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

PINOCCHIO: recent developments and plans towards the Key Science Project

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Spoke 3 General Meeting, Elba 5-9 / 05, 2024

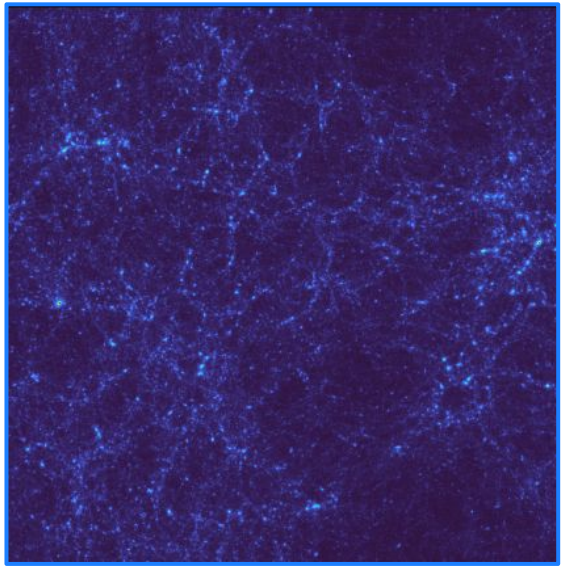
Scientific Rationale

PINOCCHIO is a code, based on Lagrangian Perturbation Theory (LPT), for simulating Dark Matter halos in cosmological boxes and past light cones (*Monaco et al. 2002, 2013; Munari et al. 2017)*

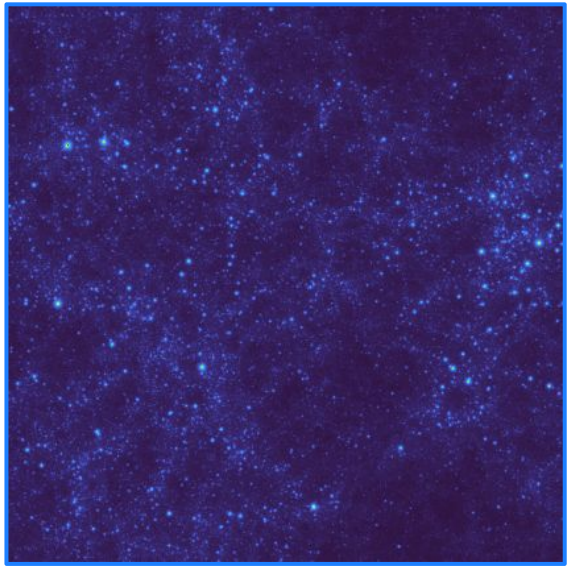
Comparison with full N-body simulations:

- ~1000 faster
- 5 – 10% accuracy in reproducing 2-point statistics, mass function and bias

