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Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

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

RAMSES GPU

Presented by:
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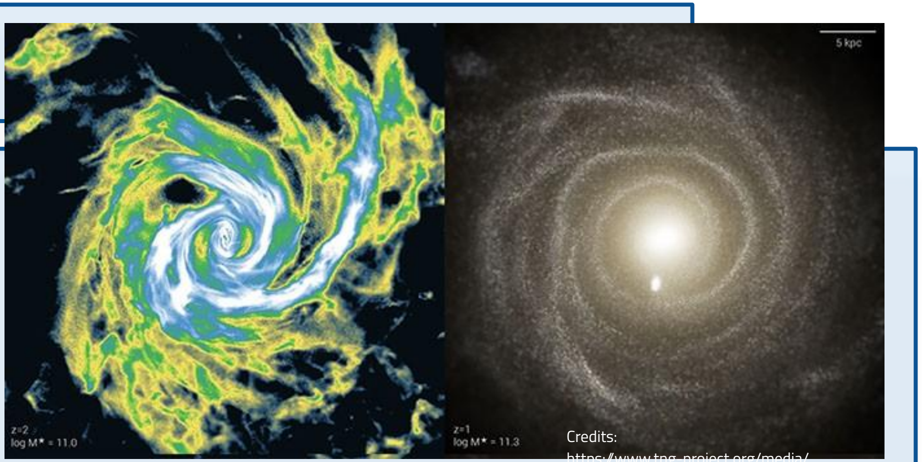
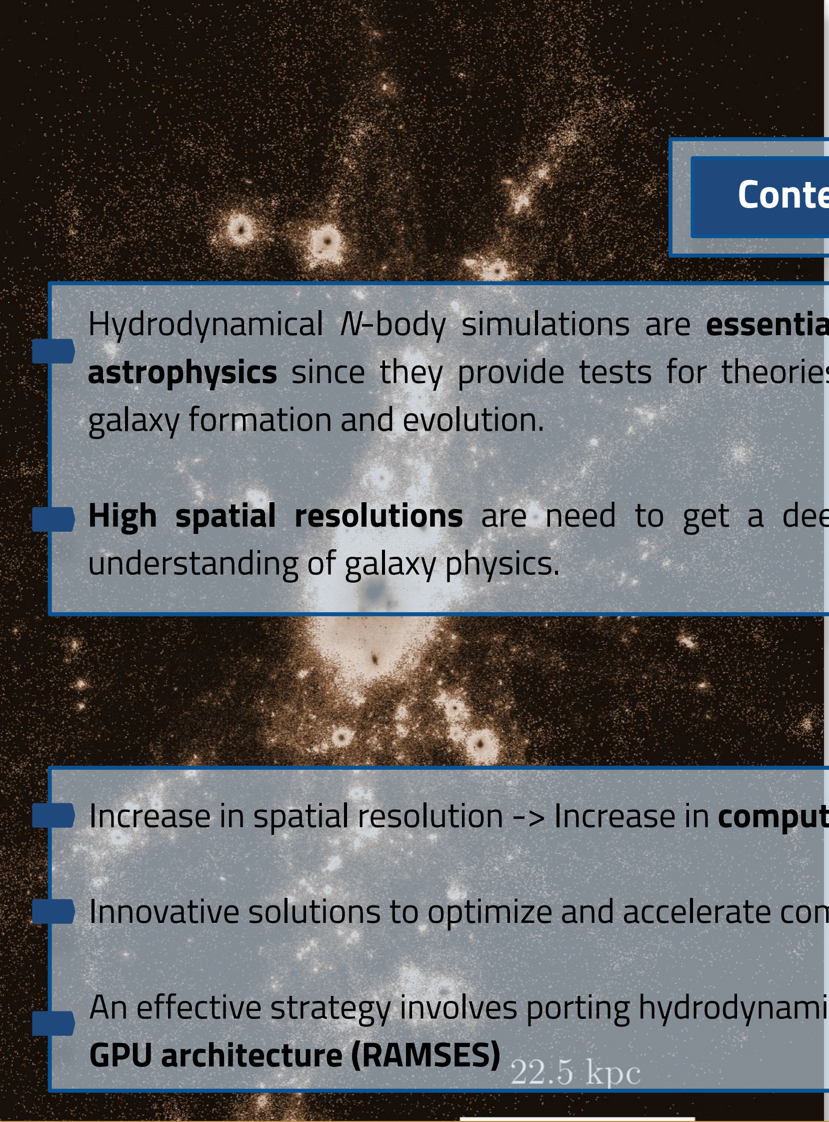
Collaborators:
Francesco Calura, Claudio Gheller, Emanuele De Rubeis,
Donatella Romano, Valentina Cesare

