3rd Annual Meeting of EUROfusion HPC ACHs

Status of BIT1 Porting to GPU and Progress on X-tork

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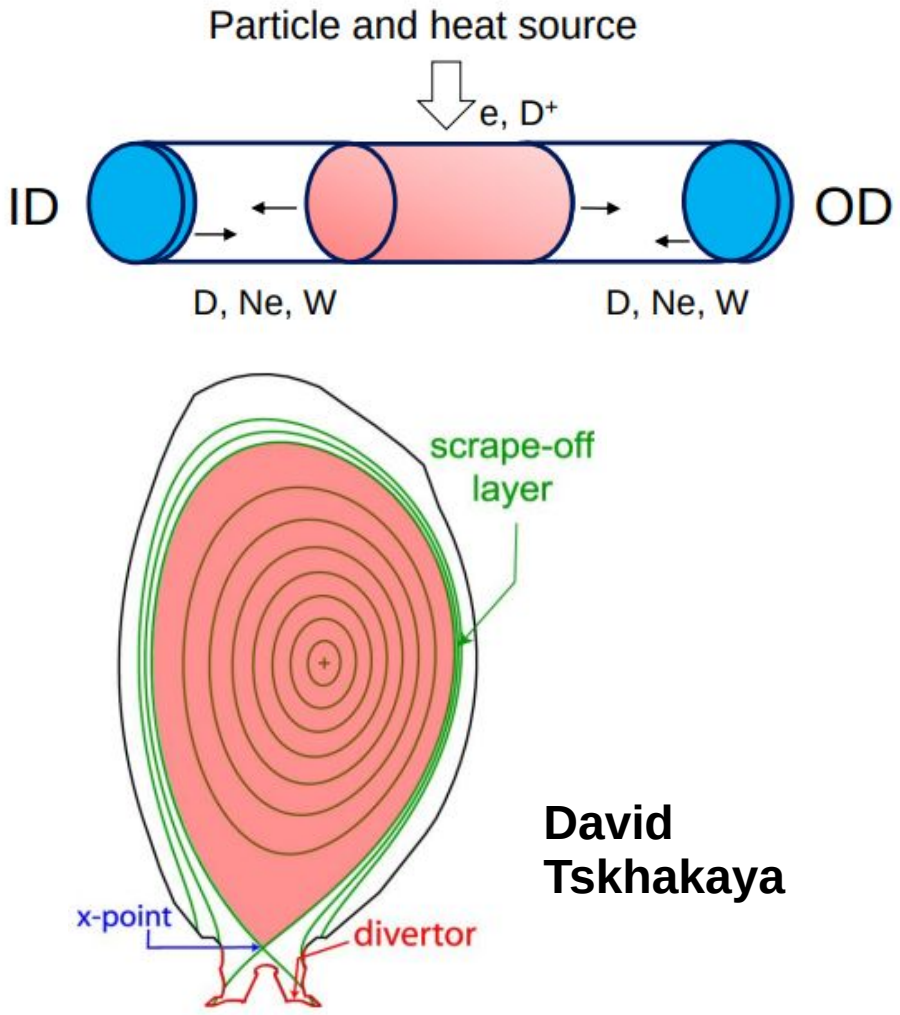
BIT1

