4th Annual Meeting of EUROfusion HPC ACHs

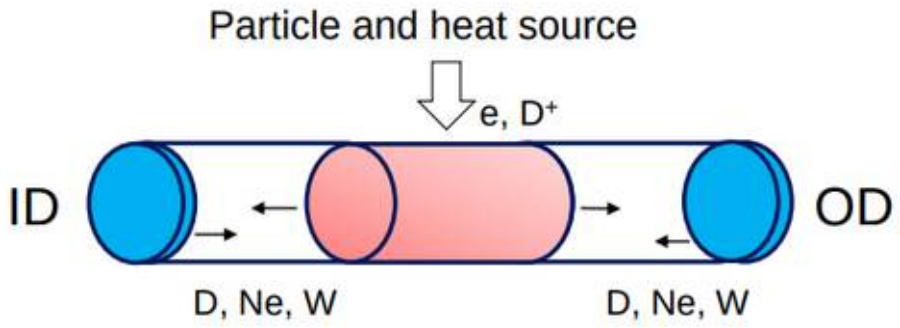
Progress on BIT1 GPU Porting

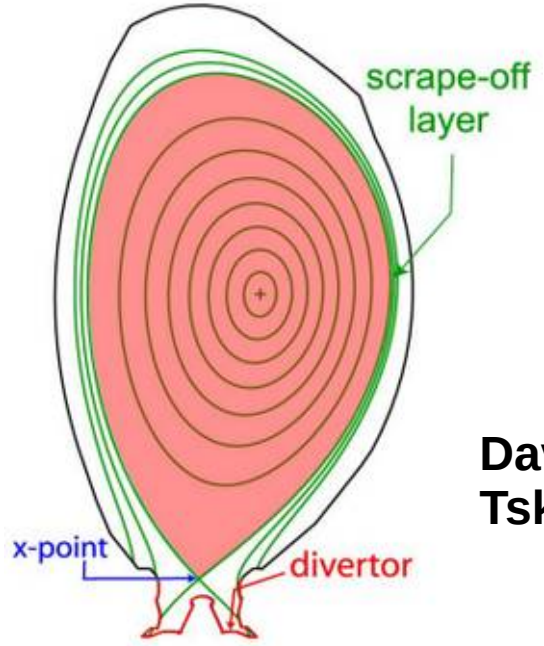
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Introduction

