
SPH EXA
PASC
Platform for Advanced Scientific Computing
SKACH
Universität Basel
sciCORE
Center for scientific computing
Universität Zürich[UZH]
CSCS
Florina Ciorba – University of Basel
Lucio Mayer – University of Zurich
Rubén Cabezón – University of Basel
March 17, 2025 – SKACH Science Day

https://github.com/sphexa-org/sphexa

FUNDING

Platform for Advanced Scientific Computing
2017-2025

SKACH
2021-2028

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SPH at EXAscale requires contributions from …

Computer Science


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Lukas Schmidt


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Yiqing Zhu


Aurelien Cavelan

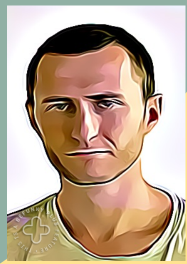

Jean G. Piccinali


Jean Favre


Danilo Guerrera


Michal Grabarcyck


Ayoub Neggaz


Joseph Touzet

Astrophysics


Rubén Cabezón


José A. Escartín


Axel Sanz

Cosmology


Lucio Mayer


Noah Kubli

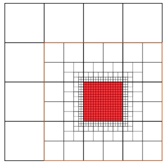

Darren Reed


Jonathan Coles

Extreme Scale Access
22,000,000 GPUh* on LUMI-G

SPH-EXA

SPH-EXA application front-end (github.com/unibas-dmi-hpc/SPH-EXA)
- Initial conditions, checkpointing, compression, parallel I/O
- Flexible combination and addition of additional physics for domain scientists
- Performance data for scheduling, load-balancing, energy-efficiency optimizations
- In-situ and post-hoc visualization
- **10'751** C++ LoC, Y= 287 CUDA/HIP → enables performance, portability, visualization



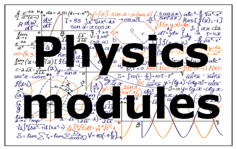
Cornerstone octree

Domain Decomposition
- Space-filling curves and octrees
- Global and locally essential octrees
- Octree-based domain decomposition
- **30'481** C++ LOC, Y= 6'840 CUDA/HIP → enables extreme scalability (weak and strong)

SPH Solvers

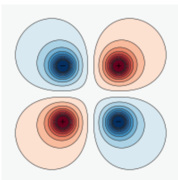
SPHYNX

ChaNGa



Modern SPH and physics implementation with key features
(astro.physik.unibas.ch/sphynx, github.com/N-BodyShop/changa)
- Generalized volume elements
- Integral approach to derivatives
- Artificial viscosity with switches
- Sub-grid physics
- **5'072** C++ LOC, Y= 2'152 CUDA/HIP→ enables accurate & robust hydrodynamics

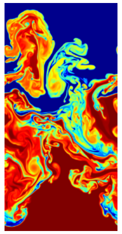
Flagship code for

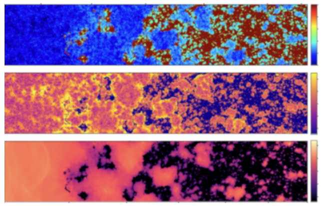


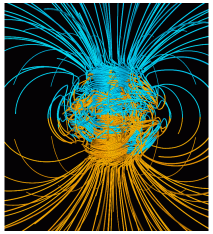
Ryoanji N-body solver

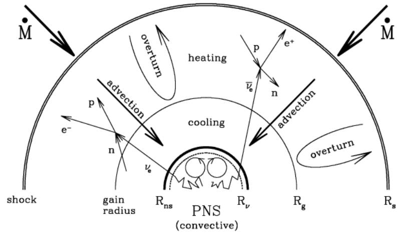
N-body Gravity-solver on GPUs with
- Cornerstone octrees
- Breadth-first traversal inspired by Bonsai (github.com/treecode/Bonsai)
- EXA-FMM multipole kernels (github.com/exafmm)
- Individual block time-steps native on GPUs
- **4'533** C++ LOC, Y= 2'137 CUDA/HIP → enables extreme scale Astro/Cosmo simulations

Current & future capability physics modules

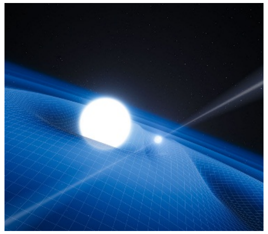

Hydrodynamics


Radiative transfer

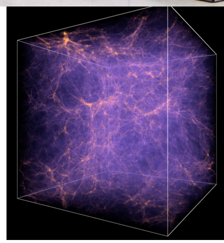

Magnetic fields



Neutrino transport


General Relativity

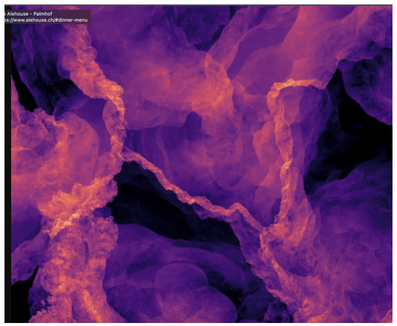

Nuclear network

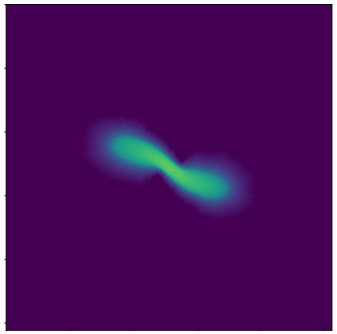

Cosmology

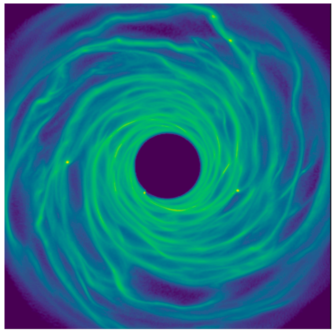
Goals

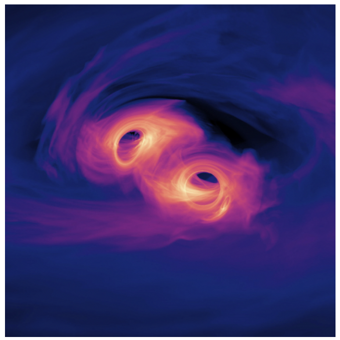
Astrophysics
- **Render highly scalable any computationally-challenging problem in astrophysics and cosmology**
- **Become the benchmark particle-based code in the field**
- **Focus on the most transformative science targets of next decade**

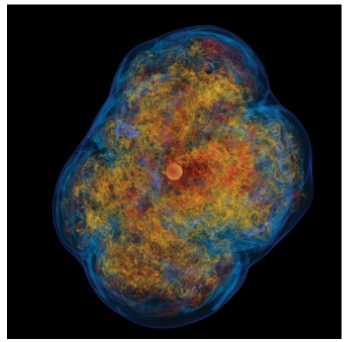
Computer Science
- **Adaptive load balancing of multiple adaptive time-steps**
- **AI-driven and AI-based performance & energy optimization**
- **Become the benchmark for domain-decomposition, load balancing, energy efficiency studies and system acceptance**


Star formation in the interstellar medium, turbulent flows


Stellar tidal disruption arounds supermassive black holes (SPH-EXA)


Protoplanetary disks and Planet formation (SPH-EXA)


Relativistic hydrodynamics: black hole mergers in astrophysical backgrounds


Core collapse Supernova

J. Nordhaus

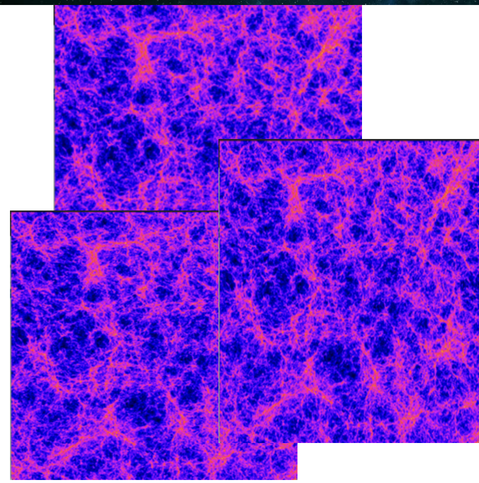
https://hpc.dmi.unibas.ch/research/sph-exa/

Self-gravity solver: novel algorithm (Cornerstone) to evaluate gravitational forces at scale on GPUs

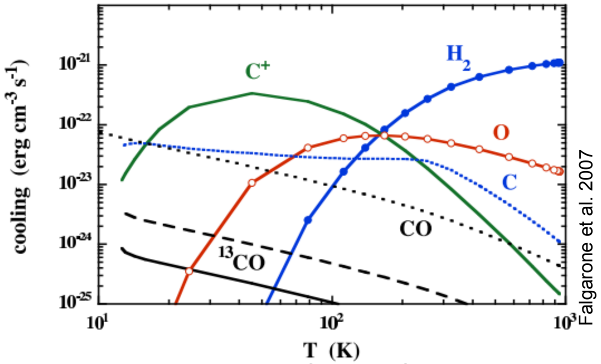
Individual particle time-steps - GPU-native block timestepping scheme

Equations of state: Ideal, Helmholtz, polytropic and tabulated nuclear EOS for explosive scenarios

