ICSC Annual Meeting

del Centro Nazionale HPC, BIG DATA
AND QUANTUM COMPUTING

Roma
Auditorium Antonianum

Cosmological simulations with the *OpenGADGET3* code

Milena Valentini, University of Trieste

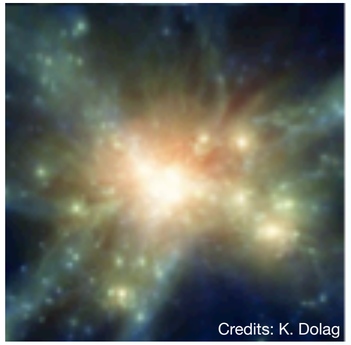
COLLABORATORS:

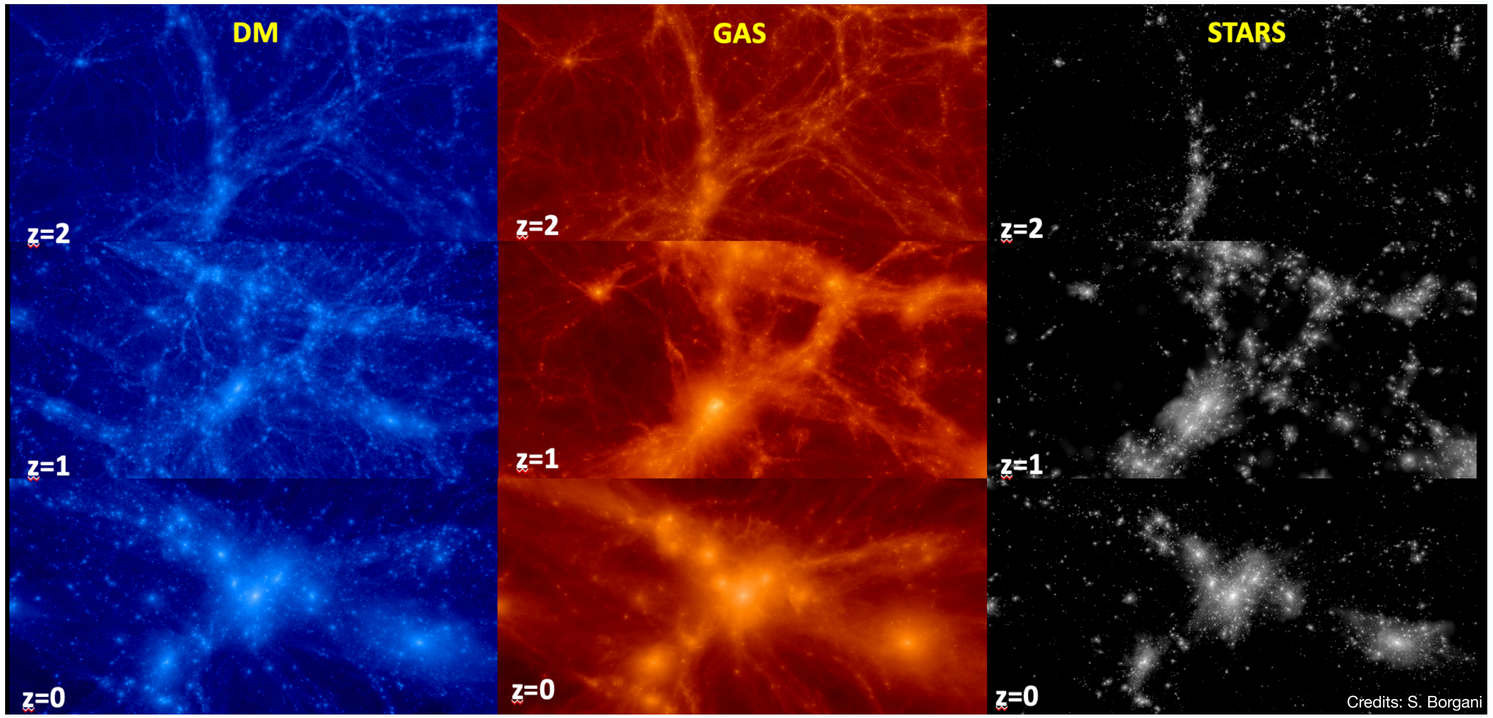
S. Borgani, L. Tornatore, K. Dolag, G. Murante, G.L. Granato, C. Ragone-Figueroa, A. Damiano, L. Sala, T. Castro, A. Ragagnin, A. Saro, G. Taffoni, M. Viel

THE *OpenGADGET3* CODE: A STATE-OF-THE-ART CODE FOR HPC

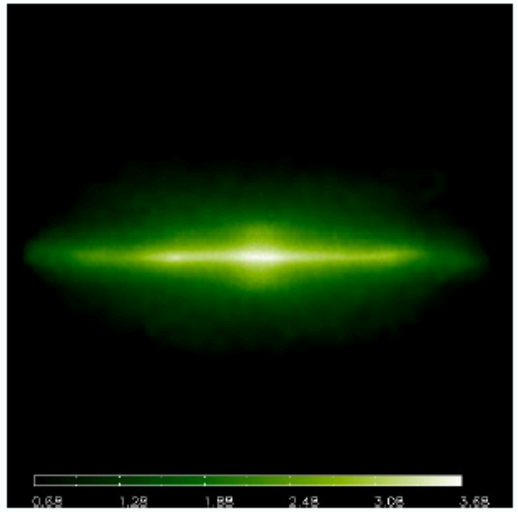
Scientific rationale

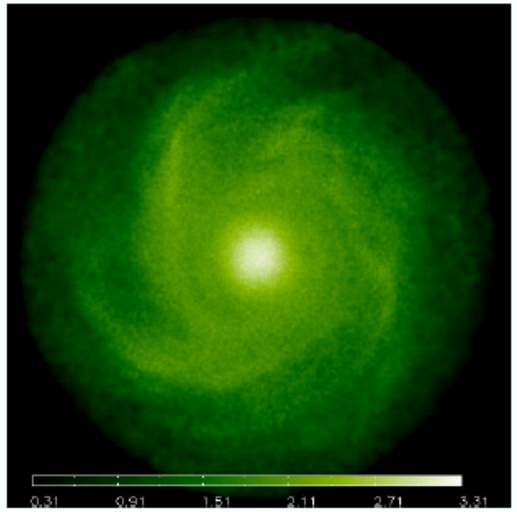
- Numerical cosmology
- Structure formation and evolution

