OpenACC Implementation of Radiative Transfer Simulation Code

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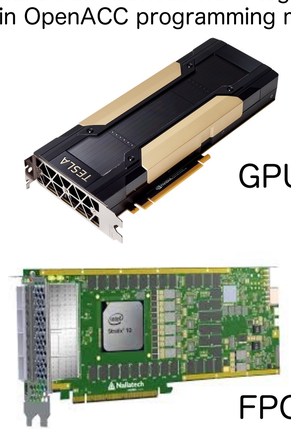
❖ Introduction

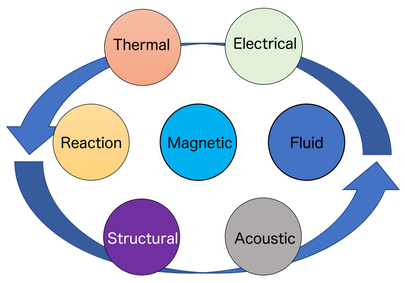
Motivation

- Realizing a way to easily use GPU and FPGA by OpenACC
  - Why OpenACC?
    - ✓high maintainability
    - ✓high portability
    - → quite friendly to application developers!
- Why GPU-FPGA coupling is needed?
  - Keyword: Multiphysics
  - Simulations with multiple interacting physical properties
    - ✓space – particle reaction
    - ✓fluid dynamics with chemical reaction
    - ✓macroscopic/microscopic hybrid simulation for molecular dynamics
  - Various computations are included within a simulation
    → Hard to accelerate simulation speed by GPU only

We aim to combine GPU and FPGA to improve simulation speed (offloading GPU non-suited computation part to the FPGA)

Make both devices work together in OpenACC programming model

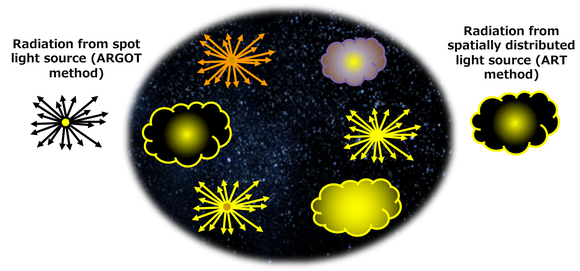




Schematic representation of Multiphisics

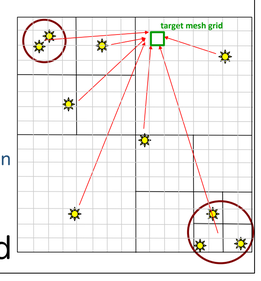
What we have to do first is…

- Investigating the performance change by converting to OpenACC
  - we implemented ARGOT code with OpenACC and evaluated its performance by comparing with those of OpenMP-based CPU implementation and CUDA-based GPU implementation
- ARGOT code: an astrophysics simulation code
  - developed in Center for Computational Sciences, University of Tsukuba
  - combining two types of radiative transfer
    - ✓ARGOT method
      - a radiative transfer from a spotlight (point source)
    - ✓ART method
      - a radiative transfer from spatially distributed light
  - CPU (OpenMP) and GPU (CUDA) implementations are already available



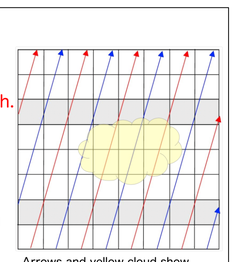
Our target application: ARGOT code (one of the Multiphisics simulations)

- is to solve the radiative transfer from point radiation sources
- builds an oct-tree data structure for the distribution of radiation sources
  - It's a 3-dimensional problem space, so it's an octave tree
  - For point of view from the target mesh , it is treated as a same light source if the light sources fall within a certain degree
    effective number of sources : N_s ➡ $\log N_s$
- is similar to Tree-Code in gravity calculation
  - suitable for the GPU
  - Each ray is assigned to each CUDA thread, and then these computations are conducted in parallel



ARGOT method

- ART method is based on ray-tracing method
  - 3D target space split into 3D meshes
  - Rays come from boundaries and move in straight in parallel with each other
- This method is not suitable for SMID-style arch.
  - Memory access pattern for mesh data is varies depending on ray's direction
    - ✓causing a decrease in cash hit ratio
  - Atomic operations are needed
    - ✓for processing the superimposition of the effects of multiple rays on the shaded mesh
    - ✓To avoid atomic operations, ray tracing along the red and blue light must be separately performed
      - causing the memory access patterns to become more scattered