Gadget



Pinocchio



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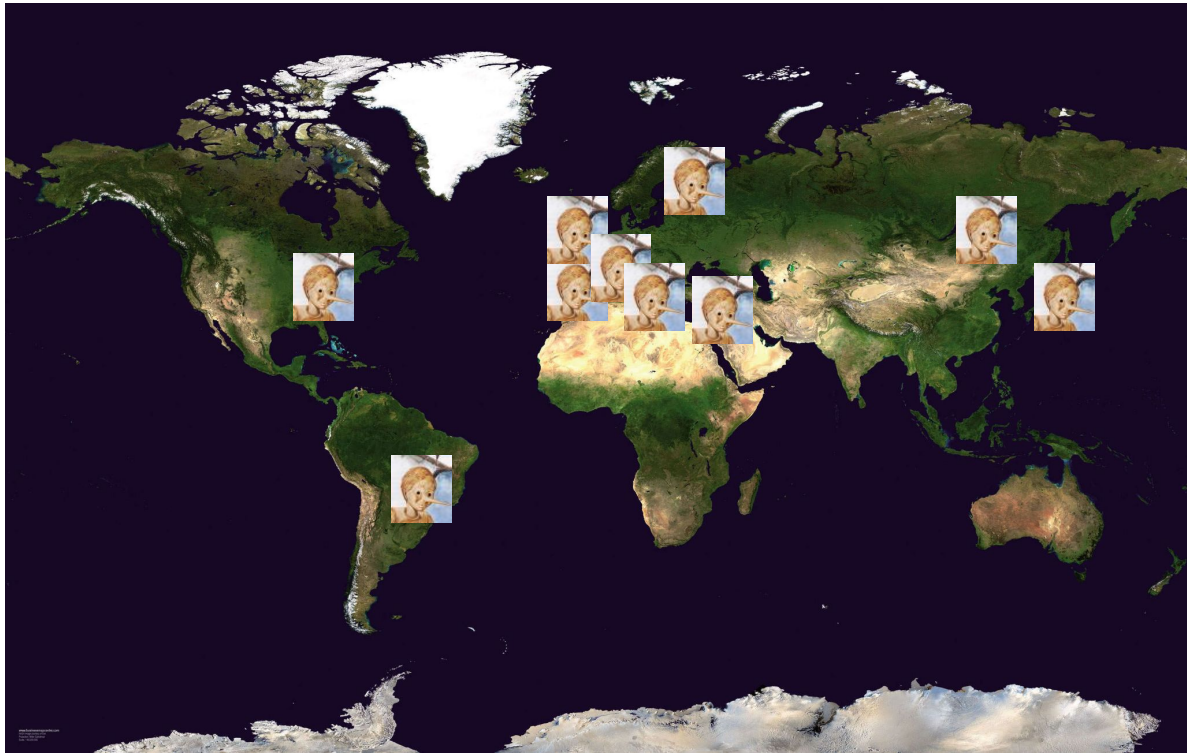


Technical Objectives, Methodologies and Solutions

- **Optimize the code and allow it to run on architectures with GPUs:**
  - **Improve code performance**: *suitable threadization? main bottlenecks ?*
  - **Identify off-loadable regions**: *what can be ported to GPUs?*
  - **Improve scientific output**: *Adopting new algorithm?*
- **Adopted solutions:**
  - **Improve** the **MPI** framework: **OpenMP**
  - **Porting** collapse times to **GPU**: **OpenMP/OpenACC**
  - **Optimize** and **investigate** a new fragmentation algorithm: **Deblending**
  - **Testing, bug fixing, testing, bug fixing… !!**

Timescale, Milestones and KPIs

04/2023 — 09/2023 — 02/2024 — 06/2024 — 12/2024 — 05/2025

MS 6

1. Familiarization with the code
2. Bug fixing
3. Identification off-loadable regions and bottleneck

MS 7

1. Threadization of collapse time with OpenMP
2. GPU offloading of collapse times with OpenMP/OpenACC

MS 8

1. Deploying stable code fully suited for LEONARDO with documentation
2. Optimization and re-engineering of the fragmentation code, the main actual bottleneck

MS 9

1. Set of demonstrative simulations with the new fragmentation and report

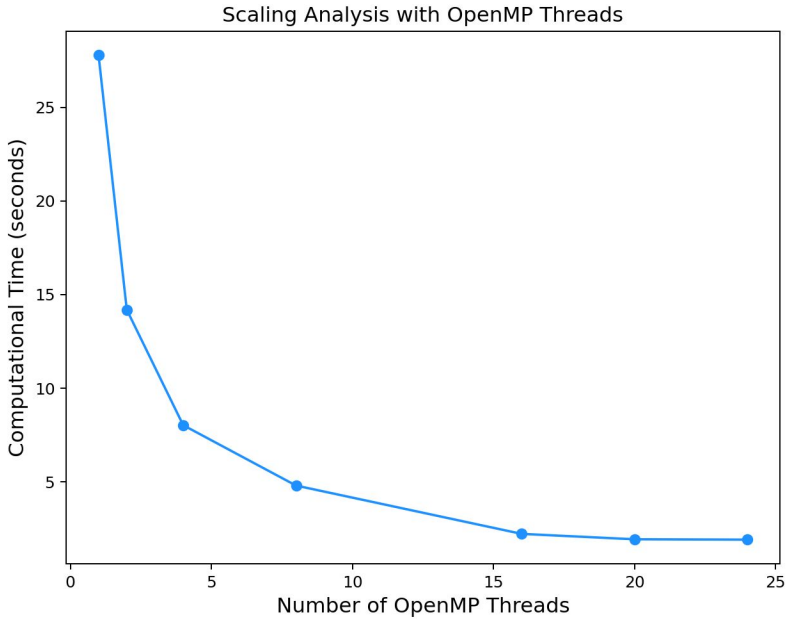
MS 10

1. 100 simulations
2. Technical paper on the code

Accomplished Work, Results

We have extended the existing parallel computing paradigm by integrating OpenMP into the collapse times calculation

