GPU porting of ASCOT5 code for Monte Carlo simulations in fusion plasmas

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5th Fusion HPC Workshop

EUROfusion Advanced Computing Hubs

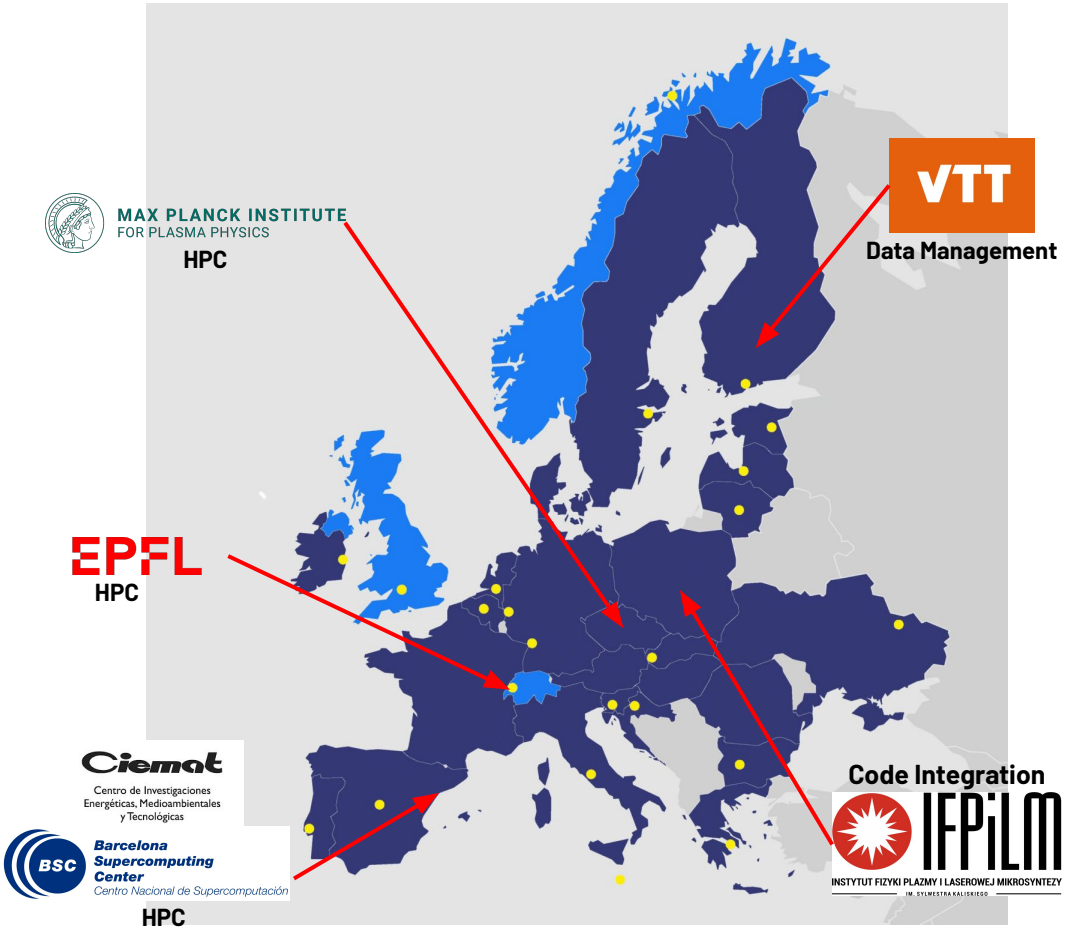
EUROfusion E-TASC – Theory and Advanced Simulation Coordination between:

- **14 TSVV** (Theory, Simulation, Validation and Verification) projects
- **5 ACH** (Advanced computing Hubs)

In particular, **3 HPC ACHs** were created in order **to help building power plants through numerical simulations**

- Extension of **HLST** (Roman Hatsky/IPP)
- Develop **efficient, reliable** tools
- **Modernize and industrialize research codes**

In order to **gain insight and predict fusion experiments** (ITER, JT60-SA, DEMO…)



How to transition towards GPU codes

Plasma simulation codes are research codes:

- mostly **CPU-only**,
- written in **C,C++ and Fortran**,
- **MPI** and/or **OpenMP**,
- **under active development** by physicists, mathematicians, etc...
- main objective: GPU porting

General porting rules:

- **least modifications** of the code/no rewrite
- "maximum" **performance**
- **portability**/no specific target

3 approaches:

Library encapsulation (e.g. Kokkos, PETSc, AmgX, BLAS/Lapack...)