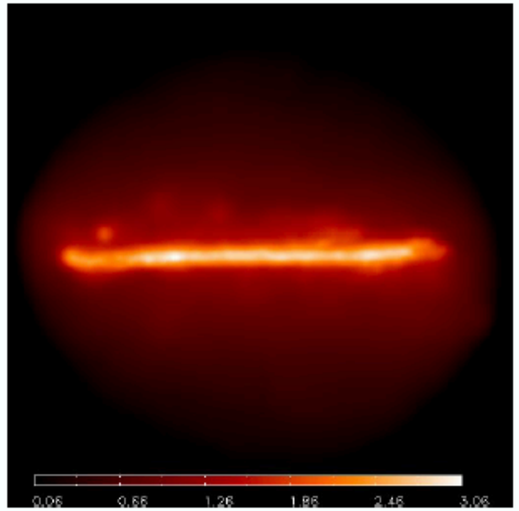

Credits: K. Dolag

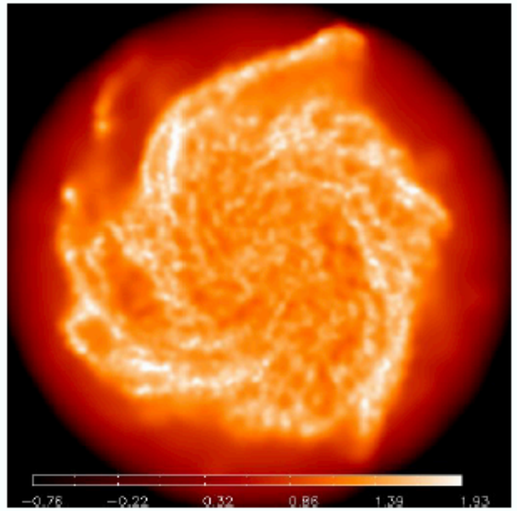


Credits: S. Borgani

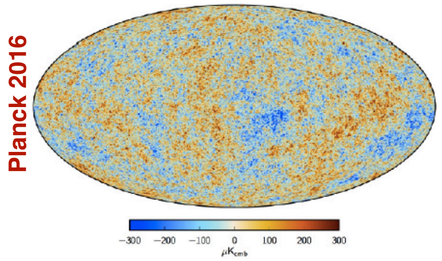








COSMOLOGICAL HYDRODYNAMICAL SIMULATIONS



Initial Conditions

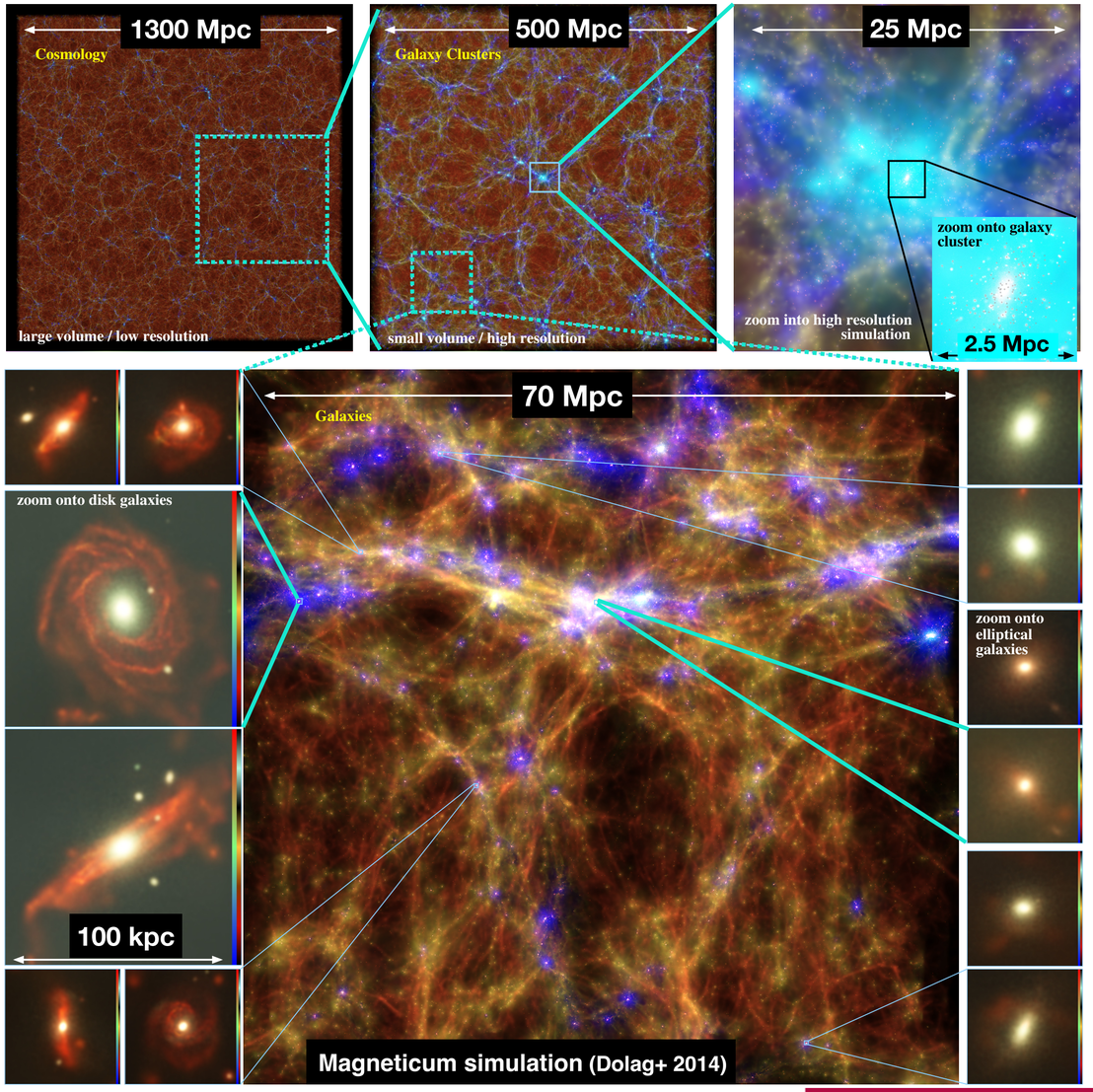
+ Gravity

Vlasov and Poisson equations

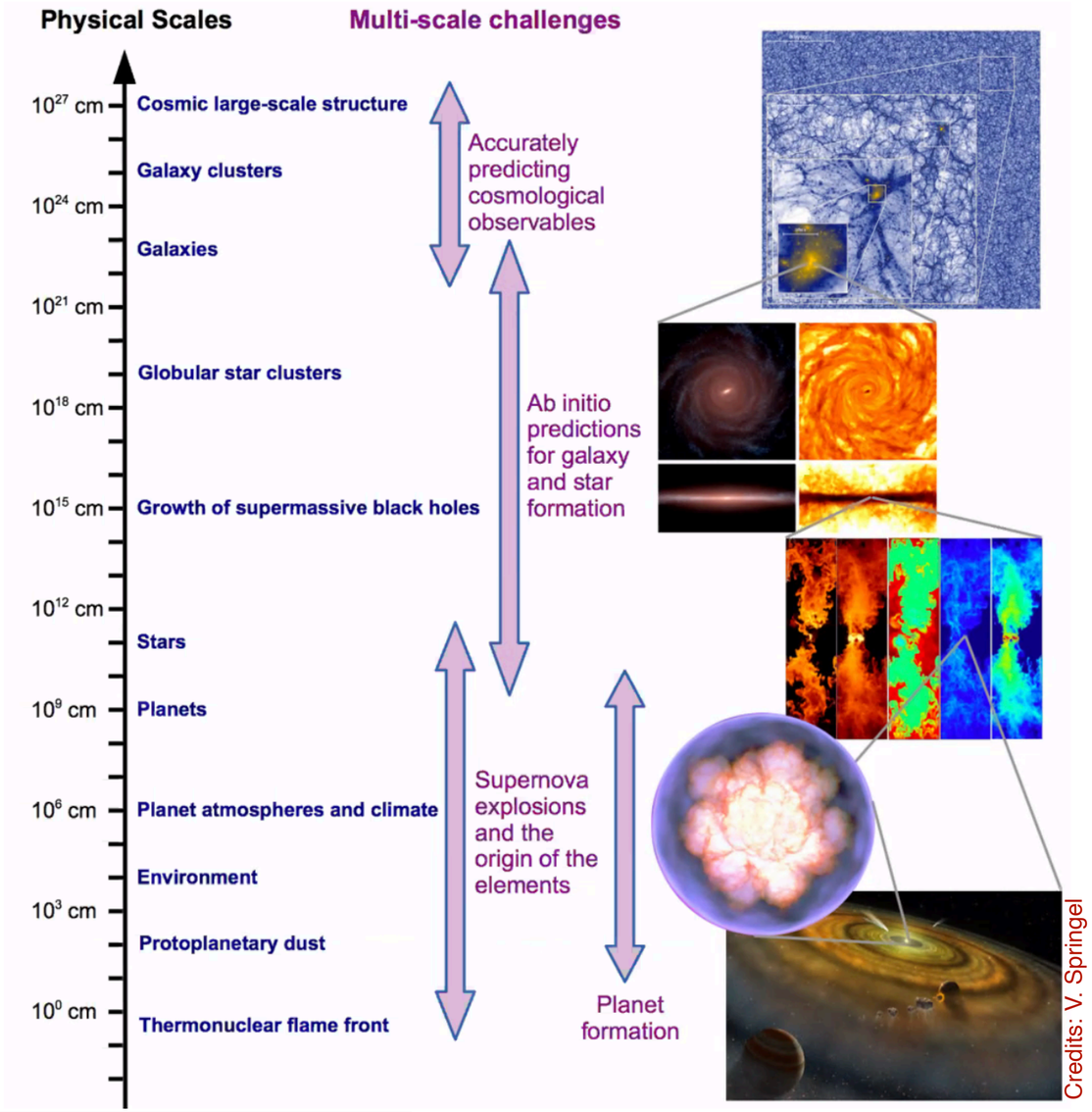
+ Hydrodynamics

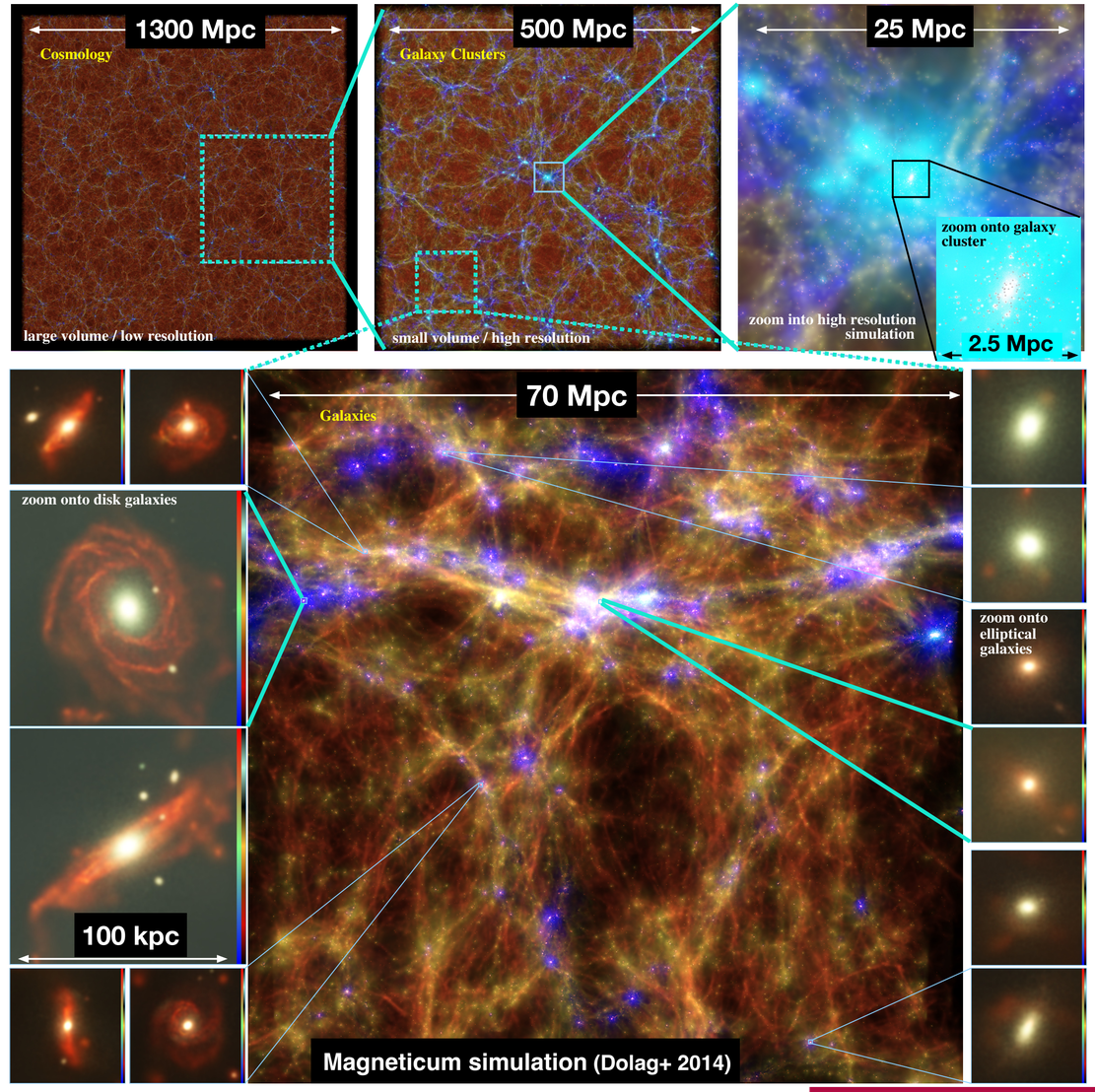
equations of the hydrodynamics and equation of state

