Sustainability of Extreme-Scale Simulations with SPH-EXA

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https://github.com/unibas-dmi-hpc/SPH-EXA

Download SPH-EXA

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SPH-EXA SKACH

Platform for Advanced Scientific Computing

TGSF: The role of Turbulence and Gravity in Star Formation

EuroHPC Joint Undertaking

Extreme Scale Access

Allocation: **22,000,000 GPUh*** on LUMI-G
Duration: 12 months, Nov.’23 – Oct.’24
*Largest allocation in Europe to date.

Objectives

Cosmology & Astrophysics

- Study the formation of pre-stellar cores and their initial mass function at unprecedented resolution — Scalability limitation for previous codes
- Study turbulent transport and mixing
- Contribute to the general theory of turbulence (Lyapunov exponents)

More natural with Lagrangian codes (for the two objectives above)

Computer Science

- Study the load imbalance, performance, and energy consumption at unprecedented scales
- Study large scale compression techniques for checkpointing, compression, and visualization

HPC research at extreme scale

Publications | News

PASC project principle investigators discussing their new astrophysical simulation code, which helped them win a large

TGSF: The role of Turbulence and Gravity in Star Formation

Definition

Sonic scale (l_s) : is the scale at which the transition from supersonic to subsonic turbulence occurs.

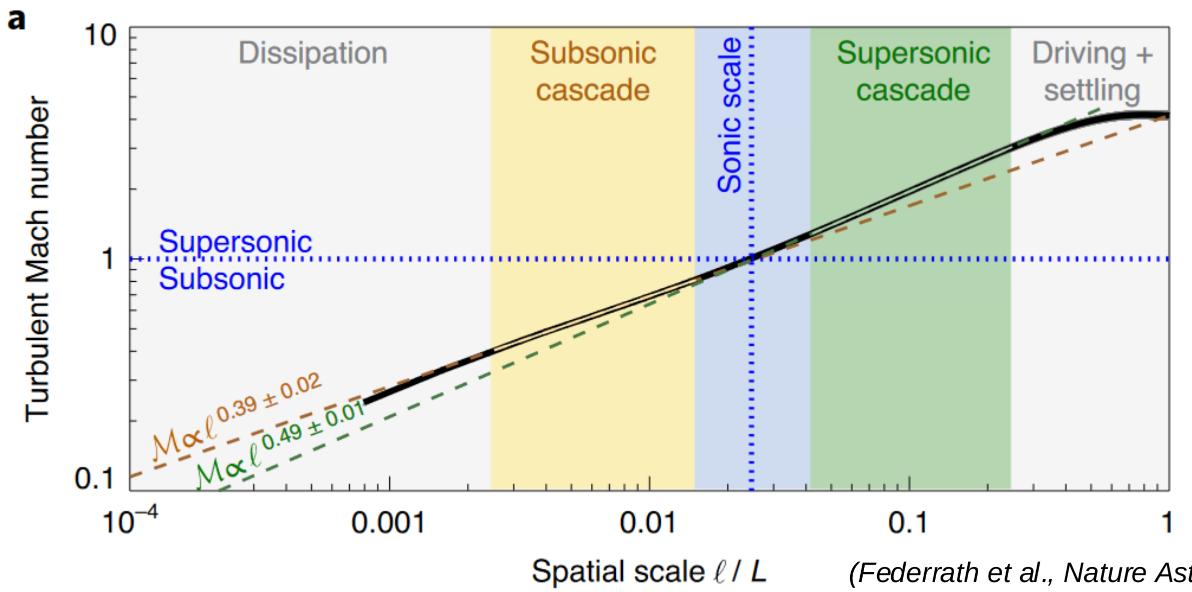
$$l_s = \phi_s L(\mathcal{M})^{-2}$$

ϕ_s encompases our lack of knowledge about the exact position of the Sonic scale. Usually taken as $\phi_s = 1$

Nevertheless, a large-scale simulation (Federrath et al. 2021) has directly measured ϕ_s to be x2.4 smaller.