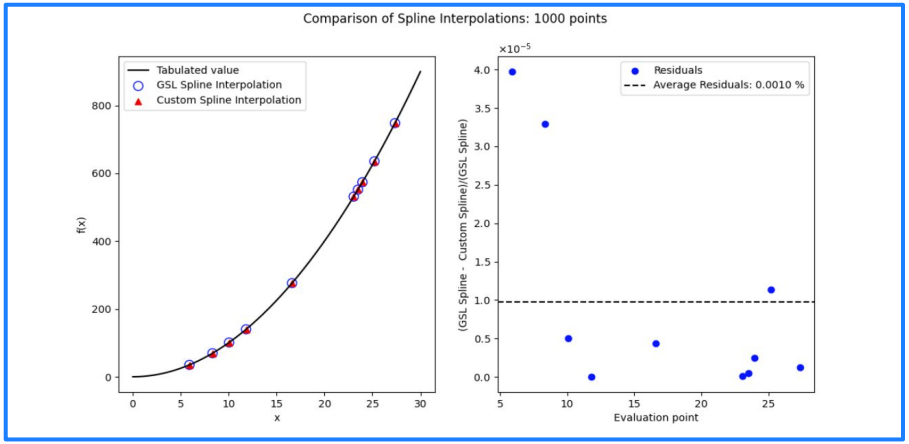
- Nearly ideal scaling up to ~20 threads per single MPI Task
- Expected nearly ideal scaling up to 36 threads
- Large Euclid Box (box ~ 4 Gpc, 4096^3 particles) computational time: ~ 8% out of ~ 40 minutes
- Computational time improvement: ~ 9x speed-up
- Thousands of mocks: ~ 50 hours less

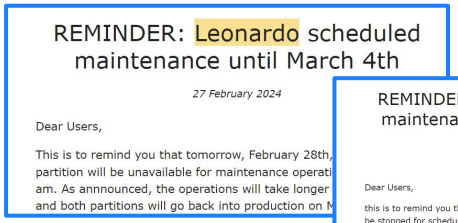


Accomplished Work, Results

Offloading of collapse times calculation on GPU with OpenMP/OpenACC

- Submission of proposal for GPU hours (ISCRA C): accepted
- Set up the environment to compile the code on LEONARDO
- Offloading implemented (needed a custom cubic spline interpolation)
- GPU offloading test out of PINOCCHIO and comparison with GSL: done
- Integration in PINOCCHIO and test on CPU: done
- Minor issues at run time still need to be fixed but..

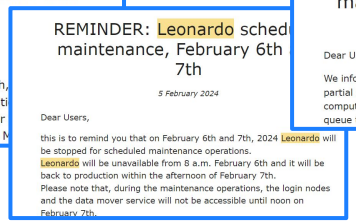



REMINDER: Leonardo scheduled maintenance until March 4th

27 February 2024

Dear Users,

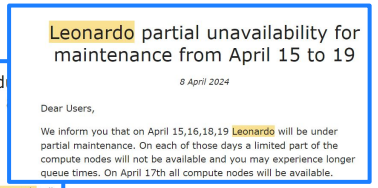
This is to remind you that tomorrow, February 28th, partition will be unavailable for maintenance operati am. As annnounced, the operations will take longer and both partitions will go back into production on


REMINDER: Leonardo sched maintenance, February 6th 7th

5 February 2024

Dear Users,

this is to remind you that on February 6th and 7th, 2024 Leonardo will be stopped for scheduled maintenance operations.
Leonardo will be unavailable from 8 a.m. February 6th and it will be back to production within the afternoon of February 7th.
Please note that, during the maintenance operations, the login nodes and the data mover service will not be accessible until noon on February 7th.