Cuda/ROCm

Pragma directives (OpenMP offload / OpenACC)

- GRILLIX — MAX PLANCK INSTITUTE FOR PLASMA PHYSICS
- GyselaX — cea irfm
- ORB5 — EPFL WARWICK MAX PLANCK INSTITUTE FOR PLASMA PHYSICS
- Soledge3X — cea irfm
- ASCOT5 — Aalto University
- CAS3D — MAX PLANCK INSTITUTE FOR PLASMA PHYSICS
- FELTOR — DTU
- GBS — EPFL
- GENE — MAX PLANCK INSTITUTE FOR PLASMA PHYSICS

ASCOT5 GPU porting

- **Outline**
  - **ASCOT5: particle orbit-following code**
  - **MPI + OpenMP CPU algorithm**
  - **GPU porting strategy**
  - **Benchmarks**
  - **Profiling**
  - **Conclusion**

ASCOT5

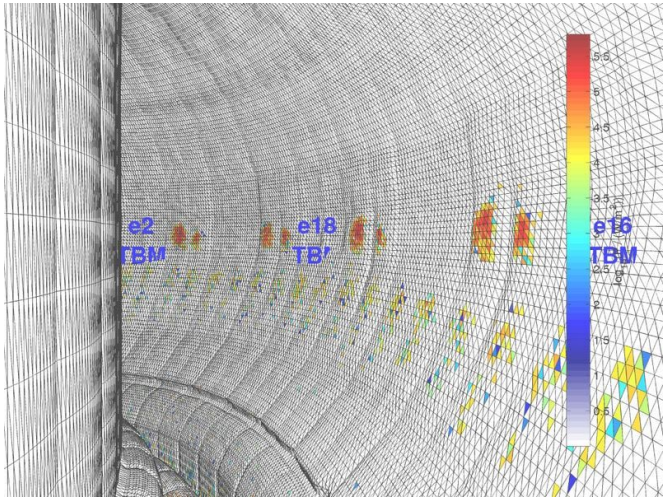
- ASCOT5 is a test **particle orbit-following** code for toroidal magnetically confined fusion devices
- The code uses the **Monte Carlo method** to solve the distribution of particles by following their trajectories.
  - The **evolution of the distribution function** for a test particle species *a* is described by the **Fokker-Planck equation**

$$\frac{\partial f_a}{\partial t} + \mathbf{v} \cdot \nabla f_a + \frac{q_a}{m_a}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_a = \sum_b -\nabla_{\mathbf{v}} \cdot [\mathbf{a}_{ab} f_a - \nabla_{\mathbf{v}} \cdot (\mathbf{D}_{ab} f_a)]$$

  and **approximated by the Langevin equation** for a large number of markers that represent the distributed function:

$$d\mathbf{z} = [\dot{\mathbf{z}} + \mathbf{a}(\mathbf{z}, t)]\, dt + \boldsymbol{\sigma}(\mathbf{z}, t) \cdot d\boldsymbol{\mathcal{W}}$$

- The particles undergo **collisions with a static Maxwellian background plasma**
- The detailed magnetic fields and the first wall can be **fully 3D**
- **MPI + OpenMP** (task-based) and **highly vectorized**



ASCOT5 CPU version

- CPU: MPI - OpenMP - Vectorized implementation:
  - The time evolutions of each particle are independent from each other
  - One + two levels of parallelism:
  - MPI: Particles distributed among tasks, fields replicated
  - OpenMP: queue based approach
  - highly vectorized using the SIMD, originally developed for KNL manycore systems as target
  - to enable multithreading, a number of worker threads, each operating on a single set of N_{SIMD} arrays, are launched and allowed to perform their simulation independently
  - swapping mechanism
    - after each iteration, particles that have reached their end condition are stored in an array for completed particles
    - a fresh particle is retrieved from a queue to continue simulation in the particular slot in the N_{SIMD} arrays