- Different physical phenomena across a **wide range of scales**: **sub-resolution models** essential

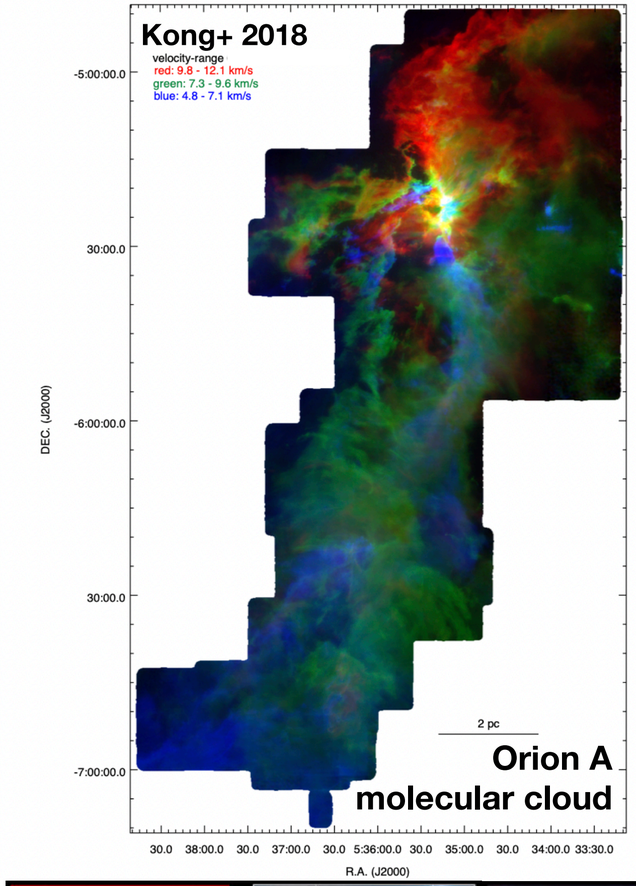


COSMOLOGICAL HYDRODYNAMICAL SIMULATIONS





WHY SUB-RESOLUTION PHYSICS: DYNAMICAL CHALLENGE





Star formation:

accretion of gas from the large scale (~Mpc)

↓

gas cooling to form HI (~kpc)

↓

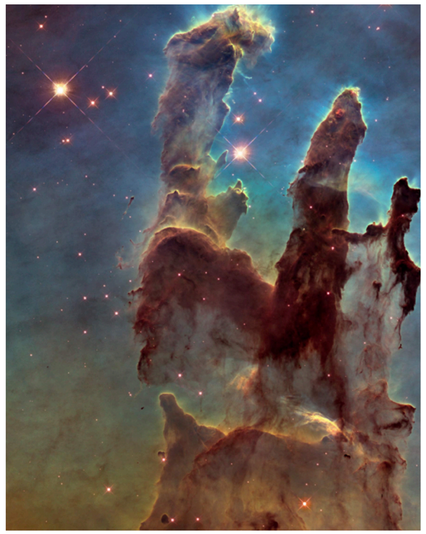
formation of molecular clouds (~10 - 100 pc)

↓

H_2 fragmentation and accretion to clumps and cores (~1 - 0.1 pc)

↓

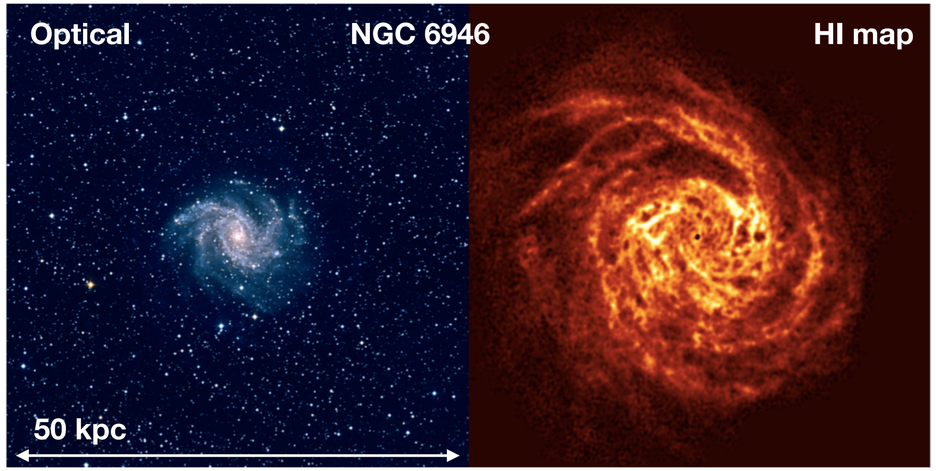
subsequent contraction of cores to form stars (~10^{-8} pc)



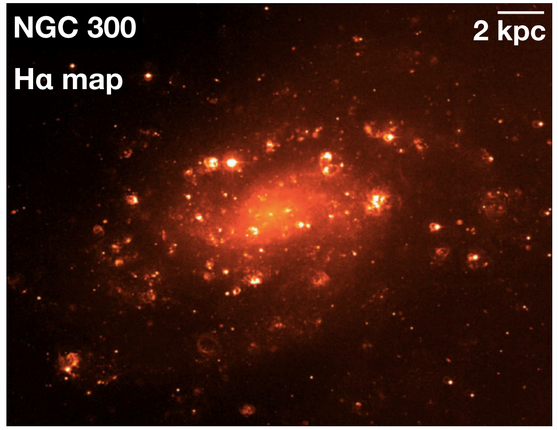
Multi-scale, multi-phase problem:

- Dynamical challenge (“coupled” physics)
- Physics on small scales is qualitatively different from physics on large scales
- Non-linear nature of galaxy formation