Leonardo partial unavailability for maintenance from April 15 to 19

8 April 2024

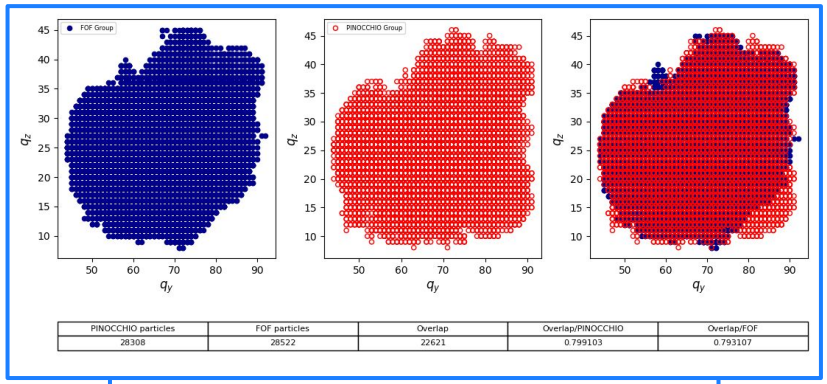
Dear Users,

We inform you that on April 15,16,18,19 Leonardo will be under partial maintenance. On each of those days a limited part of the compute nodes will not be available and you may experience longer queue times. On April 17th all compute nodes will be available.

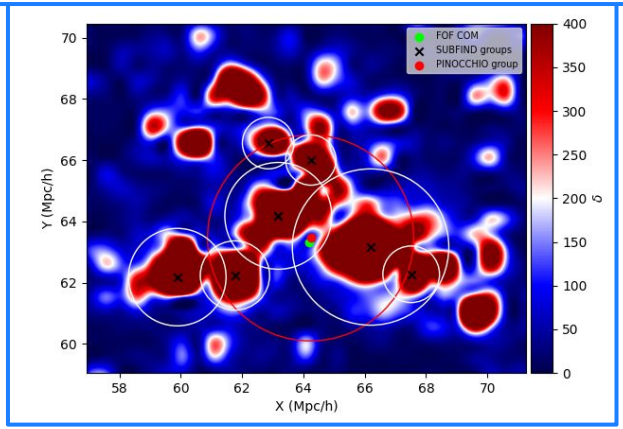
Accomplished Work, Results

Optimization and **re-engineering** of the **fragmentation** code segment

- Particle by particle **comparison** with an **N-body** code (OpenGadget3)
- **Initial condition** for the N-body generated with **PINOCCHIO**
- **Visualization** of the halos **eulerian** and **lagrangian patch**



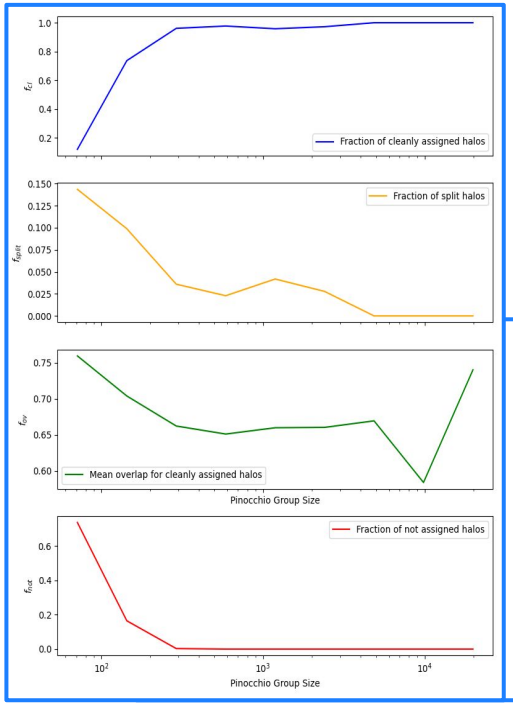
PINOCCHIO particles	FOF particles	Overlap	Overlap/PINOCCHIO	Overlap/FOF
28308	28522	22621	0.799103	0.793107