Xavier Sáez

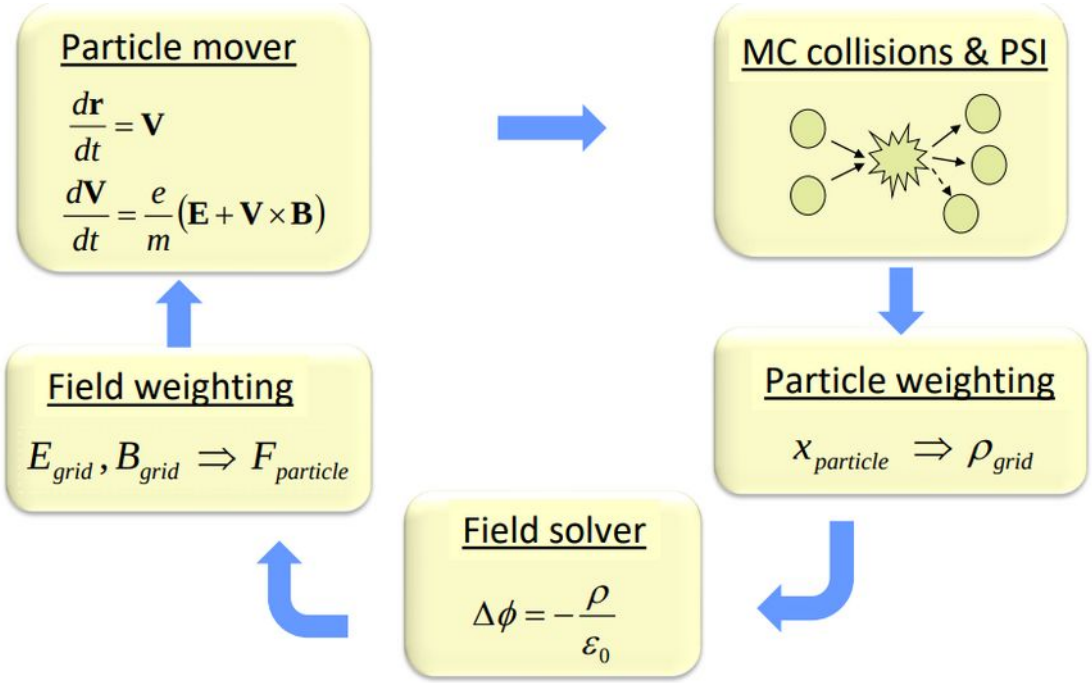
BIT1: Introduction



David Tskhakaya

- BIT1 is an electrostatic 1D3V PIC + 2D3V direct Monte Carlo code for plasma simulations.
- **Input:** Particle, heat sources, geometry and divertor material
- **Simulated particle species:** El, D (H, T), Li, He, Be, O, …
- Highly accurate → $5x10^6$ cells →capability to simulate whole SOL
- **Language:** C
- **Libraries**: No external libs
- **Parallelization**: MPI using domain decomposition

BIT1: Algorithm



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

BIT1: Project Goal

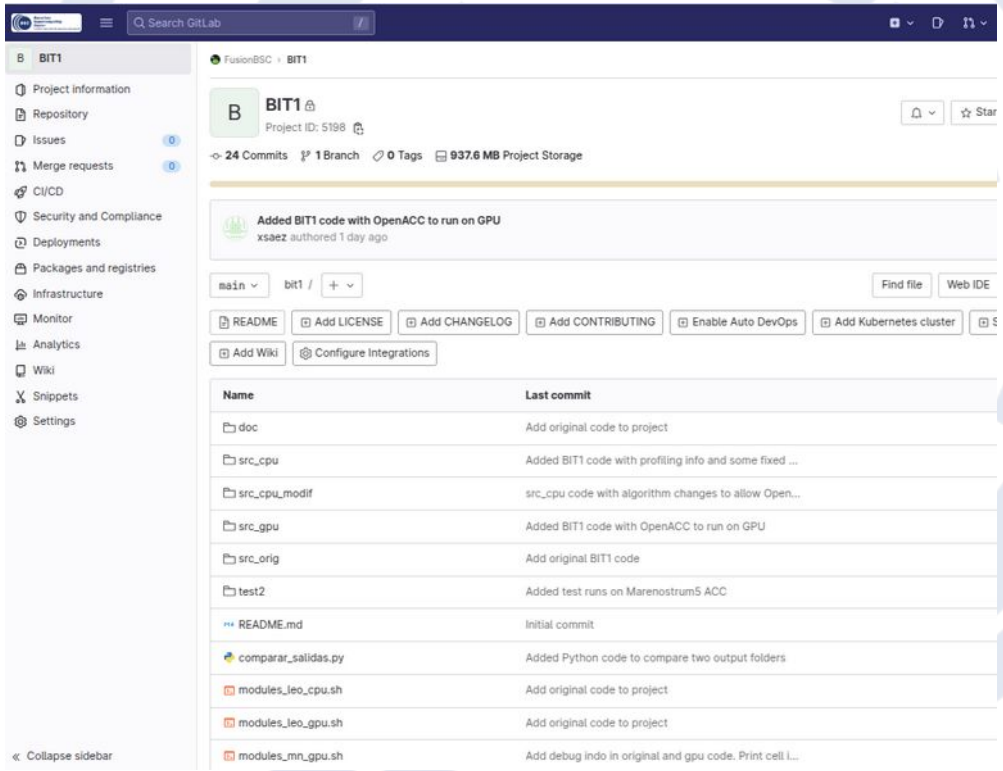
- **Main objective:** port BIT1 to GPUs using OpenACC.
  - Ensure maintainability and readability of the codebase.
  - Achieve acceleration by offloading costly routines to GPUs.

- **Sub-objectives:**
  - Introduce OpenACC directives minimally invasively.
  - Preserve usability for non-GPU experts.
  - Measure performance vs MPI-only CPU version.
  - Document issues and propose next steps.

