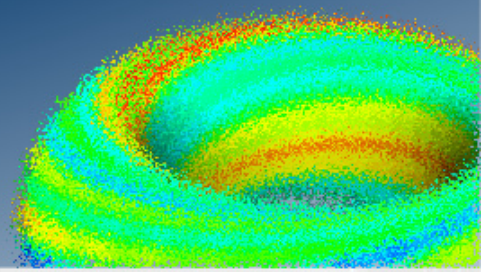
Fusion Group

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA



The Advanced Computing Hub at BSC:

Improving fusion codes following the principles of EUROfusion standard software

X. Sáez[1] , M. Garcia-Gasulla[1] , J. Vinyals[1] , C. Morales[1] , D. Vicente[1] , A. Soba[1,2] , I. Gasilova[1] , M. J. Mantsinen[1,3]

[1] Barcelona Supercomputing Center, Spain
[2] National Scientific and Technical Research Council (CONICET), Argentina
[3] ICREA, Barcelona, Spain

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EUROfusion

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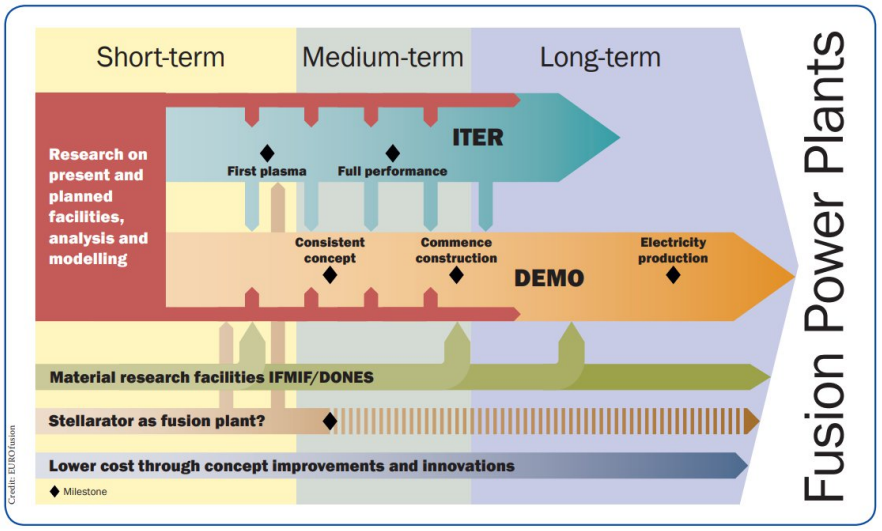
European Research Roadmap

- Provides a **clear and structured way toward commercial fusion energy**
- Is **the basis of the EUROfusion and Fusion for Energy programmes** for the realisation of Fusion Energy
- **Includes DEMO** design studies that are being conducted in Europe
- The DEMO project follows ITER with the goal of designing a commercial fusion power plant



Motivation

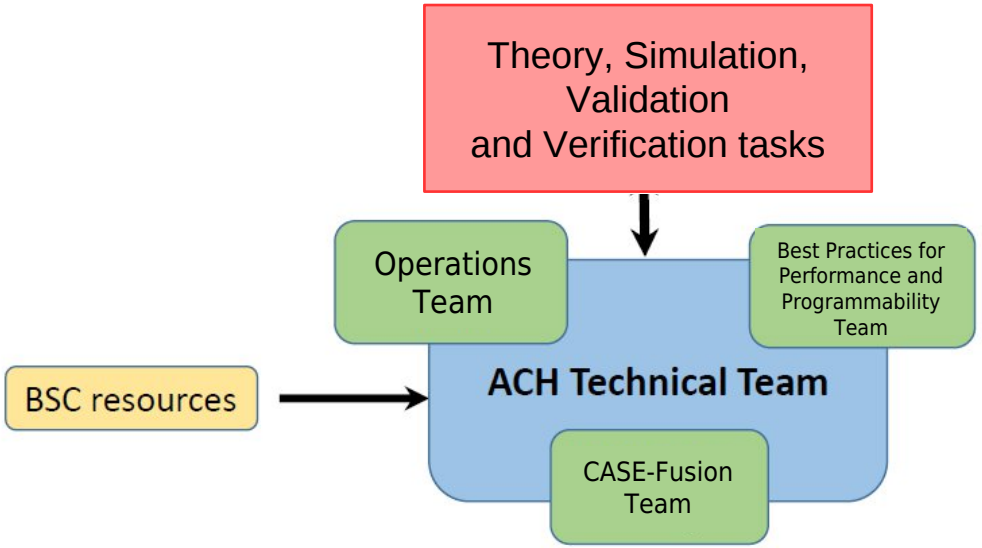
- **The step from ITER to DEMO is challenging**. DEMO design is complex in terms of the amount of systems needed to produce and control the plasma
- **Experimental data from ITER and IFMIF-DONES are essential, but not sufficient to design DEMO** with confidence in an unexplored environment to predict plasma and materials performance
- There is a need to create a high-quality suite of research codes (**EUROfusion-standard software**) to model data from existing EUROfusion facilities and to reliably extrapolate to future devices

EUROfusion ACHs

- The goal is to bring together fusion physicists, materials scientists and engineers with computer scientists within the same organisational framework to make use of high-performance computers (HPC) and accelerate the development of fusion energy
- EUROfusion has initiated coordination among theory and advanced simulation creating:
  - **Theory, Simulation, Validation and Verification tasks** (TSVV) that perform fundamental research and channel science
  - **Advanced Computing Hubs** (ACHs) that provide advanced simulation expertise and knowledge to TSVVs