Ewald summations: gravitational forces evaluation in boxes with periodic boundaries

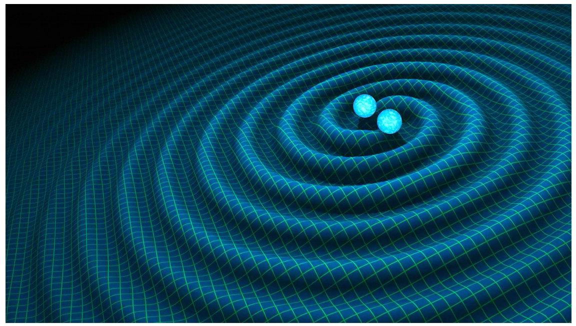


Grackle: chemistry and radiative cooling for astrophysical applications



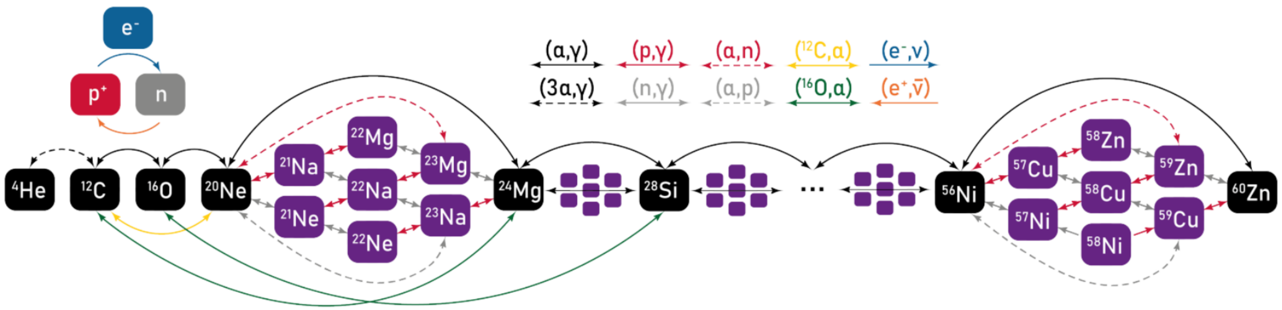
Gravitational waves: calculation of waveforms and energy emission

Sink particles (under development) for star and planet formation simulations



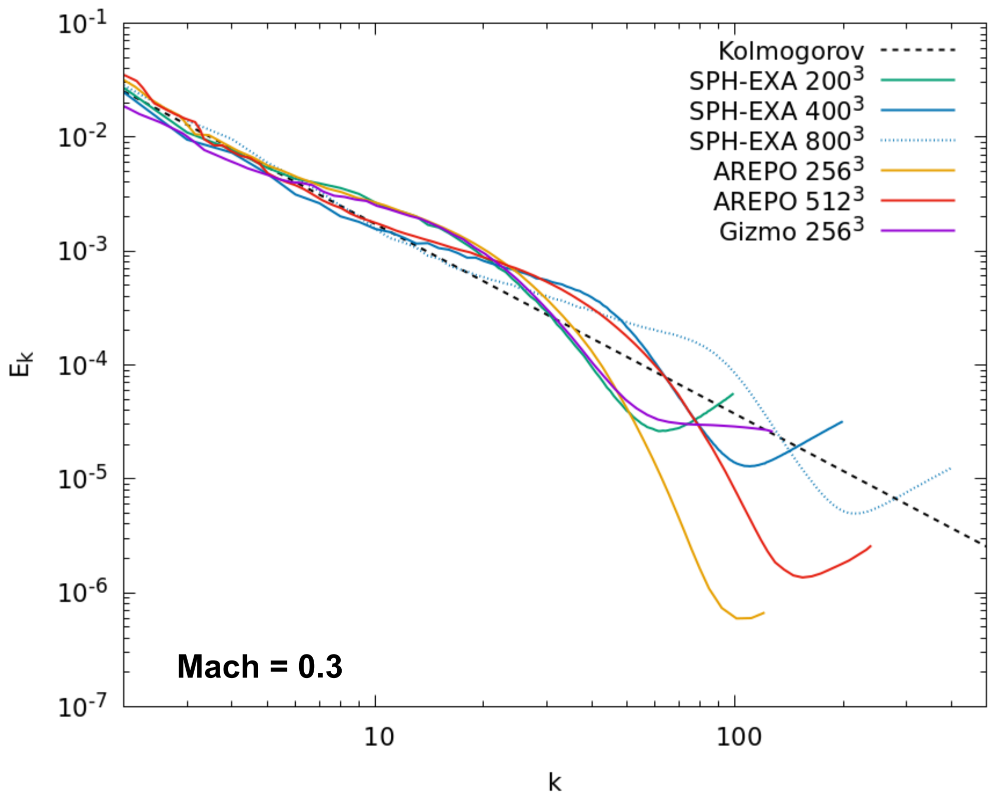
R. Hurt / Caltech-JPL

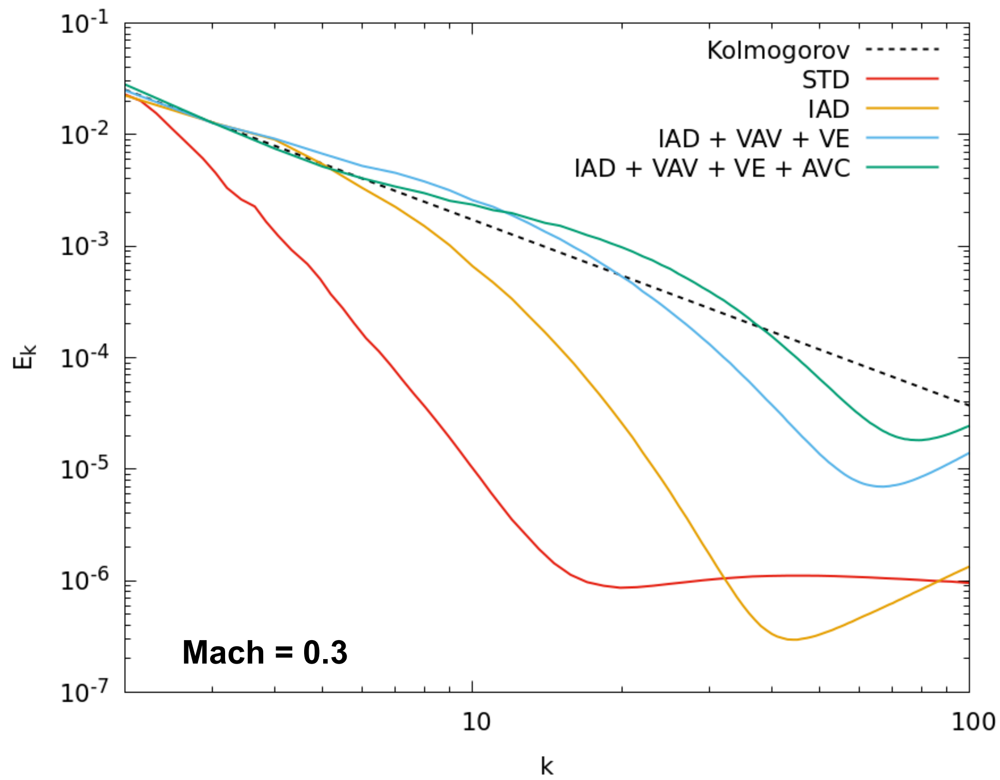
Nuclear network: energy generation and nuclear abundances from nuclear reactions



SPH-EXA combines a state-of-the-art implementation of the SPH method (volume elements, integral approach to derivatives..) with unprecedented performance to reach extremely high resolution.

This unique combination allows SPH-EXA to model notoriously hard problems such as the **subsonic turbulence cascade** as accurately as competitor grid codes





https://arxiv.org/pdf/2503.10273

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, extended to 21 Feb 25
***Largest allocation in Europe to date.**