BIT1: Execution Environment

- **Platforms used:**
  - Leonardo (A100 GPUs, HDR IB)
  - MareNostrum 5 (H100 GPUs, NDR IB)
  - Pitagora (incomplete GPU ecosystem)
- **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: 4e-14 s, 1,000 iterations.
  - Each job used 4 MPI ranks (one per GPU), and Each MPI task is explicitly 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: Preliminary Work

- **Environment setup:**
  - Creation of module-loading scripts per platform.
- **Cleanup of unused variables to remove warnings.**

```
picc  -c -O2 -noacc  bincc.c
"bincc.c",   line   13:   warning:   variable   "iisp"   was   declared   but   never   referenced
[declared_but_not_referenced]
   int        isp, iisp, i, s, p1, p2, nnp, k, sid, sod;
                     ^
```

- **Fixing segmentation fault caused by long file paths.**

```
Can't find input file /gpfs/projects/bsc21/bsc021331/BIT1/bit1-feature-GPU-OpenACC/tests/../BIT1_c8/at@N
Can't find input file /gpfs/projects/bsc21/bsc021331/BIT1/bit1-feature-GPU-OpenACC/tests/../BIT1_c8/at@@eH
```

- **Preparation for GPU port:**
  - Ensuring build consistency across supercomputers.

BIT1: CPU Version

- **Reference baseline performance:**
  - **Original BIT1 CPU:** runtime ~244.5 s.
  - **Instrumented CPU version:** runtime ~249 s (minimal overhead).
    step time ~260 ms
- **Modifications for GPU preparation:**
  - Inlining routines for GPU compatibility.

```
void chist_N()
{
 int     isp;

 for (isp=0; isp<nsp; isp++)
 {
   np_hist[isp][hist_hi2] = fnp(isp);

 }    /* end of for (isp=0...*/
}  /* END of chist_N() */
```

```
void chist_N()
{
 int     isp;
 int s, j;

 for (isp=0; isp<nsp; isp++)
 {
   //   np_hist[isp][hist_hi2] = fnp(isp);
   int j= 0;
   for (s=0; s<nc; s++)
     j += np[isp][s];
   np_hist[isp][hist_hi2] = j;
 }    /* end of for (isp=0...*/
}  /* END of chist_N() */
```

  - Replacing complex array accesses with local vars.

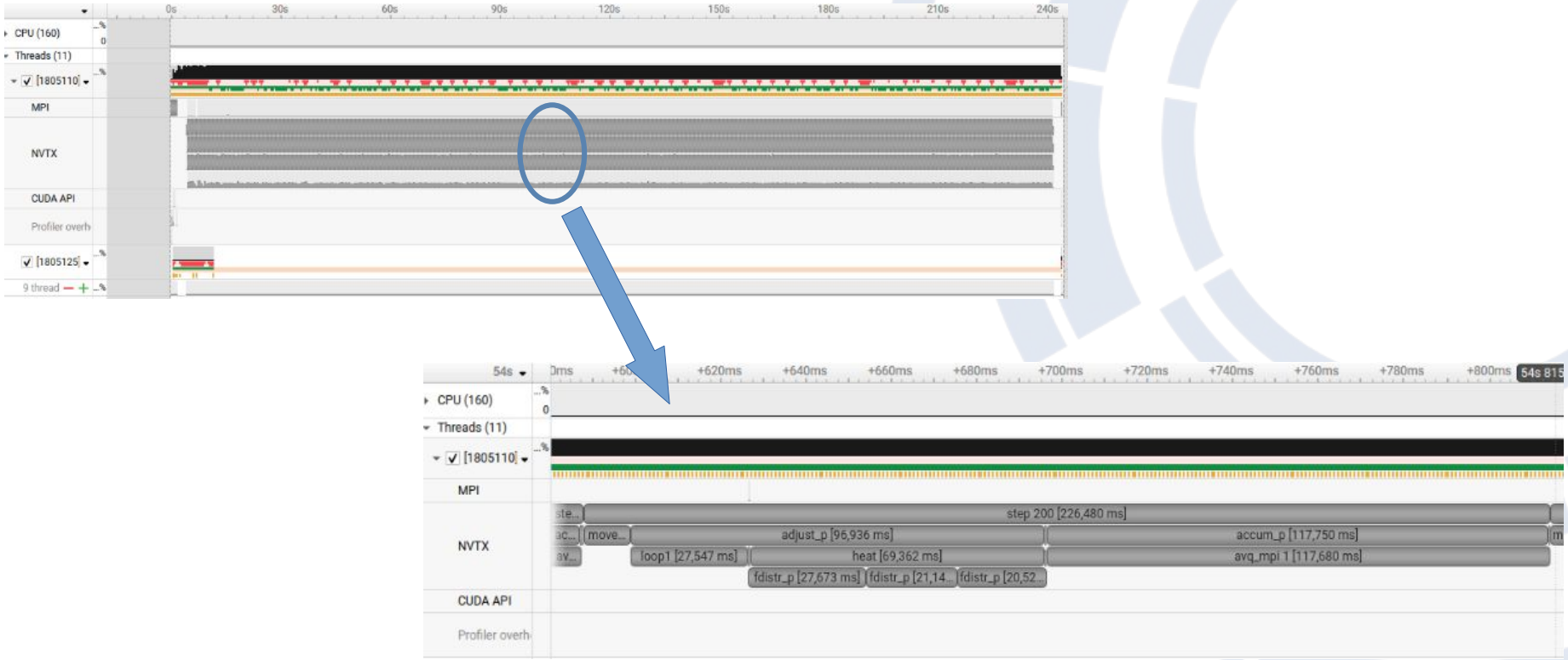
```
if (np[iisp][j])
{
  Tx[iisp][j] *= Tscale[iisp]/np[iisp][j];
  T_dif[iisp][j] *= Escale[iisp]/np[iisp][j];
}
```

```
 np_tmp = np[iisp][j];
 if (np_tmp)
{
  Tx[iisp][j] *= Tscale[iisp]/np_tmp;
  T_dif[iisp][j] *= Escale[iisp]/np_tmp;
}
```