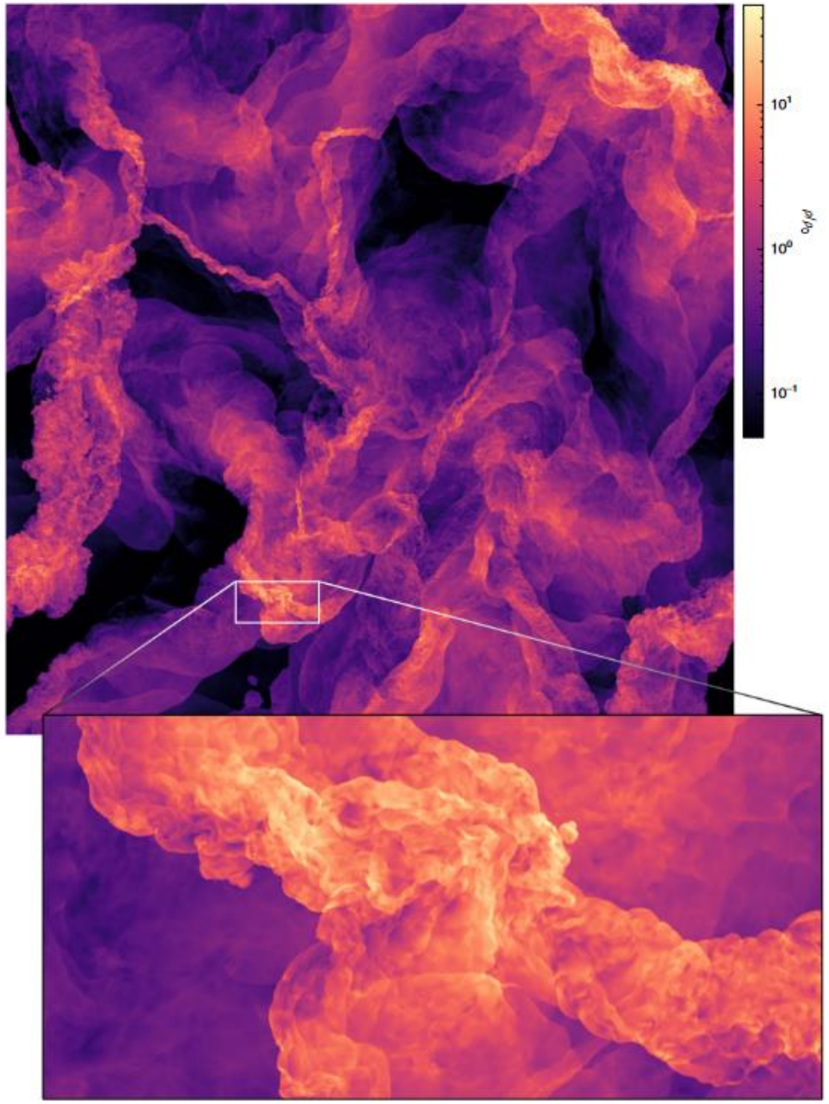
This pushes the collapse scale to smaller scales than previously considered and it has a critical relevance in the predictive power of star formation theories.

In order to test this, **self-gravity** must be included in such simulations.



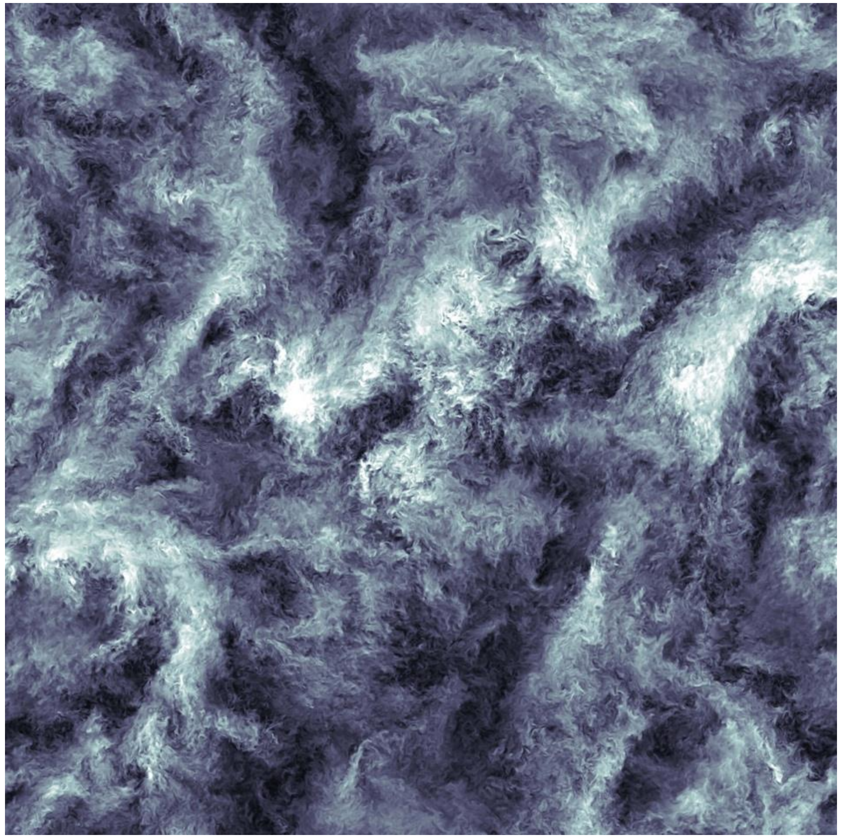
(Federrath et al., Nature Astronomy, 5, 2021)

