

GPU enabled EUTERPE

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GPU enabled EUTERPE



- HLST project MULTIKIN in 2020
- enabling GPU for EUTERPE
- different path
 - language based (Kokkos, CUDA, OpenCL, Julia)
 - directive based (OpenMP 4.5, OpenACC)
- Nils selected Kokkos for investigation
- implementing a toy problem in Fortran (one dimensional PIC solver)
- Kokkos C++ library leads to a complex Fortran layer
- not efficient without porting EUTERPE to C++
- decision last year to use OpenACC



initial approach

• calculate electrons parallel to ions on GPU

Parts on GPU

- particle pushing
- charge assignment
- particle communication
- cache sorting

Difficulties

- fractured code (many interdependent modules)
- widely used global variables (declaration and updating)
- inlineable functions and subroutines for parallel regions



Types of parallelization

- using MPI for domain decomposition
- using OpenMP for CPU compiled parts in order to use multiple cores of the CPU
- using CPU/GPU for different types of particles
- equilibrium data accessible on GPU
- introducing species specific parts
- avoid code duplication
- particle dependent subroutines
- particle communication after pushing
- time integrators need particle dependent copying and calculating of particle properties
- disable cache optimization due to doubled memory requirements



- pushing and charge assignment of ions and electrons asynchronously
- after first tests it was better to put ions to GPU instead of electrons
- Nils implemented a compile dependent distribution of particles to GPU or CPU
- since September code is maintained in Greifswald
- introduce real version of the code
- all test cases runable with debug options
- code now gives same results for all actual test cases



Outlook

- merge with current master
- production runs to check stability
- rewrite cache optimization
- remove global variables from modules
- implement more strict programming style
- employing OpenMP on more places
- execute more parts asynchronously
- data structures
- solver (PETSc) to GPU?