PLASMA PEPSC

https://plasma-pepsc.eu/

Plasma-PEPSC
Plasma Exascale-Performance Simulations CoE
PDC Summer School 2023

Stefano Markidis
Coordinator

Outline

- The Plasma-PEPSC EuroHPC CoE
- Vision
- Four Plasma Simulation Codes
- Our Approach
- Conclusions

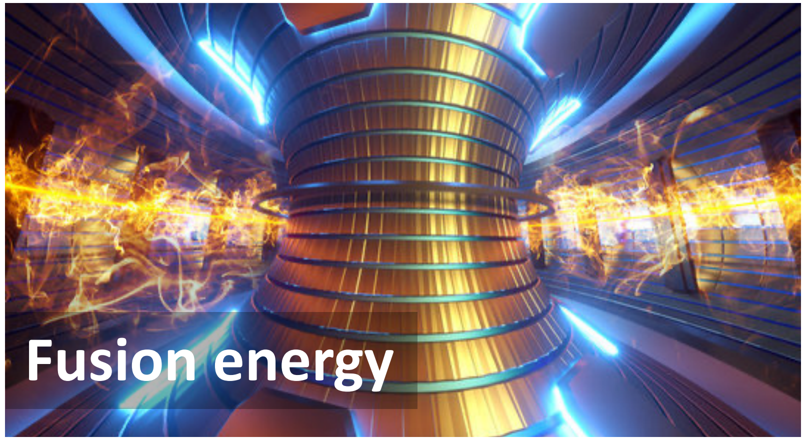

Plasma-PEPSC Kick-off Meeting
Stockholm, January 24-25, 2023
PLASMA
PEPSC

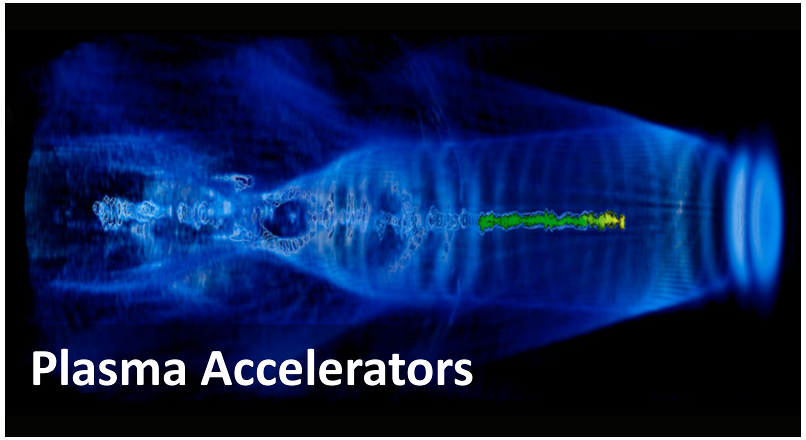
PLASMA PEPSC

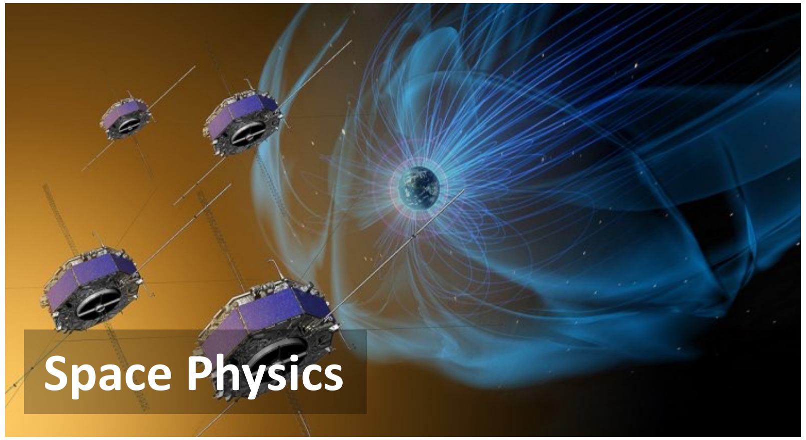
Call: HORIZON-EUROHPC-JU-2021-**COE-01** - Centres of Excellence preparing applications in the Exascale era
Duration: 4 Years. It started on Jan.1, 2023
Budget: 7.9M€