BSC-ACH

- Barcelona Supercomputing Center (BSC) has been awarded one of these ACH that will offer advanced simulation to TSVVs
- **BSC-ACH provides expert support to users regarding High-Performance Computing (HPC)**:
  - *scalable algorithms*
  - *code parallelization*
  - *performance optimization*
  - *code refactoring*
  - *GPU-enabling*
  - …

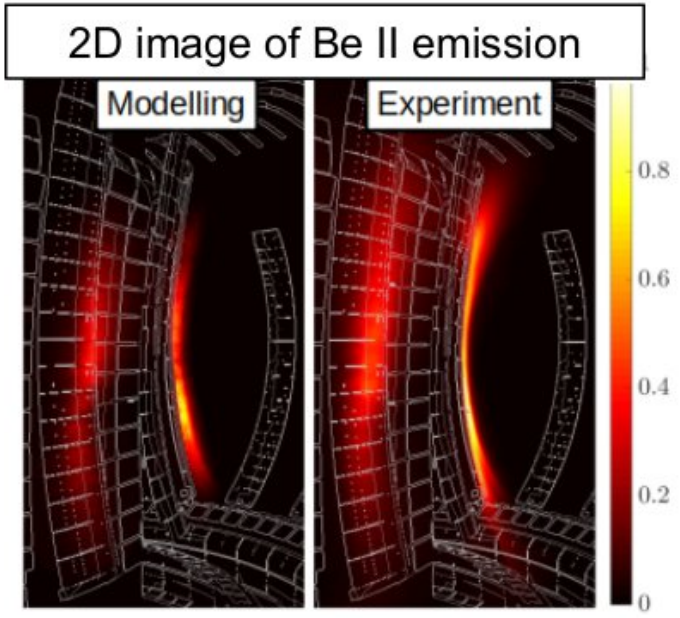


Codes assigned to BSC-ACH

Code	Work required	Code Coordinator	Groups in charge	Start
ERO 2.0	GPU porting	Dmitry Matveev, Juri Romazanov	CASE-Fusion, Best performance…	2022
SPICE2	Implementing a parallel Poisson Solver and a Parallel electric field calculations.	Michael Komm	CASE-Fusion, Operations	2022
KNOSOS	Optimization.	José Luis Velasco	Operations	2022
STELLA	Optimization.	Michael Barnes	Best performance…	2022
SOLPS	• Check the correctness of the OpenMP multi-threading • Improve compiler options and/or job submission script • Consider vectorization of the code profitable for use on Cray platforms	David Coster	Operations, Best performance…	2023
STELLA	Optimization.	Michael Barnes	Best performance…	2022
XTOR-K	GPU porting	Hinrich Lutjens	CASE-Fusion, Operations	2023
BIT1	GPU porting	David Tskhakaya	CASE-Fusion, Operations	2023
GENE-X	• Implementing the ability to access the unstructured computational grid in arbitrary order • Testing the performance of different reordering strategies	Philipp Ulbl	CASE-Fusion, Operations	2023
JOREK	Reduce memory consumption and improve performance	Matthias Hoelzl	CASE-Fusion, Operations	2023

ERO2

- ERO2.0 is a code for modelling plasma-wall interaction and global material migration in fusion devices. The migration is simulated by following 3D trajectories of Monte-Carlo test particles
- **Language:** C++
- **Parallelization:** MPI + OpenMP