Algorithm 1: CPU multithread vectorized algorithm

```
initialization;
#pragma omp parallel
while particles are alive in pack_{N_SIMD} do
    #pragma omp simd
    for particles ∈ pack_{N_SIMD} do
        move_particle;
    end
    #pragma omp simd
    for particles ∈ pack_{N_SIMD} do
        collisions;
    end
    #pragma omp simd
    for particles ∈ pack_{N_SIMD} do
        end_condition;
    end
    #pragma omp simd
    for particles ∈ pack_{N_SIMD} do
        diagnostics;
    end
    for particles ∈ pack_{N_SIMD} do
        if particle reached end condition then
            store particle and replace it by new one
        end
    end
end
```

ASCOT5 GPU version

- GPU porting strategy
  - Maintain a single version of the code
  - Ensure code portability and readability
  - Generic pragma for OpenMP/OpenACC

```
#ifndef gpu_commands
#define gpu_commands
/**
 * @brief Applies parallel execution to loops
 */
#if defined(GPU) && defined(OPENMP)
#define GPU_PARALLEL_LOOP_ALL_LEVELS\
        str_pragma(omp target teams distribute parallel for simd
#elif defined(GPU) && defined(OPENACC)
#define GPU_PARALLEL_LOOP_ALL_LEVELSstr_pragma(acc parallel loop)
#else
#define GPU_PARALLEL_LOOP_ALL_LEVELSstr_pragma(omp simd)
#endif


/**
 * @brief Maps variables to the target device
 */
#if defined(GPU) && defined(OPENMP)
#define GPU_MAP_TO_DEVICE(...) \
        str_pragma(omp target enter data map(to: __VA_ARGS__))
#elif defined(GPU) && defined(OPENACC)
#define GPU_MAP_TO_DEVICE(...) str_pragma(acc enter data copyin
(__VA_ARGS__))
#else
#define GPU_MAP_TO_DEVICE(...)
#endif
............

#endif
#endif
```

```
  GPU_LOOP_ALL_LEVELS
  for(i = 0; i < n_queue_size; i++) {
    if(p->running[i]) {
        posxyz[0] = posxyz0[0] + pxyz[0] * h[i] / (2.0 * gamma *
mass);
        posxyz[1] = posxyz0[1] + pxyz[1] * h[i] / (2.0 * gamma *
mass);
        posxyz[2] = posxyz0[2] + pxyz[2] * h[i] / (2.0 * gamma *
mass);
  }
  GPU_END_LOOP_ALL_LEVELS
```

ASCOT5 GPU version

- First implementation History-Based:
  - parallelism is expressed at a high level, emphasizing the independence of individual particles, allowing for concurrent execution of their respective histories from birth to death
  - each GPU processing unit is used to deal with the entire history of one or more particles until all of the particles have reached their end condition
  - this parallelism is implemented through a single monolithic GPU kernel

Algorithm 2: GPU algorithm - History-based

```
initialization;
#pragma acc parallel loop
for all particles ∈ {1...N_tot} do
    while particle is alive do
        move_particle;
        collisions;
        end_condition;
        diagnostics;
    end
end
```

ASCOT5 GPU version

- The original implementation is not GPU-friendly:
  - **one very large kernel**
  - events depend on the previous event
- Implement a new version by **splitting the initial kernel**:
  - **Parallelize over events** instead of particles
  - small kernels independent of each other

Algorithm 2: GPU algorithm - History-based

```
initialization;
#pragma acc parallel loop
for all particles ∈ {1...N_tot} do
    while particle is alive do
        move_particle;
        collisions;
        end_condition;
        diagnostics;
    end
end
```

Algorithm 3: GPU algorithm - Event-based

```
initialization;
while number of particles alive > 0 do
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            move_particle;
        end
    end
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            collisions;
        end
    end
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            end_condition;
        end
    end
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            diagnostics;
        end
    end
end
```

ASCOT5 GPU version

- Implement a new version by **splitting the initial kernel**:
  - **parallelize over events** instead of particles
  - small kernels independent of each other
  - pack particles

Algorithm 2: GPU algorithm - History-based

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#pragma acc parallel loop
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    while particle is alive do
        move_particle;
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    end
end
```

Algorithm 3: GPU algorithm - Event-based