Spoke 3 II Technical Workshop, Bologna Dec 17 -19, 2024

Context

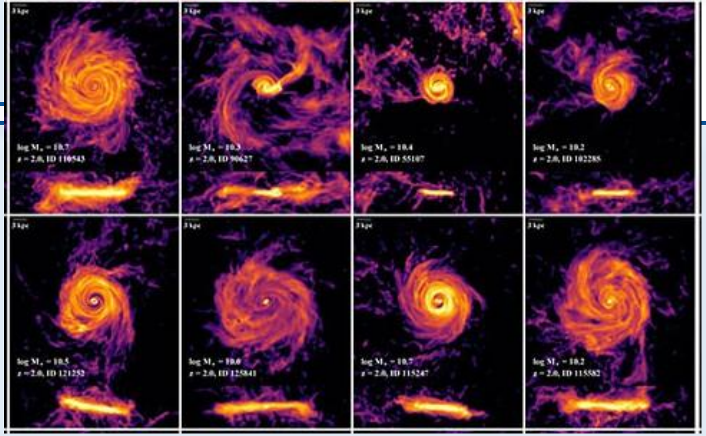


Credits: https://www.tng-project.org/media/

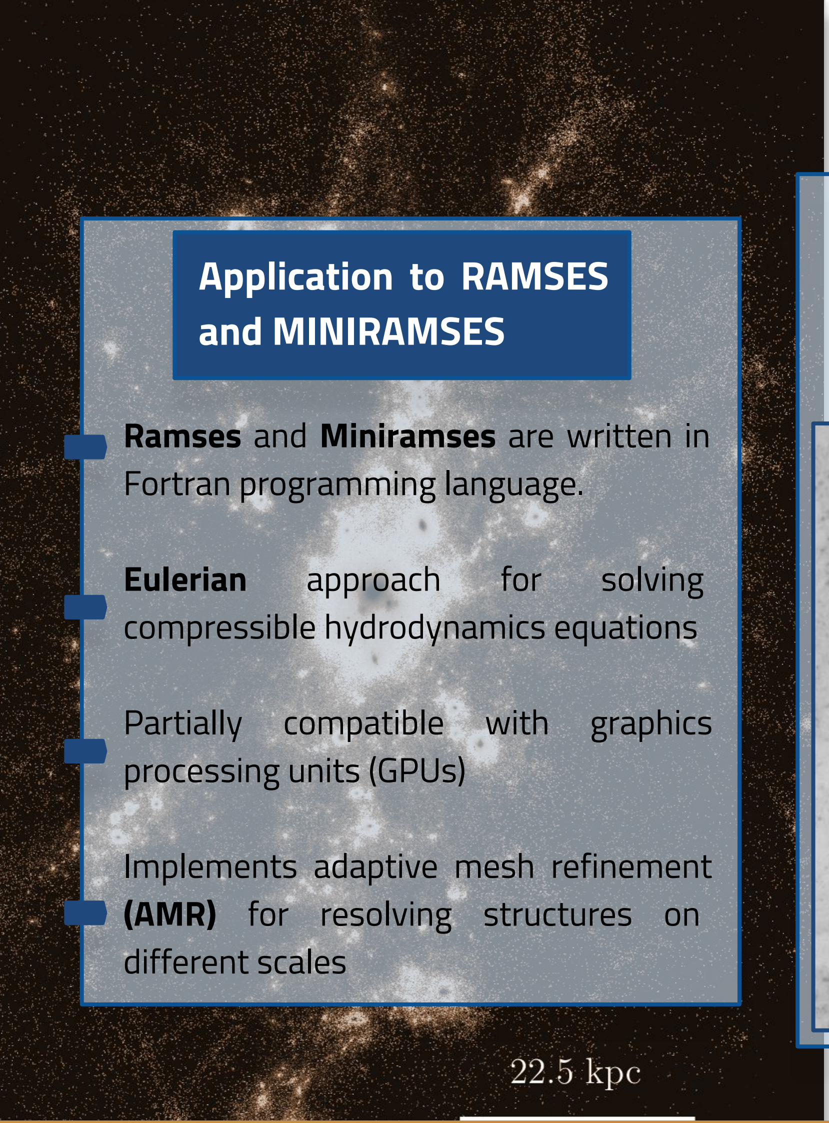


- Hydrodynamical *N*-body simulations are **essential in astrophysics** since they provide tests for theories of galaxy formation and evolution.
- **High spatial resolutions** are need to get a deeper understanding of galaxy physics.

Challenges



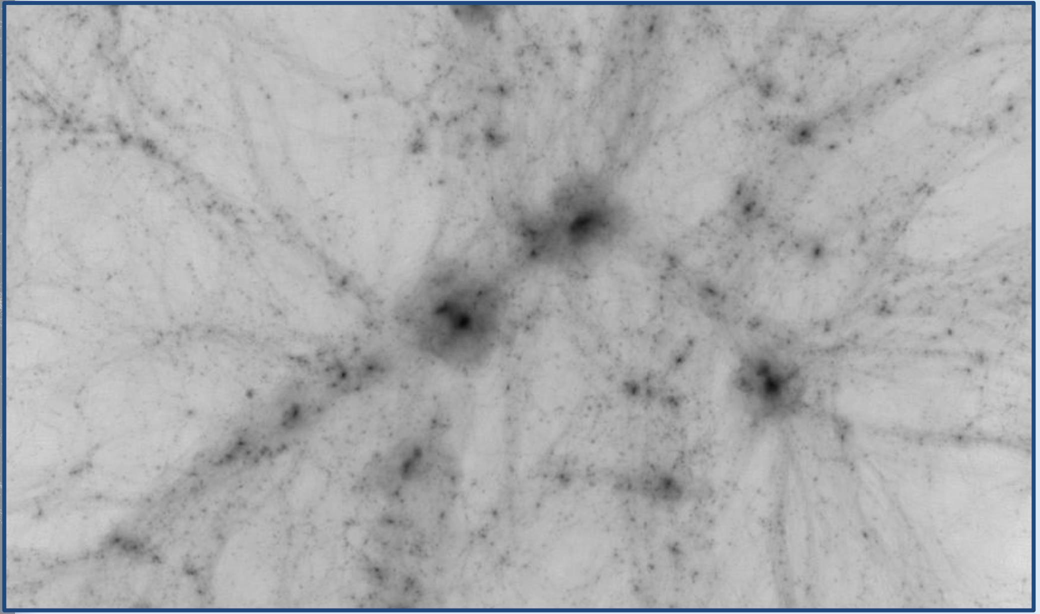
- Increase in spatial resolution -> Increase in **computational costs**
- Innovative solutions to optimize and accelerate computations.
- An effective strategy involves porting hydrodynamical codes onto **GPU architecture (RAMSES)**