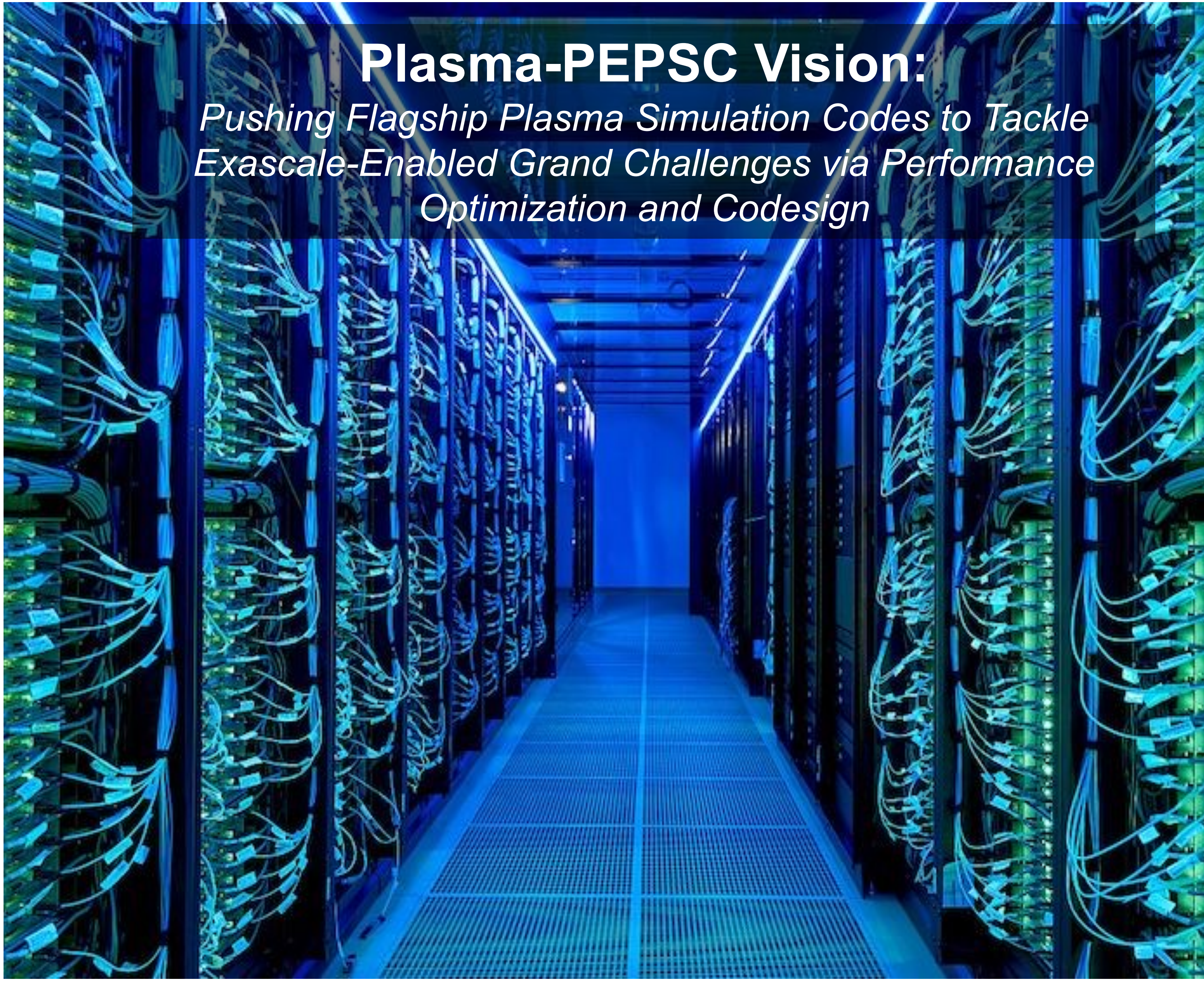
Partners:
- Academia: KTH (Coordinator), UoH, UL, TUM
- High-performance computing centers: BSC, PDC at KTH, and MPCDF at MPG.
- Research institutes and laboratories: IPP MPG, IPP CAS, FORTH, HZDR
- Industry: SIPEARL

Website: https://plasma-pepsc.eu/


Fusion energy

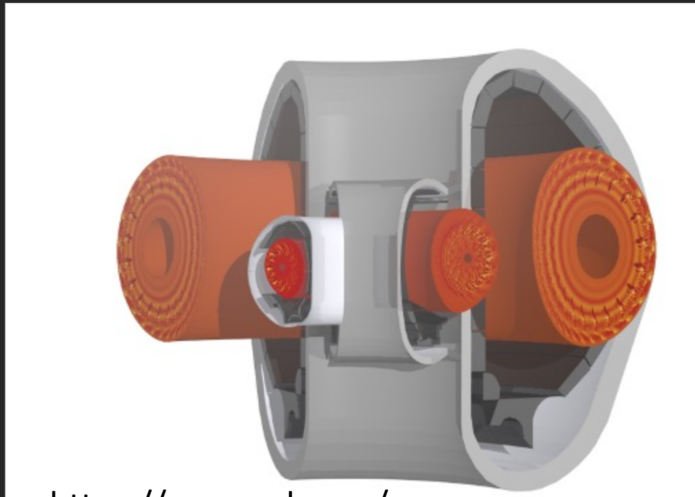

Plasma Accelerators


Space Physics


Plasma-PEPSC Vision:
Pushing Flagship Plasma Simulation Codes to Tackle Exascale-Enabled Grand Challenges via Performance Optimization and Codesign