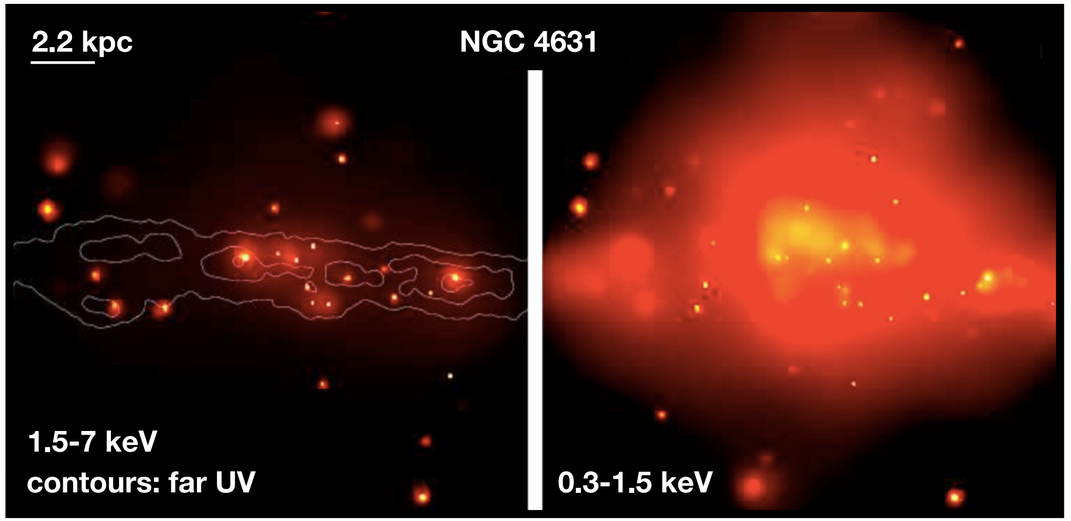
THE MULTI-PHASE INTERSTELLAR AND CIRCUMGALACTIC MEDIA



Boomsma+ 2008

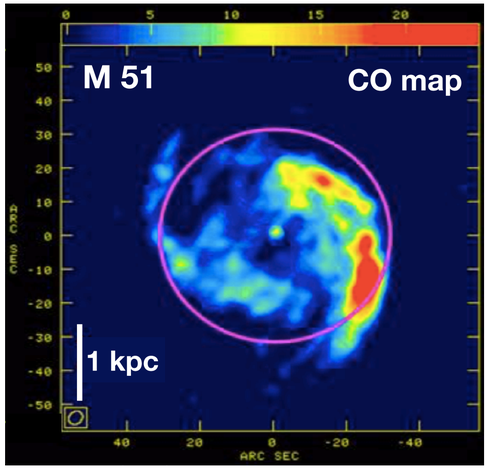


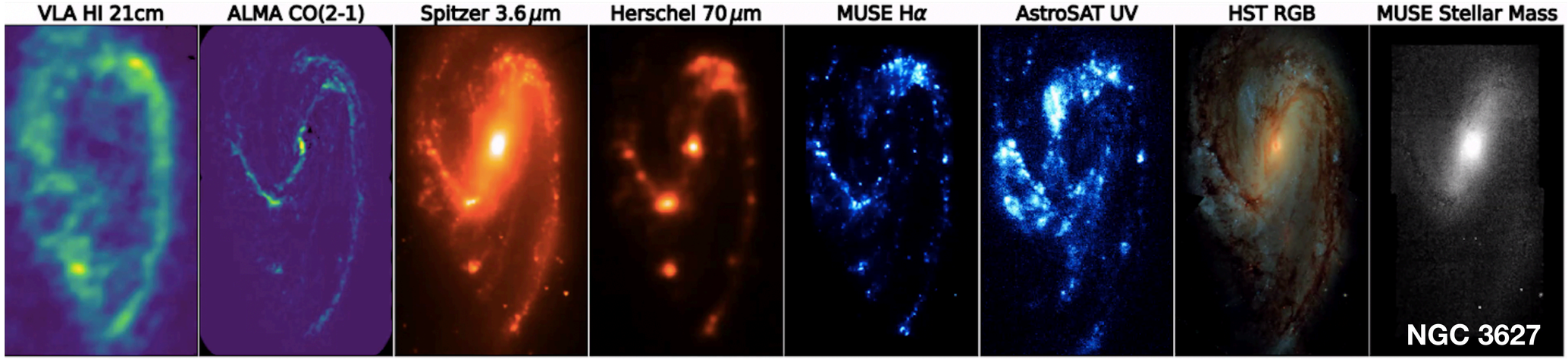
Bresolin+ 2009



Wang+ 2001

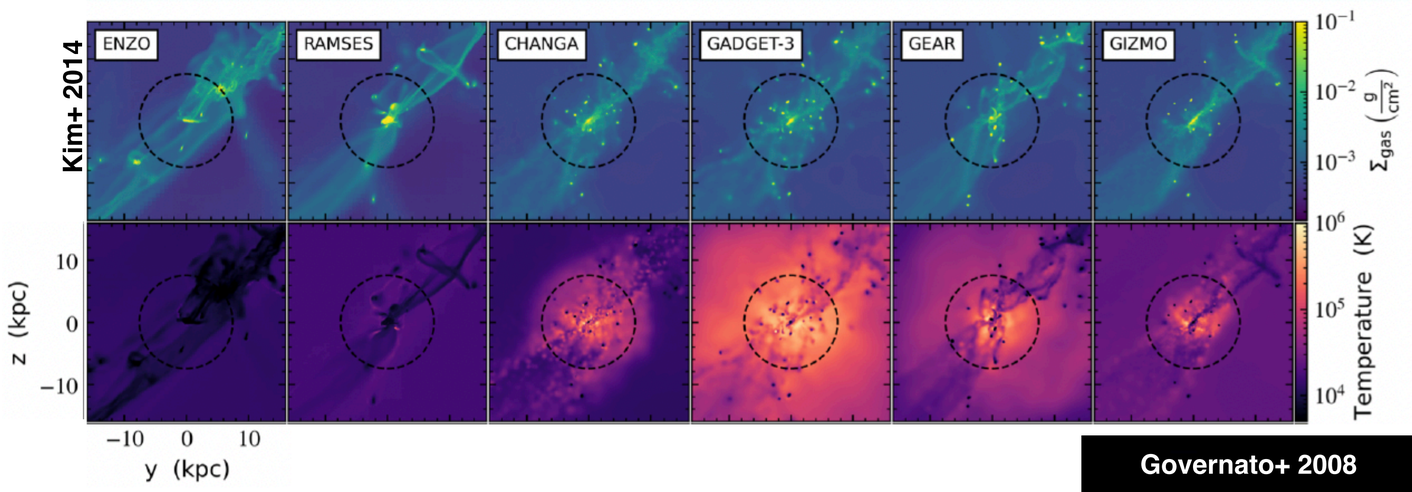
Sakamoto+ 1999



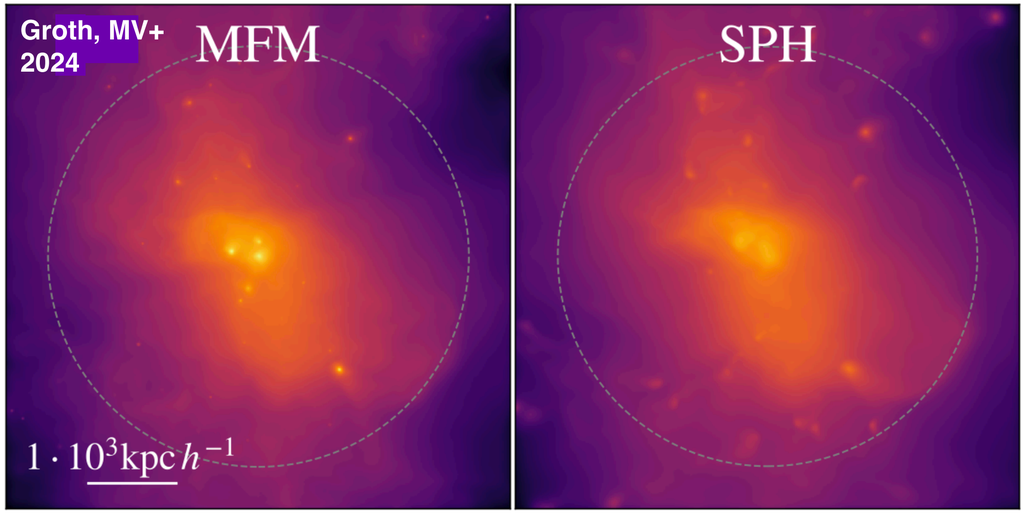


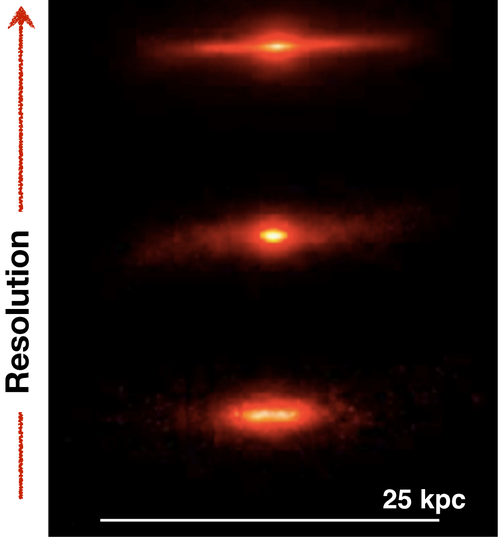
Credits: Phangs Survey

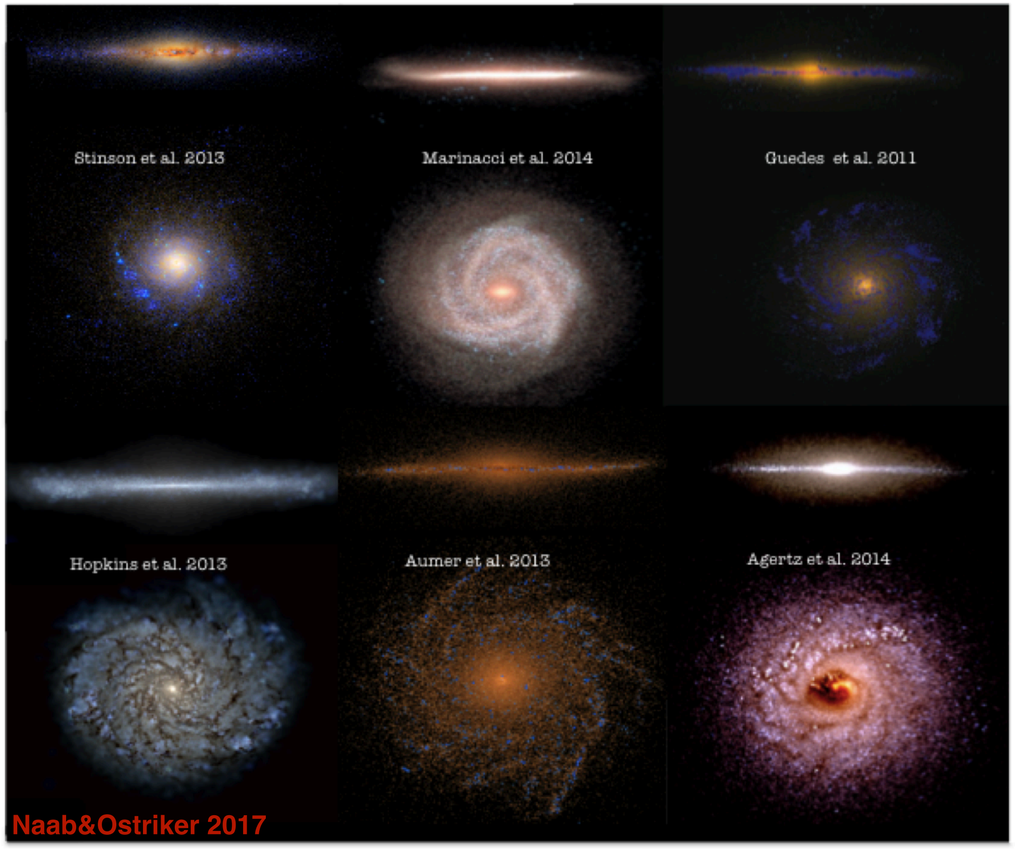
IMPACT OF NUMERICS AND SUB-GRID PHYSICS



- **Sub-resolution physics modelling** is crucial
- **Resolution** and the **hydrodynamic scheme** play a significant role







Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

THE *OpenGADGET3* CODE: A STATE-OF-THE-ART CODE FOR HPC

USM LMU UNIVERSITÀ DEGLI STUDI DI TRIESTE

The OpenGadget3 code

- **TreePM+SPH code**
- **Highly optimised code:** MPI parallelised + OpenMP
- **Two hydro solvers:** improved SPH formalism or MFM
- **Two sub-grid models** (Muppi, and one based on Springel&Hernquist 2003)
- **Several modules for sub-resolution physics:** star formation, stellar feedback, BH accretion and feedback, chemical enrichment, dust evolution, magnetic fields, cosmic rays
- **Runs on CPUs and GPUs**

MUPPI sub-resolution model

- description of a multi-phase ISM with H_2-based star formation
- thermal, kinetic, and low-metallicity stellar feedback
- improved cooling table interpolation
- stellar evolution and chemical enrichment

star formation

- angular-momentum-dependent gas accretion, dynamical friction, spin evolution
- isotropic, thermal AGN feedback + mechanical AGN feedback