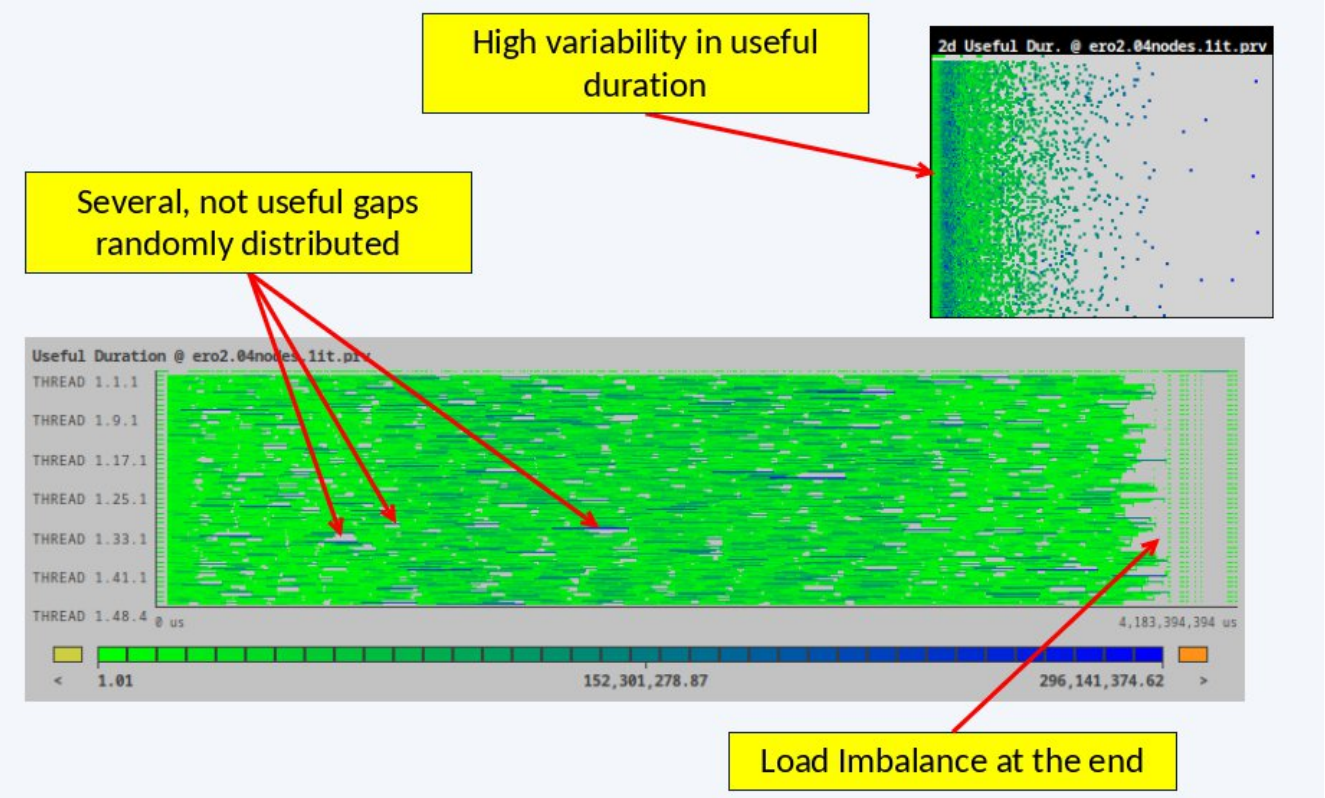
ACH tasks

- Performance analysis
- Porting to GPUs

ERO2

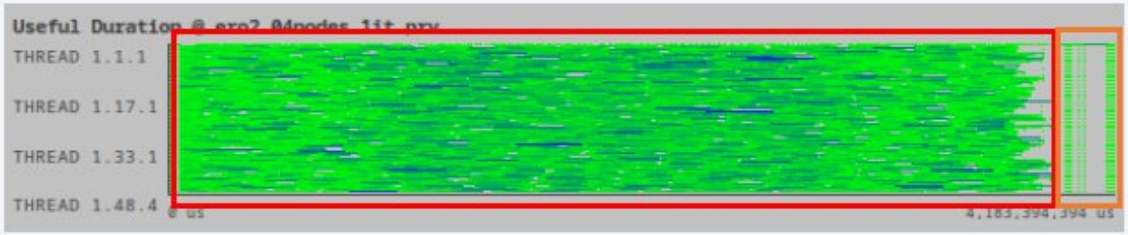
Tracing

- BSC Tools: Extrae and Paraver (http://tools.bsc.es)