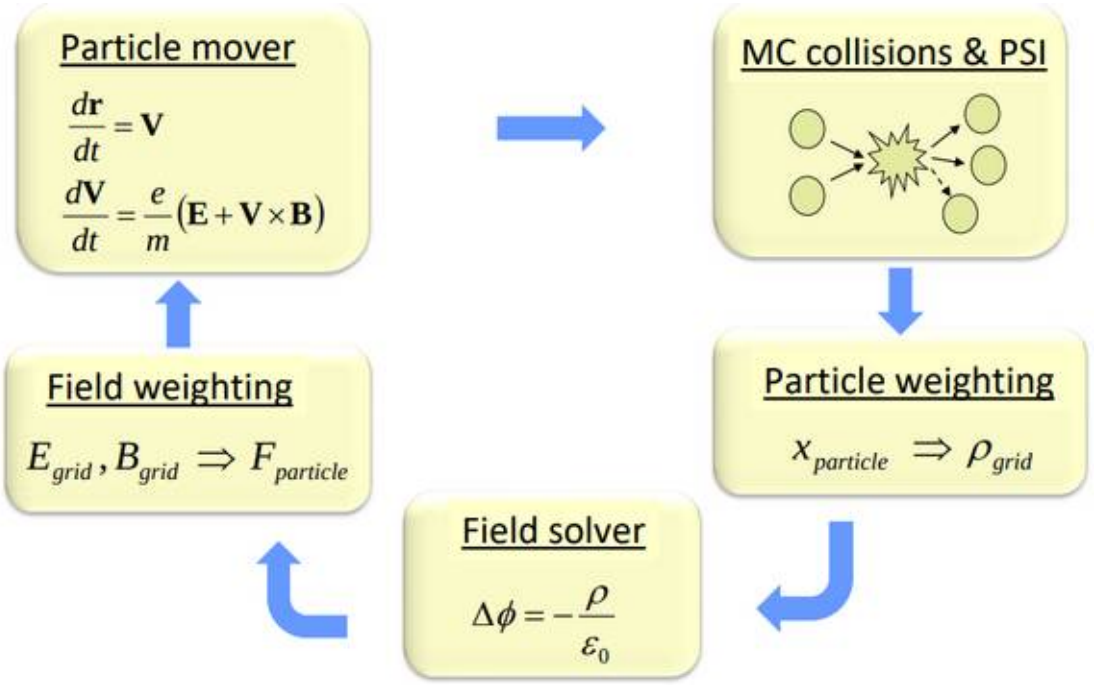




David Tskhakaya

- BIT1 is an electrostatic 1D3V PIC + 2D3V direct Monte Carlo code for plasma simulations.
- **Inputs:** Particle, heat sources, geometry and divertor material
- **Simulated particle species:** El, D (H, T), Li, He, Be, O, …
- **High spatial resolution** → $5 \cdot 10^6$ cells →capability to simulate whole SOL
- **Language:** C
- **Libraries**: No external libs
- **Parallelization**: MPI using domain decomposition

Algorithm



- BIT1 is a **Particle-in-cell (PIC) code**

Project Goal

- **Main objective:** port BIT1 to GPUs using OpenACC.
  - Ensure maintainability and readability of the codebase.
  - Achieve acceleration by offloading costly routines to GPUs.

- **Sub-objectives:**
  - Introduce OpenACC directives minimally invasively.
  - Preserve usability for non-GPU experts.

- **2026 objectives:**
  - Resolve outstanding issues.
  - Improve data management.
  - Extend GPU port.