BH

- formation and evolution of dust, and dust-assisted cooling

dust

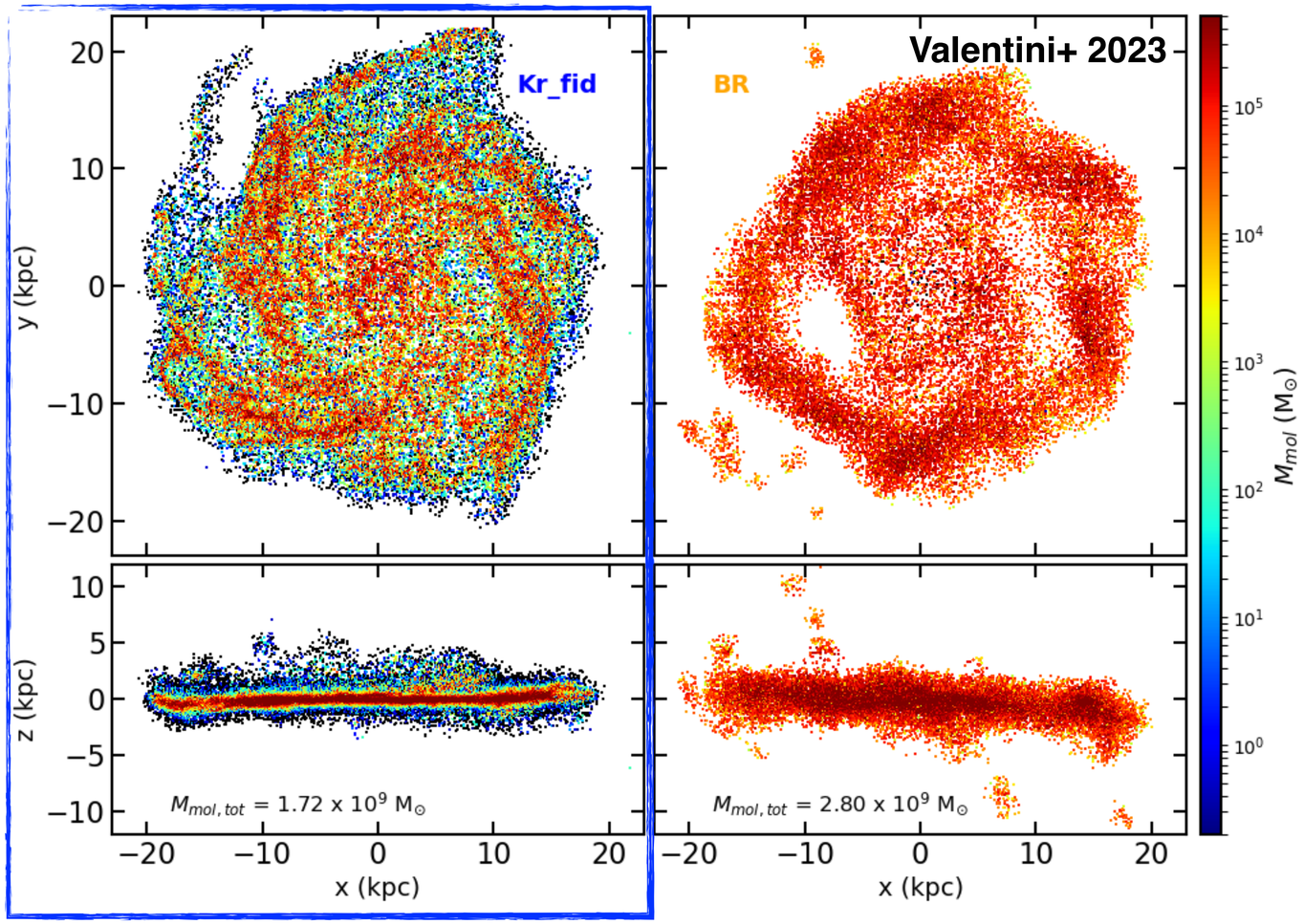
Main tasks within the WP 2 of Spoke 3

Develop Open-GADGET further:

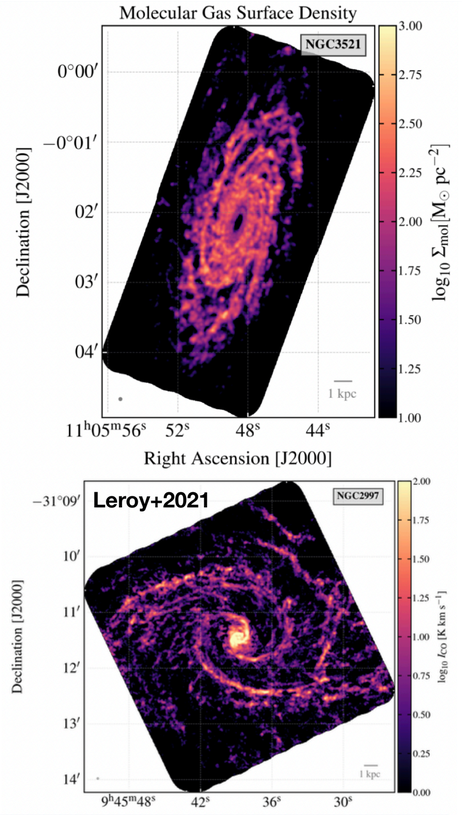
- **including additional physics modules**
- **enhancing code modularity and readability**
- **improving code performance**

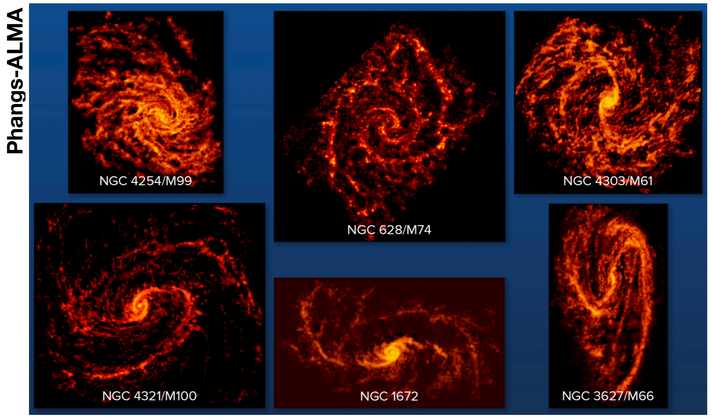
Core teams in Trieste and Munich

SUB-GRID MODELLING OF STAR FORMATION



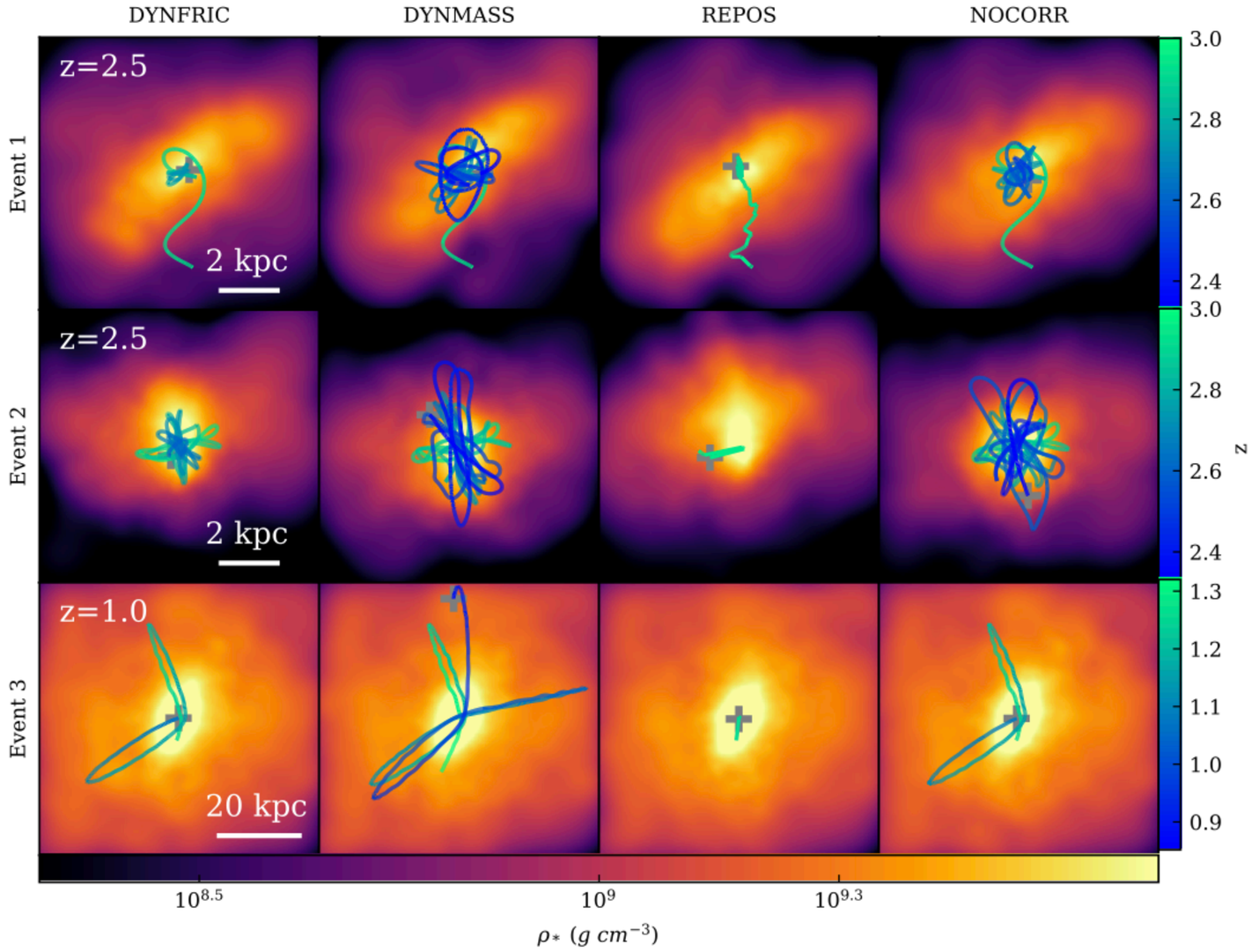
Different assumptions on the modelling of the molecular gas fraction affect the star formation rate and galaxy properties