Relevant to "Our Galaxy" and "Cradle of Life" SKAO WGs

Cosmology & Astrophysics

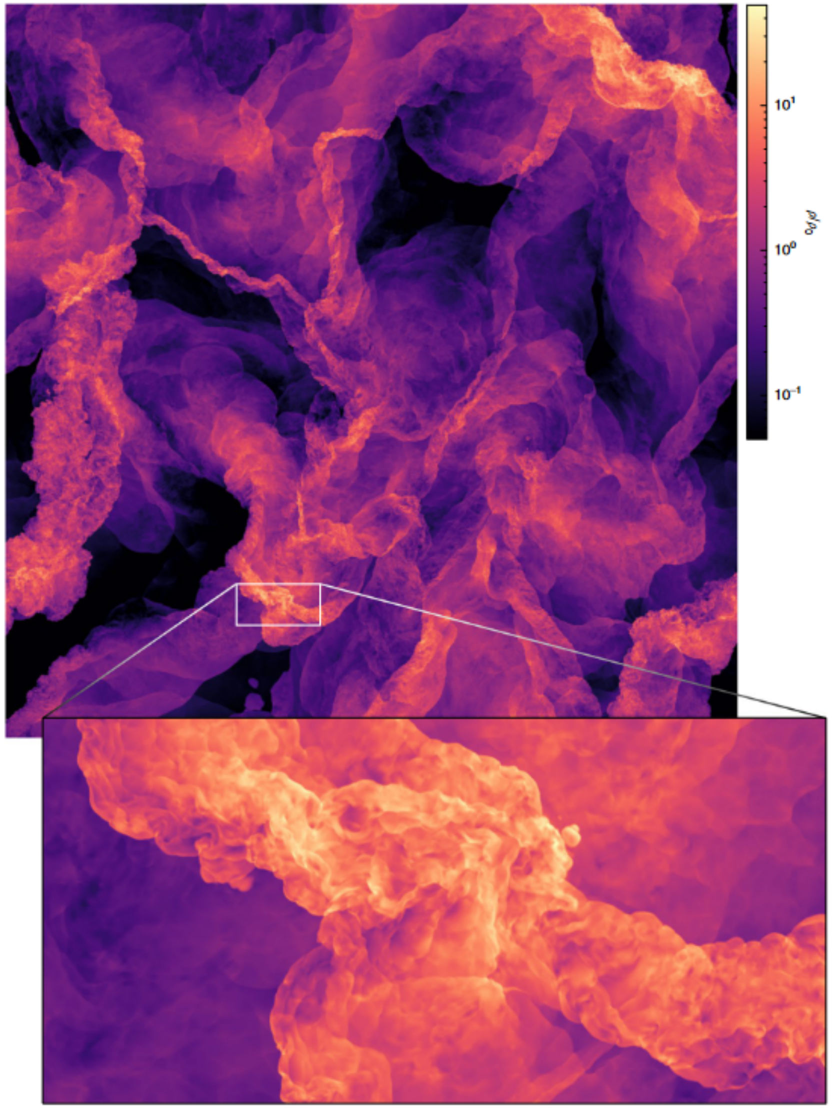
Computer Science

Objectives

- Study the formation of 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)
  - (these two: More natural with Lagrangian codes)
- Study the load imbalance, performance, and energy consumption at unprecedented scales
- Study large scale compression techniques for checkpointing, compression, and visualization
  - (these two: HPC research at extreme scale)

Publications | News

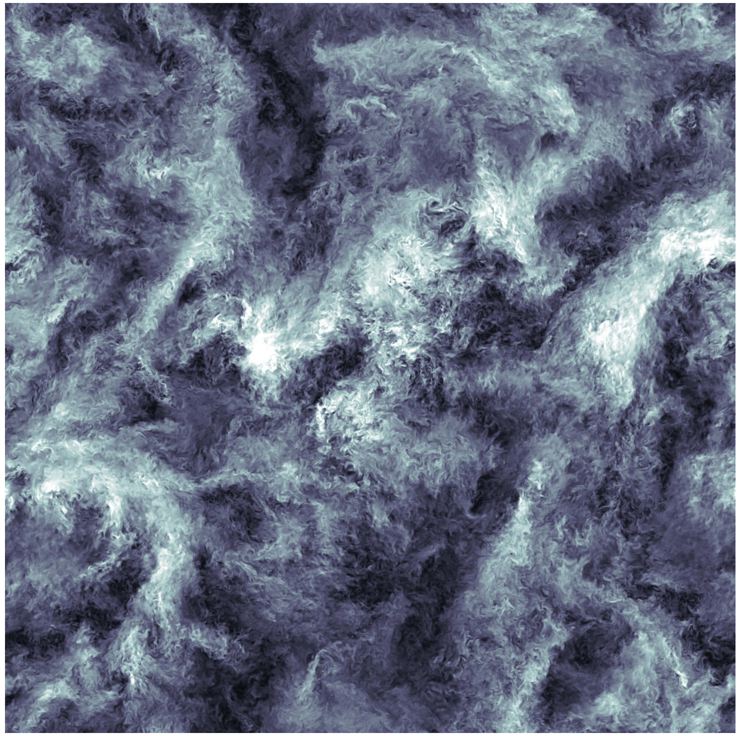
PASC project principle investigators discussing their new astrophysical simulation code, which helped them win a large allocation on LUMI-G https://bit.ly/cscs-sph-exa2



FLASH
Eulerian code
10,048^3 grid cells
Hydrodynamics + turbulence **only**
(no gravity)
CPU only (65,536 cores)
SuperMUC-Phase 1

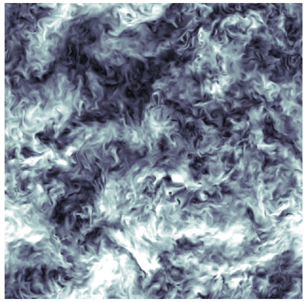
SPH-EXA

SPH-EXA
Lagrangian code
10,079^3 SPH particles
Hydrodynamics + turbulence
+ **gravity**
CPU + GPU (16,416 GPU GCDs)
LUMI-G



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)



Simulations set executed

$2{,}500^3$ → LR

$5{,}000^3$ → MR + self-gravity

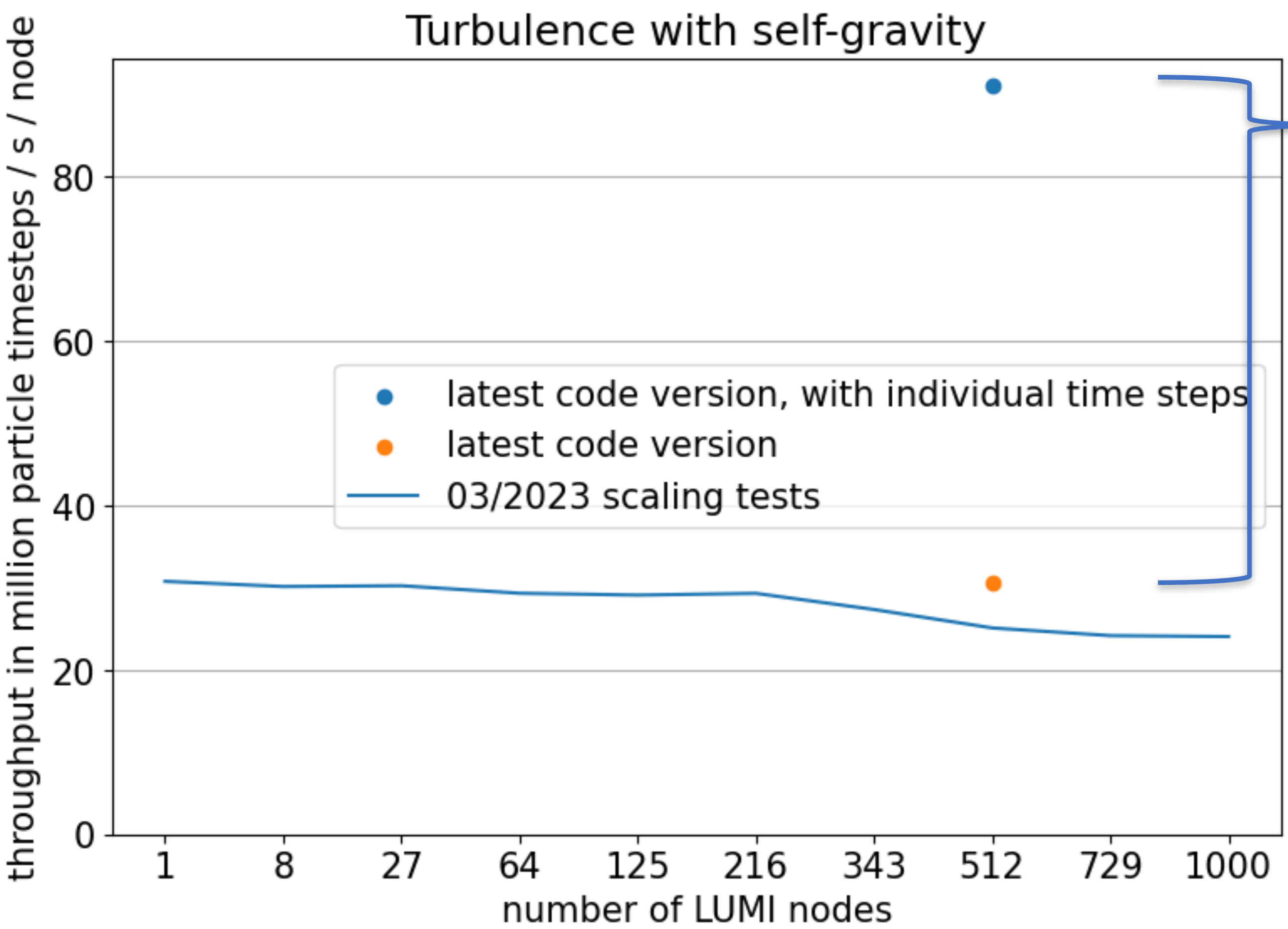
$10{,}000^3$ → HR + self-gravity

Individual time-stepping (ITS) provided a performance boost and reduced the need to use particle splitting for initial conditions. **A new set of simulations** has been executed, setting and relaxing the ICs in the target resolution.
Table: resource usage (Node-hours) comparison between planned (estimated w/o ITS) and executed (w/ ITS) simulation sets. Each LUMI-G node has 4 GPUs / **8 GCDs**.