```
initialization;
while number of particles alive > 0 do
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
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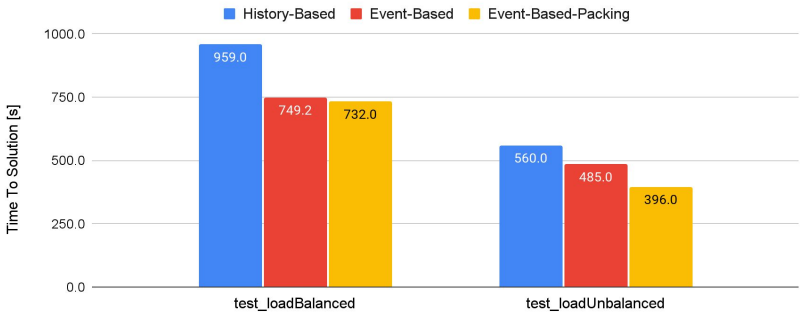
        end
    end
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            collisions;
        end
    end
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            end_condition;
        end
    end
    #pragma acc parallel loop
    for all particles ∈ {1...N_tot} do
        if particle alive then
            diagnostics;
        end
    end
end
```

Algorithm 4: GPU algorithm - Event-based - packing

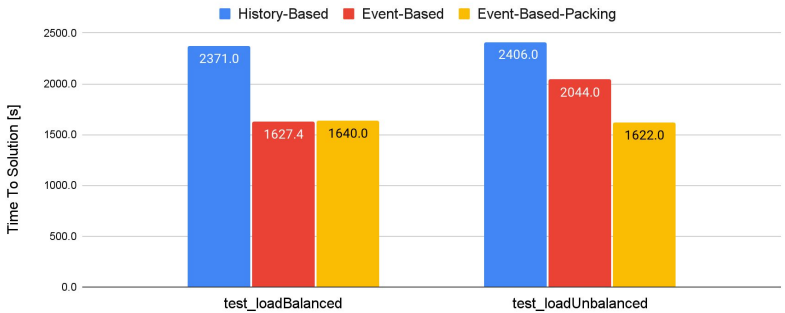
```
initialization;
N_pack ← N_tot;
while number of particles alive > 0 do
    #pragma acc parallel loop
    for packed particles still alive ∈ {1...N_pack} do
        move_particle;
    end
    #pragma acc parallel loop
    for packed particles still alive ∈ {1...N_pack} do
        collisions;
    end
    #pragma acc parallel loop
    for packed particles still alive ∈ {1...N_pack} do
        end_condition;
    end
    #pragma acc parallel loop
    for packed particles still alive ∈ {1...N_pack} do
        diagnostics;
    end