Previous Work

16

OpenACC-enabled routines

across 10 source files

~20×

Time-step speedup

260 ms → 13 ms

~7×

Application-level speedup

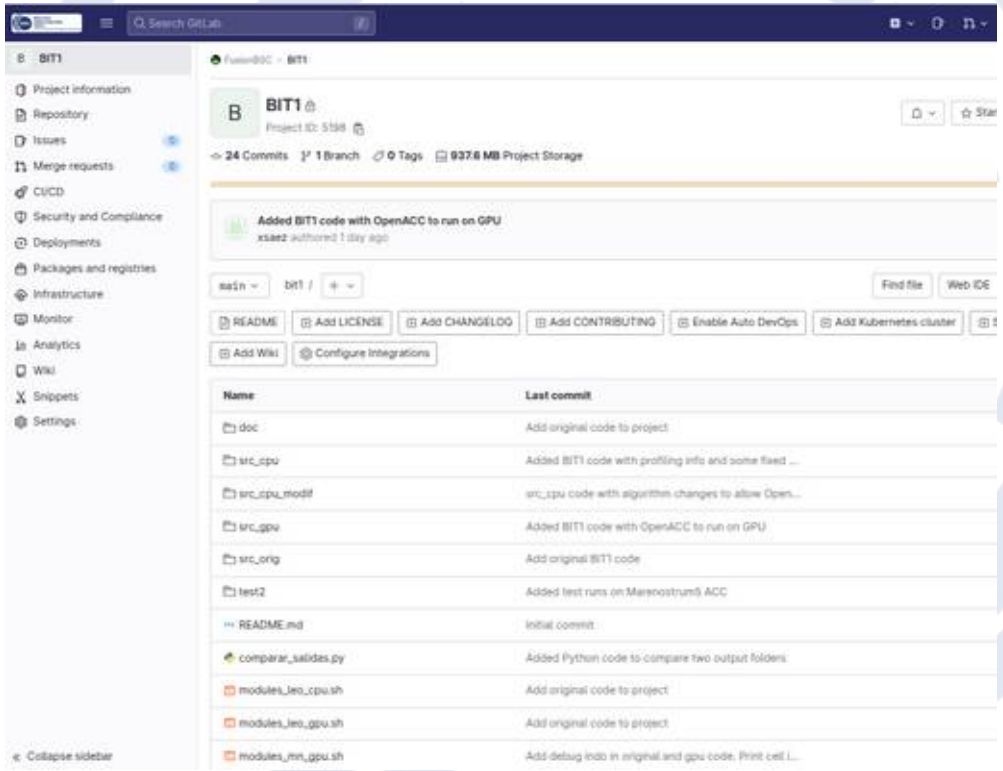
249 s → 35.8 s

- **Key lesson from the first port**
  - GPU kernels helped only after reducing excessive CPU–GPU transfers.

Execution Environment

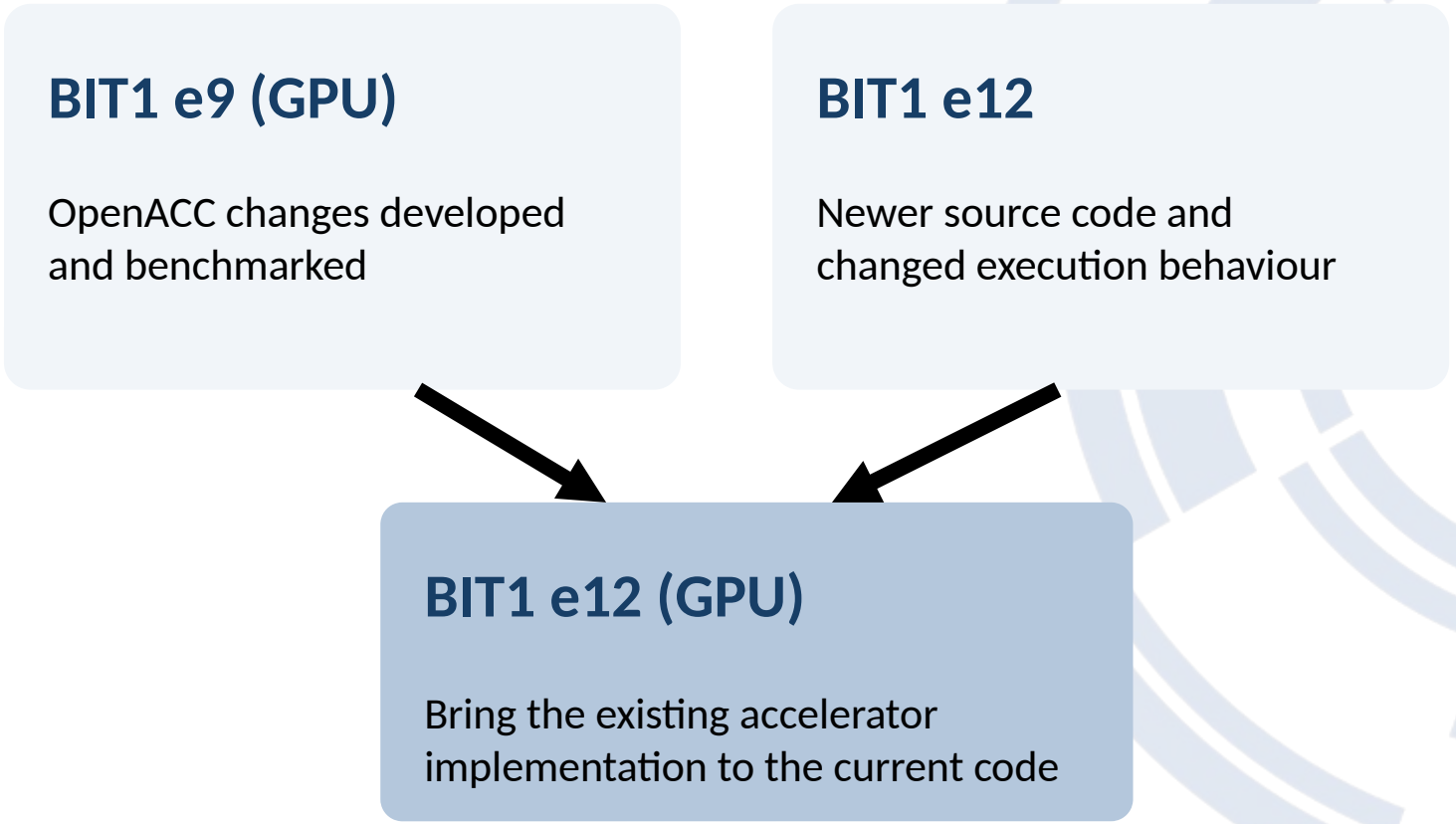
- **Platforms used:**
  - MareNostrum 5 (H100 GPUs, NDR IB)
- **Test case: DCSM_0_e21_c8.inp**
  - 1D bounded plasma with electrons, D^+ ions, and neutrals.
  - Domain: 0.1 m, 100,000 cells.
  - Time step: $4 \cdot 10^{-14}$ s, 1,000 iterations.
  - All runs used four MPI ranks; in GPU-enabled runs, each rank was bound to a dedicated GPU.
- **Profiling tools:**
  - NVTX for instrumentation.
  - Nsight Systems for GPU/CPU trace analysis.

