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EUROfusion

Presentation of ACH@MPG

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The Team

Located at IPP, Garching

- Roman Hatzky – team leader
- Ihor Holod (computational plasma physicist)
- Rafael Lago (computer scientist)
- Serhiy Mochalskyy (computational plasma physicist)
- Nils Moschüring (computational plasma physicist)
- Tiago Ribeiro (computational plasma physicist)

The team members dedicate 100% of their working time to the ACH

Workforce allocation

	2021	2022	2023	2024	2025
# of members	6	6	7	8	8
Commitment in ppm	36	72	84	96	96

We plan to hire in 2023 and 2024:

- Software quality (SWQ) expert
- Expert in GPU-programming and particularly porting of codes to GPUs

Huw Leggate from DCU will (probably) join the team with 12 ppm

Profile of the ACH

- Focus on Category I: HPC
- Team members have 100 % commitment
- Long-term support of the TSVVs over their lifetime
- Continuation of the HLST core team tasks with its HPC support
- Bringing together the demands of the users on the one side and system and vendor people on the other side → “ticket meetings”
- Embedded in the “Numerical Methods in Plasma Physics” division of IPP
- Provision of algorithm development
- Performance engineering support

HPC Support

Continuation of current HLST support:

- Parallelise codes using the OpenMP and/or MPI standards
- Improve the performance of existing parallel codes both at the single node and inter-node levels
- Support for high performance parallel I/O
- Choose or adapt algorithms and numerical library routines to improve applications for the targeted computer architectures
- Support the transfer of codes to new processor architectures like GPU and ARM

Support for EUROfusion HPC users

- Give advice to the EUROfusion HPC user community based on experience gained from specific project work
- Provide guidance to young scientists on available training activities in HPC including on upcoming new computer architectures
- Assess the “MARCONI-Fusion” tickets submitted by users to the user support of CINECA
- Monitor and improve the performance of the “MARCONI-Fusion” supercomputer

Improvement of the efficiency of algorithms

Try to reduce the number of FLOPs needed to solve a given problem as much as possible → usage of highly efficient parallel algorithms

- Identify the simplest model problem of a given numerical problem in a simulation code → reduction of complexity
- Select and implement the most efficient algorithms for a given problem on a specific hardware

With more efficient algorithms it is possible to gain orders of magnitude in speed-up!

Such an effort takes time (years), needs the relevant know-how and requires the collaboration of many specialists

Algorithm development

- Affiliation with the "Numerical Methods in Plasma Physics" (NMPP) division of IPP (≈ 30 members)
- Specialization on specific classes of algorithms e.g.:
  - Structure preserving numerical methods for ODEs and PDEs
  - Time integration techniques
  - Iterative solvers in particular multigrid
  - Gyrokinetic methods for PIC codes

Become a hub between state-of-the-art algorithm development in computational plasma physics and the demands of the TSVVs

Performance-engineering support

Structured process with three stages:

- Analysis and identification of code patterns
- Construction of a simplified quantitative model of the performance, e.g. the “roofline model”
- Validation of the performance model by comparing its predictions with direct “experimental” measurements, i.e. benchmarks with different performance tools

Iterative refinement of the performance model

Evolve a reduced but consistent model of the compute-intensive parts of a code

EUROfusion standard software

Develop and maintain specific HPC libraries and interfaces for HPC software packages within the ACH:

- Good software engineering practice
- High-quality code documentation
- Professional dissemination of software
- Excellent support of users

Contribution to TSVVs own research software development:

- Help developers to comply with coding and documentation
- Teach developers good software engineering practices

Cooperation with ACH

- Close collaboration with the developers is mandatory and should be established by personal meetings, video conferences and e-mail
  → project coordinators have to be prepared and accessible

- Changes and improvements to the codes can be done only in agreement with and with the support of the code developers

- The provided support is flexible and problem-oriented within the framework of the project
  → flexible adaptation to problems which may occur

“Rules of conduct”

- The team should not be misused for doing the job of the developers:
  - low level programming work, e.g. clean-up work
  - implementation of new physics
- The ACH should be informed about other collaborators which work/worked on the performance improvement of the code
- Important contributions of ACH members should be credited by co-authorship when applicable
- The code developers keep the responsibility for their codes:
  → The code changes have to be finally accepted by the developers

The ACH does not lecture the code developers!

Summary

- Our experience: Eleven years of HLST support
- 50 % of permanent positions enable a long-term support
- Continuation of HPC support, including porting to modern architectures like GPU or ARM
- Support from the NMPP department of IPP to develop state-of-the-art algorithms for the demands of the TSVVs
- Implementation of state-of-the-art algorithms for the codes of the TSVVs
- Performance-engineering support