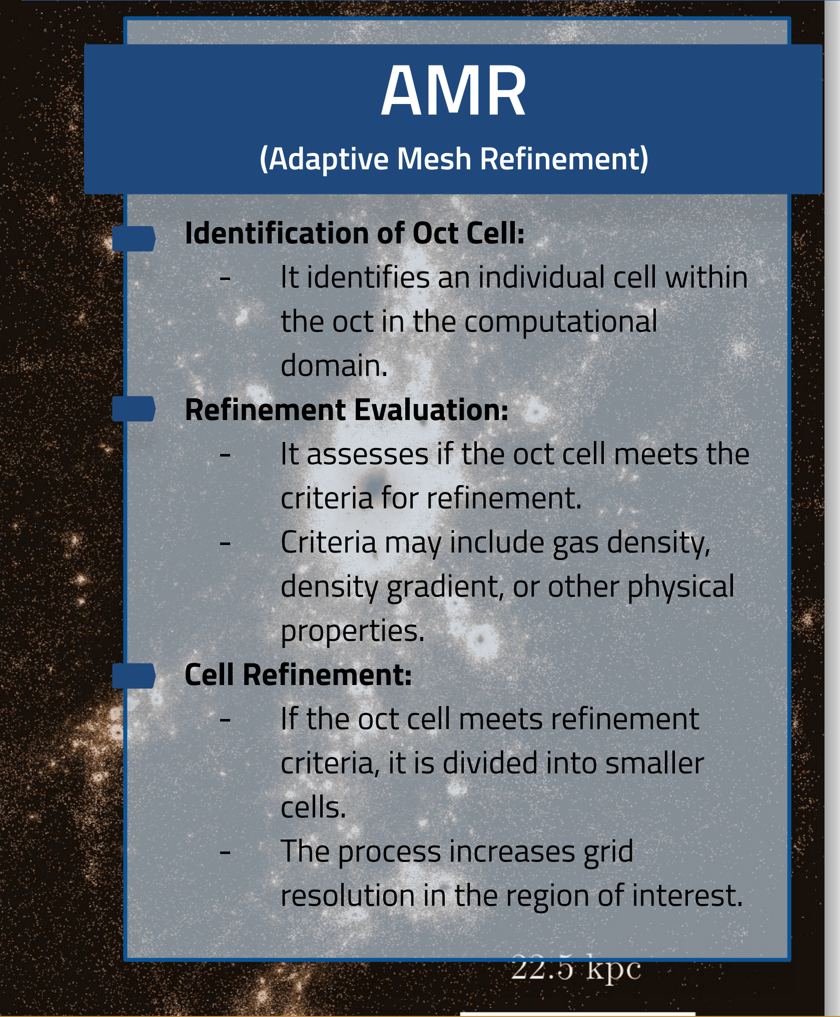


Application to RAMSES and MINIRAMSES

- **Ramses** and **Miniramses** are written in Fortran programming language.
- **Eulerian** approach for solving compressible hydrodynamics equations
- Partially compatible with graphics processing units (GPUs)
- Implements adaptive mesh refinement **(AMR)** for resolving structures on different scales

MINIRAMSES is an optimized version of Ramses featuring an enhanced grid memory management system, which facilitates memory access and substantially (?) increases the potential for efficient GPU integration of the code.





AMR

(Adaptive Mesh Refinement)

Identification of Oct Cell:

- It identifies an individual cell within the oct in the computational domain.

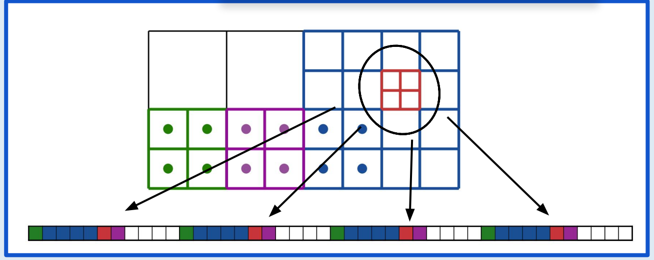
Refinement Evaluation:

- It assesses if the oct cell meets the criteria for refinement.
- Criteria may include gas density, density gradient, or other physical properties.

Cell Refinement:

- If the oct cell meets refinement criteria, it is divided into smaller cells.
- The process increases grid resolution in the region of interest.

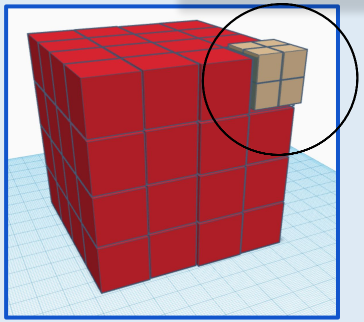
RAMSES



Example of classical AMR working

During cells refinement, new born cells belonging to the same oct are saved in non-contiguous parts of the memory.

MINIRAMSES



Introduces the new macrostructure: of super-oct in cell refinement.

ocs in super-octs are saved in contiguous memory locations. Cell adjacent in space close in memory