  - Splitting large loops for better parallel analysis.

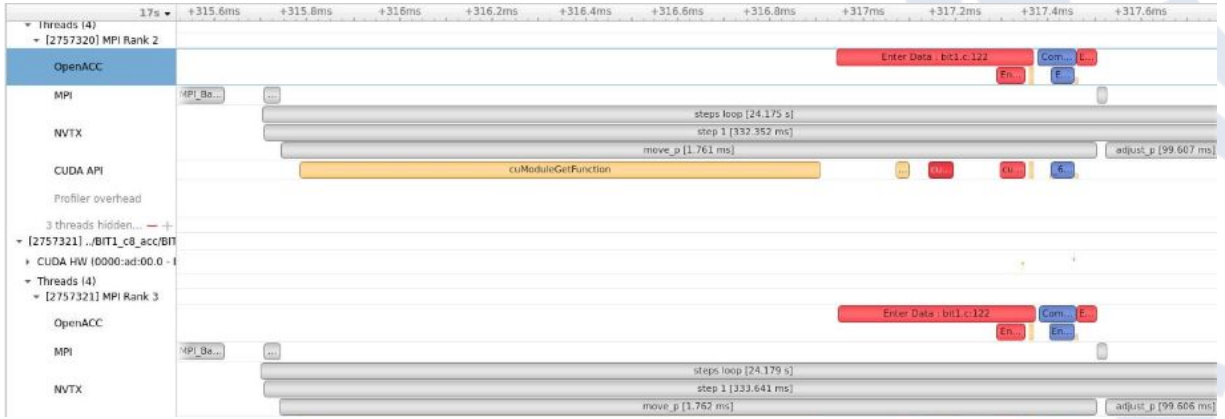
BIT1: CPU Version (2)

- **Trace:**
  - Execution flow of main PIC loop.
  - Time spent in particle mover and field solver.
  - Profiling used to identify GPU porting targets.



BIT1: First GPU Approach

- **Initial GPU-enabled routines:**
  - move0 (particle mover).
  - arrj (particle-to-cell assignment).
- **Results:**
  - move0 accelerated from 43.6s → 2.16s (20×).
  - Overall runtime worsened (0.87× speedup).
- **Reason: excessive CPU–GPU transfers.**
  - Led to strategy of porting all routines in test case.