Final properties (e.g. morphology) of simulated galaxies help in supporting or disfavouring different models to estimate the star formation rate

BLACK HOLE DYNAMICS IN COSMOLOGICAL SIMULATIONS



Damiano, Valentini, Borgani+ 2024

→ New approach to correct for the effect of **unresolved dynamical friction** on the orbits of BH in cosmological sims:
increased efficiency in centering BHs and accurate spiraling of BH orbits during mergers

Correcting for unresolved dynamical friction provides good BH centering, reduces wandering BHs, captures fairly BH-BH mergers

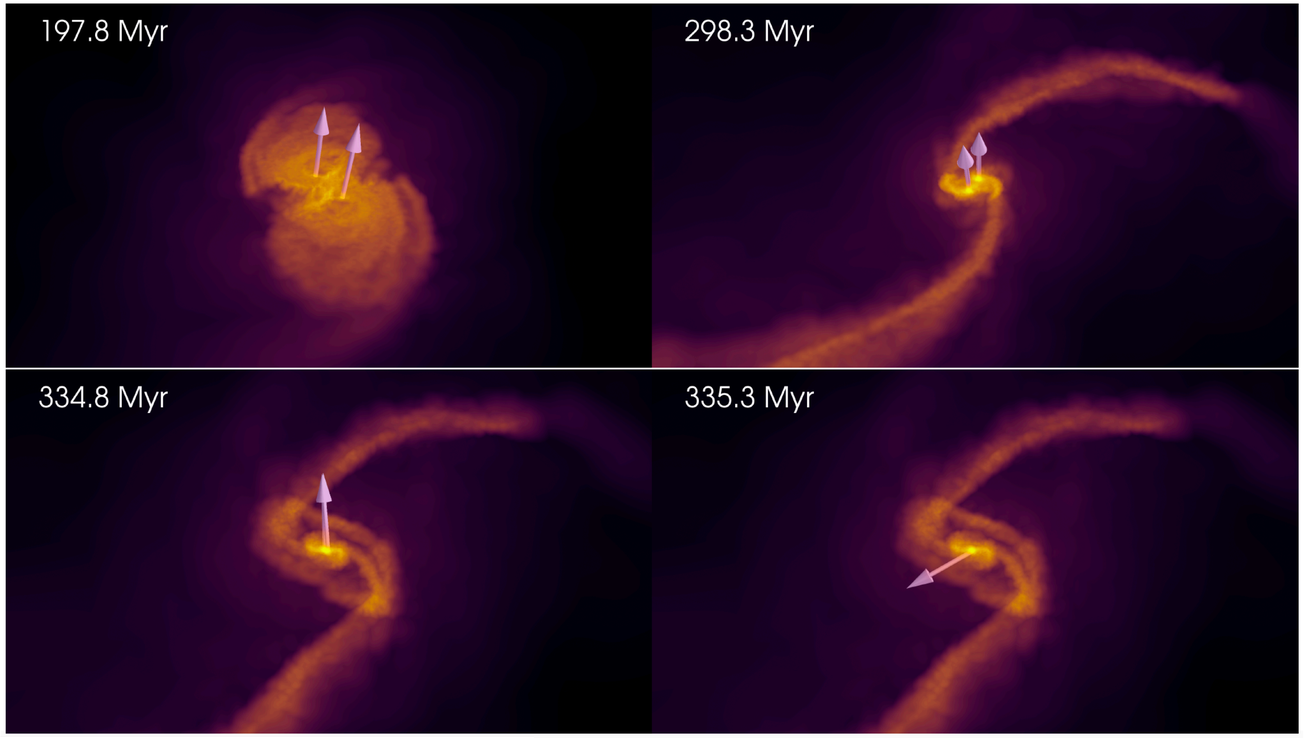
Adopting different numerical prescriptions for BH re-positioning has an impact on BH dynamics, AGN feedback, BH-BH mergers

MODELLING THE EVOLUTION OF THE BLACK HOLE SPIN

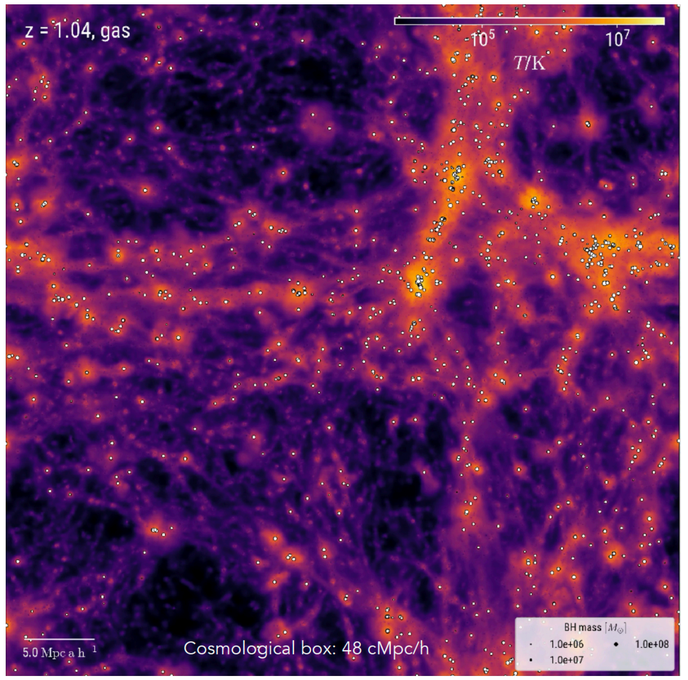
Sub-resolution accretion disc links BH accretion on resolved scales to BH spin evolution

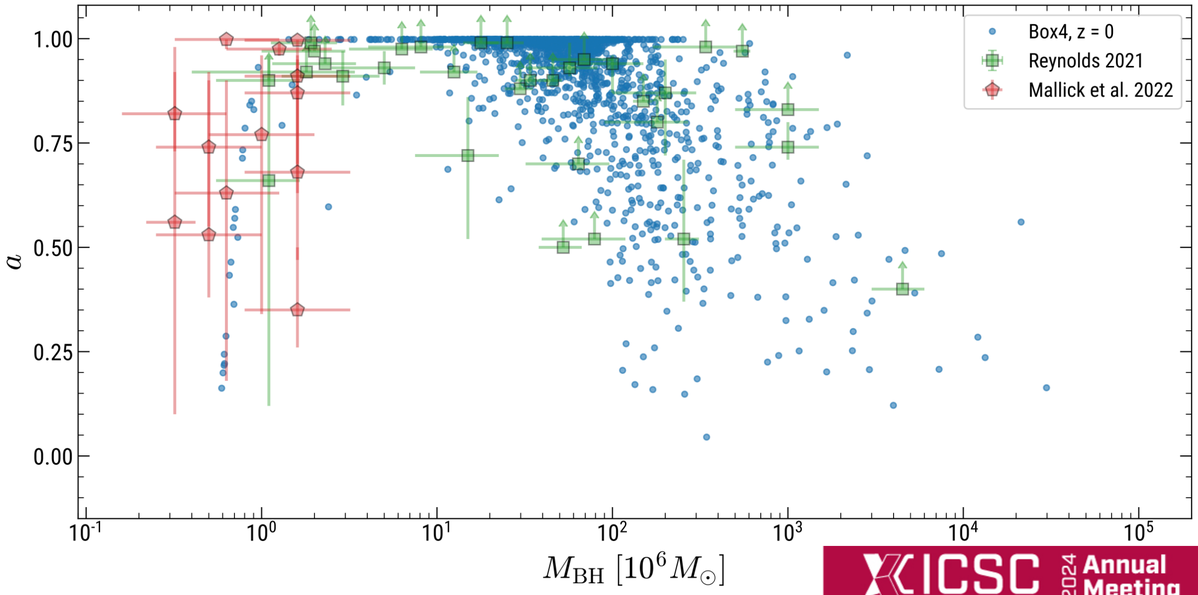
BH spin direction and magnitude → angular momentum of accreting gas
and mergers with other spinning BHs

BH radiative efficiency dependent on BH spin



Sala, Valentini+ 2024



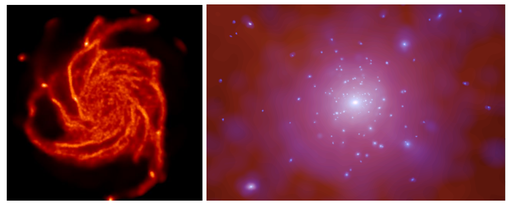


KEY SCIENCE PROJECTS WITHIN ICSC - SPOKE 3

EAGER: Evolution of gAlaxies and Galaxy clustErs in high-Resolution cosmological simulations

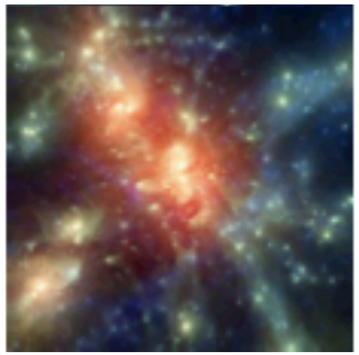
Main **scientific goal** of the project:

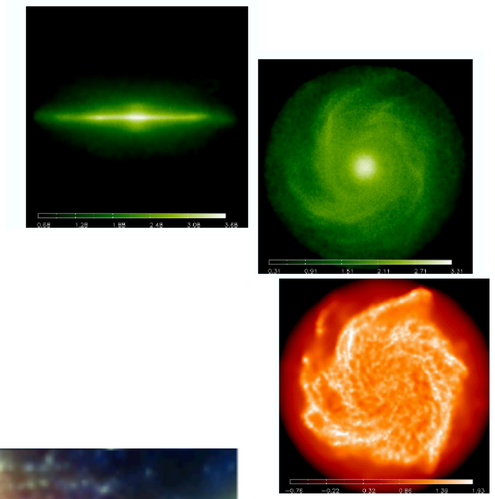
- investigate the connection between **super-massive BHs and host galaxies**, and the large-scale environment