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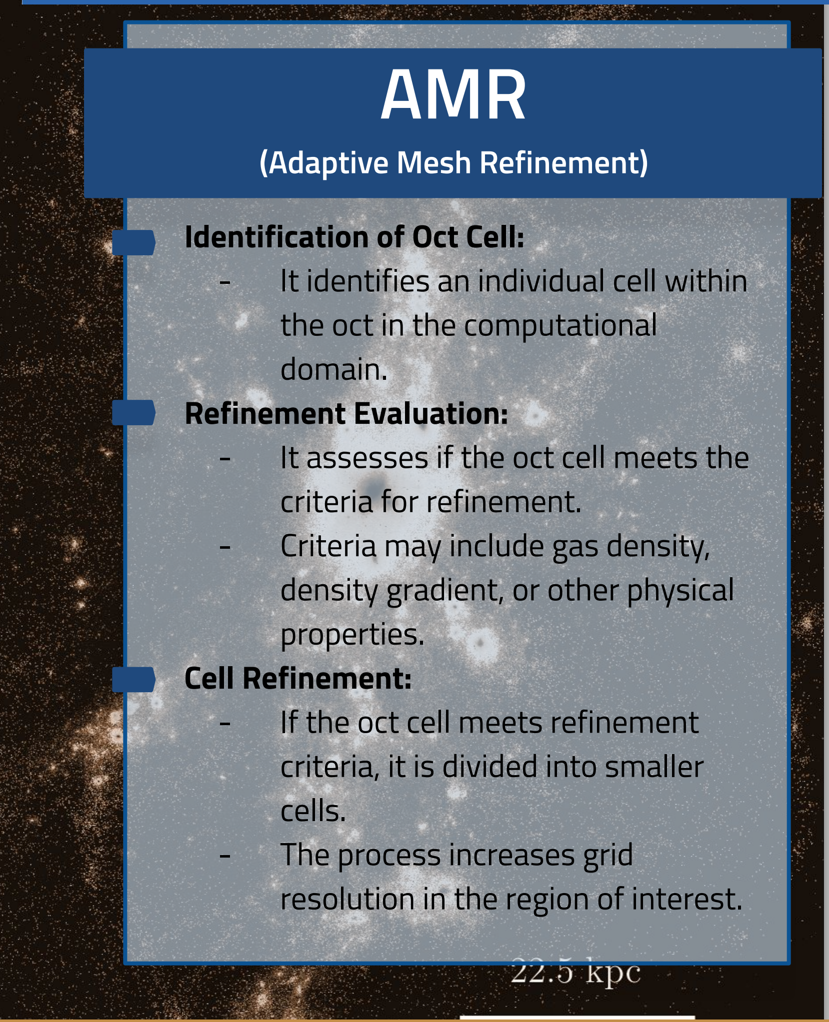
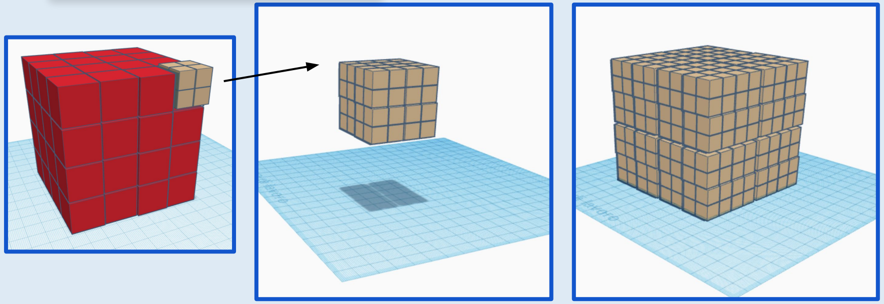


Super-oct



The **superoct** is a **large cube** composed of smaller sub-cubes, known as octs. Its **hierarchical structure** functions similarly to grid refinement, with each successive level increasing the number of octs along each edge by a factor of 2. As a result, the edge length of the superoct at a given level contains double the number of octs compared to the previous level.

Superoct level (**n**) from 0 to 5. In 3d, number of octs per superoct is 8^n

n = 4 ---> octs per superoct = 4096
n = 5 ---> octs per superoct = 32768
The larger n, the better the changes for an optimal porting

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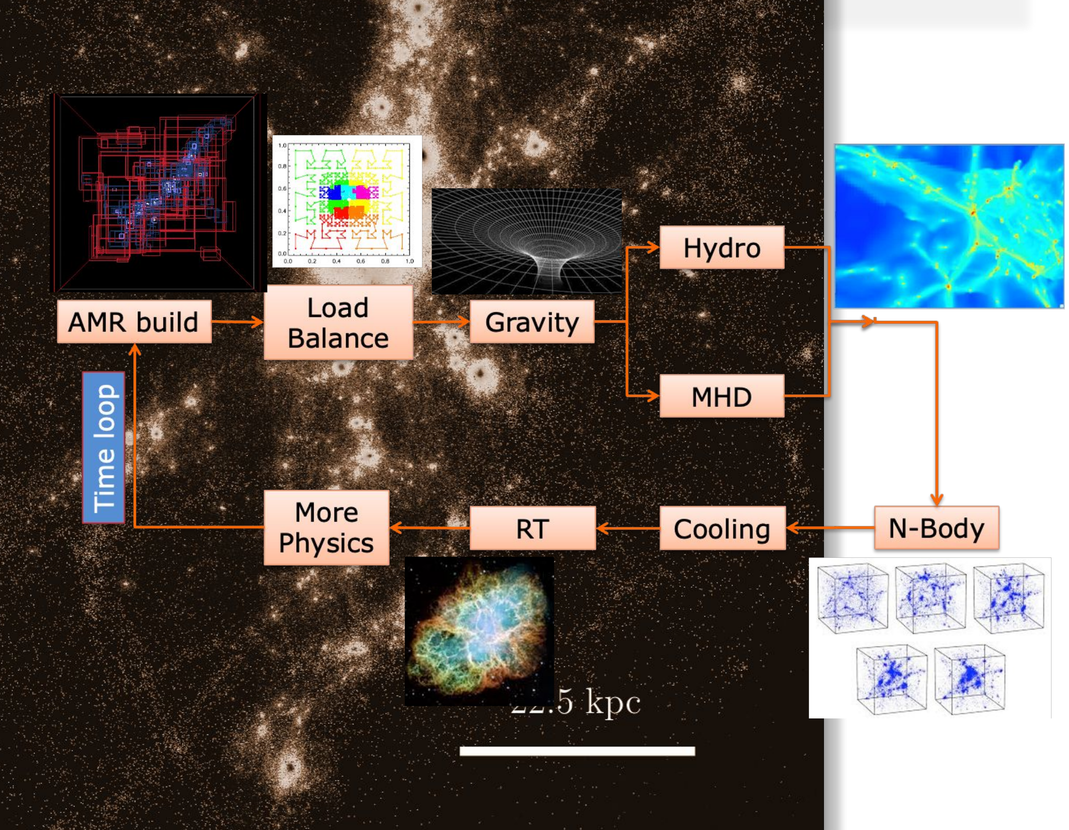
Basic functioning of (MINI)RAMSES



AMR build
Load Balance
Gravity
Hydro
MHD
N-Body
Cooling
RT
More Physics
Time loop

Adaptive Mesh Refinement (AMR):

the grid resolution is dynamically adapted to match the simulation's needs. Regions of interest are refined for higher resolution

Load Balancing:

RAMSES optimizes computational resources by distributing the workload evenly across processing units.