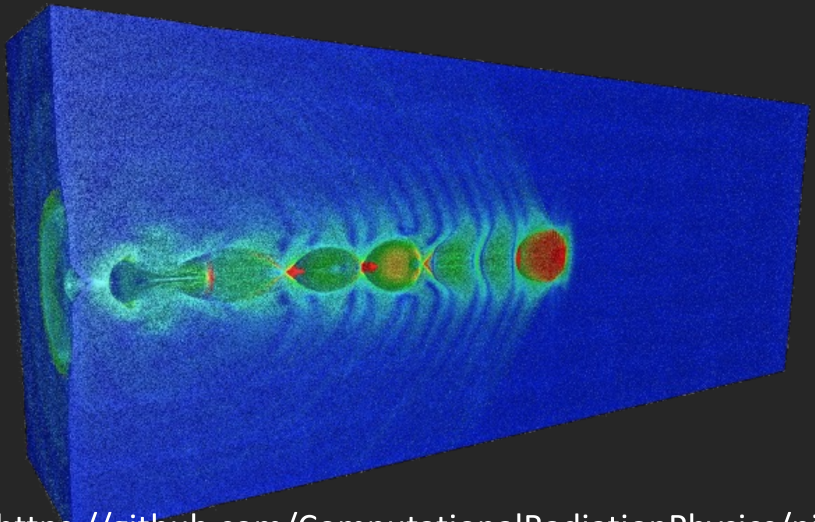
Plasma-PEPSC Flagship Codes

GENE / GENE-X



https://genecode.org/

PIConGPU

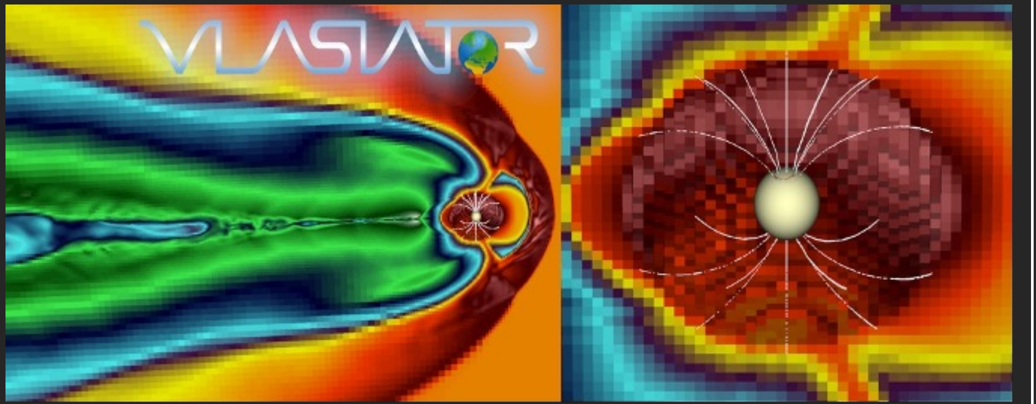


https://github.com/ComputationalRadiationPhysics/picongpu

BIT

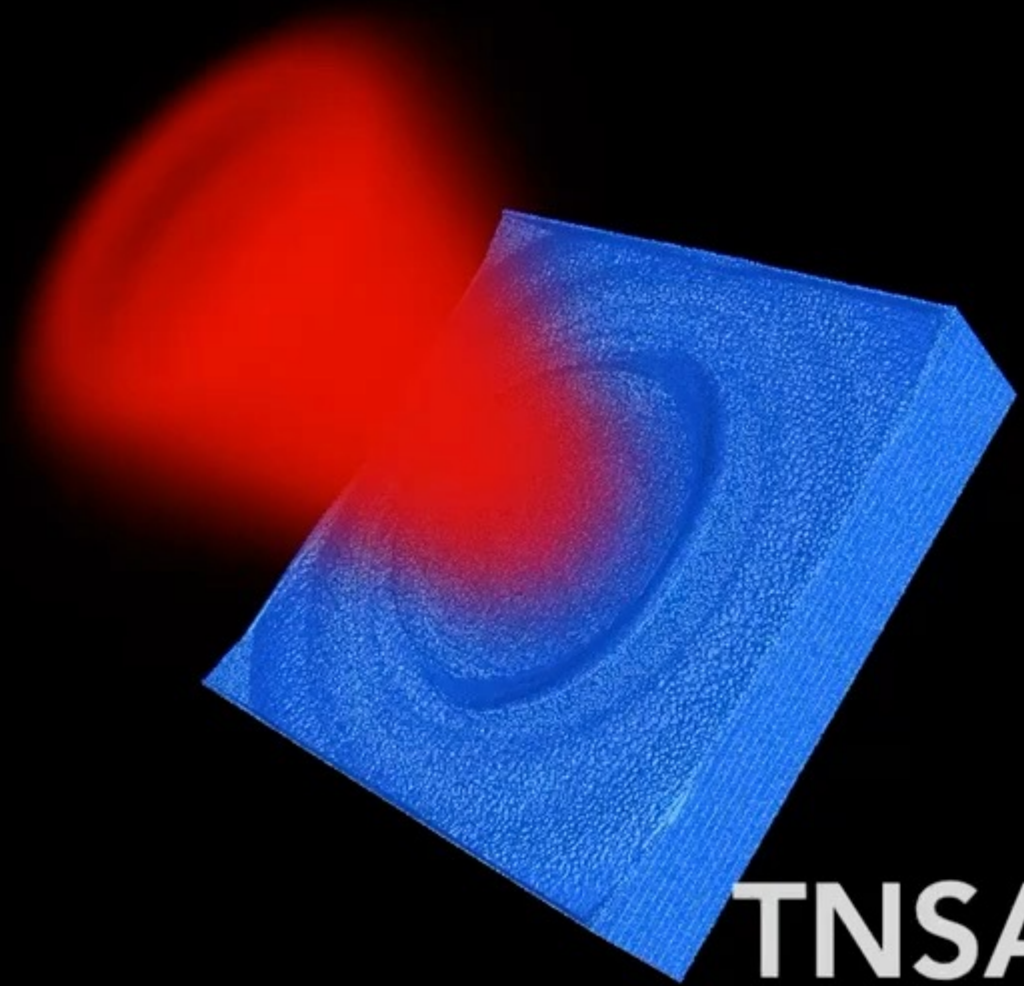
https://repo.tok.ipp.cas.cz/tskhakaya/bit1