Resolution	Physical Time (s)	Nodes	Estimated (Nh)	Measured (Nh)	Measured ITS + Opt. (Nh)	Simulation Type
$2'520^3$	0→0.875	128	11'654	30'131	NA	Hydro+Turbo+Gravity
$2'500^3$	0→1.250	64	NA	NA	5'855.66	Hydro+Turbulence
$5'040^3$	0→0.040	192	11'654	20'800	NA	Hydro+Turbulence
$5'000^3$	*0→0.040*	*512*	NA	NA	*325.40*	Hydro+Turbulence
$5'000^3$	*0→0.875*	*512*	($5'040^3$) 224'400	*NA*	*76'400.35*	Hydro+Turbulence
$5'000^3$	0→1.250	512	NA	NA	112'439.89	Hydro+Turbulence *
$5'000^3$	**1.250→1.328**	**512**	NA	NA	**15'658.24**	**Hydro+Turbo+Gravity** *
$10'079^3$	*0→0.040*	*1'024*	*220'000*	*NA*	*NA*	*Hydro+Turbulence*
$10'000^3$	0→0.040	1'000	NA	NA	7'086.94	Hydro+Turbulence
$10'000^3$	0→0.072571	1'000	NA	NA	22'251.67	Hydro+Turbulence *
$10'000^3$	*0→1.250*	*1'024*	*5'442'198*	**13.86× less than initial plan**	**Est. 392'473.00**	Hydro+Turbo
$10'000^3$	*1.250→1.328*	*1'024*	*437'620*	NA	Est. 31'560.00	Hydro+Turbo+Gravity

Mach=4, physical time ≥ 0.75 seconds

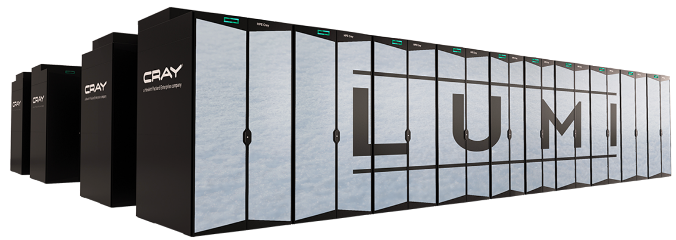
5'000³ particles	1.250→1.328 s	512 nodes	with individual time steps (●)	15'658.24 Nh	Hydro+Turbo+Gravity*



MR with 5000³ particles hydrodynamics + turbulence with self-gravity, from 1.250 to 1.328 seconds of physical time finished in **30 hours** on **512 nodes** on LUMI-G using individual time steps.

These results in 3x improvement in throughput with individual time steps (●) vs. global time steps (●).

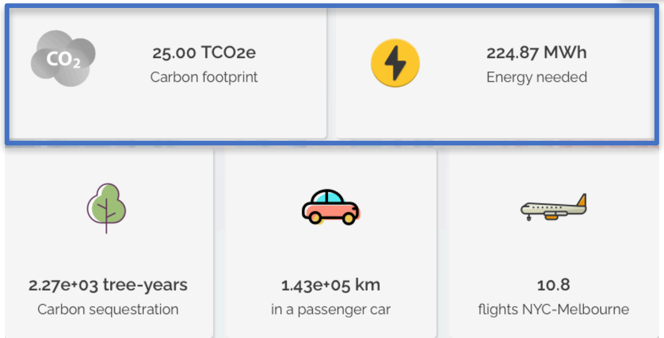
— scaling tests of earlier code versions with hydro+turbo+self-gravity without individual time steps.

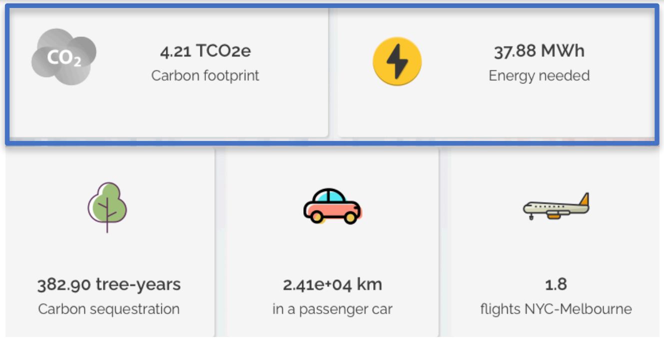


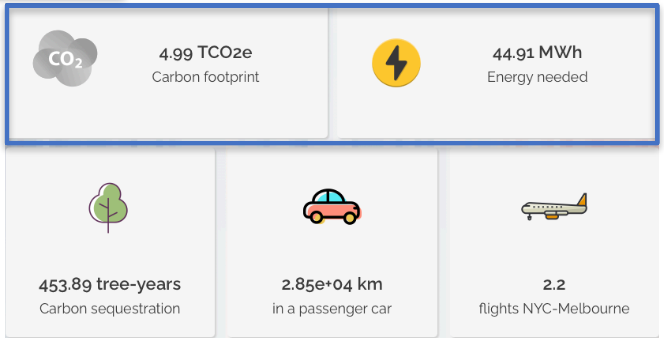
Sebastian Keller (CSCS)

TGSF: The Energy Cost for Selected Simulations

LUMI is carbon neutral and very energy efficient (PUE 1.03)







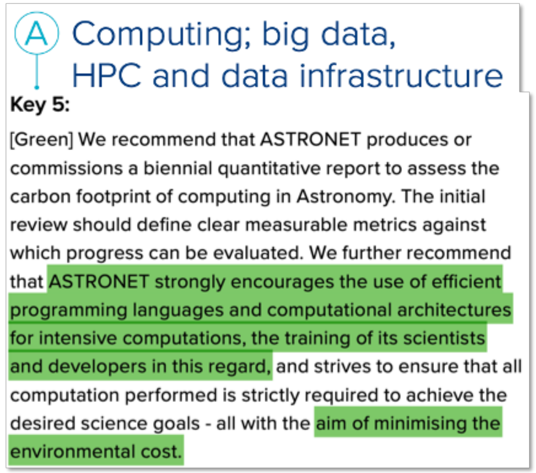
https://www.green-algorithms.org

- Mid resolution TGSF run w/ ITS
  - **$5'000^3$** particles
  - 548'021 time-steps executed
  - 4'096 MPI ranks on **512 nodes**
  - Reaching 0→1.25 physical seconds and needing **112'439.89 Nh**
- Mid resolution TGSF run w/ ITS + self gravity
  - **$5'000^3$** particles
  - 41'069 time-steps executed
  - 4'096 MPI ranks on **512 nodes**
  - Reaching 1.250→1.328 physical seconds and needing **15'658.24 Nh**
- High resolution TGSF run w/ ITS
  - **$10'000^3$** particles
  - 5'320 time-steps executed
  - 8'000 MPI ranks on **1'000 nodes**
  - Reaching 0→0.0725 physical seconds and needing **22'251.67**

7 Sustainability and accessibility

A strong priority of the European Astronomy community is to see questions of sustainability, ethics, equality and diversity considered as part of decision making processes. The key recommendations are:

- Astronomy projects should include environmental footprint assessments and reduction plans regarding construction and management of facilities, travel and computing, to follow (at the least) the European timeline towards carbon-neutrality.