Gravity:

Gravity field is computed based on the matter distribution.

Hydro:

The hydrodynamic equations describing the fluid motion are solved

N-body:

the trajectories of collisionless particles (e.g., dark matter) are evolved using the leapfrog algorithm.

Cooling:

Cooling processes to account for energy loss

More physics:

Additional physics as wids, star formation etc.

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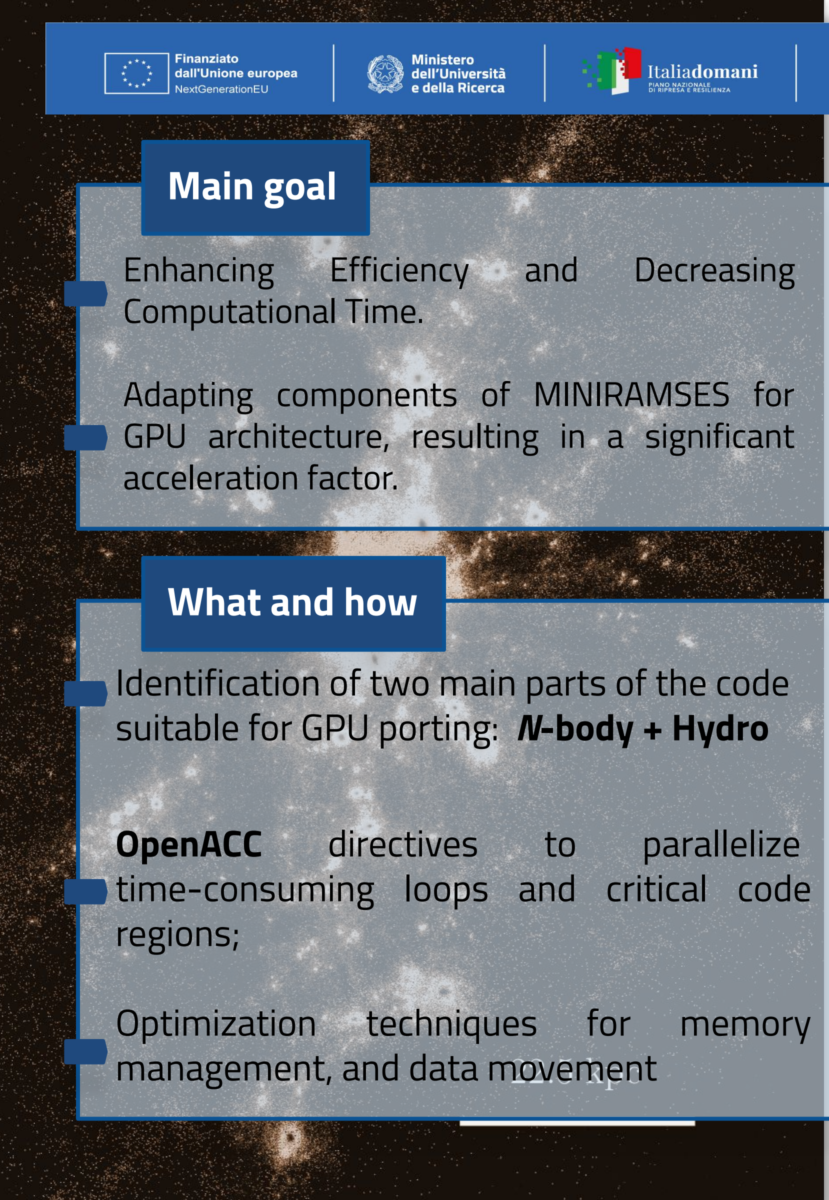

Main goal

- Enhancing Efficiency and Decreasing Computational Time.
- Adapting components of MINIRAMSES for GPU architecture, resulting in a significant acceleration factor.

What and how

- Identification of two main parts of the code suitable for GPU porting: ***N*-body + Hydro**
- **OpenACC** directives to parallelize time-consuming loops and critical code regions;
- Optimization techniques for memory management, and data movement

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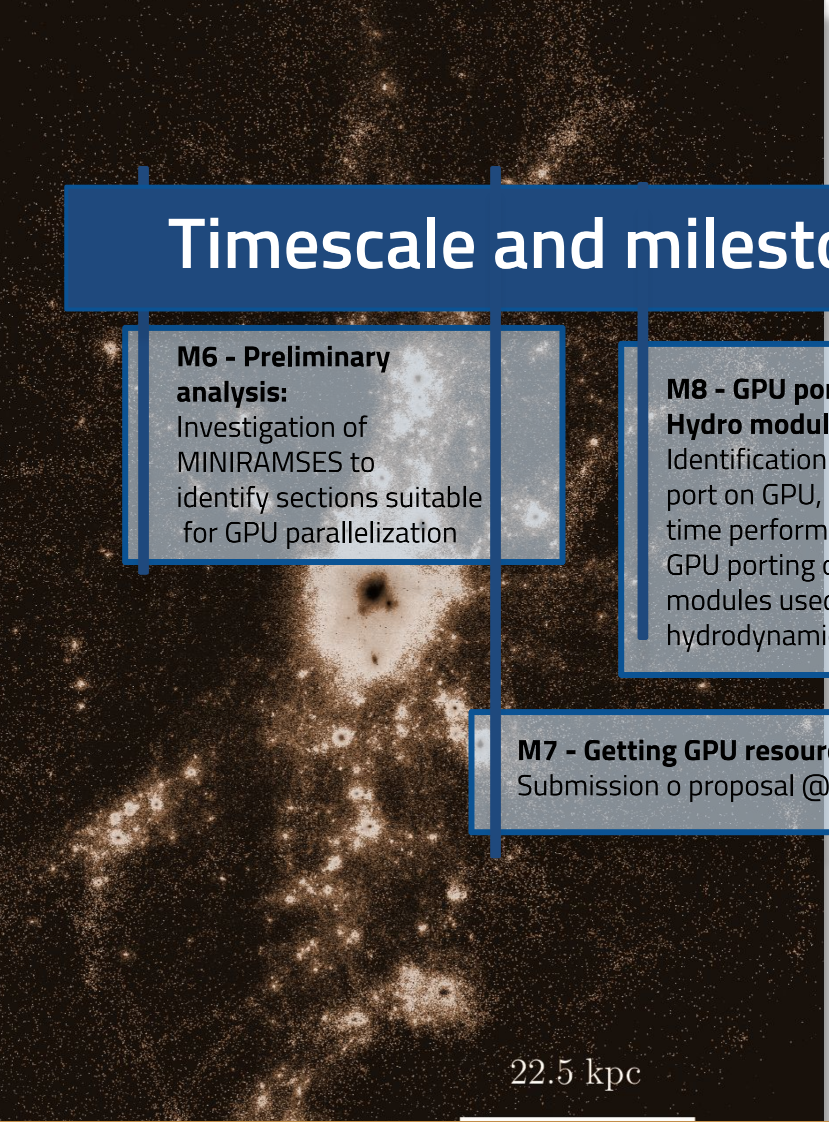
Timescale and milestones