    if (N_pack − N_running > α · N_tot) then
        pack particles;
        N_pack ← N_running;
    end
end
```

Benchmarks

- Benchmark:
  - Collisional full-orbit simulation of prompt-losses of fusion alpha particles
  - 2D wall; ITER-like but circular equilibrium interpolated with cubic splines
  - 2D wall rectangular, coulomb collisions, gyro orbit, simulation time = 0.0001s, fixed time step
  - **Leonardo**: A100, nvhpc/23.1
  - Comparison of three GPU implementations on GPU A100
    - Event-based packing algorithm is most efficient in all cases
    - Impact of Packing:
      - test_loadBalanced: Minimal impact due to majority of particles reaching end of simulation
      - test_loadUnbalanced: Significant impact with speedup of up to 1.41 compared to history-based algorithm and up to 1.22 compared to event-based one.



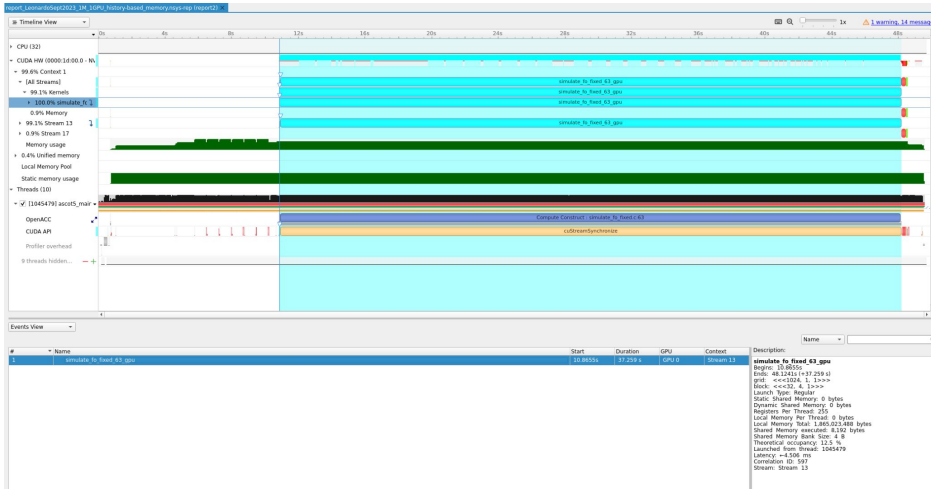
Comparison of the 3 particle-following GPU implementations - 1 Millions markers - 1 A100

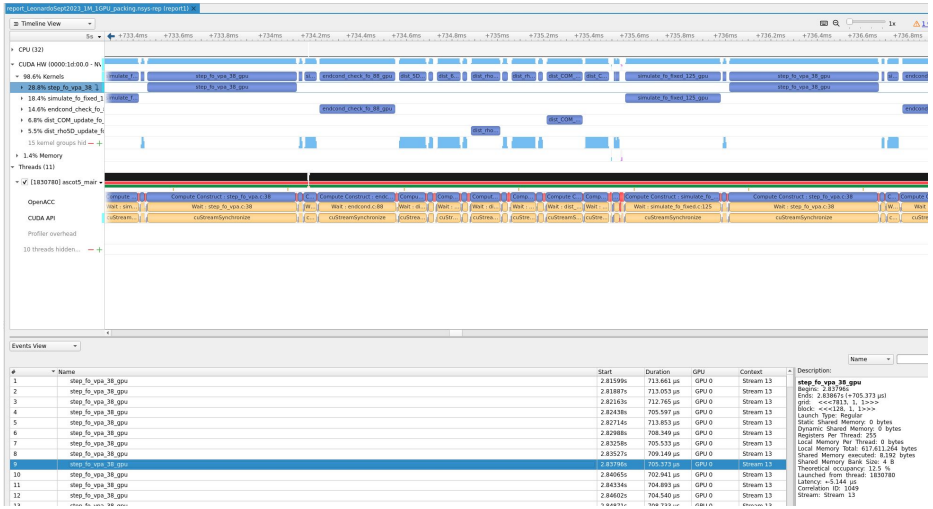


Comparison of the 3 particle-following GPU implementations - 10 Millions markers - 4 A100

Profiling Nsys

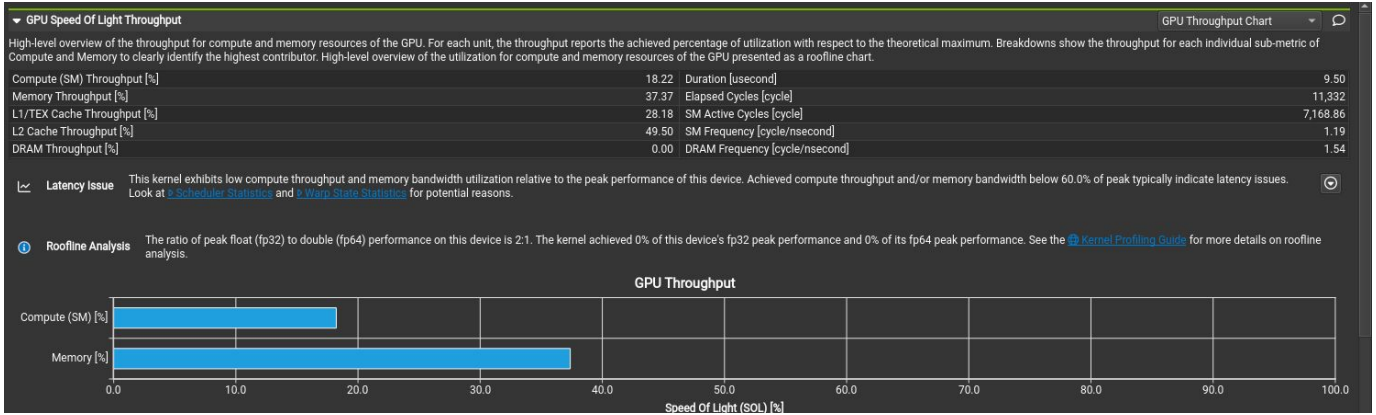