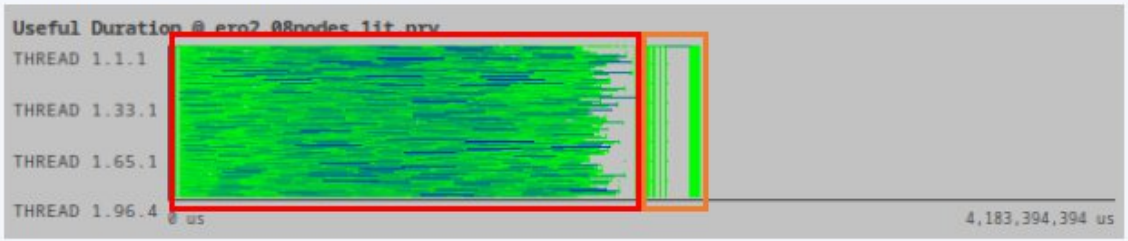


ERO2

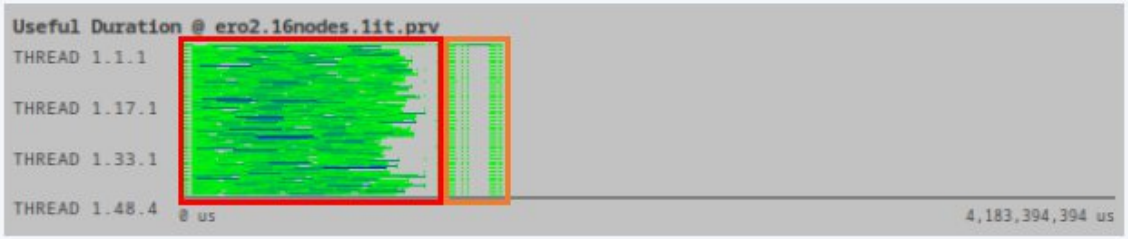
4 nodes



8 nodes



16 nodes

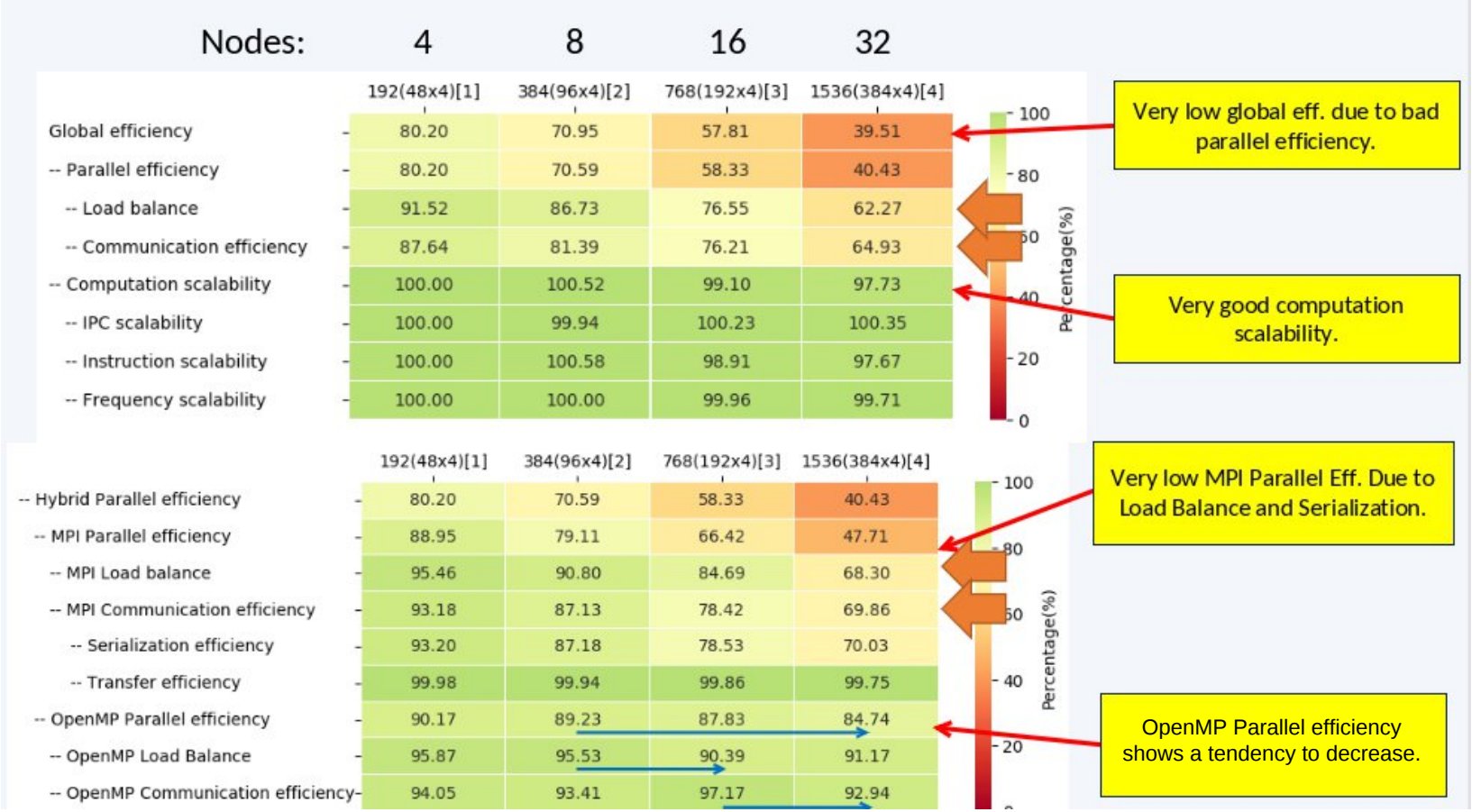


32 nodes

- Gathering phase does not scale.
- Computation seems to scale.
- Load imbalance increases.