M6 - Preliminary analysis: Investigation of MINIRAMSES to identify sections suitable for GPU parallelization

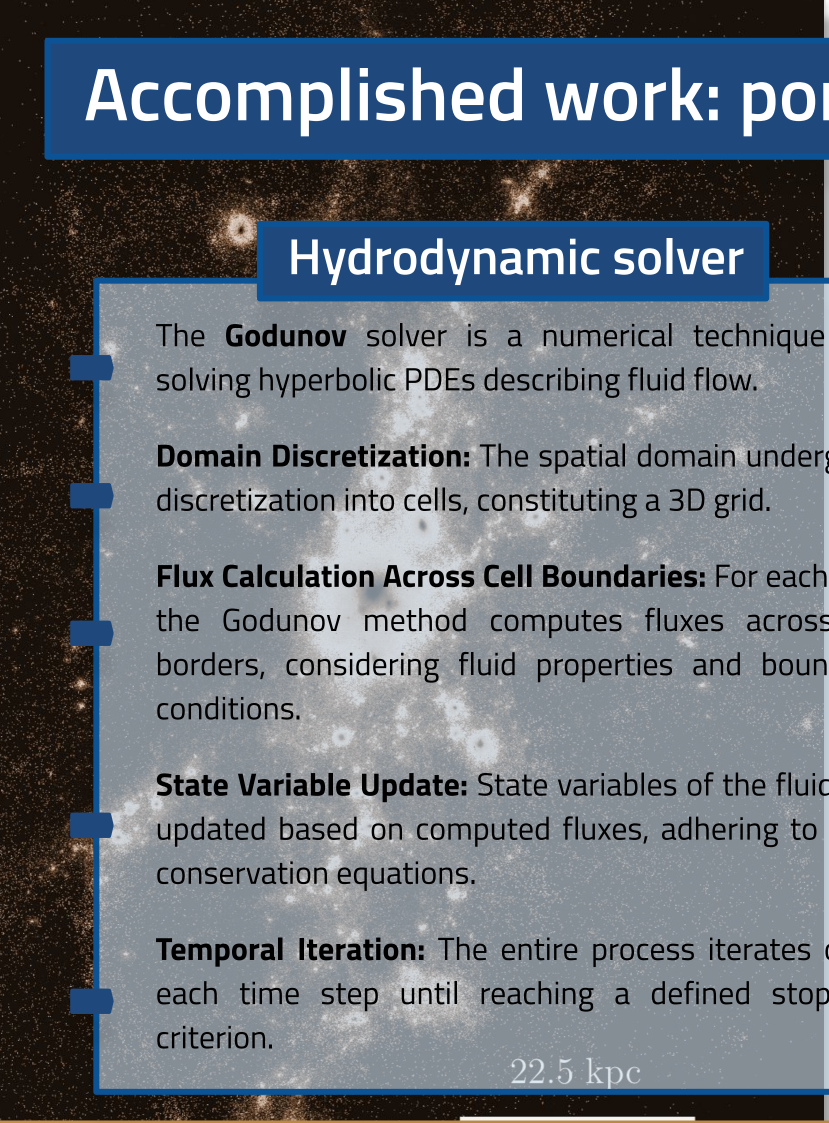
M7 - Getting GPU resources: Submission o proposal @Cineca

M8 - GPU porting of Hydro modules: Identification of modules to port on GPU, evaluation of time performances. Gradual GPU porting of individual modules used in hydrodynamics.

M9 - Tests Tests and performance evaluations before and after. Evaluation of initial performance and identification of any issues or bugs.

M10 - Memory management of hydro modules: Identification of strategy for memory management. Optimization of the code on GPU to maximize performance

Accomplished work: porting of the hydro solver



Hydrodynamic solver

- The **Godunov** solver is a numerical technique for solving hyperbolic PDEs describing fluid flow.
- **Domain Discretization:** The spatial domain undergoes discretization into cells, constituting a 3D grid.
- **Flux Calculation Across Cell Boundaries:** For each cell, the Godunov method computes fluxes across its borders, considering fluid properties and boundary conditions.
- **State Variable Update:** State variables of the fluid get updated based on computed fluxes, adhering to flow conservation equations.
- **Temporal Iteration:** The entire process iterates over each time step until reaching a defined stopping criterion.