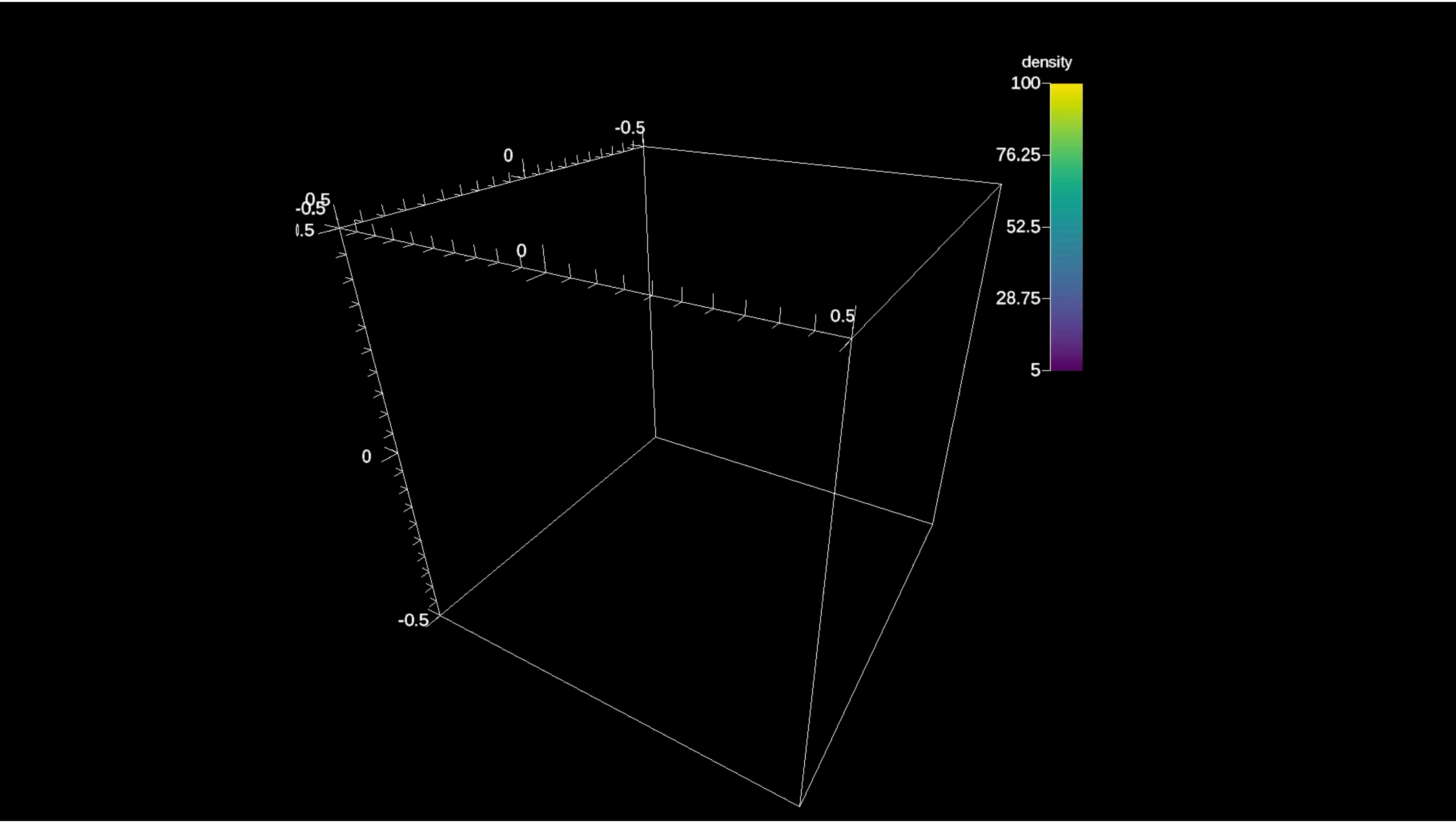


A Computing; big data, HPC and data infrastructure

Key 5:

[Green] We recommend that ASTRONET produces or commissions a biennial quantitative report to assess the carbon footprint of computing in Astronomy. The initial review should define clear measurable metrics against which progress can be evaluated. We further recommend that ASTRONET strongly encourages the use of efficient programming languages and computational architectures for intensive computations, the training of its scientists and developers in this regard, and strives to ensure that all computation performed is strictly required to achieve the desired science goals - all with the aim of minimising the environmental cost.

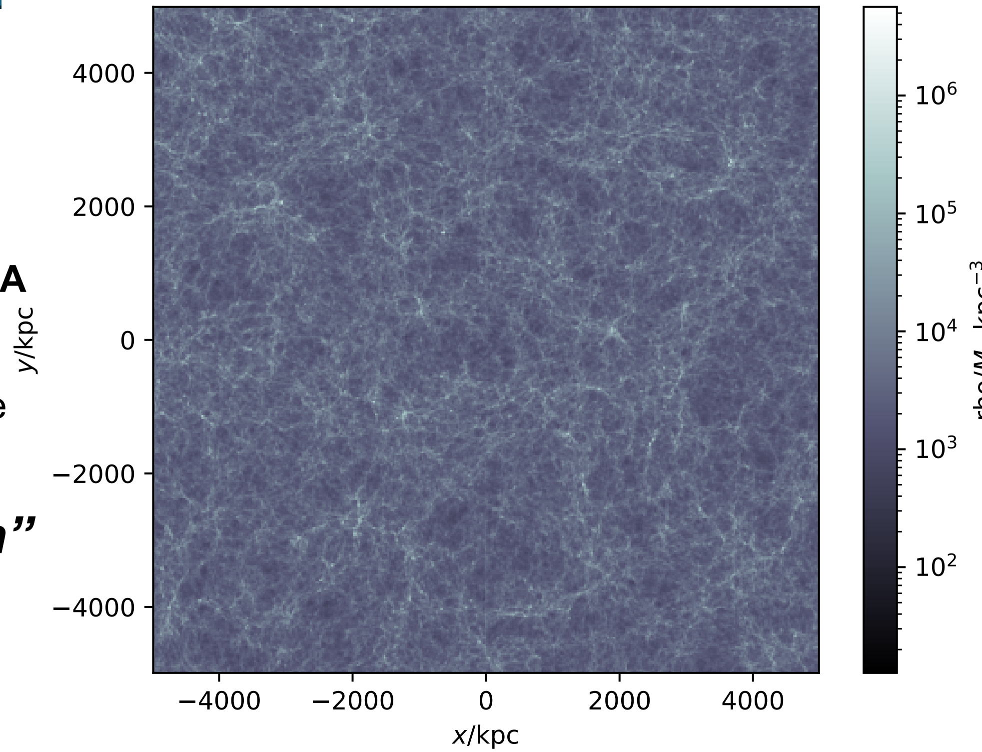
https://www.astronet-eu.org


density
100
76.25
52.5
28.75
5
-0.5
0
0.5
0
-0.5
0.5
0
-0.5

A1. Radiative cooling and chemical network reactions via GRACKLE (already implemented on CPU, porting to GPUs ongoing)
A2. Different particle species (in progress both for CPU and GPUs)
A3. Sub-grid models for star formation and Supernova feedback (to be ported from legacy code ChaNGa)
A4. Thermal and metal diffusion (to be ported from legacy code ChaNGa)
A5. Ewald summations for periodic boundary conditions (already implemented)
A6. Co-moving coordinates
A7. Adaptive time-stepping (to be done)

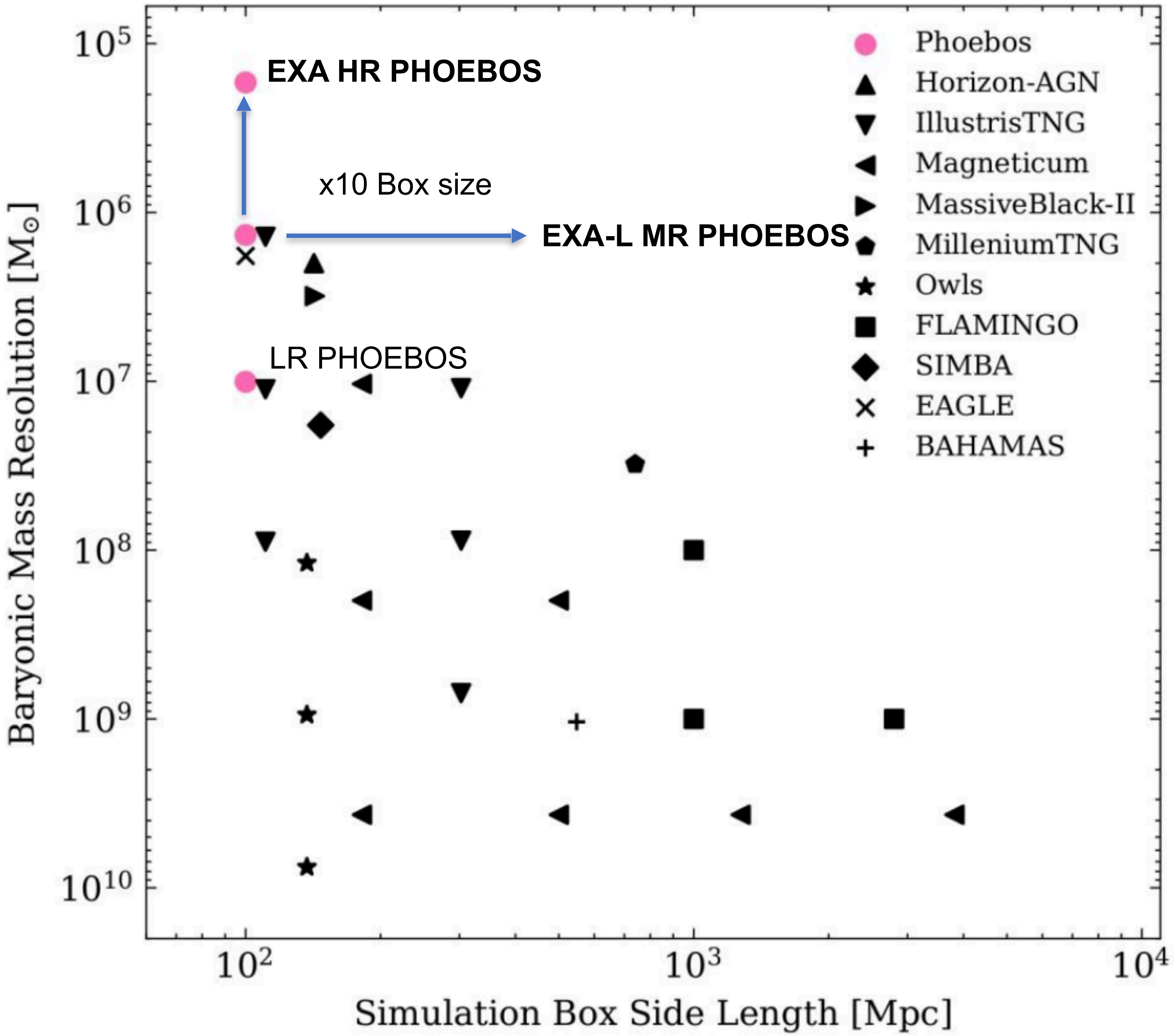
Phoebos suite of runs (current)
Run with ChaNGa code
Cosmological Hydrodynamical Volumes with 100 Mpc boxes