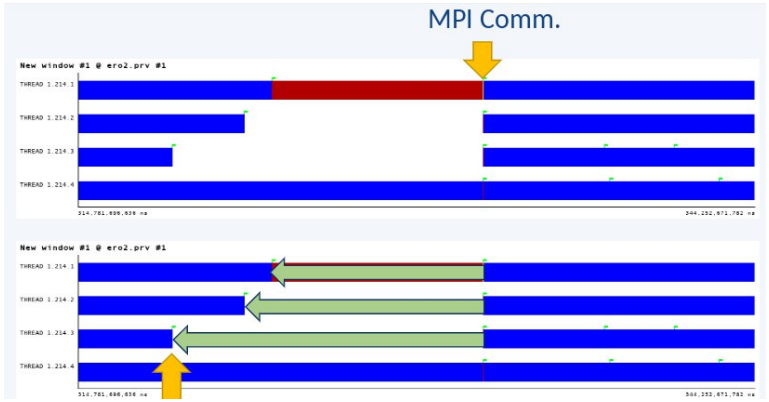
ERO2

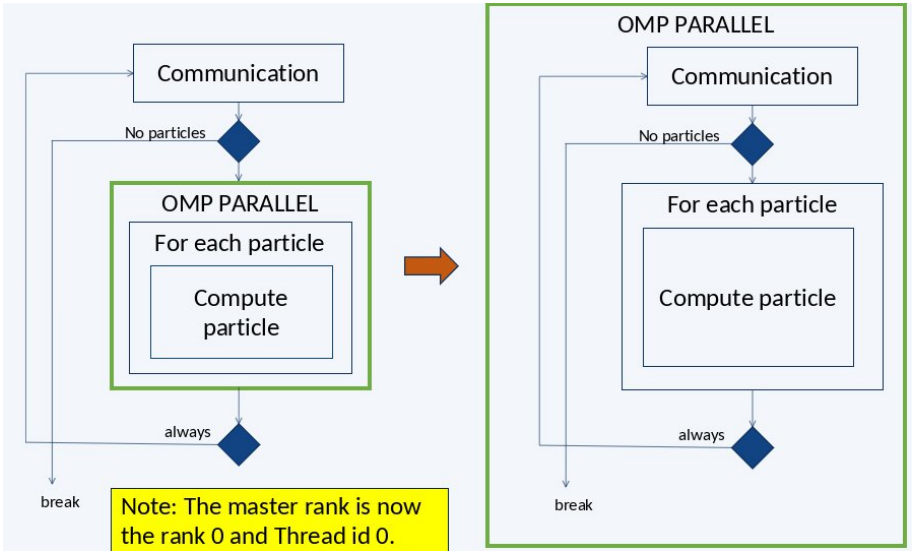
Global efficiency metrics



ERO2

Optimization





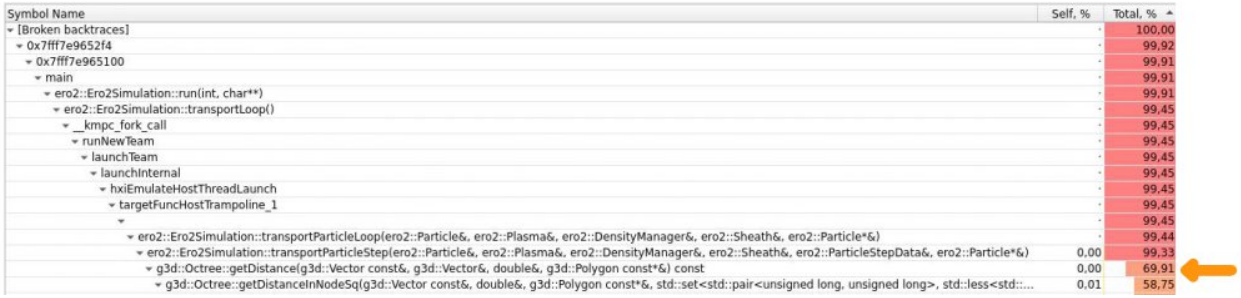
- Include MPI communication inside the OpenMP parallelization, so new work can be started when threads start idle

ERO2

Porting to GPU

- OpenACC
  - The compiler is responsible for generating kernel and managing data transfers
- Find top time-consuming routine ⇒ octree distance search

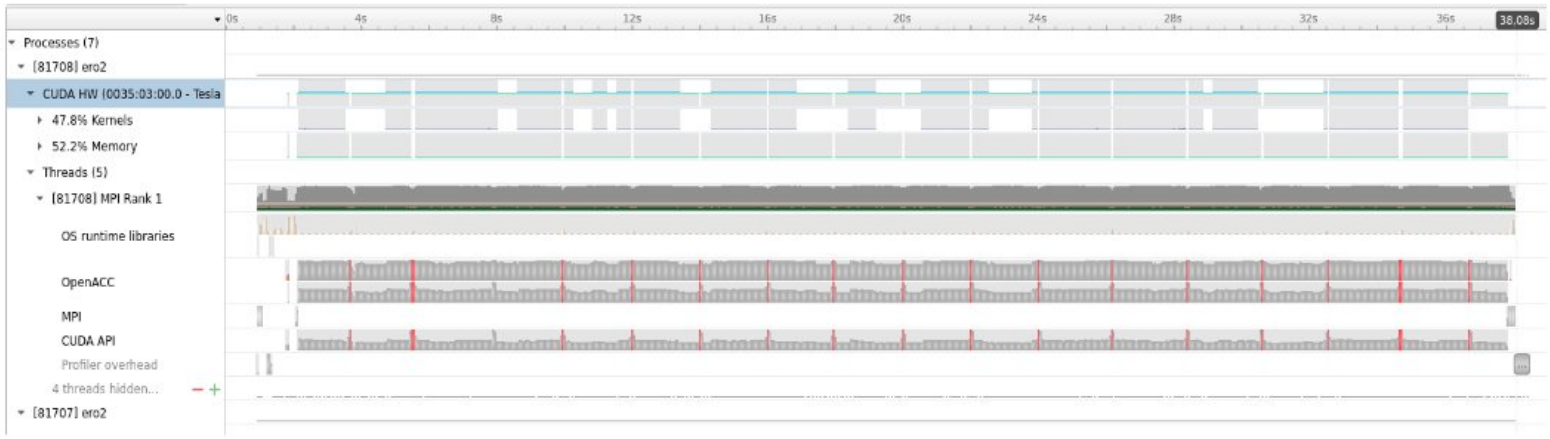
  Intel VTune (https://www.intel.com)



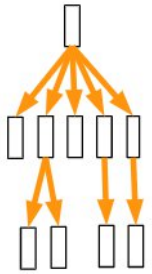
- Issues:
  - C++-style loops are not supported
  - Polymorphism is not supported
  - Routine calls within parallel loops can be problematic
  - …
- However, it is not as ideal as it was initially expected
  - OpenACC has lacks with C++
  - The feedback from error messages is not very clear

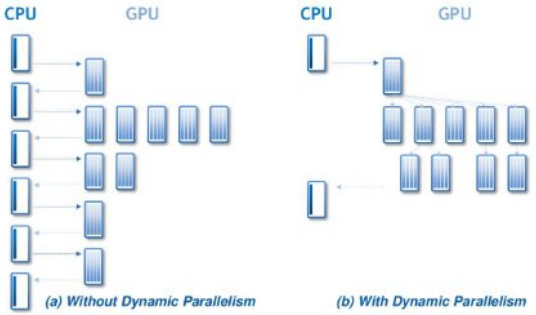
ERO2

- NVIDIA Nsight (https://developer.nvidia.com/nsight-visual-studio-edition)