Arrows and yellow cloud show rays and gas to compute reactions, respectively

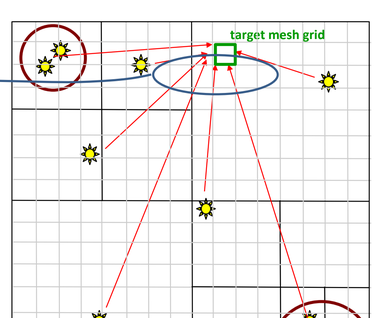
ART method

❖ OpenACC implementation

Loop optimizations

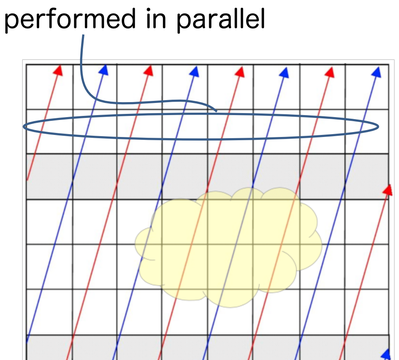
- Parallel regions are specified like OpenMP
  - Replace #pragma omp parallel for with #pragma acc parallel loop
    - ✓The CUDA implementation is based on the OpenMP implementation, so the parts that are offloaded to the GPU should be equivalent.
    - ✓Function calls in parallel regions should be OpenACCed with #pragma acc route seq.
- Add asnyc clause for asynchronous execution
- The parallel granularity is set based on the block size and number of threads of the CUDA implementation
  - Set num_gang and vector_length

Each ray is mapped to a thread, and radiative transfer is performed in parallel



Each ray is mapped to each thread, and radiative transfer from point sources is performed in parallel.

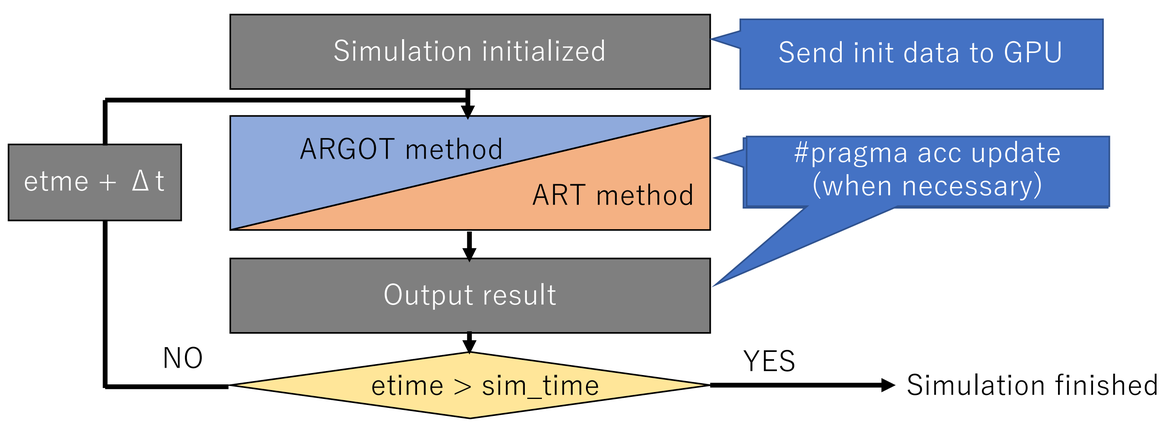
ARGOT method



ART method

Data management

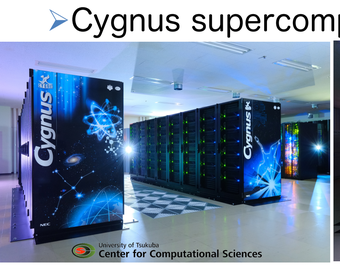
- Data transfer is implemented to be equivalent to the CUDA implementation
  - At initialization, use #pragma acc enter data copyin() to send data to GPU memory
    - ✓#pragma acc update host() is used only for processes that need to be run on the host (pulling the necessary data from the GPU)
    - ✓#pragma acc update device() is used to update the GPU memory with the host's updated data
  - As with Loop optimizations, async clause is added to asynchronous execution

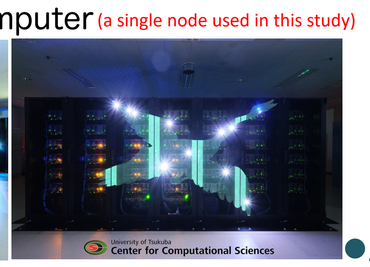


Simulation flow of ARGOT code

❖ Performance comparison

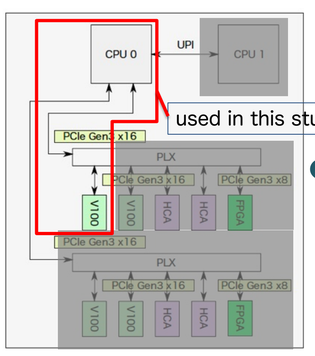
- Evaluation testbed
  - Cygnus supercomputer (a single node used in this study)

