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Mercury-Arxes: next steps toward high-resolution planet formation simulations

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Scientific Rationale

- The ***exploration of the Solar System*** continuously provides new clues and constraints on which to expand and test our understanding of how it formed.
- JWST and incoming space-based and ground-based facilities are projecting us into a new era of architectural and compositional ***characterization of exoplanetary systems***.
- Italy has a leading role in the scientific design of the exoplanetary mission **Ariel** by ESA and is contributing to the Solar System missions **Juno** and **Uranus Flagship** by NASA.
- Italy is pioneering exoplanetary studies around double white dwarfs with ***gravitational waves*** with the **LISA** mission by ESA
- The study of planet formation requires a ***systems approach*** accounting for the physical and compositional dimensions of the problem, both in terms of planets and their native disk environment.

To support these endeavors and understand the roots of the great diversity of characteristics of the planetary systems we know, modern ***planet formation codes*** needs to be:

- ***Multi-physics*** and capable of tracking the multiple components of protoplanetary disks.
- ***HPC-capable*** to tackle the increasing complexity and details of the simulations.

Technical Objectives, Methodologies and Solutions

MERCURY ArXes

Mercury-Arχes (Turrini+2019,2021) is the multi-language n-body code of **Arχes**, the INAF suite of planet formation and astrochemistry codes:

- Builds on the Mercury n-body code (Chambers 1999; FORTRAN77) and the WHFAST library (Rein & Tamayo 2015; C99).
- Integrates planet formation libraries to track the *growth*, *migration* and *interactions with the disk gas* of planetary bodies (Turrini+2019, 2021 + Polychroni+2023; Fortran2003).
- *Parallelized and vectorized* (SIMD) with OpenMP, porting designed so that the parallel and serial version produce the same results.

Technical Objective: *porting Mercury-Arxes to GPU computing*

Methodology: *pragma-based approach, Agile development process*

Present Adopted Solution: *OpenACC standard*

Timescale, Milestones and KPIs

M8-M9: team expansion; implementation of new OpenACC design and scalability testing

Goals:

- Training of new team members on HPC and GPU computing
- Improve gain w.r.t. OpenMP on CPU version and usability w.r.t. first release

KPIs:

- Hiring of two new technological researchers in the team

- Improvement of computational density per data transfer ratio

Milestone: Release of second GPU-enabled version

M10: assess possibility of unified porting in OpenMP; finalize porting to GPU of Mercury-Arxes

KPI: Comparative assessment of global performances between OpenACC and OpenMP

Milestone: Release of final GPU-enabled version

Accomplished Work, Results

M6: Release of first GPU-enabled version (https://www.ict.inaf.it/gitlab/PlanetaryFormation/arxes)

M7: Application on real scientific use case with gain on OpenMP version (Turrini+2023, A&A)

M8:

- hiring of two technological researchers in the team:
  - ***Paolo Simonetti*** (WP1+ WP5; INAF-OATS)
  - ***Danai Polychroni*** (WP1+ WP5; INAF-OATO)

- Kick-off training on HPC and GPU computing
- Identified design with higher computational density per data transfer also usable as training ground
- Development of new physical library for Mercury-Arxes based on GroMiT (validation ongoing)
- Definition of KSP OPAL for testing Mercury-Arxes for deployment in large-scale simulation campaigns

Next Steps and Expected Results

M8:

- Complete HPC and GPU computing training
- Validate integration of new physical library based on GroMiT
- Implementation of new OpenACC-based design

M9:

- Benchmark of performance and scalability w.r.t. to first release and CPU-only version
- Finalization of second GPU-capable version