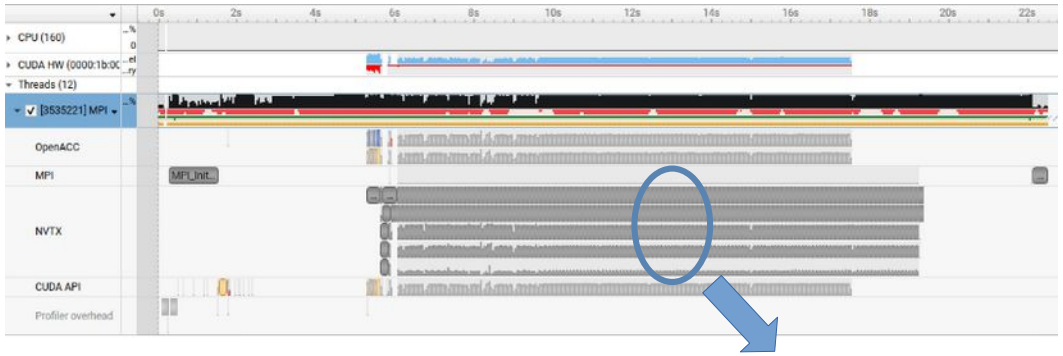


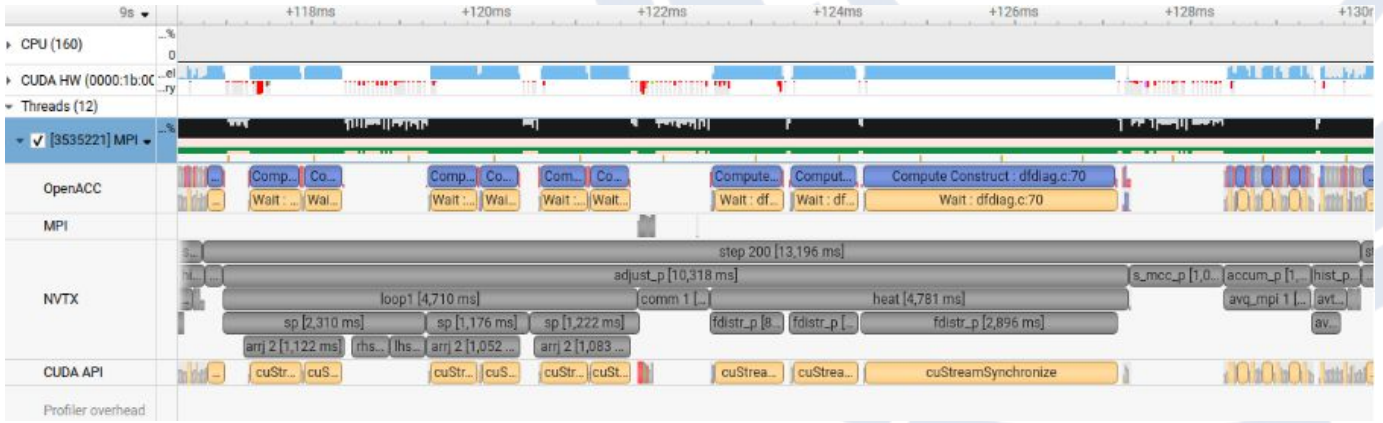
BIT1: GPU Version

- **GPU-enabled routines:**
  - 16 routines across 10 source files.
- **Substantial redesign of arrj for parallel execution.**
- **Performance:**
  - Total runtime improved from 249 s to 35.8 s (~7× faster).
  - Step time improved from 260 ms to 13 ms (~20× faster).
- **Most runtime now spent on GPU kernels.**

BIT1: GPU Version (2)

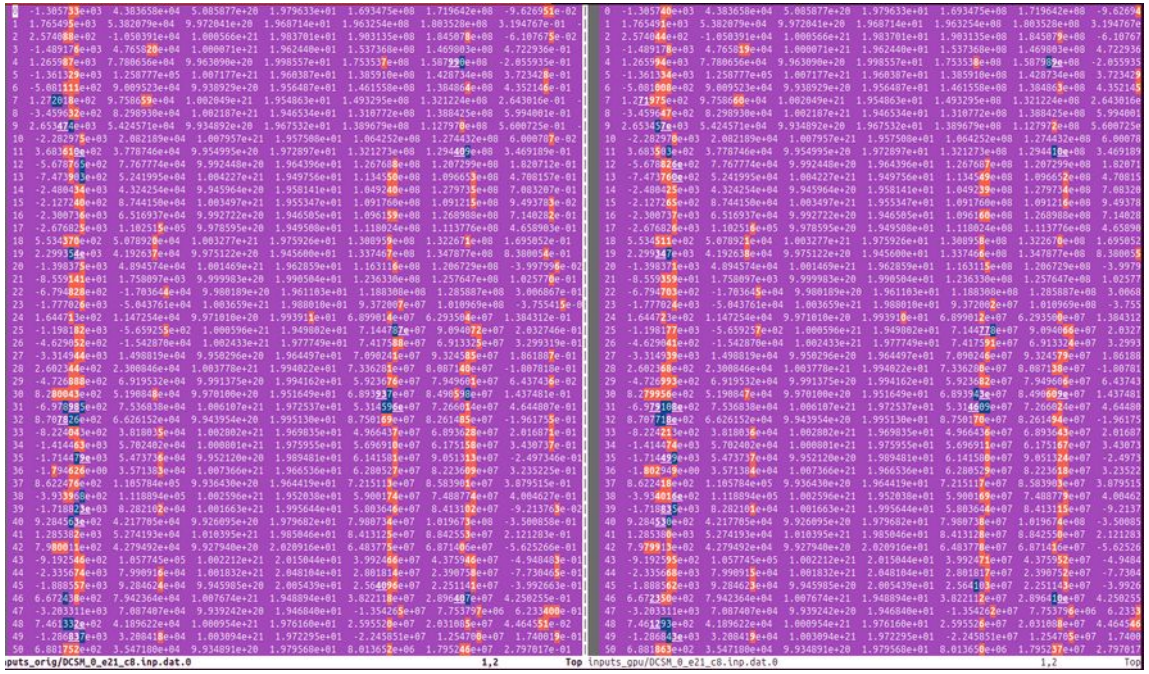
- **Trace:**
  - Dominance of GPU kernels over CPU execution.
  - Greatly reduced host–device transfers.
  - Balanced overlap of MPI communication.