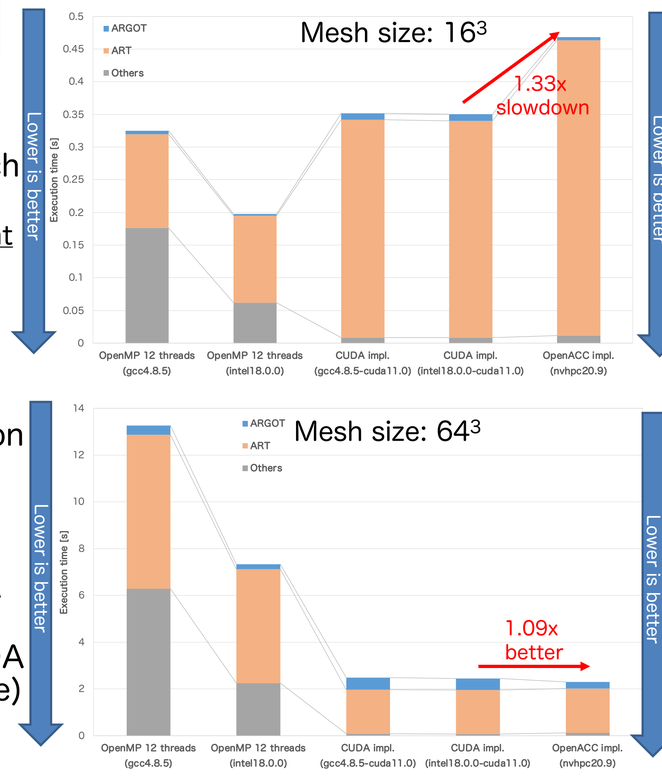


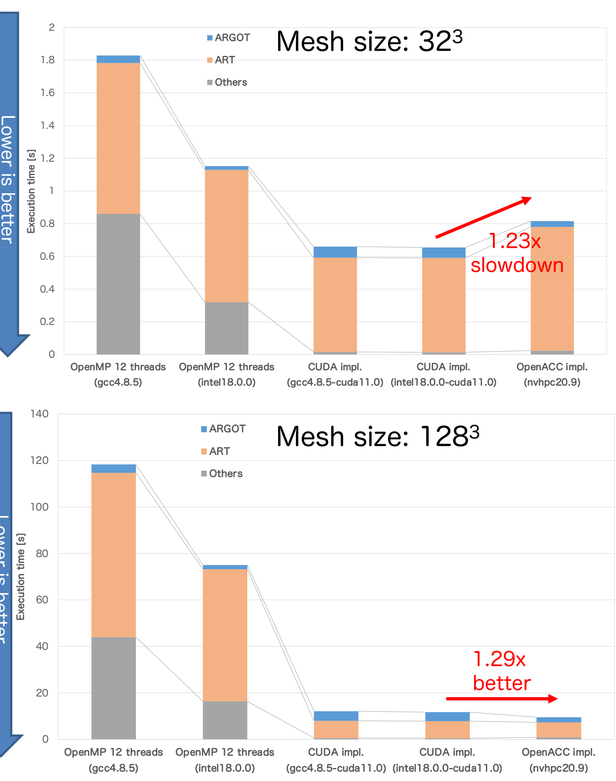


- Others
  - solving chemical reactions and the radiative heating and/or cooling of each mesh
    - ✓Computation of a mesh highly independent from one another, which is why the GPU implementation can accelerate their execution
- ARGOT method
  - The larger the mesh size, the more noticeable the performance degradation of the CUDA impl. (this is because of cudahostalloc)
- ART method
  - Small mesh size: 73% ~ 76% of CUDA impl. Performance
  - Large mesh size: almost same as CUDA impl. (1.1x better when 128^3 mesh size)

Hardware specification	
CPU	Intel Xeon Gold 6126 x 2
Host Memory	192 GiB (16 GiB DDR4-2666 ECC RDIMM x 6 chan. x 2)
GPU	NVIDIA Tesla V100 (PCIe Gen3 x16) x 4
GPU Memory	32 GiB CoWoS HBM2 @ 900 GB/s with ECC
Software specification	
OS	CentOS 7.9
Host Compiler	gcc 4.8.5, Intel compiler 18.0.0 (for OpenMP impl.)
CUDA Toolkit	CUDA 11.0.221 (for CUDA impl.)
OpenACC Compiler	NVIDIA HPC SDK 20.9







❖ Conclusion and future work

- What we did is...
  - as a preliminary evaluation for the realization of GPU-FPGA integration with high usability, we implemented the ARGOT code by OpenACC and evaluated the performance of OpenMP-based CPU implementation and CUDA-based GPU implementation
  - we confirmed that...
    - ✓For small mesh size: OpenACC-based implementation achieved up to 77% of the performance CUDA-based ARGOT code implementation
    - ✓For large mesh size: OpenACC-based implementation achieved up to 1.29x better performance compared to CUDA-based ARGOT code implementation
- Next step is...
  - to evaluate multi-node versioned OpenACC implementation's performance by comparing to OpenMP and CUDA implementations

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