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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA

ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Parallelizing the Mercury-Arxes code using OpenACC: an update

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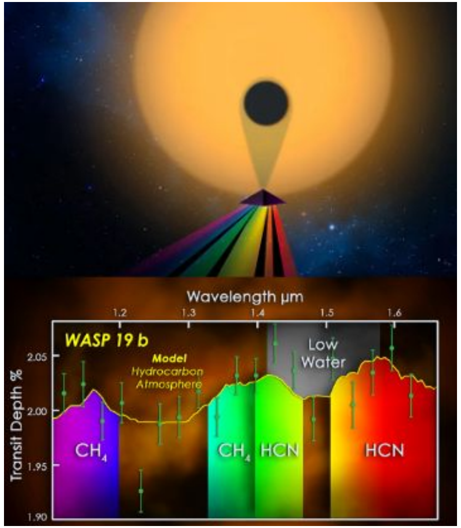
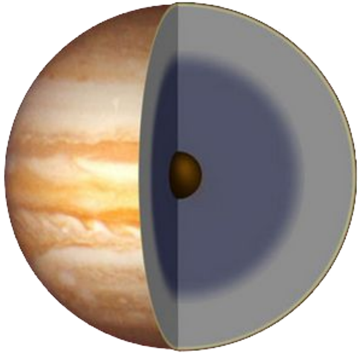
Scientific rationale

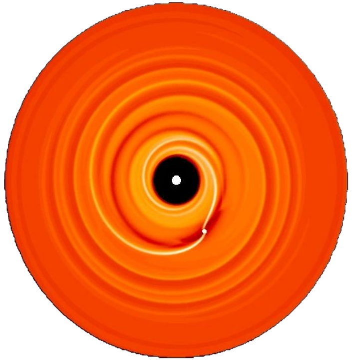
1. Chemical composition of the atmosphere from observations

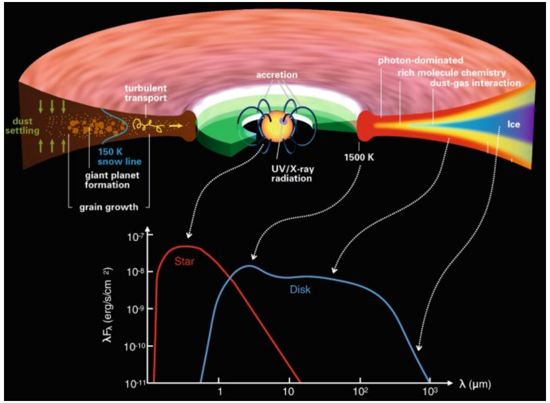




2. Chemical composition of the whole body from the atmosphere (gas giants)

3. Formation & evolution from chemical composition





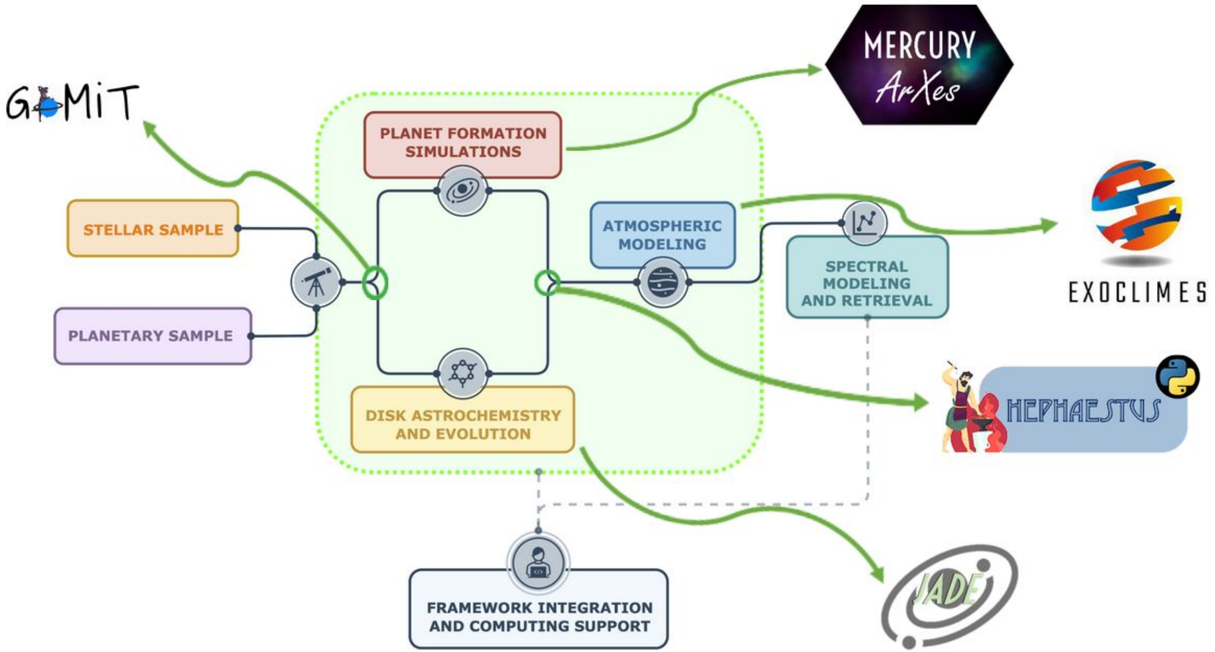
4. Understand planetary formation in a cosmic context