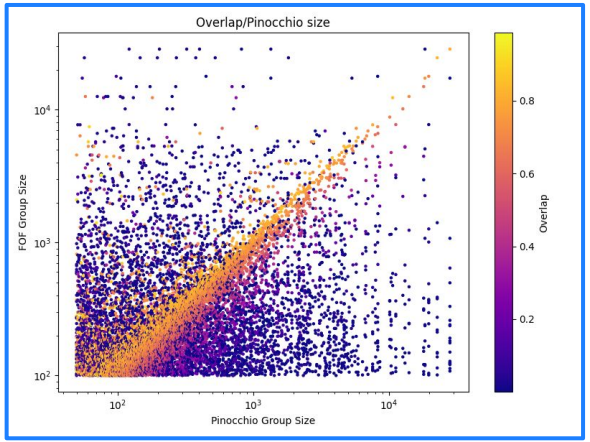


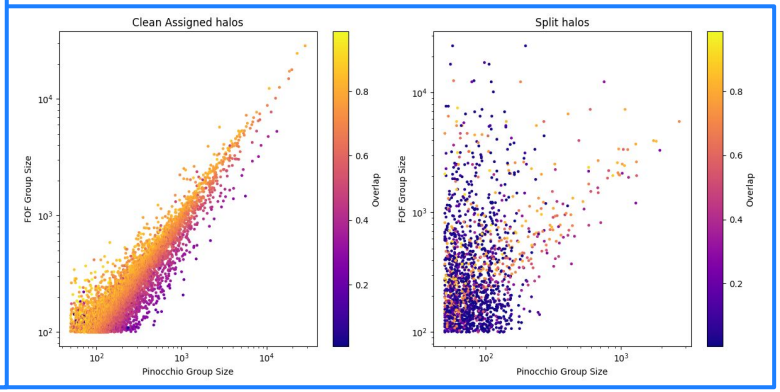
Accomplished Work, Results

Optimization and **re-engineering** of the **fragmentation** code segment

- **Estimation** of PINOCCHIO **accuracy** in building up the halos compared to **FOF** halo finder
- **Overlap matrix** and **fraction statistics**







Key Science Project: EuMocks

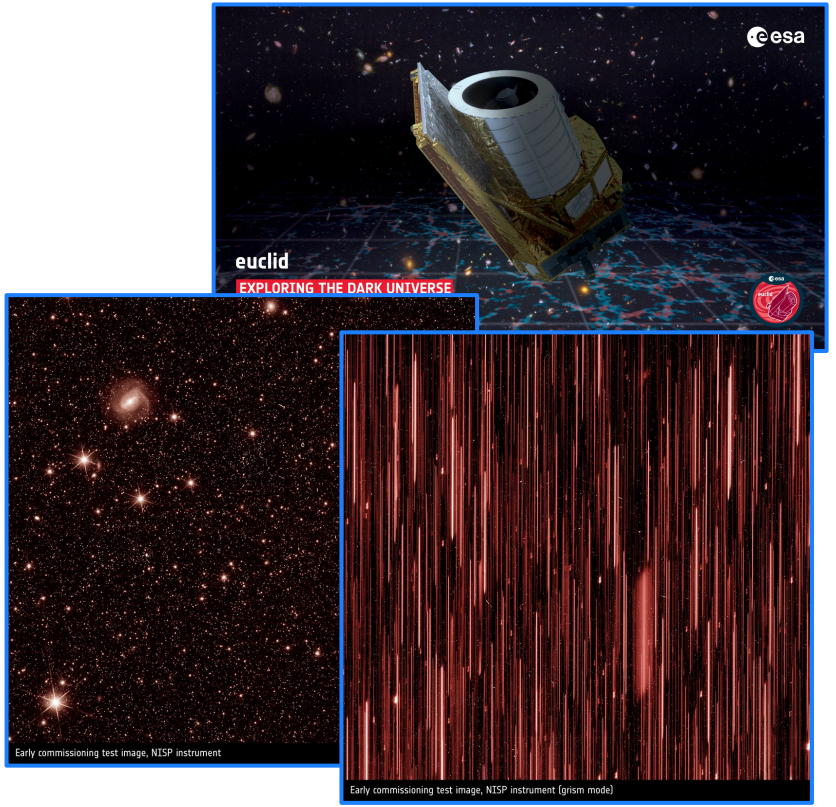
Euclid will survey the universe down to redshift z~2, **mapping the large-scale structure** (~15,000 sq deg of the sky) to measure its geometry and growth rate to shed light on dark sector