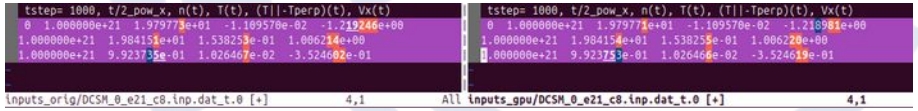




BIT1: Floating-Point Differences

- **GPU results differ slightly from CPU outputs:**
  - Due to different operation ordering in parallel execution.
  - Floating-point arithmetic differences between CPU/GPU.
- **All outputs provided for validation in the repository.**

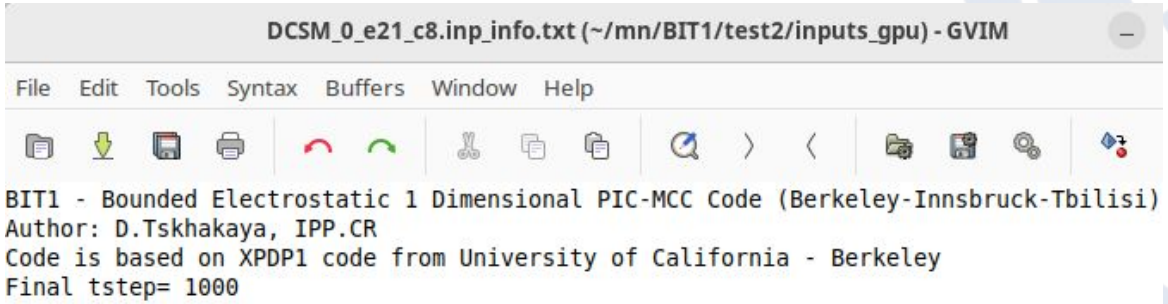




BIT1: Segmentation Fault After Completion

- **Observed crash after simulation ends:**
  - Occurs after all files are written.
  - Likely related to memory deallocation.
- **Does not affect correctness.**
  - Requires future debugging for clean execution.

```
=== Execute gpu version ===
time mpirun -n 4 ./wrap_nsys.sh ../src_gpu/BIT1 inputs_gpu/DCSM_0_e21_c8.inp
Max. number of particles per cell per species: 0  2000 1  2000 2  2000
[as03r5b31:3535221:0:3535221] Caught signal 11 (Segmentation fault: address not mapped to object at address 0x42058058)
Generating '/scratch/tmp/31995526/nsys-report-9ded.qdstrm'
```



BIT1: Conclusion

- **The main objective of porting BIT1 to GPUs using OpenACC was achieved,** with a maintainable and readable codebase preserved and GPU execution successfully demonstrated on a test case.

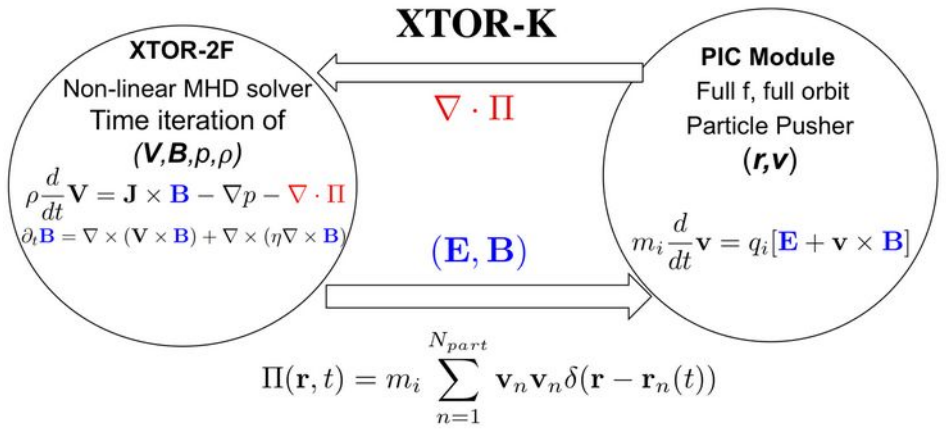
- **Next steps:**
  - **Fix finalization segmentation fault.**
  - **Extend GPU port with OpenACC:**
    - Continue adding OpenACC directives to the remaining code paths → decide new test cases.
    - Improve host–device data management:
      - Use manual control of data regions instead auto-managed memory.
      - Overlap communication and computation where possible.
  - **Perform a deep GPU redesign**