Accomplished work: porting of the hydro solver

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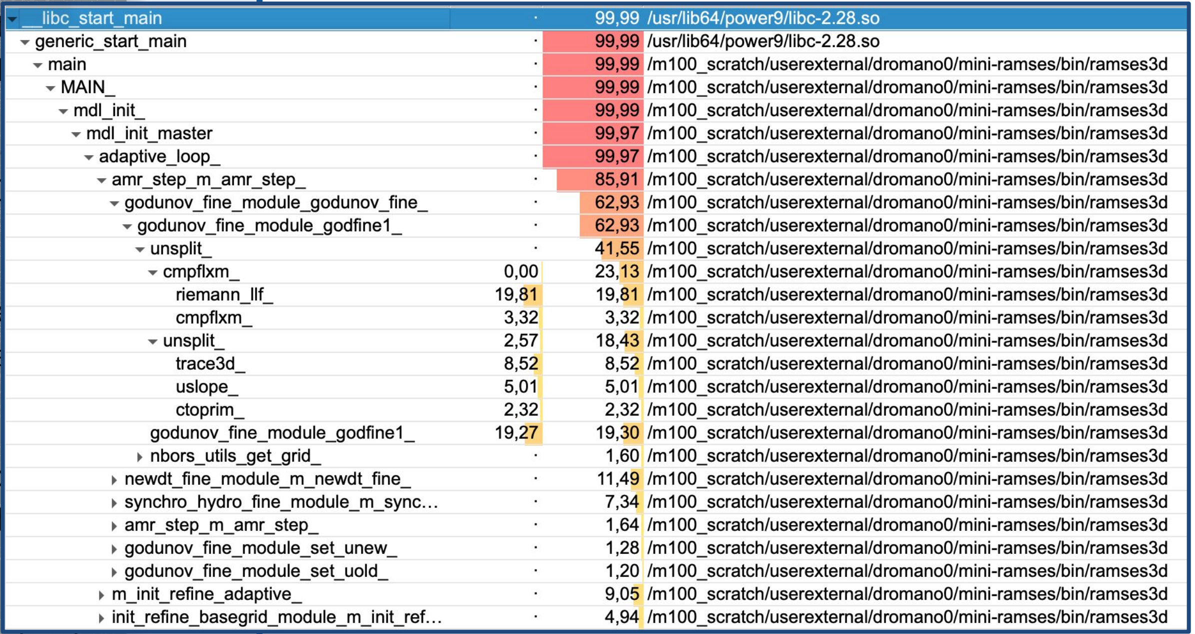
Temporal Iteration: The entire process iterates over each time step until reaching a defined stopping criterion.

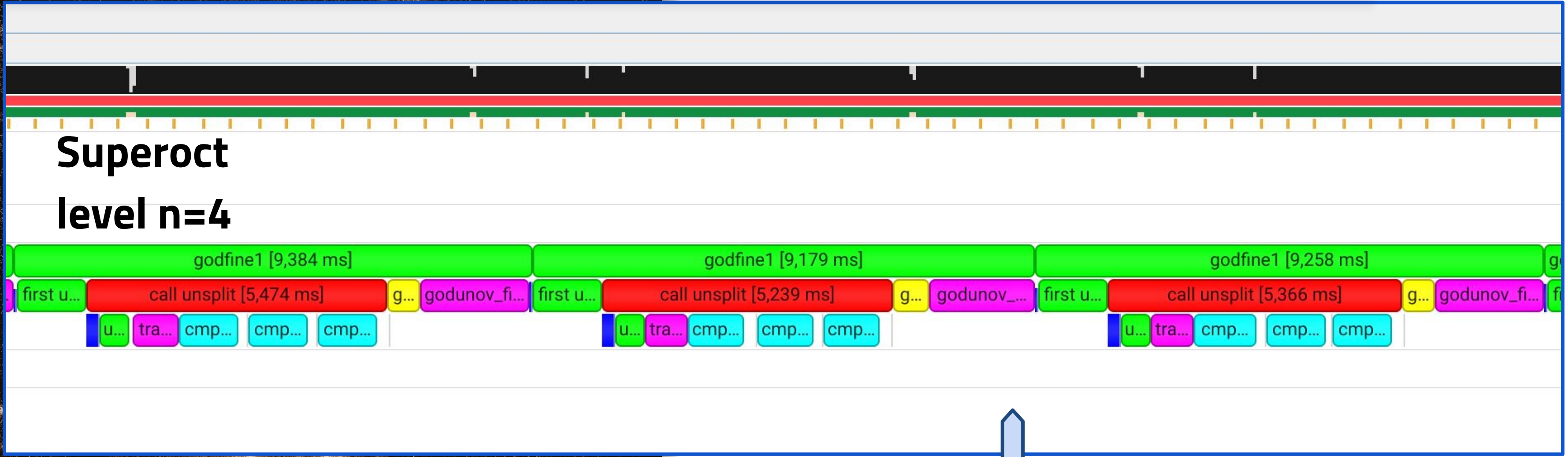
run over 1 CPU



__libc_start_main	·	99,99	/usr/lib64/power9/libc-2.28.so
generic_start_main	·	99,99	/usr/lib64/power9/libc-2.28.so
main	·	99,99	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
MAIN_	·	99,99	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
mdl_init_	·	99,99	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
mdl_init_master	·	99,97	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
adaptive_loop_	·	99,97	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
amr_step_m_amr_step_	·	85,91	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
godunov_fine_module_godunov_fine_	·	62,93	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
godunov_fine_module_godfine1_	·	62,93	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
unsplit_	·	41,55	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
cmpflxm_	0,00	23,13	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
riemann_llf_	19,81	19,81	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
cmpflxm_	3,32	3,32	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
unsplit_	2,57	18,43	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
trace3d_	8,52	8,52	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
uslope_	5,01	5,01	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
ctoprim_	2,32	2,32	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
godunov_fine_module_godfine1_	19,27	19,30	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
nbors_utils_get_grid_	·	1,60	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
newdt_fine_module_m_newdt_fine_	·	11,49	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
synchro_hydro_fine_module_m_sync…	·	7,34	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
amr_step_m_amr_step_	·	1,64	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
godunov_fine_module_set_unew_	·	1,28	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
godunov_fine_module_set_uold_	·	1,20	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
m_init_refine_adaptive_	·	9,05	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d
init_refine_basegrid_module_m_init_ref…	·	4,94	/m100_scratch/userexternal/dromano0/mini-ramses/bin/ramses3d