- Next steps
  - OpenACC + CUDA interoperability
  - CUDA Dynamic Parallelism: Recursive search into Octree





SPICE2

- Particle-In-Cell (PIC) code dedicated to performing simulations of particles in a fixed magnetic and self-consistent electric field for the study of plasma deposition near castellated plasma facing components
- **Language:** Fortran
- **Parallelization:** MPI

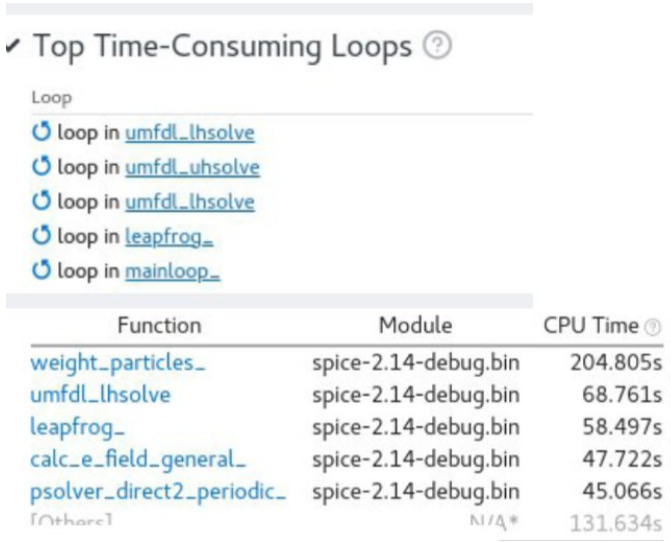
ACH tasks

- Implementation of 2D parallel Poisson solver that the number of cores in simulations can be increased to at least 128
- Implementation of a parallel routine for E-field calculation
- General improvement of the code

SPICE2

Profiling

- Intel Tools : VTune and Advisor
  (https://www.intel.com/content/www/us/en/developer/tools/oneapi/vtune-profiler.html)

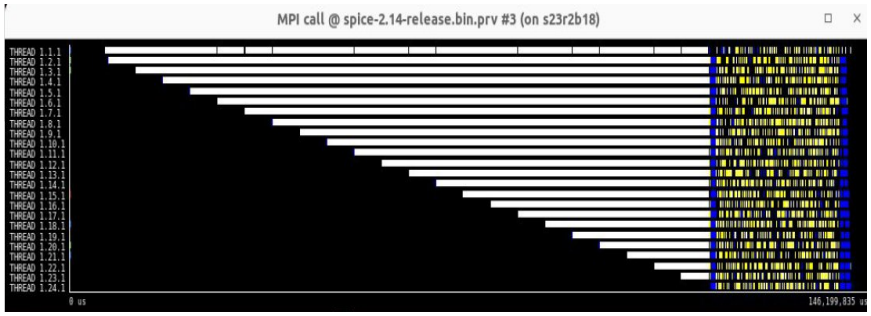


- By modifying the most consuming parts of the code, we achieve small improvements

SPICE2

Tracing

- BSC Tools: Extrae and Paraver (http://tools.bsc.es)

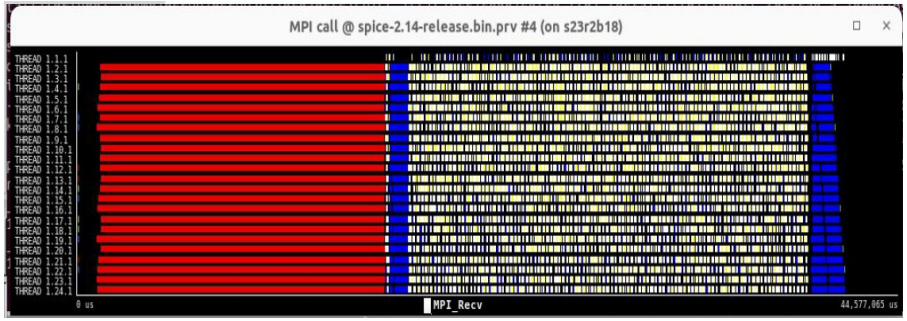


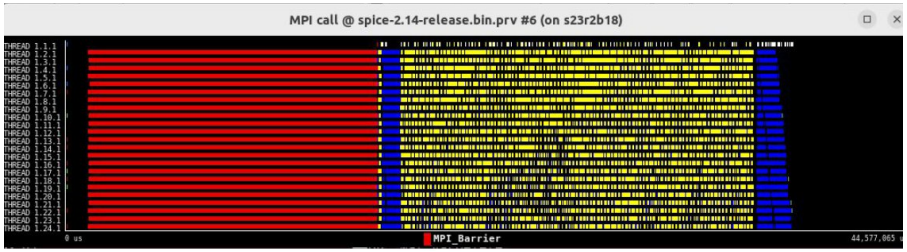
- All processes write to the same file at the beginning of the simulation
- Each process waits 6*their_rank seconds to start writing