Exa HR Phoebos and Exa-L MR-Phoebos; Future Runs with SPH-EXA
10x times higher resolution and 10x larger volumes (Gpc scale)
New milestone:
resolve galactic scale physics in a representative volume of the Universe



Relevant to *"Cosmology"*, *"Epoch of Reionization"* *and "HI galaxy science" and "Extragalactic Continuum"* SKAO WGs

EXA-PHOEBOS: Cosmological hydrodynamical simulation at Ultra High Resolution



From Gensior et al. (2024): first zoom-in cosmological simulations survey study showing that the HI morphology can be used to probe and constrain the underlying physics of star formation and feedback in galaxy formation

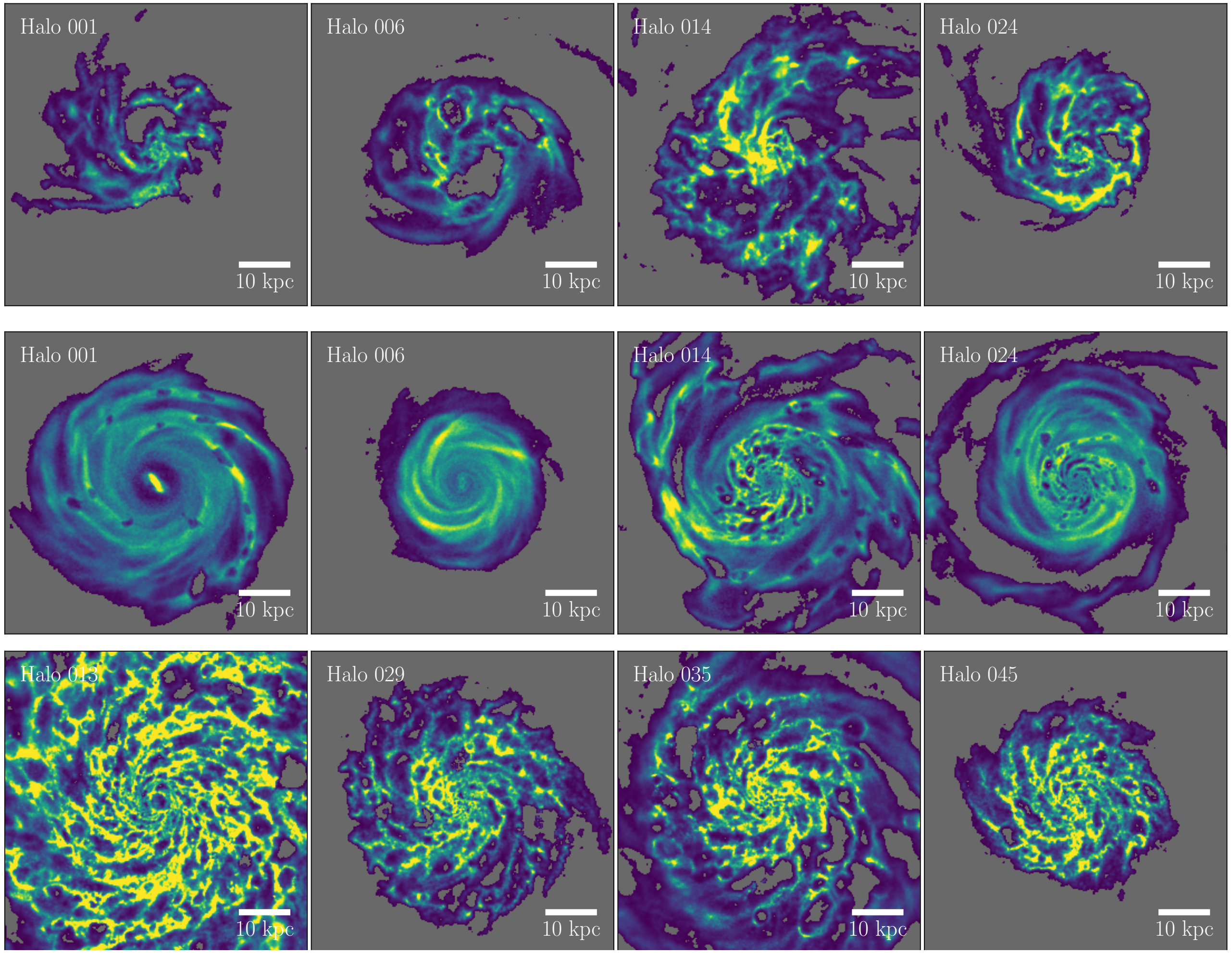
EMP-*Pathfinder*

$\epsilon_{\rm ff} = 20\%$

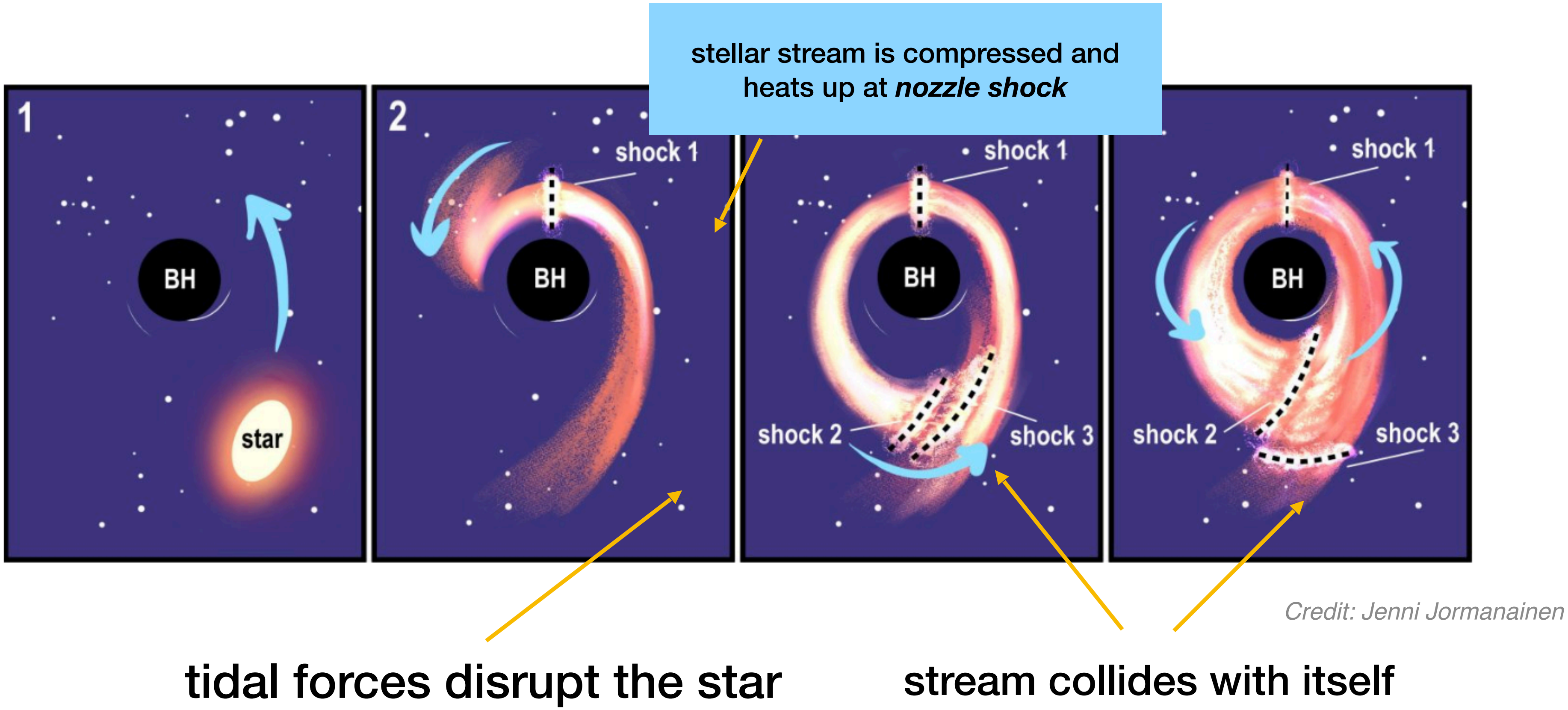
EMP-*Pathfinder*

$\epsilon_{\rm ff} = f(\alpha_{\rm vir}, \mathcal{M})$

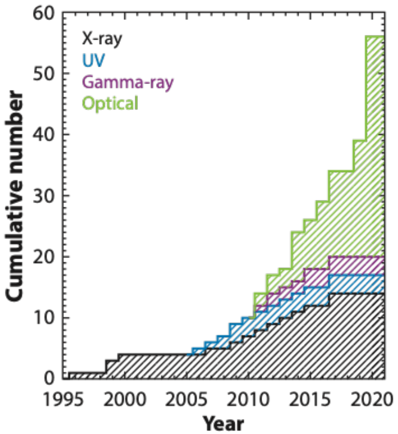
FIREbox

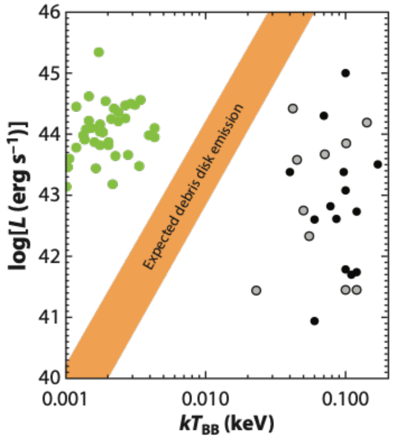


Relevant to SKAO WG “Transients”



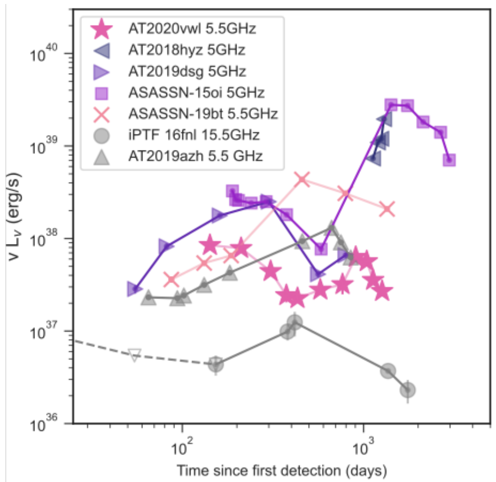
Observational properties; TDEs detected in optical/UV, X-rays, radio!