Scientific rationale

OPAL KSP: a pipeline of codes to self-consistently model how a planet looks like from its history:

- Chemical composition of the protoplanetary disk
- Planetary formation & migration
- Atmospheric chemistry
- Synthetic spectra

In the context of the italian contribution to the Ariel Dry Run



The OPAL Project

OPAL KSP: a pipeline of codes to self-consistently model how a planet looks like from its history:

- **Chemical composition of the protoplanetary disk**
- **Planetary formation & migration**
- **Atmospheric chemistry**
- **Synthetic spectra**

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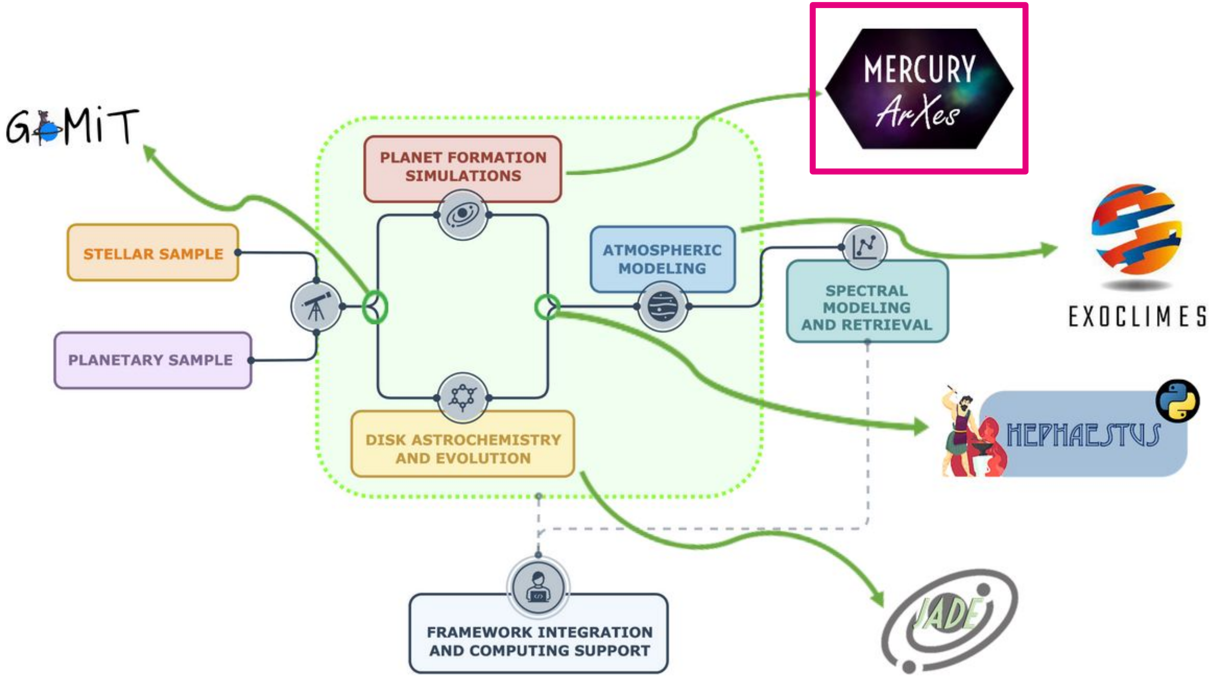