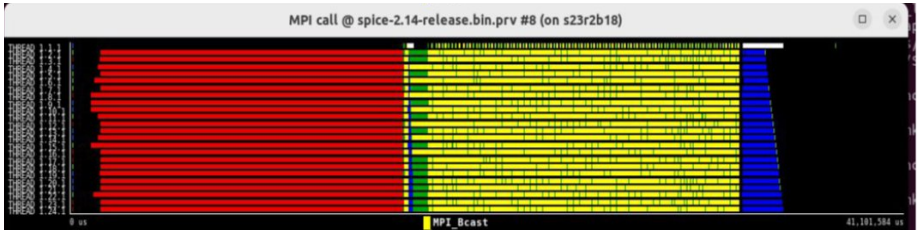
- We updated the code to only do one writing on the process with rank 0 and the others processes wait on a Barrier

SPICE2

Optimizing





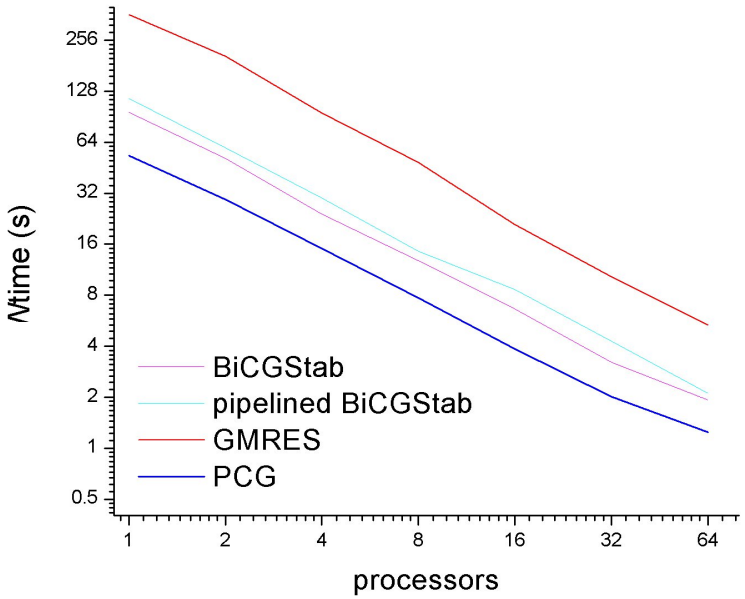


- The potentials are sent to all the processes from rank 0 with Point-to-Point (P2P) calls
- The density vector is calculated on process 0 and sent to all the processes with P2P
- Code updated to send the potentials with the MPI_Broadcast collective
- Code updated using MPI_Reduce collective to compute the density vector

SPICE2

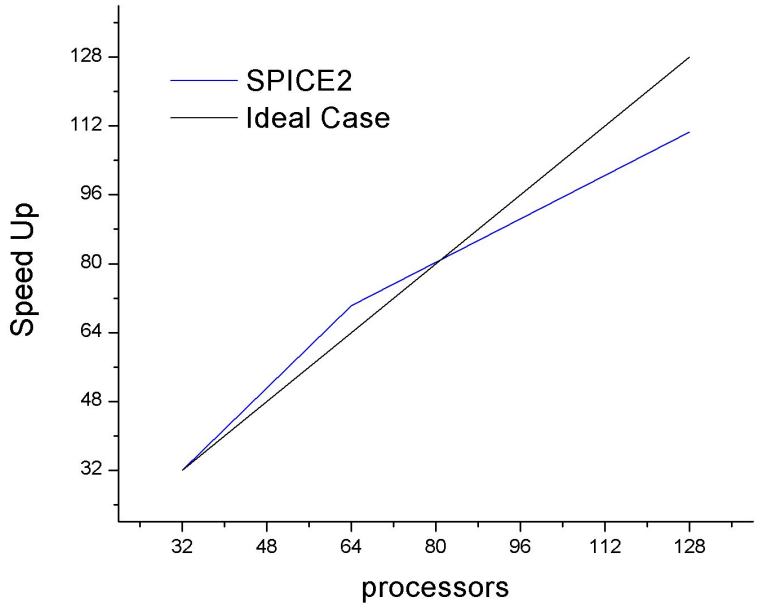
Implementation (Poisson solver)

- **Current implementation:** Direct solver based on LU decomposition using the UMFPACK and BLAS libraries
- **Limits**: good scaling up to 32 cores (memory limit of the system) and a grid limit of ~ 4000 cells in one dimension
- **Solution**: use a KSP linear solver based on PETSc library (https://petsc.org). Several options of solvers were explored
- The best time is obtained for Conjugate Gradient with Jacobi preconditioner solver



SPICE2

- **Results:**
  - Speed up of the whole code with the new solver included
  - Good performance up to 128 processors
  - Loss of scalability for more than 256 processor, but the code can now run over 512 processors, solving domains of 10000x4000 cells (Marconi)



KNOSOS

- Code that calculates neoclassical transport in low-collisionality plasmas of 3D magnetic confinement devices by solving the radially local drift-kinetic and quasineutrality equation
- **Language:** Fortran
- **Parallelization:** MPI