XTOR-K

Eduardo Cabrera

XTOR-K: Introduction

- XTOR-K is a fully implicit, HPC-oriented hybrid fluid–kinetic model that incorporates a Particle-in-Cell (PIC) Boris–Buneman particle pusher applied to one or more populations of kinetic ions. This enables the simulation of couplings between the Alfvénic spectrum and ion kinetic effects.
- It couples in a self-consistent manner the time advance of a complete set of bi-fluid equations in full tokamak geometry (thermalized plasma electron and ions background) with a 6D PIC method accurately integrating the trajectories of selected ion populations, making accessible new families of instabilities which are not allowed in a simplified framework such as magnetohydrodynamics.

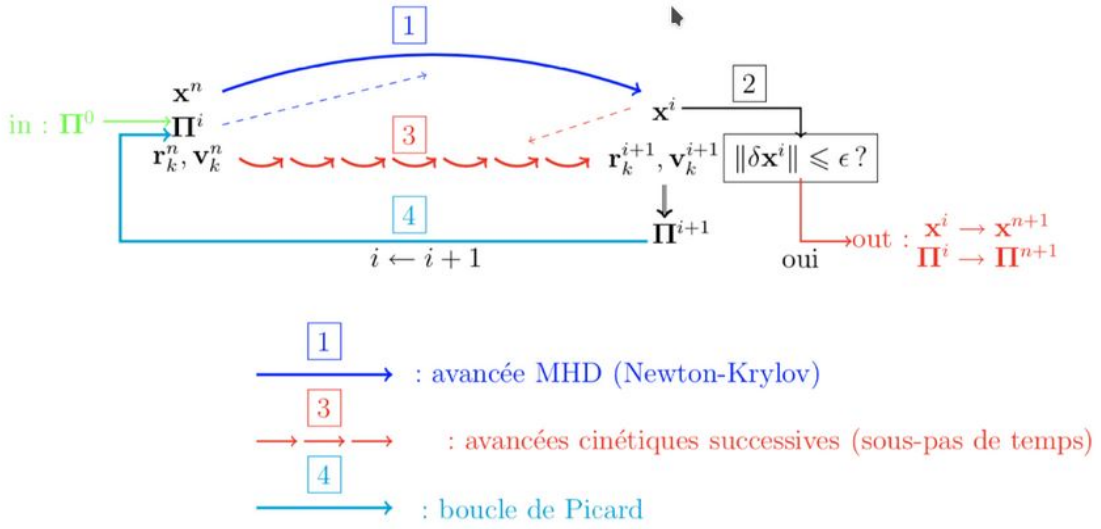


Hinrich Lütjens

- It is implemented in Fortran2008, parallelised with MPI and OpenMP already.

XTOR-K: Project Goal

- **Motivation:**
  - The kinetic component dominates the overall computational cost.
  - It relies on a PIC time-advance scheme.
- **Goal: Porting the kinetic components to GPU**
  - Reduce time spent in kinetic routines → Improve overall scaling.
  - Significantly increase the number of markers per simulation → Reduce the numerical noise inherent to the PIC method.



XTOR-K: Profiling & Bottlenecks

- **Profiling tool:**
  - Application Performance Snapshot (APS) from Intel VTune.
  - Runs performed on MareNostrum 5 (H100 GPUs, NDR InfiniBand)
- **Profiling results:**
  - Sligntly low vectorization → addressed using appropriate compiler flags
  - Main hotspots identified:
    - interpolate_eb_fields (most time-consuming routine).
    - moveRZ (calls interpolate_eb_fields multiple times).
    - OpenMP barrier synchronization overhead.
- **Conclusion:**
  - GPU porting targets these bottlenecks.