From MW-like galaxy, to Ellipticals and small boxes,

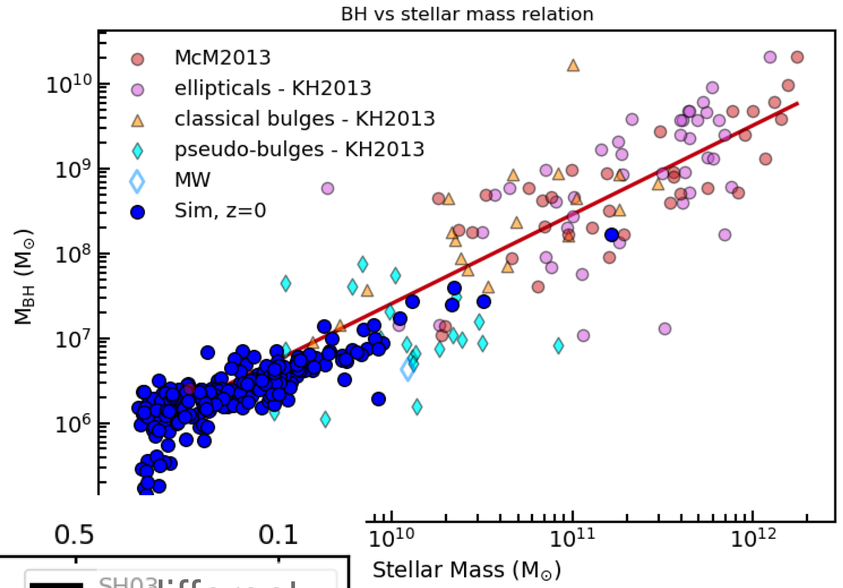
to galaxy clusters and large volumes

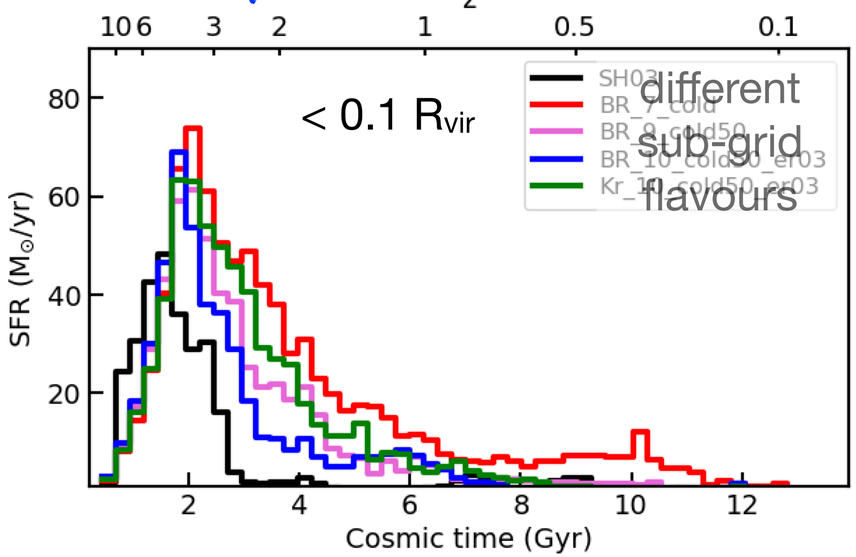




Spiral

Massive elliptical





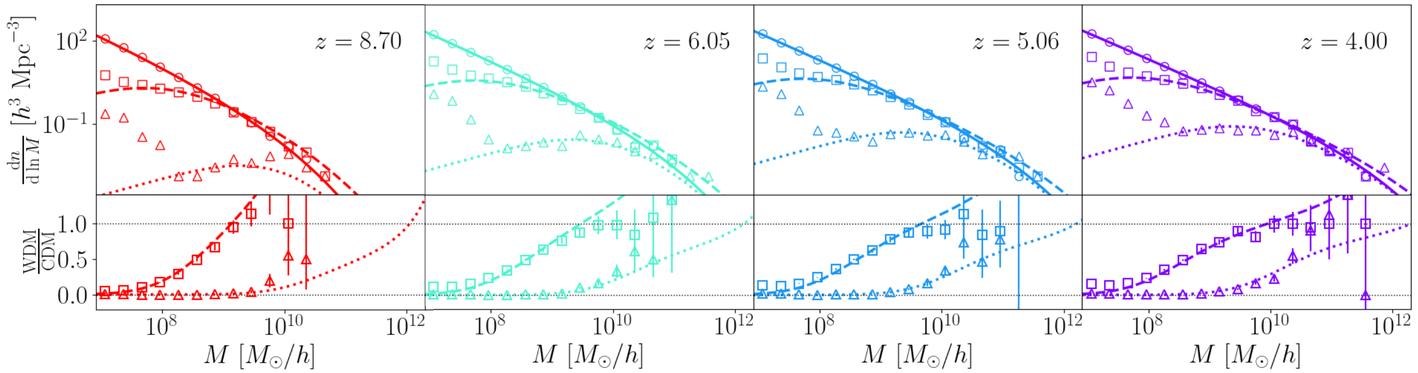
KEY SCIENCE PROJECTS WITHIN ICSC - SPOKE 3

SLOTH: Shedding Light On dark matter wiTH cosmological simulations

Main **scientific goals** of the project:

- theoretical understanding of primordial structure formation
- characterisation of the nature of dark matter
- exploitation and reliability of galaxy clusters as cosmological probes

Halo mass: FOF; universal function: Sheth-Tormen
ΛCDM: $a = 0.707, p = 0.3$
WDM 1 keV: $a = 1.000, p = 0.300$, window = smooth-k, $c_{M(R)} = 3.3, \beta = 4.8$
WDM 3 keV: $a = 0.707, p = 0.300$, window = smooth-k, $c_{M(R)} = 3.3, \beta = 4.8$



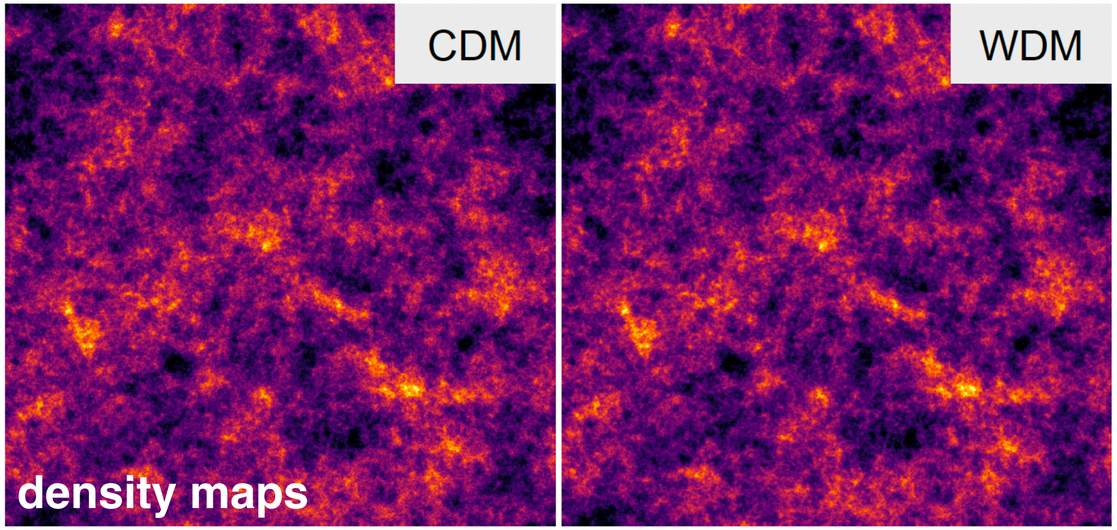
CINECA

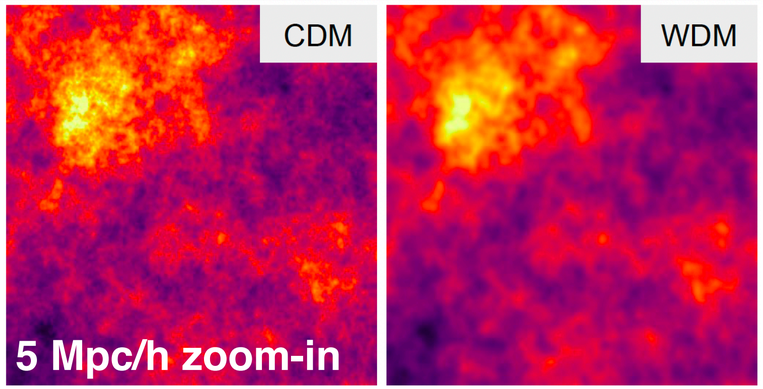
EuroHPC Joint Undertaking

Project Scope and Plan - Leonardo Early Access Program (LEAP)

Call for Leonardo Early Access Program

Simulations of warm dark matter (WDM): first results on a (10 Mpc/h)³ box w/ 1024³ particles





Valentini M., Castro T., Borgani S., Viel M., Tornatore L., Ragagnin A., Dolag K., Parimbelli G., Murante G., Dakin J.

