for periodic particle bin **sorting** to improve locality and cache reuse. Note rearrangement of data structure is expensive.
- Particle search by geometric bin hashing into 2D uniform Cartesian grid holding short list of triangles.

- **Heuristic:** First check whether particle is still in **same triangle**.
- Particle binning or **sorting** (by triangle number) $\rightarrow$ require custom allocator for optimized **prefix sum** scan by Nvidia Thrust library
Optimization for GPU (2)

• Asynchronous data transfer between CPU/GPU
  – Expect particle data to fill GPU device memory
  – dynamic pinning of host buffers
  – preallocated (small) device buffers to perform transpose operations on GPU
  – employ multiple streams to overlap
  – Implemented using F2003 abstract type, abstract procedures customized for transpose operation of different data structures
  – CUDA events for synchronization and timing
• Asynchronous (non-blocking) electron push on GPU
• Concurrently push ion particles on multi-cores using OpenMP
• Dynamic load balancing of particles assigned to GPU and GPU. However, nearly all particles assigned to Volta GPU.
Future Development

• Texture cache may not be necessary for Volta with combined L1 cache
• Avoid transpose by using data structure optimized for GPU
• Over-subscribe device memory for particle data, concurrently overlap data movement with GPU push
• new particle-mesh library under development to avoid replicating all field data
Vectorized Push Kernel for KNL

- Developed by NESAP Postdoc (Tuomas Koskela) for Cori/KNL and still developed by ALCF Postdoc

- Vectorized version for KNL (with SoAoS) to push groups of particles

- Vectorized version of code performs poorly when ported using OpenACC on GPU:
  - long loops split up as **simpler loops** to be recognized for vectorization by compiler
  - **temporary vectors** increase register usage and decrease parallelism on GPU
Atomic Update

• Need atomic 64-bit floating point (FP64) updates for particle charge deposition on background grid and for diagnostics
• Avoid collision hazard by replicating arrays for OpenMP threads

• Kepler GPU has hardware support for atomic FP32 updates, but uses atomic 64-bit compare-and-swap to emulate atomic update for FP64

• Pascal and Volta GPUs have hardware support for atomic update of FP64 with significantly improved performance
Strong Scaling of XGC

• XGC has been scaled to 2048 nodes (over 40% of full machine) on Summit with about 90% parallel efficiency

• The CPU + GPU version is over 10X faster compared to not using the GPU

• Using same number of GPUs on Titan (12288 nodes), the Summit version is over 3X faster
Strong scaling of XGC on Summit

XGC1 Performance: Strong scaling on DIII-D mesh
(13K ions and 13K electrons per mesh cell, with collisions)

SUMMIT
42 CPU cores per node
4-way SMT per core
6 GPUs per node

CPU only
CPU+GPU, no OpenACC
CPU+GPU, w/OpenACC

Average Seconds per Timestep

Compute Nodes

256 512 1024 2048

1024 512 256 128 64 32 16 8

14.3x 12.3x 14.3x 12.2x 13.2x 11.0x 11.3x

eff: 0.91 0.76 0.72

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Comparison of Titan vs Summit

XGC1 Performance: Strong scaling on DIII-D mesh
(13K ions and 13K electrons per mesh cell, with collisions)
Porting challenges

- **Compiler**, system software, tools for profiling and debugging
- **Need stable system**
- Concern about race condition in OpenMP threads launching OpenACC kernels
- OpenACC has separate pool of device memory (optimization feature)
- Band solver on GPU can reduce data movement
- Load balancing between particle push, collision kernel (number of local mesh vertices), amount of GPU device memory
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Questions?
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