Vlasiator



https://github.com/fmihpc/vlasiator

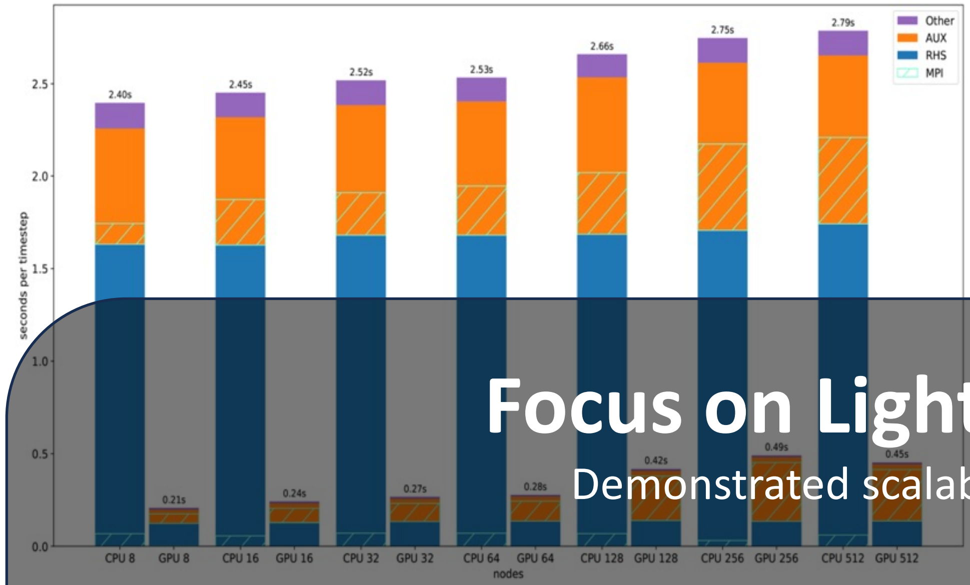
PIConGPU
ISAAC

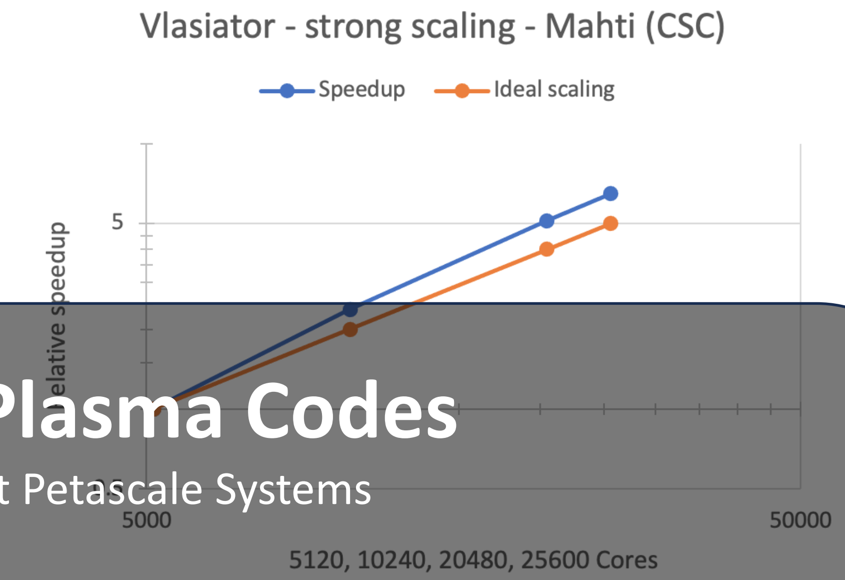


TNSA

TARGET NORMAL SHEATH ACCELERATION

GENE Scaling





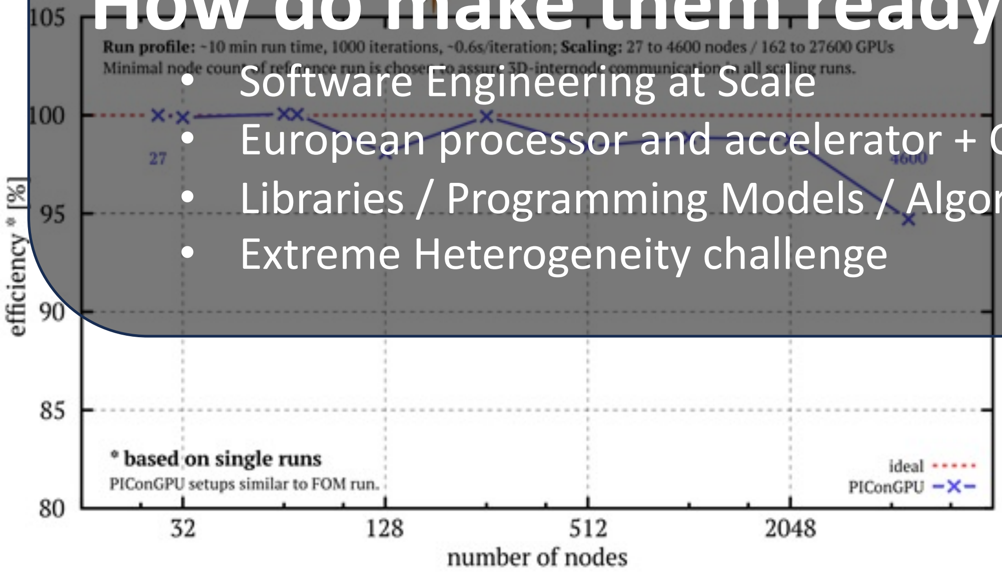
Focus on Lighthouse Plasma Codes

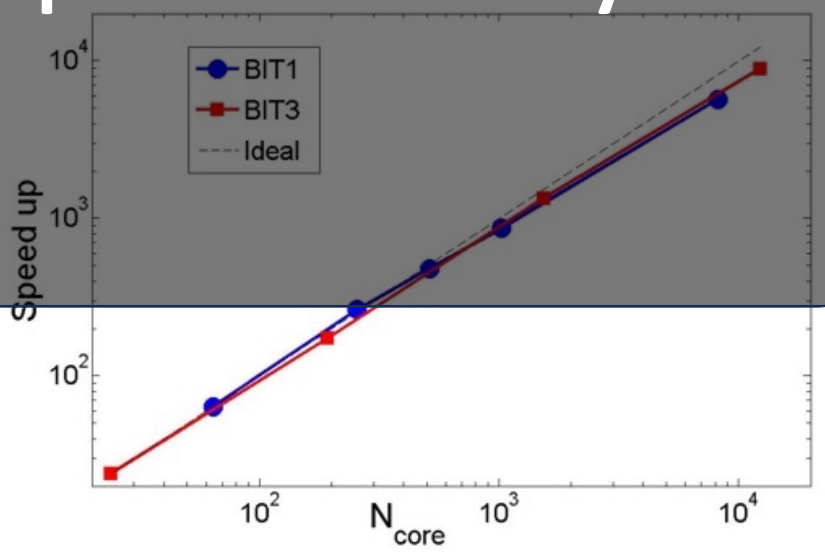
Demonstrated scalability of current Petascale Systems

How do make them ready for European Exascale Systems?

- Software Engineering at Scale