Detections of TDEs

Luminosity vs Temperature for UV / optical (green) and X-ray-detected (black) TDEs

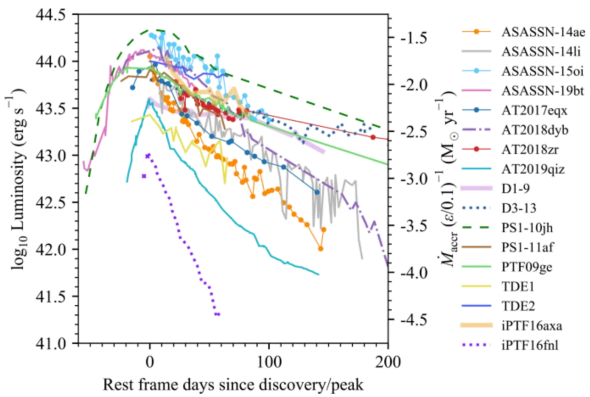


Credits to Goodwin et al. 2024

- ~100 TDEs have been detected
- LSST will greatly improve this
- bimodal distribution of spectrum
- emission mechanism not fully clear
- probably UV and optical through shocks, X-rays through accretion disk

Radio emission

- Peaked synchrotron spectrum that evolves to lower frequency with time
- Visible for years (much longer than optical/X-ray emission)
- Half of TDEs show a radio follow-up
- Synchrotron emission (from outflows and jets)
- origin not well understood
- very rarely relativistic jet

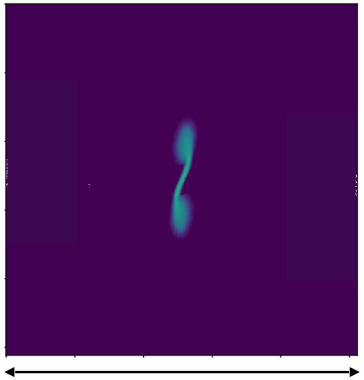


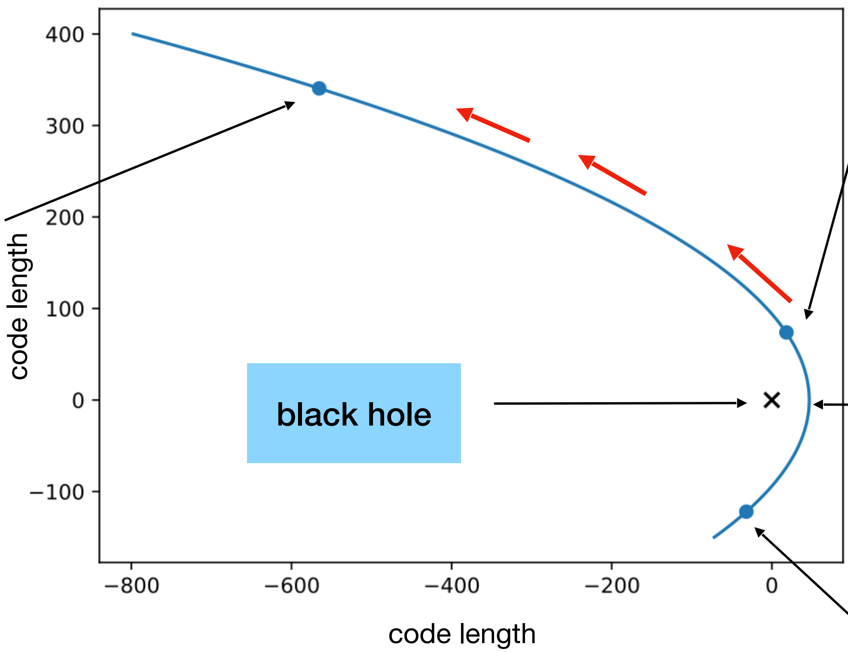
Credits: Gezari (2021)

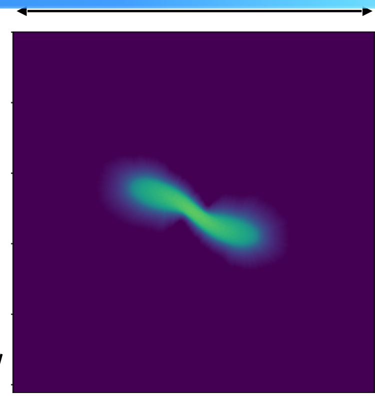
Light curves and corresponding mass accretion rates (van Velzen et al. 2020)

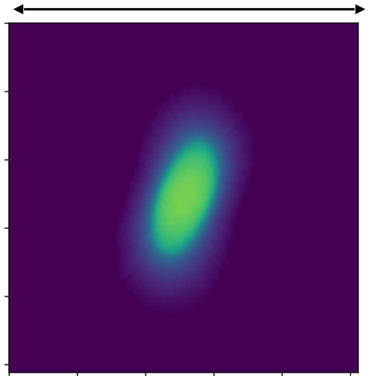
SPH-EXA simulations (Collaboration with Christopher Nixon (Leeds, UK) and Eric Coughlin (Syracuse University, USA)

- Black hole (10^6 M_star) modeled by Newtonian potential or relativistic Einstein potential
- Star is assumed to be a polytrope with tidal radius = pericentre distance
- The star starts on a parabolic orbit with pericentre distance >> Schwarzschild radius