- **GitLab Repository: FusionBSC/BIT1**
  - All codes, tests, results and traces are available.



BIT1 evolution

- **Avoid maintaining a GPU branch disconnected from the developers' current source**



Current Status

- **Code integration**
  - Existing OpenACC changes integrated into the e12 codebase.
  - The GPU-enabled e12 version compiles and runs the test case.
- **Numerical behaviour**
  - Results differ from the CPU reference.
  - Numerical acceptance criteria not yet established.
- **Performance**
  - No additional speedup has been demonstrated in this period.
- **Code availability**
  - The updated GPU version is available in a new branch of the official BIT1 repository.



Investigating outstanding issues

- **Crash after simulation ends**
- **Numerical differences:**
  - Original CPU-only e9 and e12 already differ!
  - Looking into source changes to identify potential causes

e9

```
for (i=np[iisp][j]-1; i>=0; i--)
{
   s = x[iisp][j][i];
   srho[iisp][j]   += 1.0 - s;
   srho[iisp][j+1] += s;
}
```



e12

```
for (i=0; i<np[iisp][j]; i++)
{
   s = x[iisp][j][i];
   srho[iisp][j]   += 1.0 - s;
   srho[iisp][j+1] += s;
}
```

Changing the particle traversal order can affect floating-point accumulations due to rounding errors, and these small differences may propagate over subsequent time steps

Investigating outstanding issues (2)

- **Numerical differences:**
  - Original CPU-only e9 and e12 already produce different results!
  - Further differences are observed when OpenACC is enabled in e12.
  - Do not attribute all output differences to GPU offloading before separating the e9→e12 effects.

- **Define numerical acceptance criteria**
  - Identify the relevant physical quantities to compare.
  - Agree on acceptable numerical differences (tolerances) with the BIT1 developers.
  - Consider the statistical variability inherent in PIC/Monte Carlo simulations

Conclusion

- The work focused on integrating the existing GPU port into the latest BIT1 version and investigating the observed numerical differences.

- **Next steps:**
  - **Representative cases:**
    - Select scientific cases to profile new execution paths and extend GPU coverage where useful.
  - **Numerical validation:**
    - Define CPU/GPU acceptance criteria (density profiles, field quantities, particle statistics, physical consistency, …)
    - Regression tests
    - Investigate remaining robustness issues.
  - **Production performance:**
    - Select a production case
    - Analyze application performance, host-device data transfers, memory usage and GPU utilisation.

Thanks for your attention !