- European processor and accelerator + Quantum
- Libraries / Programming Models / Algorithms
- Extreme Heterogeneity challenge

PIConGPU Scaling

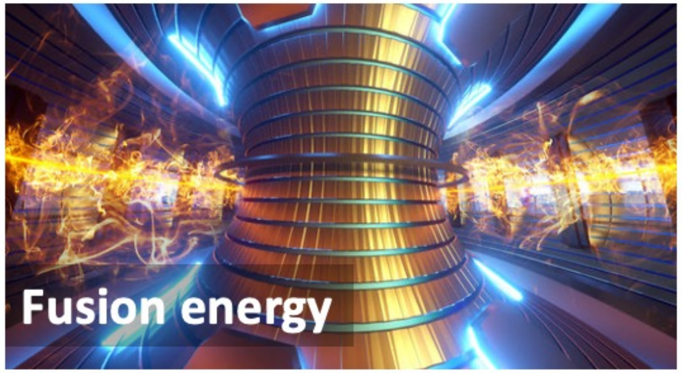


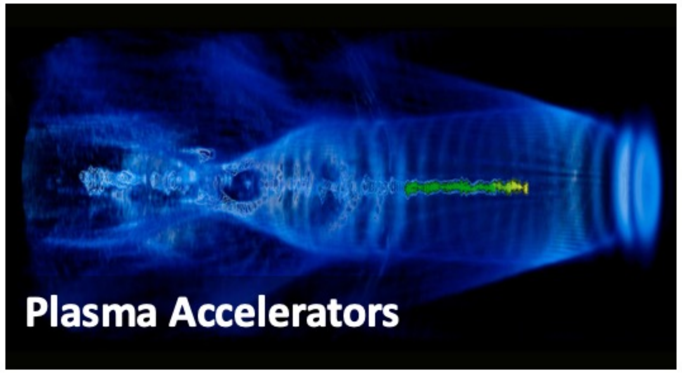


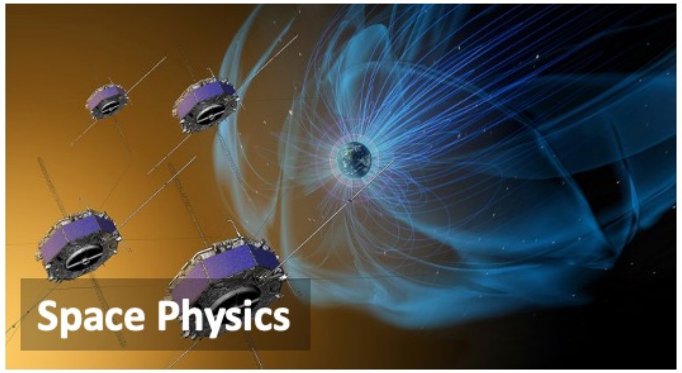
BIT Scaling

Five Technical WPs

WP1 - *Plasma Simulations – Codes and Grand Challenges*







WP2 - *Co-design of Plasma Simulation Codes with the European Processor and Accelerator*