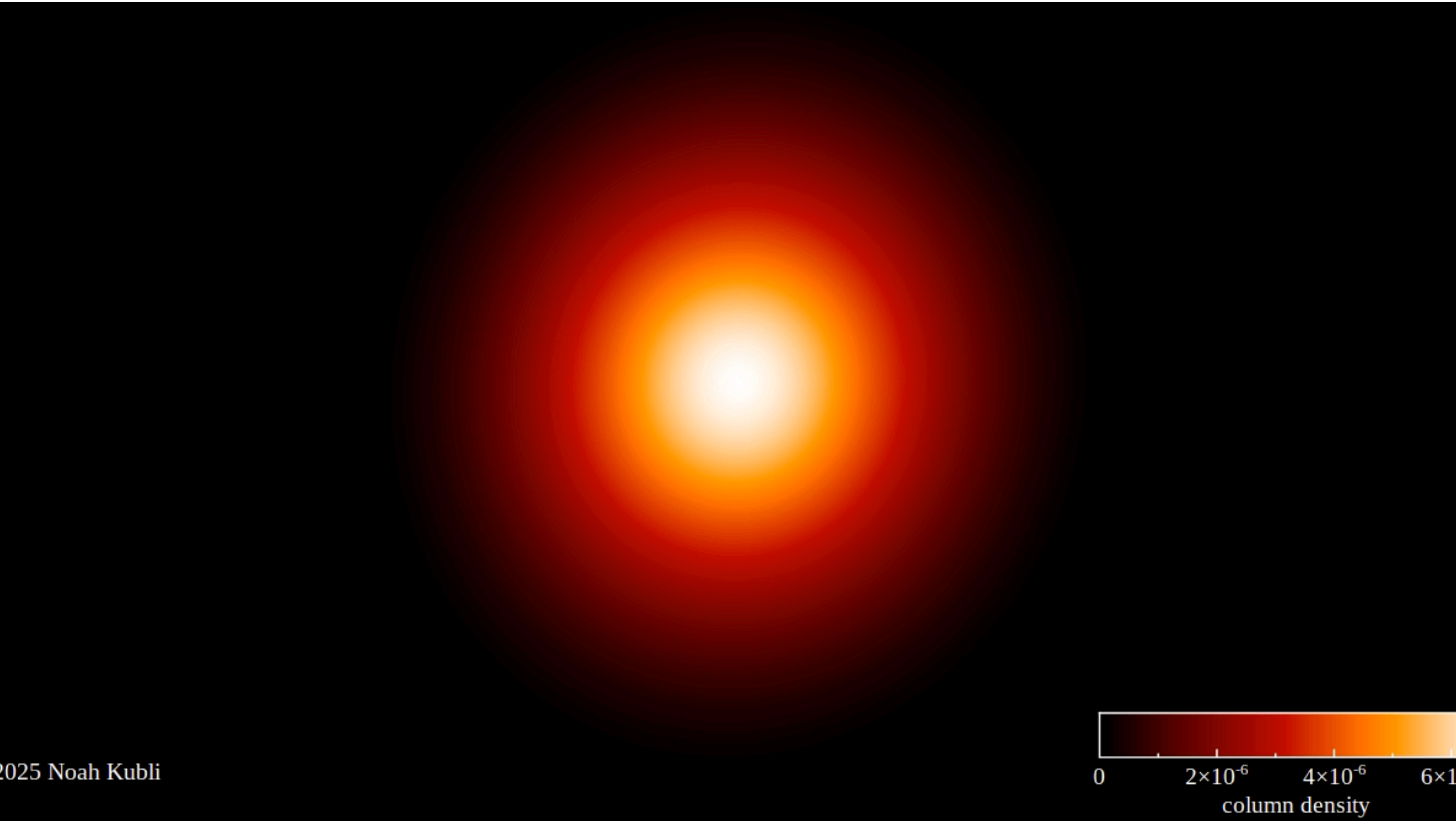




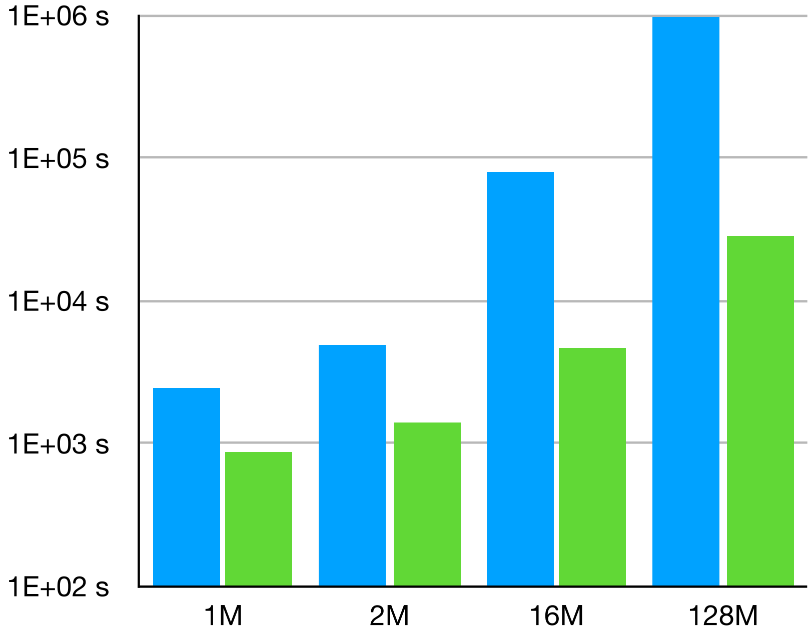




Plots from our simulation with SPH-EXA.
1 code length ~ 1.5 * 10^{11} cm

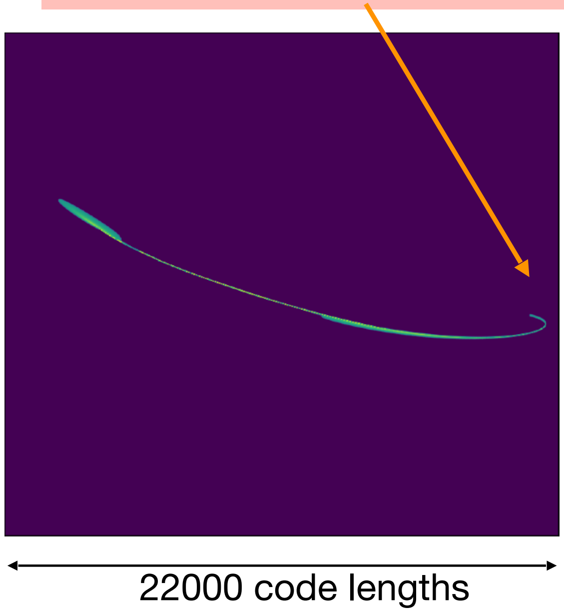

2025 Noah Kubli
0
2×10-6
4×10-6
column density

SPH-EXA outperforms previous simulation codes



Time needed for simulations.
Blue: Fancher et al. 2023;
Green: our runs with SPH-EXA on PizDaint (single node with 4 GPUs)

The bound part is coming back; soon the stream will collide with itself

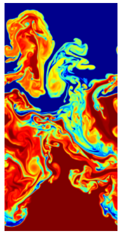


Longer term evolution after second pericentre passage (SPH-EXA)

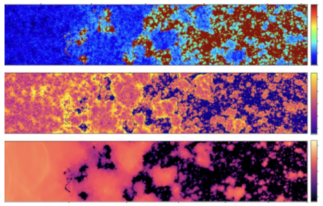
- Investigate gravitational collapse of the stream; should have a crucial dependence on adiabatic index
- Consider different polytropic models for star
- Achieve much higher resolutions (~100b particles, GPU and efficient node-parallelism greatly beneficiary, **ideal for SPH-EXA**).
- Simulate long-term evolution (multiple physical months) including relativistic precession to model late emission, orbit circularisation etc.

SPH-EXA: A Versatile Framework for Advancing SKAO Science Cases

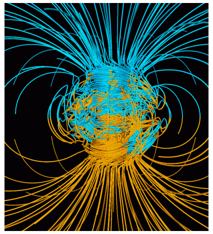
Current & future capability physics modules



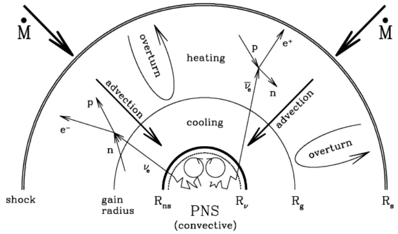
Hydrodynamics



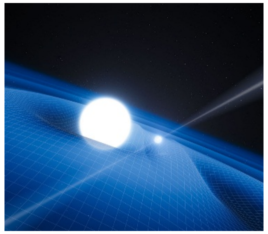
Radiative transfer



Magnetic fields

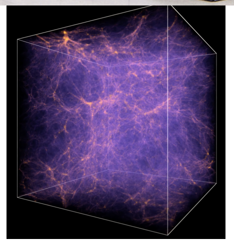


Neutrino transport



General Relativity

Nuclear network



Cosmology

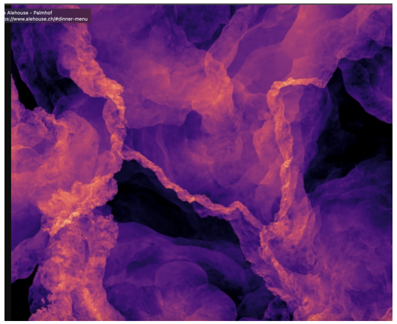
Goals

Astrophysics

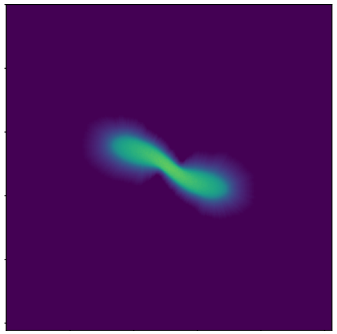
- Render highly scalable any computationally-challenging problem in astrophysics and cosmology
- Become the benchmark particle-based code in the field
- Focus on the most transformative science targets of next decade

Computer Science

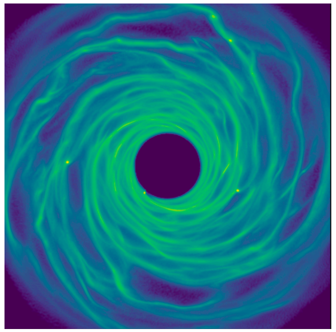
- Adaptive load balancing of multiple adaptive time-steps
- AI-driven and AI-based performance & energy optimization
- Become the benchmark for domain-decomposition, load balancing, energy efficiency studies and system acceptance



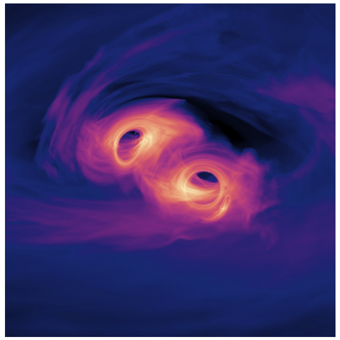
Star formation in the interstellar medium, turbulent flows



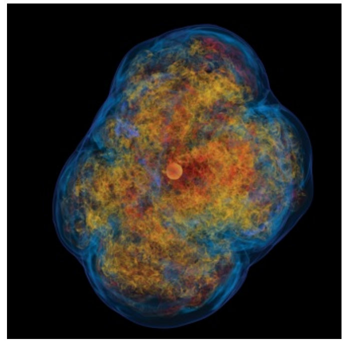
Stellar tidal disruption arounds supermassive black holes (SPH-EXA)



Protoplanetary disks and Planet formation (SPH-EXA)



Relativistic hydrodynamics: black hole mergers in astrophysical backgrounds



Core collapse Supernova

J. Nordhaus

https://hpc.dmi.unibas.ch/research/sph-exa/