Starting point and objectives

MERCURY ArXes

- hybrid symplectic integrator
- Mercury-Arxes (Turrini+21): branched out version tailored to study planetary formation:
    - based on Mercury 6
    - viscous interaction with a time-evolving disk
    - management of merging trees
    - improved keplerian evolution (see later)
- Current typical simulation: <10 gravity-source *planets*, >10^4-10^5 non gravity-source *particles*

GOAL: have all the *particles* (~10^5) as gravity-sources

- especially important at the beginning of the simulation, when most of the mass is in *particles*

Methodology

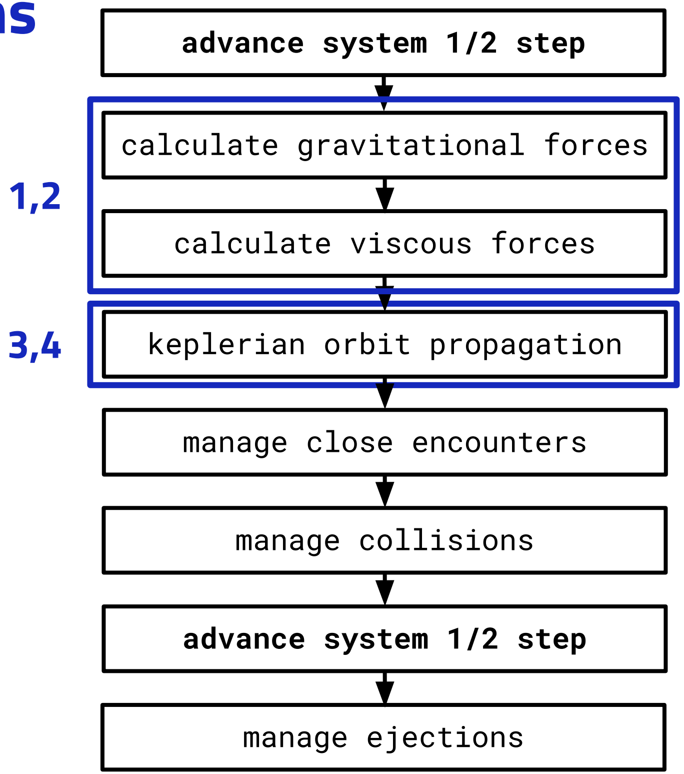
- To achieve our goal, high level of parallelism is needed
- Parallelization performed moving most of the main loop on GPU using OpenACC
- ~~Parallelization of the rest of the code using openMP~~ inefficiencies due to openACC/openMP joint usage minimizes gain -> ditched in favor of GPU-only parallelism

Mercury-Arxes main loop:

advance system 1/2 step
↓
calculate gravitational forces
↓
calculate viscous forces
↓
keplerian orbit propagation
↓
manage close encounters
↓
manage collisions
↓
advance system 1/2 step
↓
manage ejections