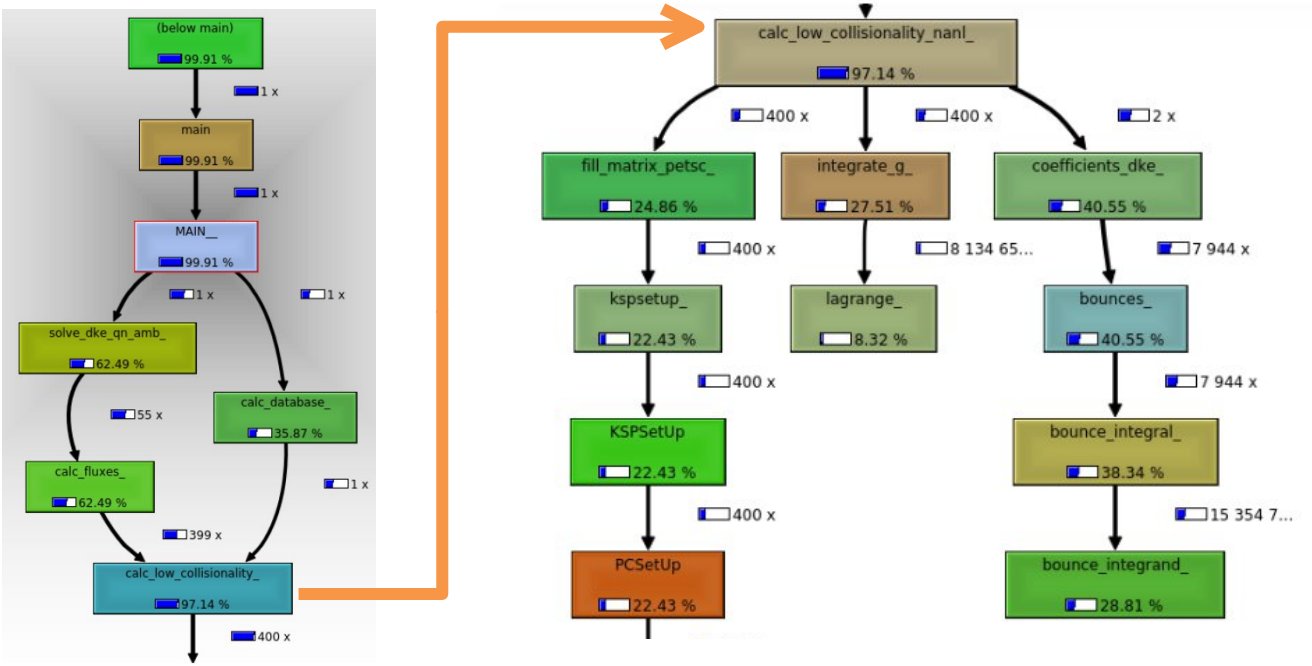
ACH tasks

- Overall performance assessment
- Optimize application

KNOSOS

Profiling

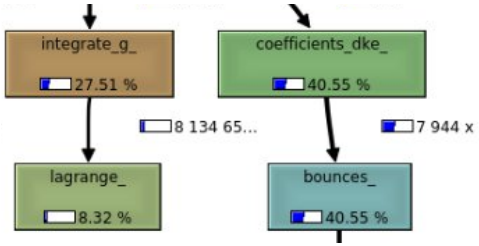
- There is a high load imbalance between MPI ranks, which seems to be produced by different number of iterations in subroutines ⇒ feedback from developers
- Discover that parallelization relies on launching “independent” calculations ⇒ **improving sequential version would translate to an overall improvement in the MPI version**
- Firstly, identify the most time consuming parts of the code with Valgrind (https://valgrind.org)



KNOSOS

Optimization

- Introduce a new parallelization level using OpenMP in `coefficients_dke` routine
- It was found that different instances of the BOUNCES subroutine could be performed in parallel without producing data conflicts between iterations
- **Result**: Execution time was reduced from 15 sec (sequential) to 10 sec (using 4 OpenMP threads)
- We repeat the process with `integrate_g` routine. However, the improvement was negligible




```
!$OMP PARALLEL DO FIRSTPRIVATE(Q)
  DO ipoint=1,npoint
     iw =i_w(ipoint)
     ila=i_l(ipoint)
     CALL BOUNCES(iw,z1(iw),t1(iw),B1(iw),hBpp1(iw),vd1(:,iw), &
          &          zb(iw),tb(iw),Bb(iw),hBppb(iw),vdb(:,iw), &
          &          z2(iw),t2(iw),B2(iw),hBpp2(iw),vd2(:,iw), &
          & 1./lambda(ila),ipoint.EQ.1,nq,Q,&
          & zlw(ipoint),tlw(ipoint),zrw(ipoint),trw(ipoint))
     BI1(ipoint)=Q(1)
     BI2(ipoint)=Q(2)
     BI3(ipoint)=Q(3)
```

Conclusions

- The Advanced Computing Hubs have an ambitious mission to accomplish in a small time window
- The creation of EUROfusion-standard software needs close collaboration between developers and computer science professionals
- We have shown some examples of our work, with different degrees of success to build trustable software capable to run efficiently in HPC systems
- In some cases, the best solution does not accomplish the objectives or the wishes of the developers

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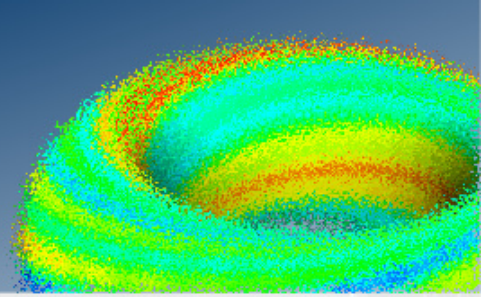

Thank you

fusion.bsc.es

@Fusion_BSC

fusion@bsc.es

xavier.saez@bsc.es