- EPI Processor
- EPI Accelerator
- Quantum Computing

WP3 - *Algorithms and Libraries for Extreme-Scale Plasma Simulations*

- MPI
- Load-balancing
- Resilience & Fault-tolerance

WP4 - *Extreme Data Analytics for Plasma Simulations*

- Parallel I/O
- In-situ data analysis
- Compression

WP5 - *Accelerated Plasma Simulations on Heterogeneous Systems*

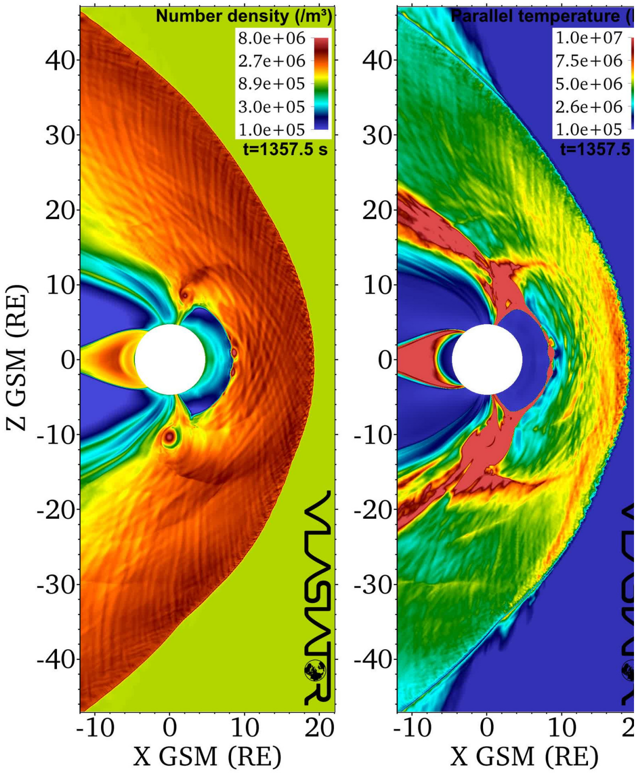
- Redesigning Algorithms, Porting, and Optimization for Accelerators
- Application Data Placement and Migration for Heterogeneous Memories

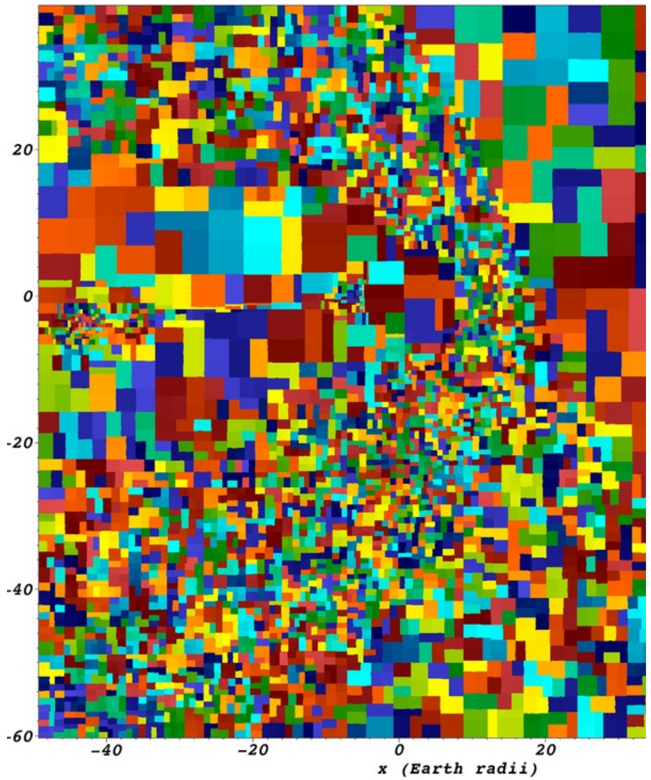
Software Engineering at Scale – Impact the Community

- Ensuring deployment of four codes on the EuroHPC systems
  - Automatic deployment with CASTIEL 2
  - Performance regression tests
- Continuous-Integration
- Documentation and user-support
- Requirement handling
- Bug tracking