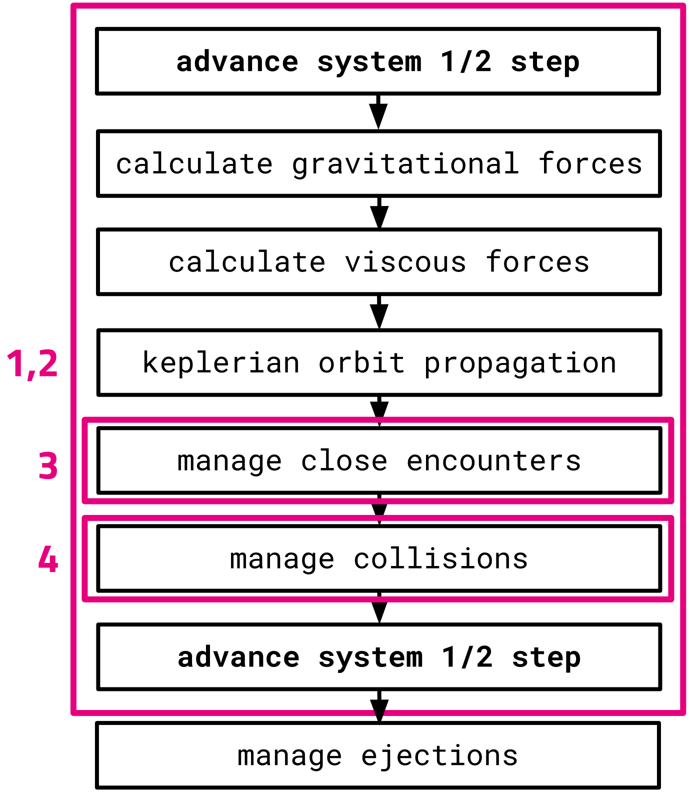
Current status: previous interventions

1. merged gravitational and non-gravitational forces in one routine
2. ported force calculation on GPU
3. translated the keplerian orbit propagation routines from C to Fortran
4. ported keplerian orbit propagation on GPU



Current status: new interventions

1. single data region for nearly the entire main loop
2. restructured the main loop for efficiency and serviceability
3. close encounters management moved to GPU
4. optimized data transfer to the collision routine (still on CPU)



Main results

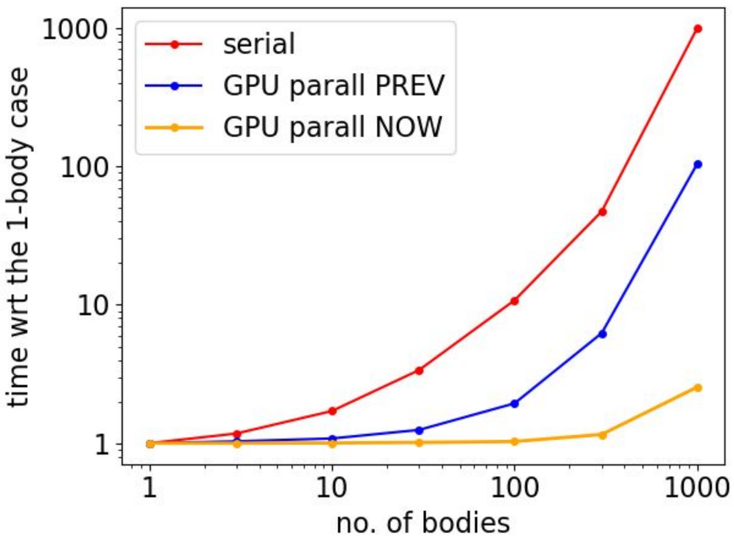
- speedups up to a factor 300 (for n° of body up to 10^3 over 10^3 yr integration)
- substantially improved serviceability of the code: now it is completely written in fortran

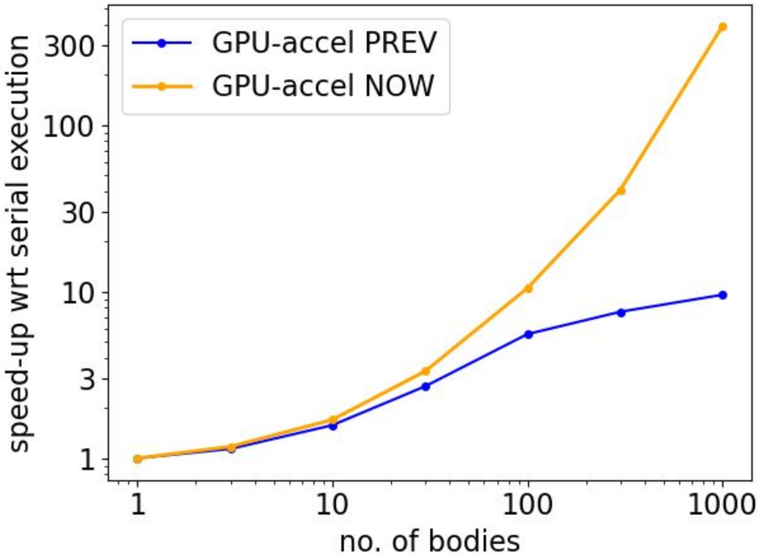
Factors positively impacting performances:

1. more careful data management
2. moved inefficiently compiled code with nvfortran to GPU
3. removed legacy instructions (e.g. on cometary forces)

Main results

Competition between overhead time and parallel execution

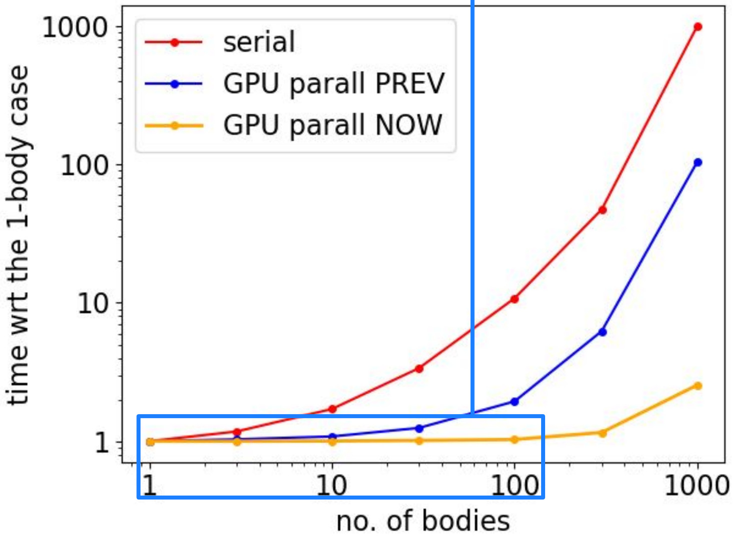


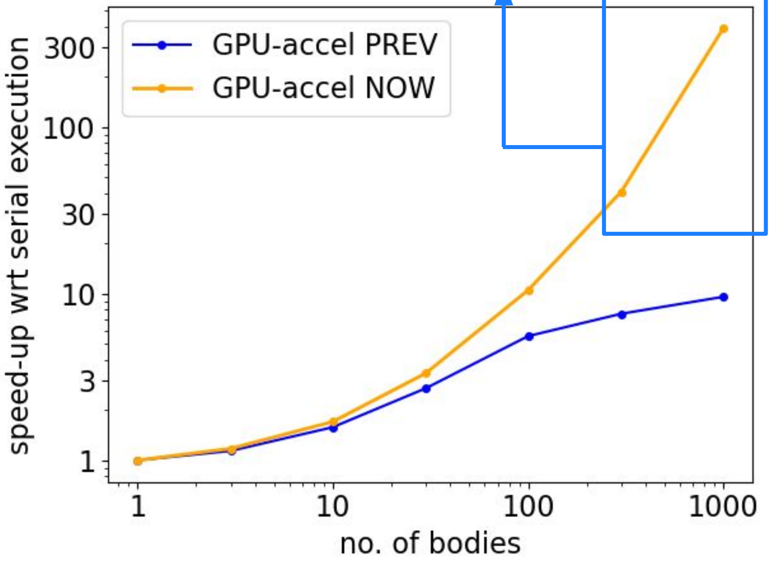


Main results

Better management of the overheads: no speed loss on low-number simulations

Large gains in high-number simulations due to parallelization of close encounters





Targets

M9 (oct. '24)

- analysis of interfaces & capabilities of different OPAL models ✅
- identification of final design strategies for the porting of Mercury-Arxes to GPU ✅

Intermediate M (apr. '25)

- completion of the first part of the OPAL simulation campaign ✅

M10 (ago. '25)

- completion of the OPAL simulation campaign
- full porting of Mercury-Arxes to GPU
- final release of the parallelized Mercury-Arxes

KPIs

M9 (oct. '24)
- initial report on Mercury-Arxes performance ✅
- release of the alpha version of the GPU-parallelized Mercury-Arxes ✅

Intermediate M (apr. '25)

M10 (ago. '25)
- full release of OPAL library of models
- final report on Mercury-Arxes performance

KPIs

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Intermediate M (apr. '25)

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95% completion towards full parallelization

Final steps

1. try to parallelize collisions (to avoid the residual inefficiencies on data transfers and CPU execution, marginal gains only)
2. final polishing for user friendliness
3. comparative performance assessment and release