TGSF: The role of Turbulence and Gravity in Star Formation



FLASH
Eulerian code
$10{,}048^3$ grid cells
Hydrodynamics only (no gravity)
CPU only (65,536 cores)

SPH-EXA
Lagrangian code
$10{,}079^3$ SPH particles
Hydrodynamics + gravity
CPU + GPU (16,416 GPUs)



Gas density contrast distribution of ISM turbulence. (Federrath et al., Nature Astronomy, 5, 2021)

Velocity field distribution of subsonic turbulence. 3000^3 particles (SPH-EXA team, 2023)

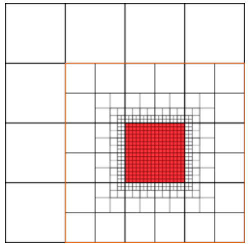
SPH-EXA: Smoothed Particle Hydrodynamics at Exascale

SPH-EXA is a *scalable* smoothed **p**article **h**ydrodynamics simulation framework **interdisciplinarily co-designed** by computational physicists and computer scientists to exploit **Exa**scale supercomputers.

SPH-EXA: Framework Components

SPH-EXA application front-end

Parallel I/O and test case setup (ICs)

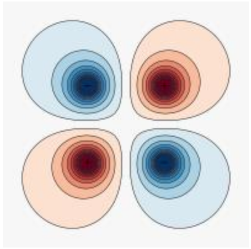


Cornerstone

Octree and domain decomposition framework

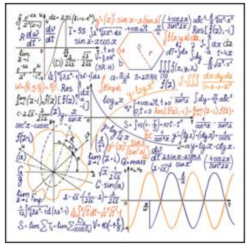
SPH

Hydrodynamics solver



Ryoanji

N-body gravity solver



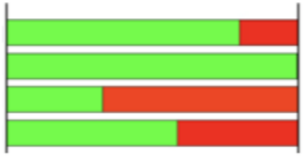
Physics modules

Radiative cooling
Nuclear reactions
Star formation
Stellar feedback

SPH-EXA: Optimization Strategy

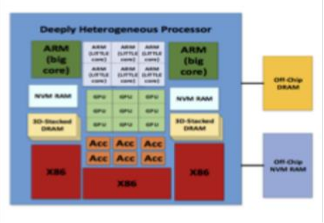
Scalability

weak, strong



Scheduling & Load-balancing

dynamic, adaptive asynchronous execution



Heterogeneity

portability on various CPU and GPU architectures

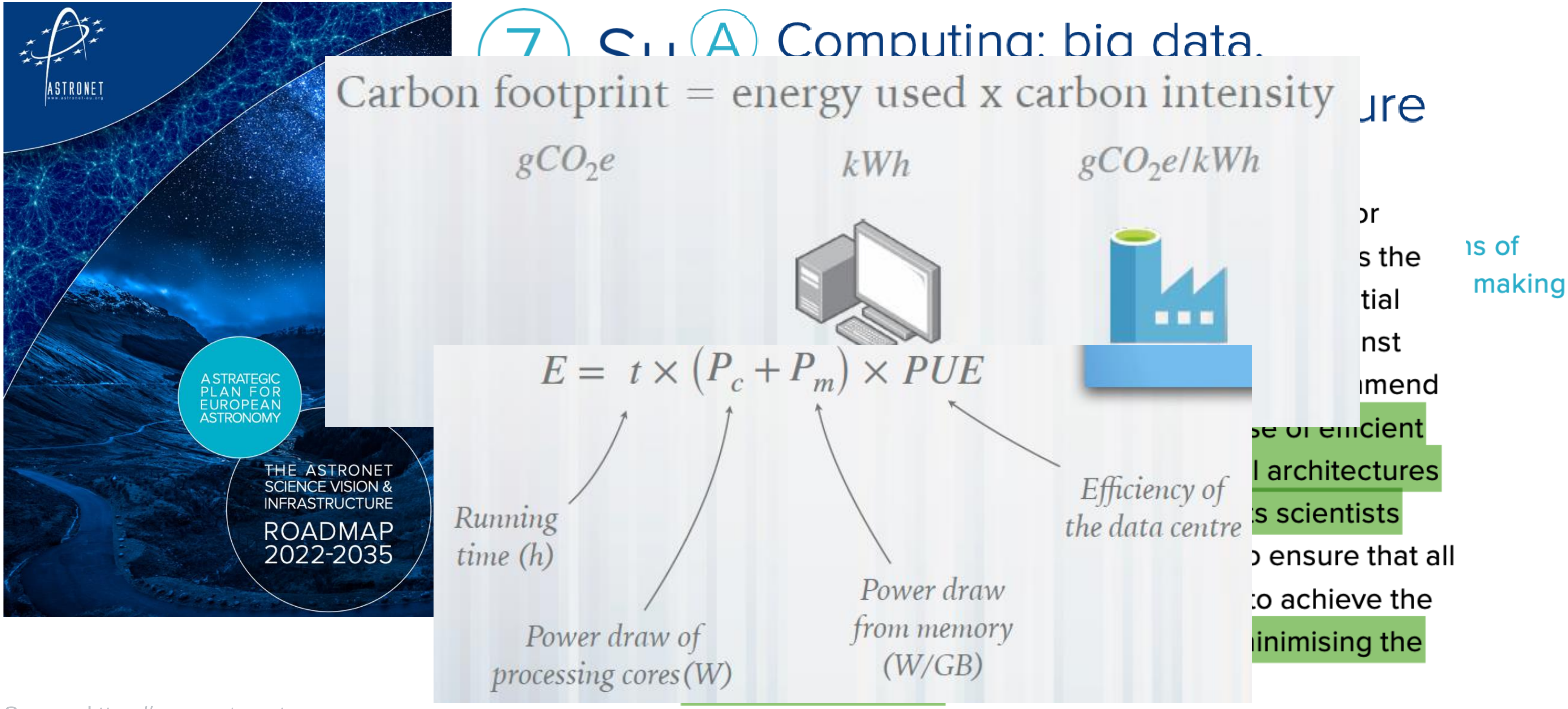
Fault-tolerance

silent error detection and recovery

Energy

measurement reporting efficiency

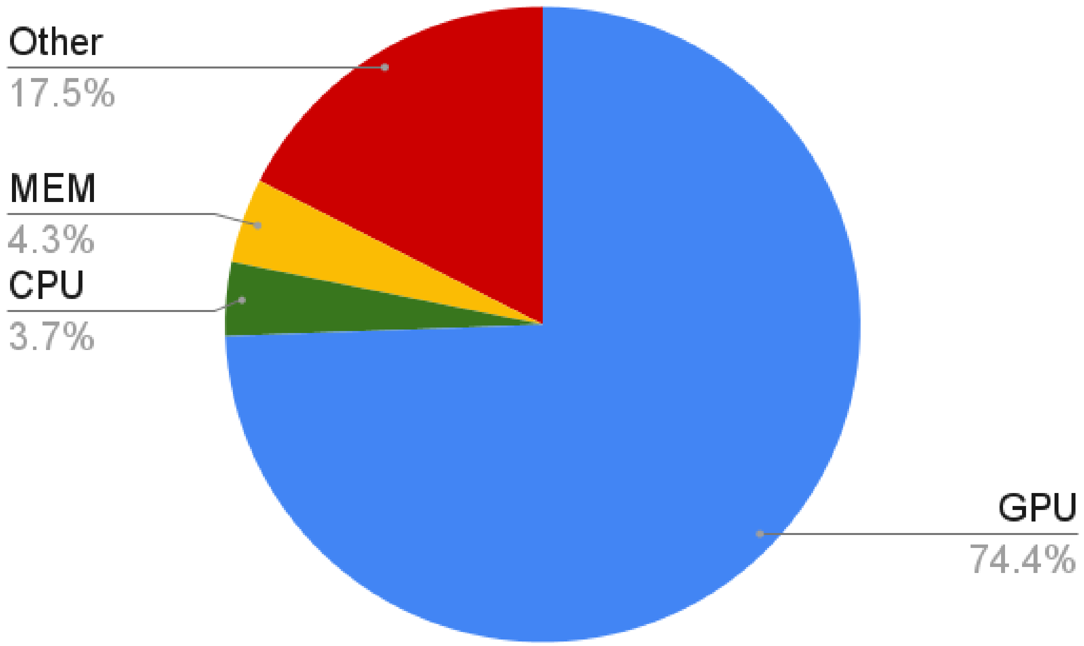
Sustainable Computing Motivation – Astronomy and Astrophysics