- **Lower Local Memory Use**: Event-based packing uses multiple smaller kernels, reducing local memory demands versus the history-based version.
- **Efficient Data Transfer**: Minimal data transfer overhead as all kernels run on the GPU.
- **Optimized Memory Access**: Contiguous, coalesced memory access through packing enhances efficiency.
- **Reduced Loop Bounds**: Through packing step, dynamic loop bounds improve runtime performance, with only ~30% particles active per timestep.



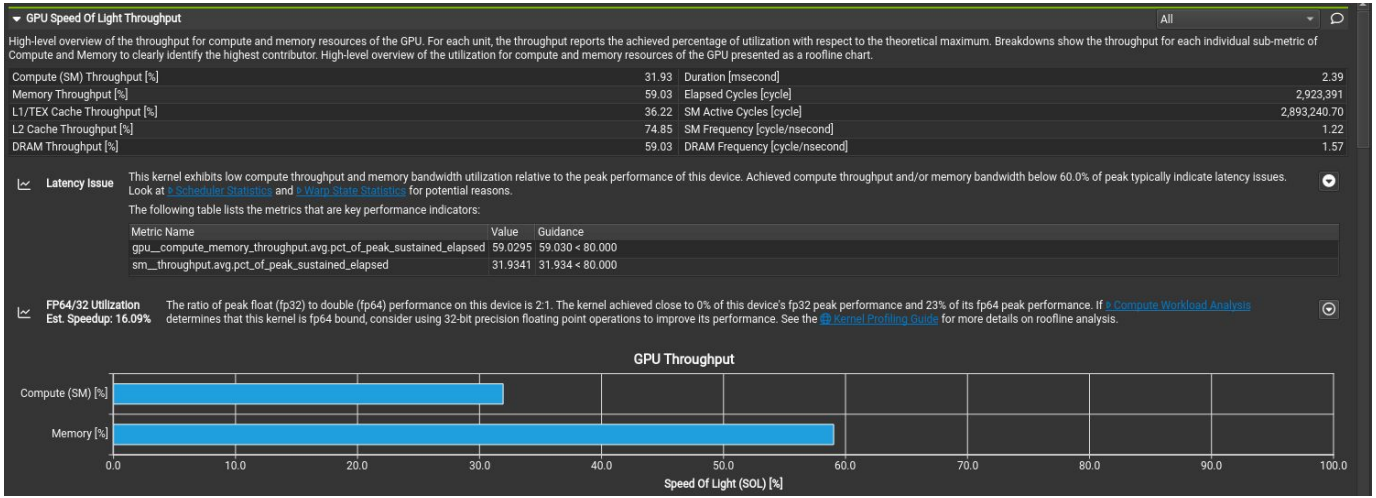


Profiling Nsight-Compute

- HistoryBased



- EventBased



Benchmarks

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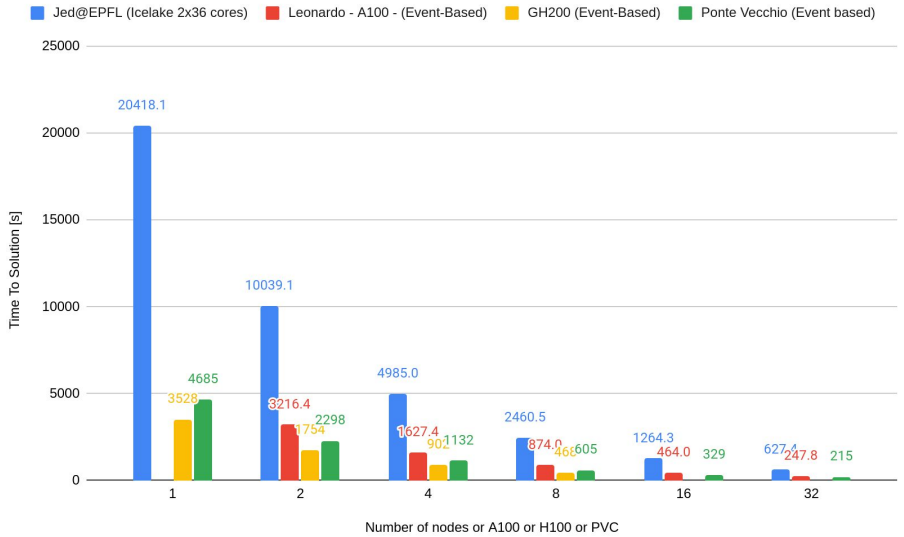
  - 2D wall; ITER-like but circular equilibrium interpolated with cubic splines
  - 2D wall rectangular, coulomb collisions, gyro orbit, simulation time = 0.0001s, fixed time step
  - **Jed**: 2x Platinum 8360Y, intel/2021.6.0
  - **Leonardo**: A100, nvhpc/23.1
  - **NVIDIA Grace Hopper Superchip engineering sample early access courtesy of NVIDIA**
  - **Intel Ponte-Vecchio 600W (2 tiles) engineering sample early access courtesy of INTEL**



Profiling

- EventBased version:
  - kernels mostly memory-bound