TECHNICAL WORK FOR FRONTIER HPC

Assessing scalability, targeting performance issues

1. GPU scalability

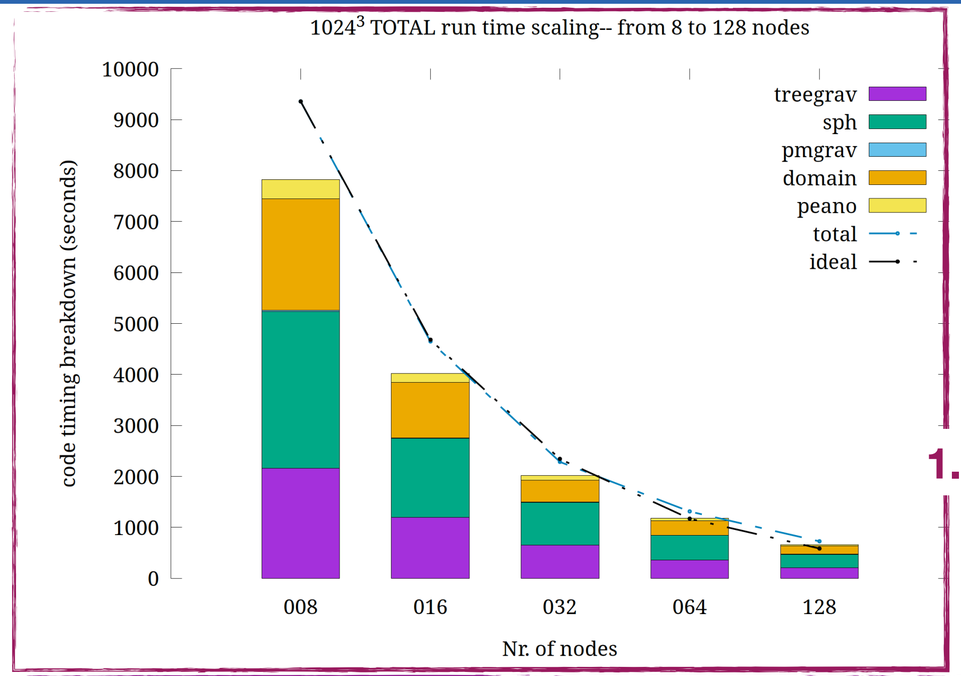
OpenGadget has most of the modules running on GPUs

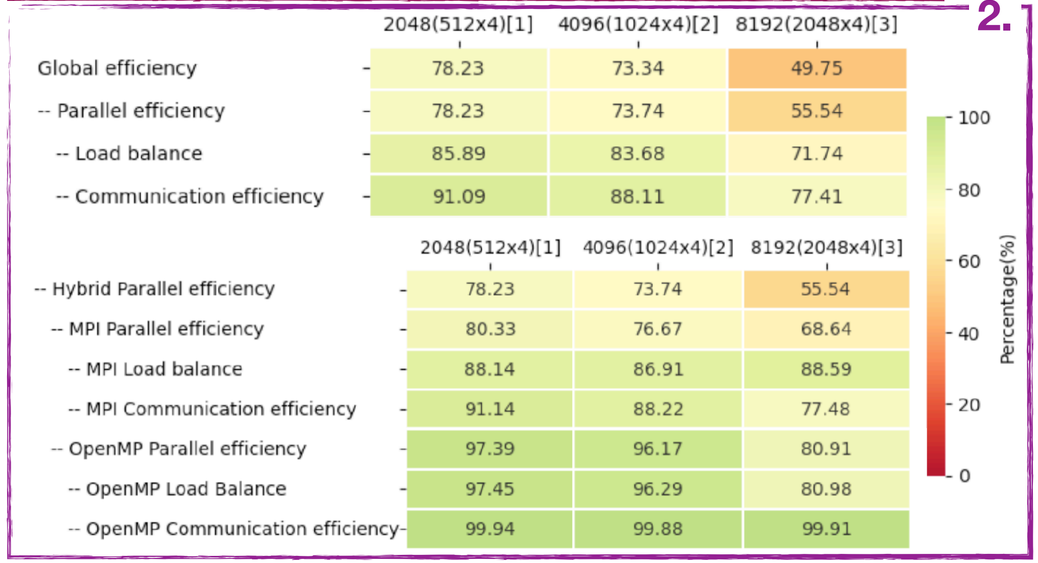
We are assessing in detail the scalability of this implementation in order to highlight the blocking factors, mitigate their impact or turn to new strategies with greater parallelisms

Collaboration with **Exact Lab (via Cascade Fundings)** to improve the efficiency of the existing GPU performance of OG3 exact lab

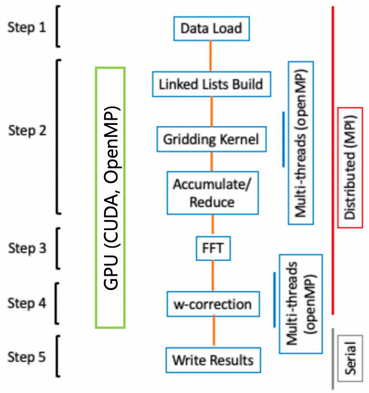
2. Performance issues

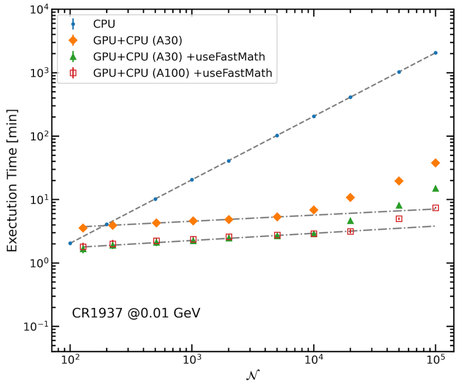
Detailed profiling with the **POP** and **SPACE Centers of Excellence**

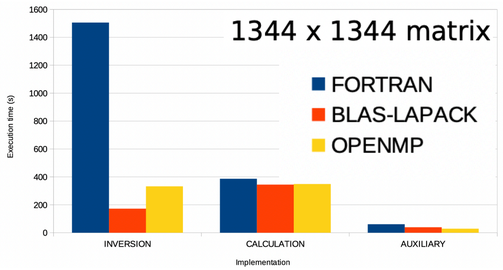


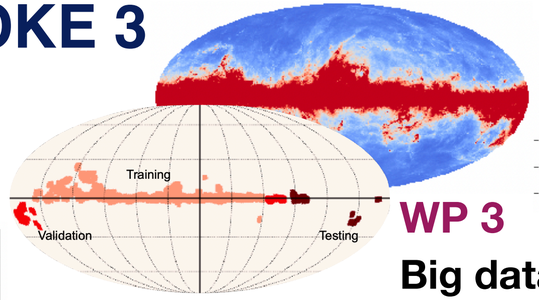


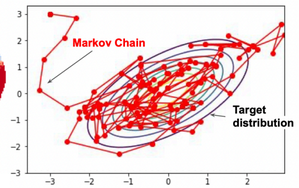
OUR EFFORT IN WORK PACKAGE 2 WITHIN SPOKE 3

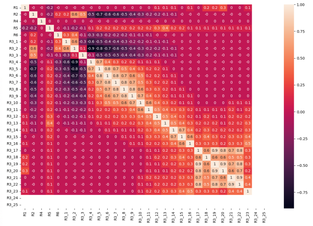












WP 1

Porting of codes and algorithms **on GPUs**

WP 2

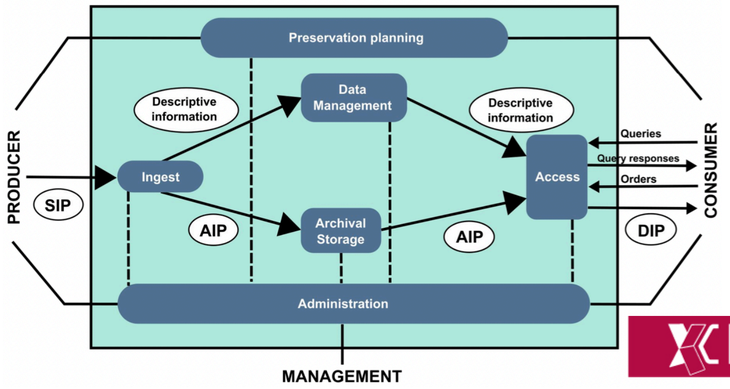
Optimisation and functionality extension **of codes** running **on GPUs**

WP 3

Big data processing and **visualization**, by adopting innovative approaches (e.g. Artificial Intelligence, inference via Bayesian statistics) for the **analysis of** large and **complex data volumes**, and efficiently exploiting HPC solutions

WP 4

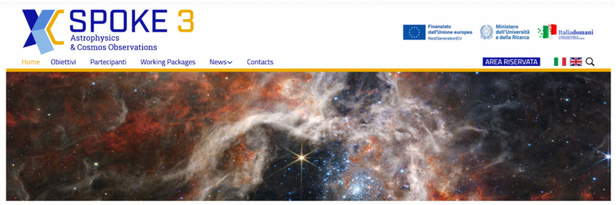
Big Data Managing, **Storage and Archive**: creation of web application for data management and of tools to move data



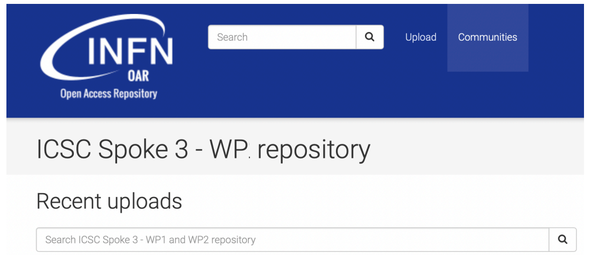
WP 5

Managing, maintaining and deploying an integrated environment which provides the **tools** for the efficient development of the community work

Website



Spoke repository



CONCLUSIONS

- **Cosmological** hydrodynamical **simulations** are a key tool to study galaxy formation and evolution, but different **sub-resolution prescriptions** affect final results
- Entered the era of HPC and fully exploiting the growing computational power from HPC facilities: our code is rather complete as for the inclusion of physical processes implemented, and computationally efficient
- Our OpenGADGET3 code is able to smoothly scale on state-of-the-art exascale infrastructures, and to efficiently exploit CPUs and GPUs
- Code soon to be released: it will contribute to allow us to study structure formation with unprecedented detail

Thank you!