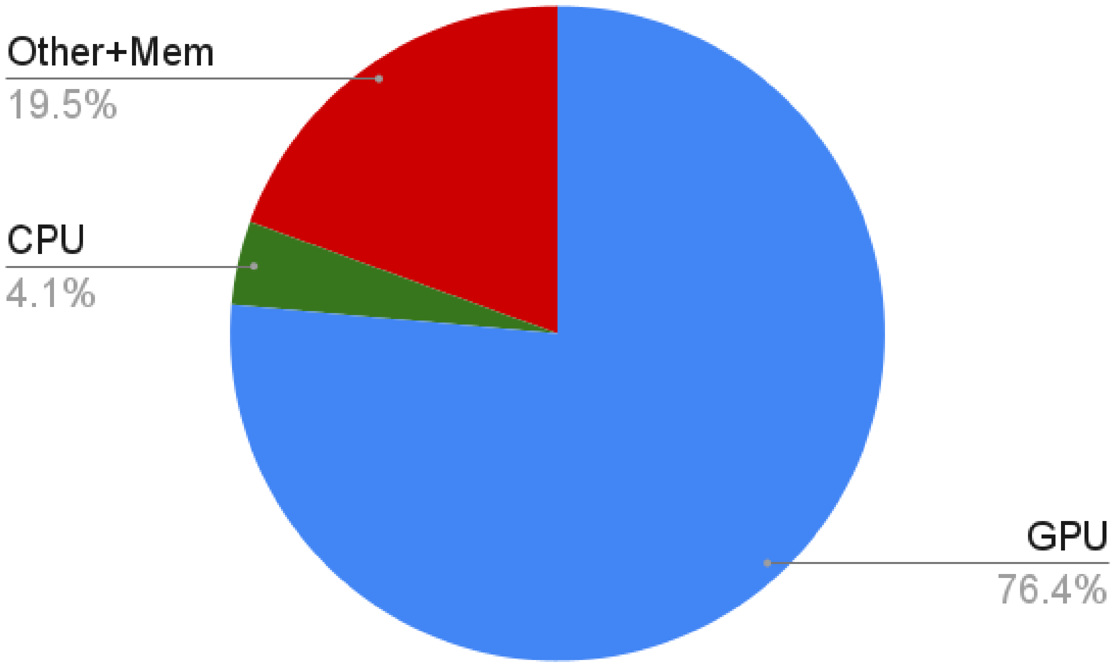
Source: https://www.astronet-eu.org

Energy Measurement and Reporting: Device Breakdown

Turbulence on LUMI-G AMD MI250X 32 MPI Ranks

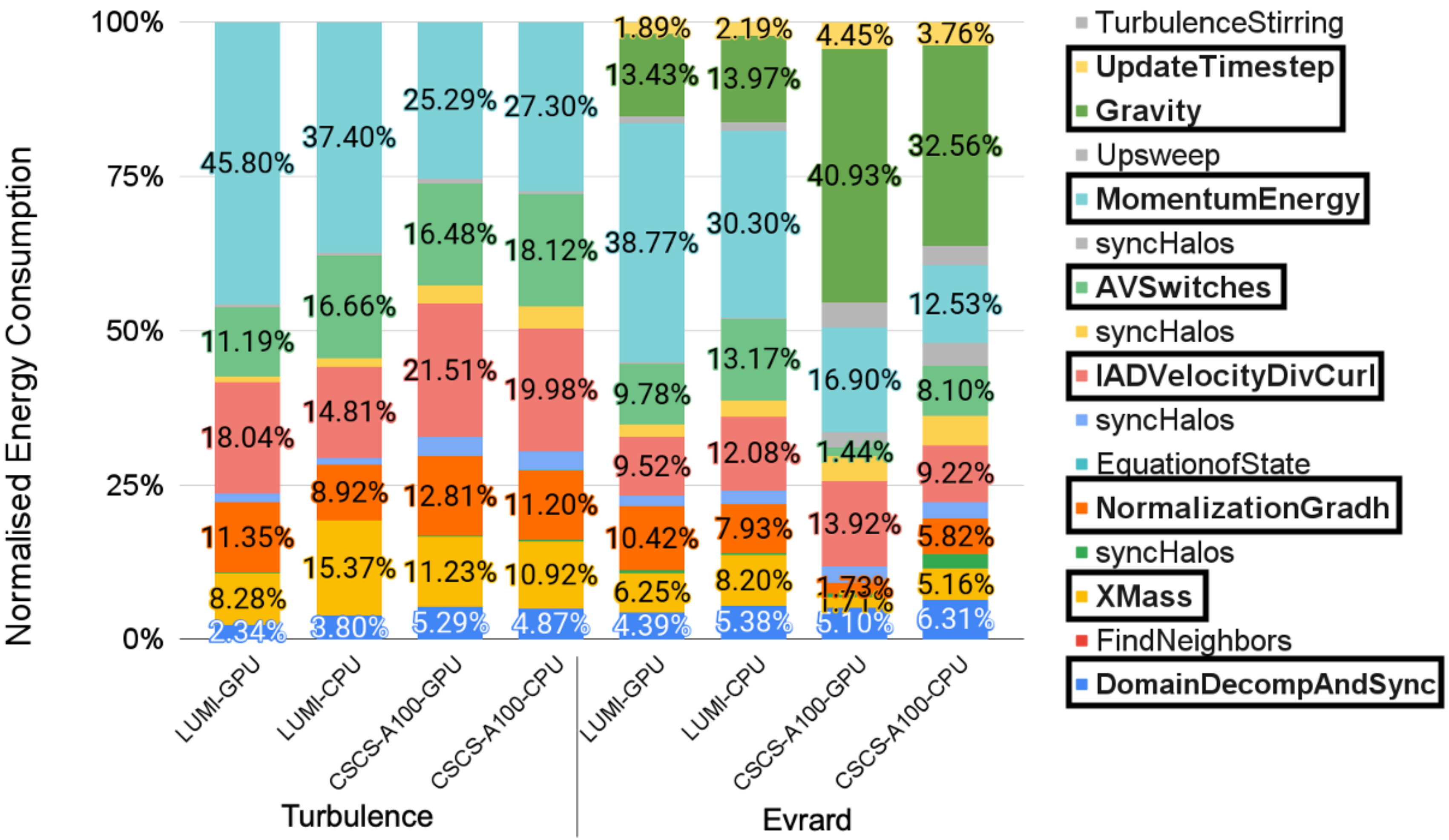