Libraries & Algorithms – The Building Blocks

Dynamic Load Balancing in Vlasiator

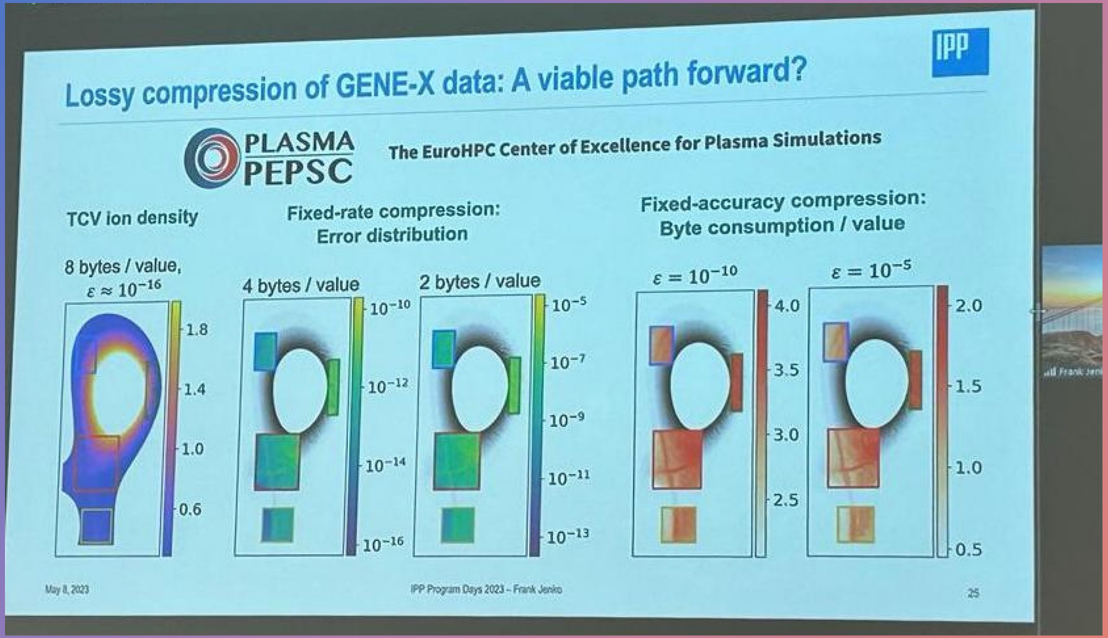


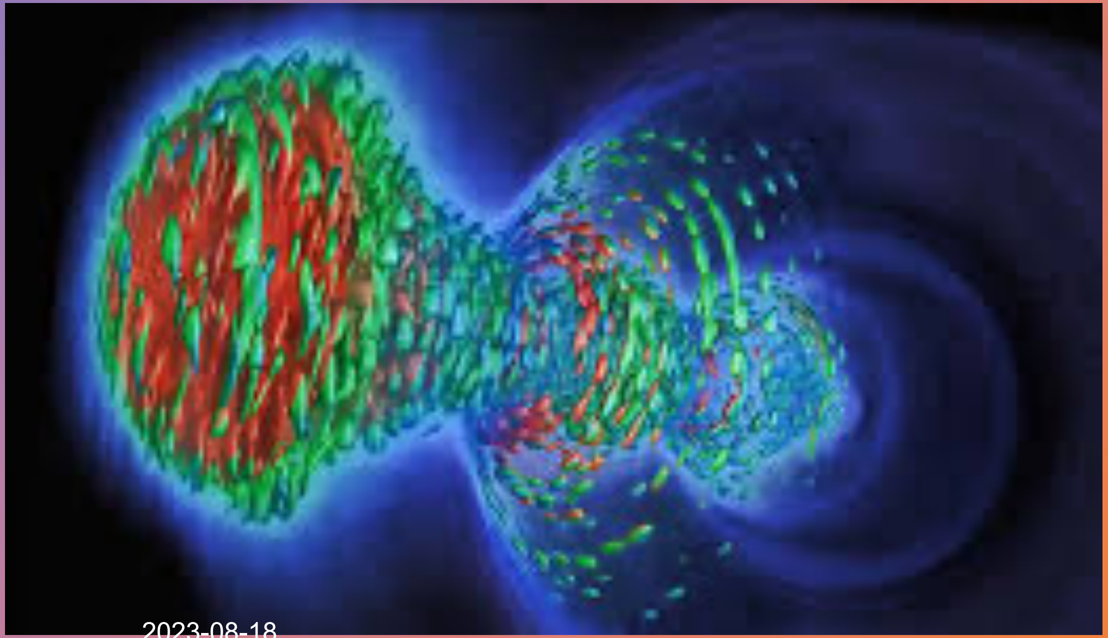


- Modern MPI features applications
    - MPI Sessions for Malleability
    - Persistent Collective for enhanced performance
- Load Balancing
    - Critical performance bottleneck
- Resilience and Fault-Tolerance Libraries
    - Key technology also for autoscaling/elasticity

Accelerators & Diverse Memories

- Current good coverage for Nvidia GPUs
  - Need better support for AMD GPUs
  - We can rely on Alpaka (HZDR) – abstraction level for different accelerator and multicore
- Adaption of code to efficient usage of GPUs
  - One code relies heavily on sorting
- Disaggregated memories for workflows





Simulation Results - Data Deluge

- We deal with data from kinetic data – not just fluid data from each grid points
  - Distribution functions and particle information – often interested in a small population
- Compression (also lossy) and low precision where possible
  - This impacts on results and requires validation
- In-situ data analysis and visualization
  - ADIOS-2
  - ISAAC (HZDR)

Codesign – Providing feedback to EPI

- **European Processor:** SiPearl ARM Processor
- **European Accelerator:** RISC-V Vector Accelerator with BSC as leader
- Providing performance data for the development of the European processors

Quantum Computing & Plasma Simulations

- What are the impact and the role of quantum computing in plasma simulations?
- Hybrid QC-HPC workloads
- Quantum-inspired algorithm

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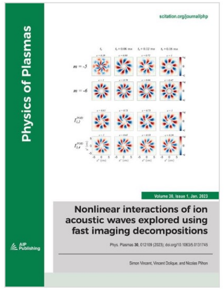

REVIEW ARTICLE | JANUARY 27 2023

Quantum computing for fusion energy science applications

Special Collection: Papers from the 2021-2022 Sherwood Fusion Theory Conferences

I. Joseph ; Y. Shi ; M. D. Porter ; A. R. Castelli ; V. I. Geyko ; F. R. Graziani ; S. B. Libby ; J. L. DuBois

Check for updates

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Note: This paper is part of the Special Topic: Papers from the 2022 Sherwood Fusion Theory Conference.