XTOR-K: CPU code

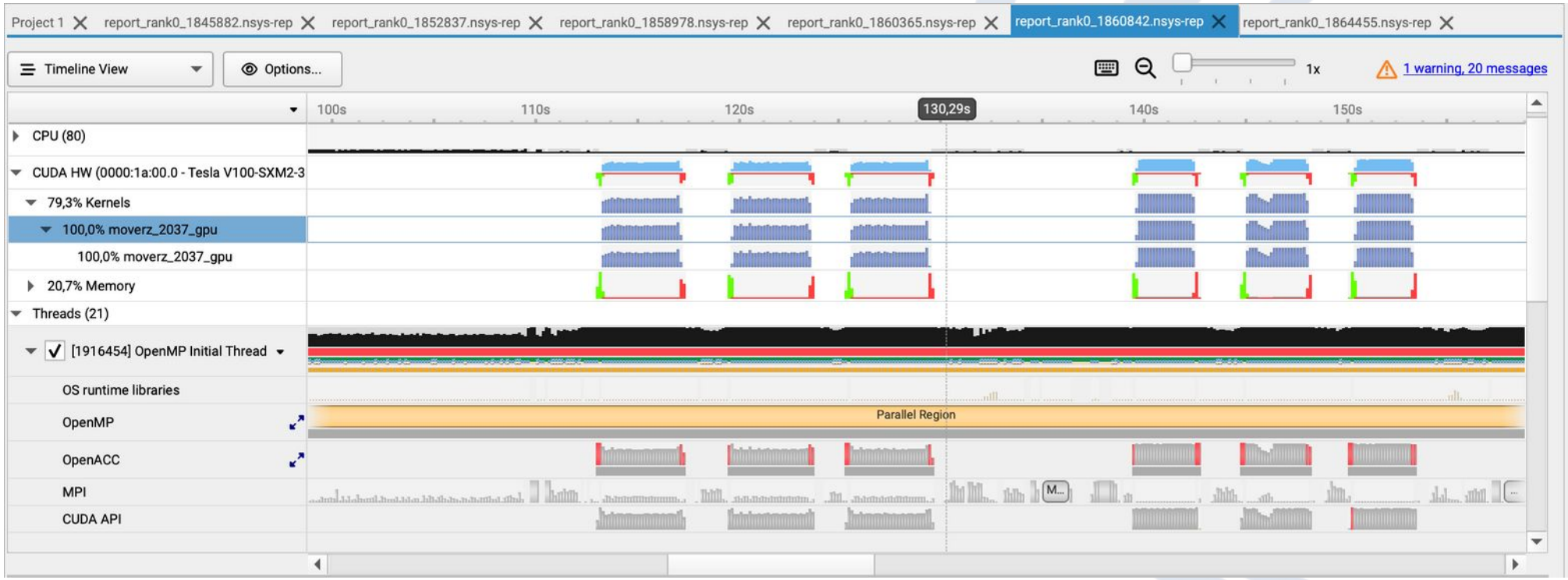
- **Ensuring a stable bug-free CPU version**
- **Identified and fixed issues when compiling with newer Intel compiler version**
  - PETSc type mismatches (e.g. ierr must be PetscErrorCode, not PetscInt).
  - Incorrect use of REAL for array indices → Replaced with proper INTEGER indices.
  - Division-by-zero errors when accessing ghost-point indices at domain boundaries.
  - Makefile compilation order issues → Reordered modules so dependencies are compiled first.
  - Mismatch between routine definitions and their implementations (argument list).
- **Outcome**
  - Stable and validated hybrid MPI/OpenMP CPU version ready.

XTOR-K: GPU Porting

- **Initial Approach:**
  - Tested OpenMP offloading option → more than 3x slower than CPU.
- **Final Approach**
  - Adoption of OpenACC.
  - Porting of 6 kinetic subroutines: particlepositioninfo, interpolate_eb_fields, particleshaperz, depositmoments, inirun and **moveRZ**.
  - **Issue:** Loops often too small (≤64 iterations) for efficient GPU parallelism.
  - **Revised Strategy:**
    - Parallelize only the outermost loop in moveRZ (# particles).
    - Execute the routines it calls serially on the GPU.
    - Transfer all required data (CPU -> GPU) prior to executing moveRZ routine.
- **Work completed:**
  - Full moveRZ routine successfully ported to GPU.
  - Additional routines (fullebeparmappingrz and fullparticleadvance) from non-kinetic part were ported.
  - Data transfer between CPU ans CPU streamlined.
  - Redundant MPI barriers calls removed.

XTOR-K: Performance Results

- **The GPU version outperforms the CPU version.**
- **Achieved simulations with up to 100 million particles per GPU → Not feasible on CPU nodes.**
- **GPU porting now enables large-scale simulations that were not feasible on CPU-only systems.**



XTOR-K: Future work

- **Ongoing Work:**
  - Porting projectedmomentsmappingrtheta subroutine using cuFFT and cuBLAS.
  - **Issues:** ~30 missed deallocations detected with compute-sanitizer tool.
  - **Critical issue:**
    - Argument-passing inconsistency: 3D array passed as 4D.
    - Fortran requires exact matching of array dimensions.
    - This inconsistency currently blocks completition of the GPU port.
- **Next steps:**
  - Clarification has been requested from developers regarding whether this array mismatch is intentional to evaluate alternatives.
  - Complete GPU port of the remaining routines.
  - Further optimization needed for data transfers.

Thanks for your attention !