Turbulence on CSCS Nvidia A100 32 MPI Ranks

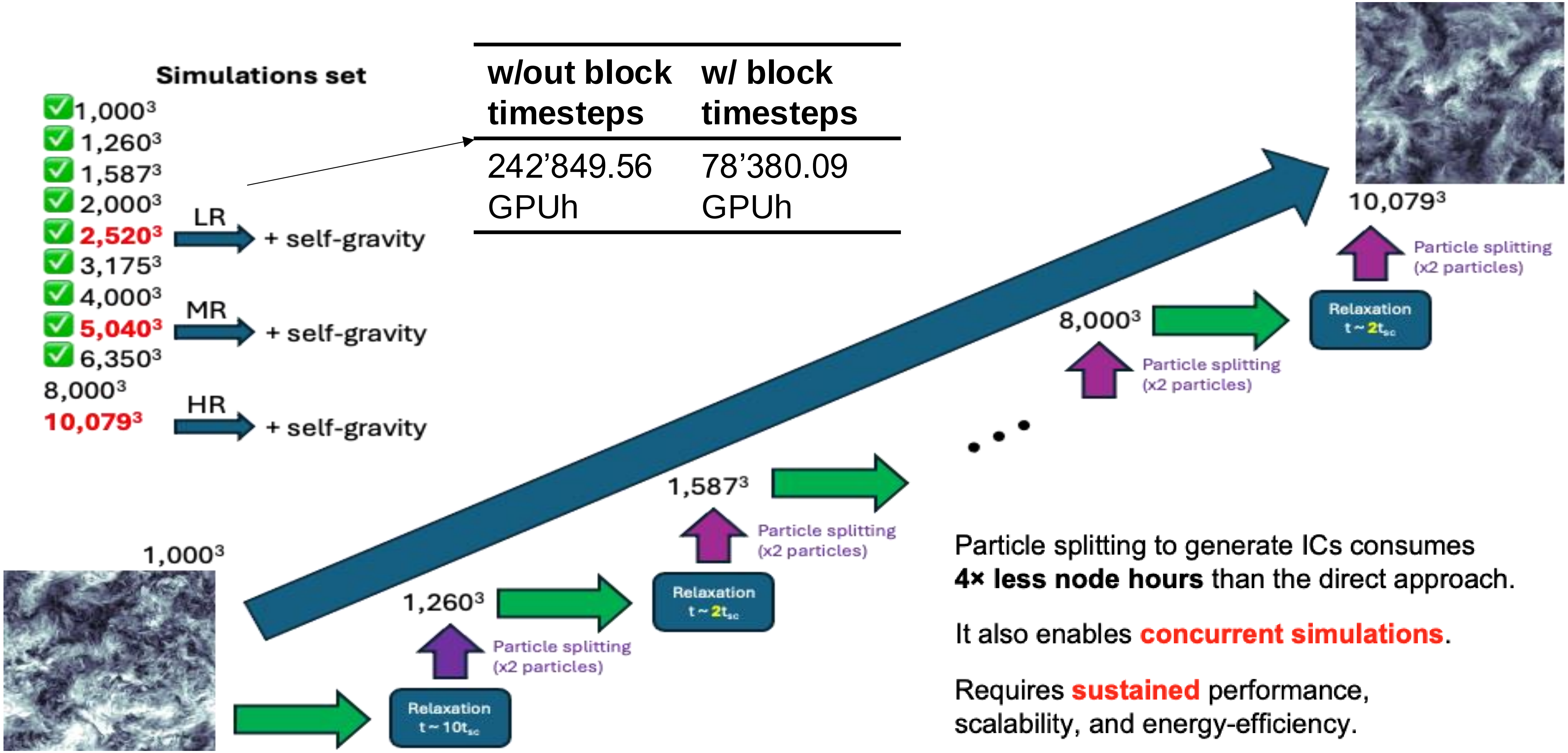


Energy Measurement and Reporting: Functional Breakdown

Code functional breakdown, 100 time-steps, 32 MPI Ranks on 4 LUMI-G Nodes and 8 CSCS-A100 Nodes



TGSF Simulation Plan



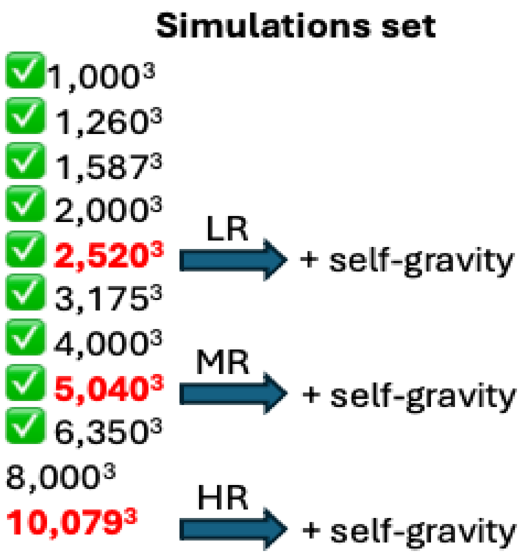
w/out block timesteps	w/ block timesteps
242’849.56 GPUh	78’380.09 GPUh

Particle splitting to generate ICs consumes **4× less node hours** than the direct approach.