Physics of Plasmas 30, 010501 (2023)
https://doi.org/10.1063/5.0123765 **Article history**

A quantum-inspired method for solving the Vlasov-Poisson equations

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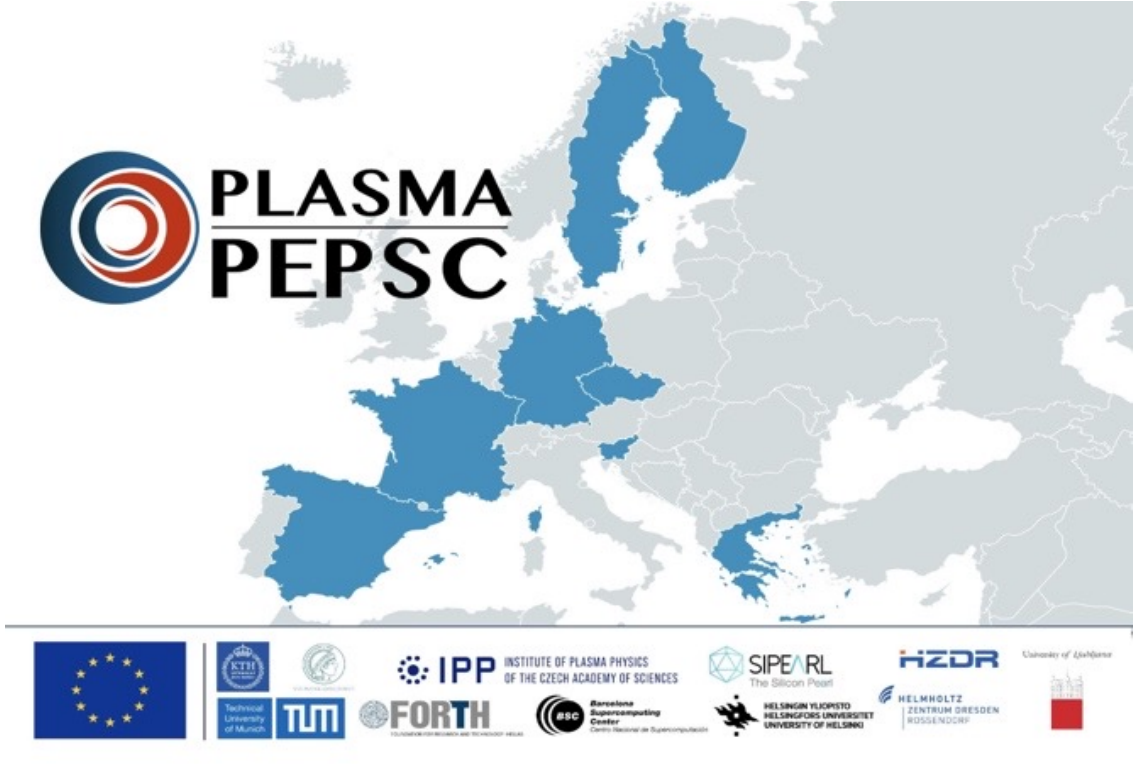
Plasma Science and Fusion Center, Massachusetts Institute of Technology, 77 Massachusetts Av., Cambridge, MA 02139

(Dated: May 25, 2022)

Kinetic simulations of collisionless (or weakly collisional) plasmas using the Vlasov equation are often infeasible due to high resolution requirements and the exponential scaling of computational cost with respect to dimension. Recently, it has been proposed that matrix product state (MPS) methods, a quantum-inspired but classical algorithm, can be used to solve partial differential equations with exponential speed-up, provided that the solution can be compressed and efficiently represented as an MPS within some tolerable error threshold. In this work, we explore the practicality of MPS methods for solving the Vlasov-Poisson equations in 1D1V, and find that important features of linear and nonlinear dynamics, such as damping or growth rates and saturation amplitudes, can be captured while compressing the solution significantly. Furthermore, by comparing the performance of different mappings of the distribution functions onto the MPS, we develop an intuition of the MPS representation and its behavior in the context of solving the Vlasov-Poisson equations, which will be useful for extending these methods to higher dimensional problems.

Conclusions

- We are a new EuroHPC center of excellence for plasma simulations at Exascale
  - Four lighthouse plasma codes: BIT, GENE, PIConGPU, and Vlasiator
  - Addressing challenges at exascale: software engineering at scale, extreme heterogeneity, data deluge problem, algorithms, and libraries



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EuroHPC
Joint Undertaking

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PEPSC