  - multiple branch divergences in end_condition kernel involving lower Memory SOL due to thread divergence

Main kernels	*%*
move_particle	64.8
diagnostics	9.6
end_condition	6.5
collisions	5.8
copy_particles_structures	5.5
sorting	< 0.1
packing	< 0.1

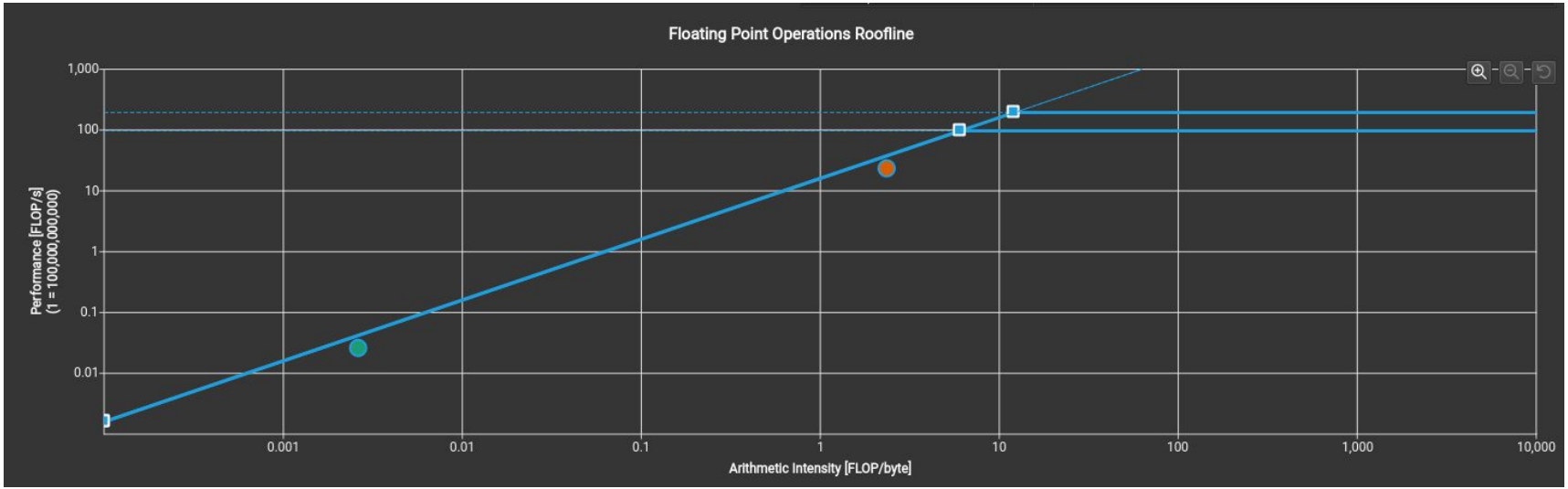
TABLE I. RELATIVE WEIGHTS OF THE DIFFERENT STEPS OF THE SIMULATION ON A100. % VALUES ARE AVERAGED SIMULATING 1 MILLION PARTICLES WITH THE ASCOT5 EVENT-BASED-PACKING ALGORITHM

Main kernels	*Memory SOL (%)*	*Compute SOL (%)*
move_particle	68	30
diagnostics	80	26
end_condition	36	12
collisions	40	56

TABLE II. TEST_LOADBALANCED, SPEED OF LIGHT - 1 MILLION PARTICLES WITH THE ASCOT5 EVENT-BASED-PACKING ALGORITHM

Profiling

- Roofline



Conclusion

- **Successful GPU Transition**: ASCOT5 was efficiently ported from CPU to GPU using a directive-based strategy, ensuring code consistency.
- **Optimized Algorithms**: Three strategies were tested, with event-based-packing achieving the best performance due to improved load balancing and reduced thread divergence.
- **Significant Speedup**: Event-based-packing on H100-96GB shows up to 6x speedup over a dual Intel Xeon CPU node.
- **Future Work**: Conduct new tests incorporating enhanced physical models.