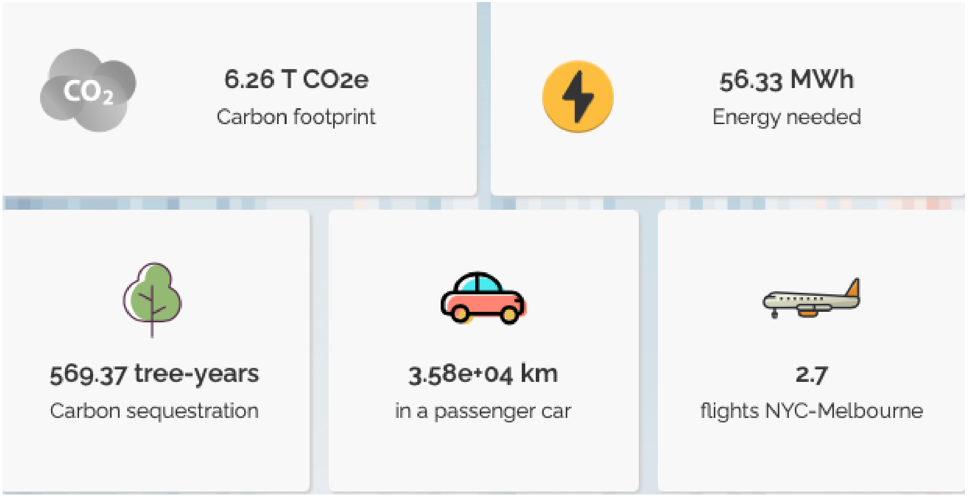
It also enables **concurrent simulations**.

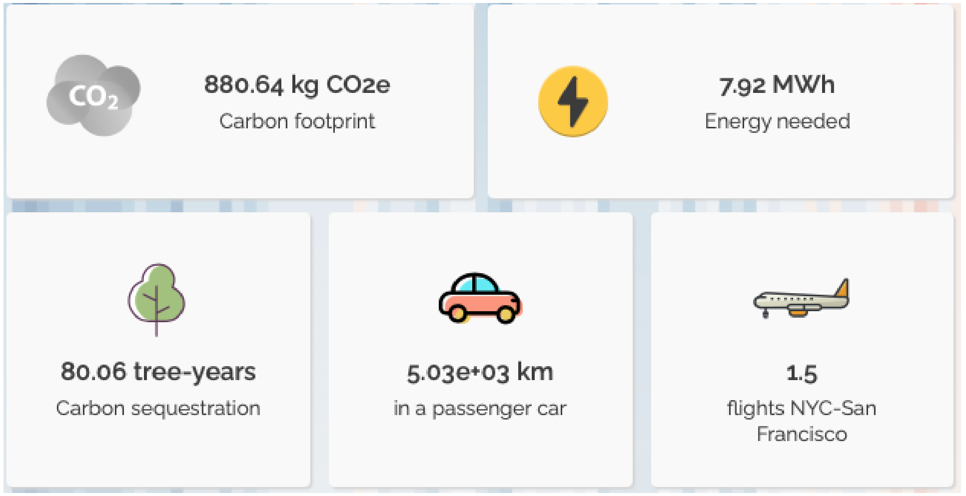
Requires **sustained** performance, scalability, and energy-efficiency.

TGSF Low-Resolution Simulation Energy Measurements

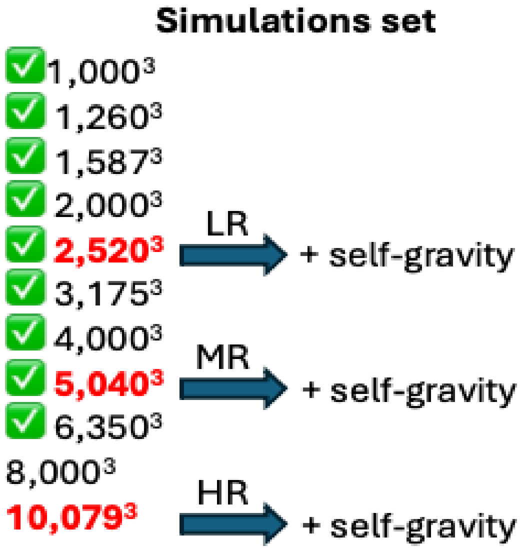


- Total of 35 jobs.
  - 6 failed and 29 successful.
- Succesful jobs = 242’849.56 GPUh
  - Measured value.
- Failed jobs = 34’082.44 GPUh
  - Calculated value.





TGSF Low-Resolution Simulation Energy Measurements



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Measured energy breakdown of successful jobs per device