Control of **systematic errors** will be the issue to tackle to provide convincing and potentially groundbreaking results

Key Science Project goal: **3500 simulations** (**~4Gpc with ~10^{12} particles**), **resolving halos of ~10^{11} M_{sun}/h**, in a past-light-cone covering **half of the sky** starting at **z=3**

Development is needed (Spoke3 + Spoke1, PRIN PNRR 2022):
SCIENCE:
- improve and optimize **the reconstruction of halos**
- implement a **Particle-Mesh** code to move halos (instead of 3LPT)
- add **lensing** and relativistic effect

CODING:
- port on **GPUs** specific code segment
- improve the **fragmentation**



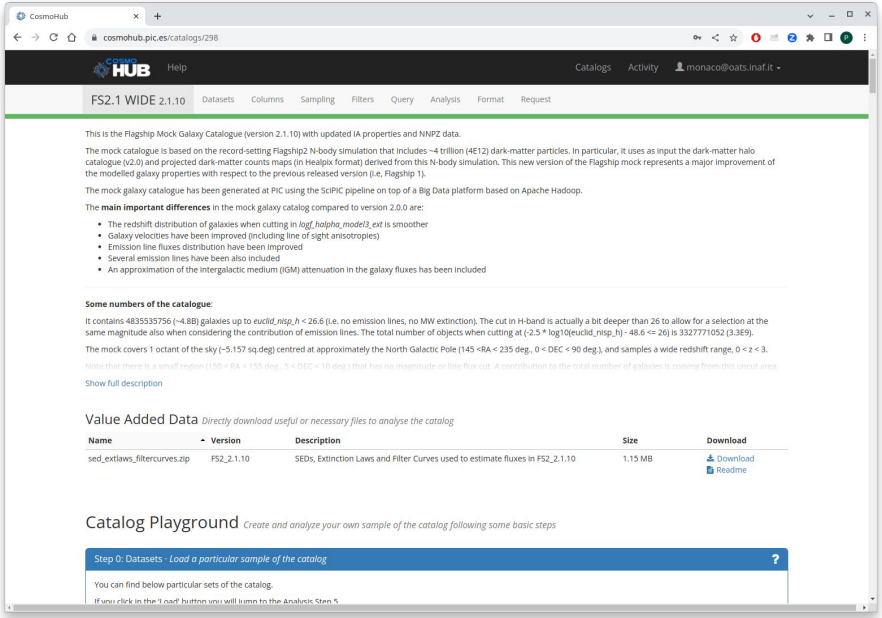
Key Science Project: EuMocks

Massively parallel code, every step must be optimized before burning so much computing time

Computing time: ~30,000,000 core hours
Memory: ~128 TB
Storage: >~1PB

Petabyte-scale output **to be offered to the community**
-> National / Interoperable Data Lake

example: Cosmohub.pic.es



Key Science Project: EuMocks

2023 | **2024** | **2025** | **2026**

launch
July 2023

DR1 data
Sept 2024

DR1 public
Sept 2025

DR2 data
Sept 2026

Milestone 7 | Milestone 8 | Milestone 9 | Milestone 10

ICSC
year 1

ICSC
year 2

ICSC
END

ICSC resources available

code development.....

available simulations.....

Sept 2024:
available simulations
in the data lake?

March 2025
code ready

March 2025
data lake ready

August 2025
first 100 sims

August 2026
3500 sims

KPI | **KPI** | **KPI**

Next Steps and Expected Results

- **Application to the upcoming CINECA GPU HACKATHON (with *David Goz and Giovanni Lacopo*):**

  - **Finalizing** and **optimizing** the already in place **GPU** version of the collapse time calculation

  - **Porting** on **GPU** the **FFT calculation** using cuFFT

- **Optimization and re-engineering of the fragmentation code segment:**

  - **Fine tune** the present physical based threshold for **particle accretion** and **halo merging**

  - **Introduce** a halo **concentration** proxy in order to minimize the **LPT displacements** errors

- **Adopt a new format for the PINOCCHIO scientific output**

  - **FITS catalog** obtained at a post processing phase with a **custom developed code**