63% of the time is spent by the hydrodynamical solver (godfine1)

Accomplished work: porting of the hydro solver



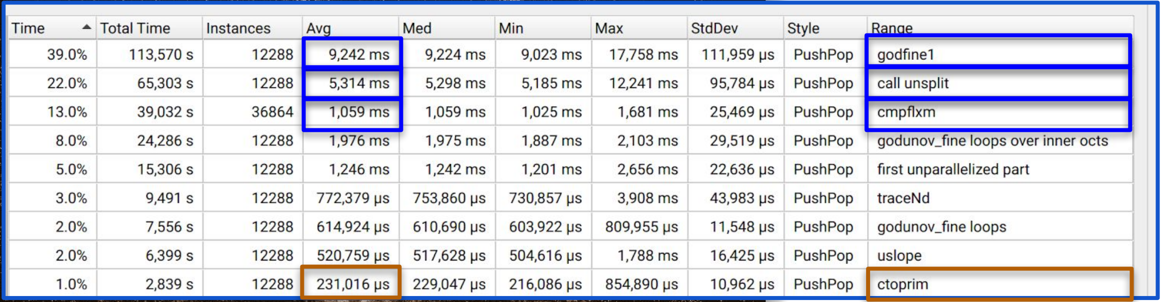
Full CPU run (1CPU)
Sedov3d test: Explosion of a supernovae in a constant medium.
Only hydro, no gravity.

Major of the computational time is spent during the **call unsplit()**

Each call to godfine1 solves hydrodynamics for one super-oct

About time

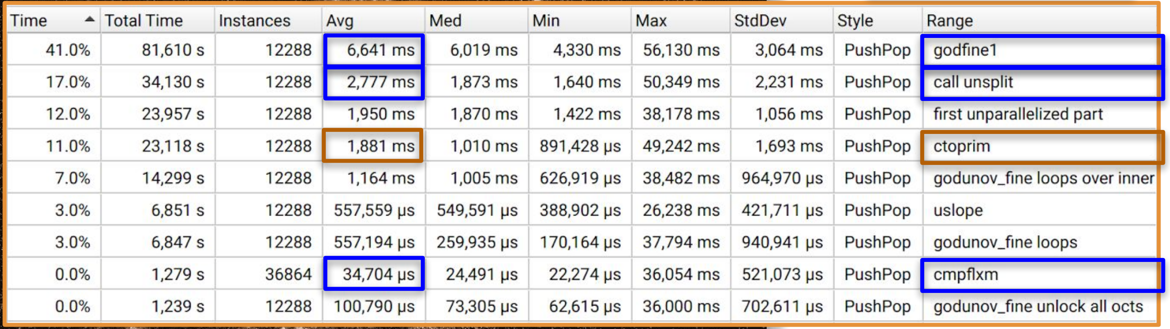
full CPU



Time	Total Time	Instances	Avg	Med	Min	Max	StdDev	Style	Range
39.0%	113,570 s	12288	9,242 ms	9,224 ms	9,023 ms	17,758 ms	111,959 μs	PushPop	godfine1
22.0%	65,303 s	12288	5,314 ms	5,298 ms	5,185 ms	12,241 ms	95,784 μs	PushPop	call unsplit
13.0%	39,032 s	36864	1,059 ms	1,059 ms	1,025 ms	1,681 ms	25,469 μs	PushPop	cmpflxm
8.0%	24,286 s	12288	1,976 ms	1,975 ms	1,887 ms	2,103 ms	29,519 μs	PushPop	godunov_fine loops over inner octs
5.0%	15,306 s	12288	1,246 ms	1,242 ms	1,201 ms	2,656 ms	22,636 μs	PushPop	first unparallelized part
3.0%	9,491 s	12288	772,379 μs	753,860 μs	730,857 μs	3,908 ms	43,983 μs	PushPop	traceNd
2.0%	7,556 s	12288	614,924 μs	610,690 μs	603,922 μs	809,955 μs	11,548 μs	PushPop	godunov_fine loops
2.0%	6,399 s	12288	520,759 μs	517,628 μs	504,616 μs	1,788 ms	16,425 μs	PushPop	uslope
1.0%	2,839 s	12288	231,016 μs	229,047 μs	216,086 μs	854,890 μs	10,962 μs	PushPop	ctoprim

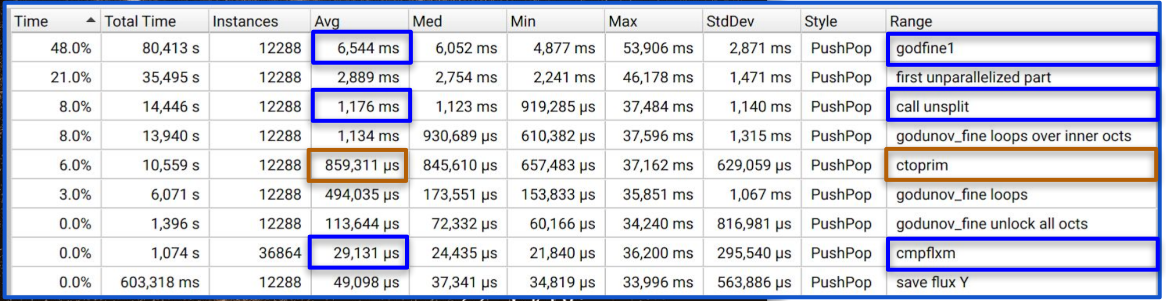
intermediate

superoct level 4



Time	Total Time	Instances	Avg	Med	Min	Max	StdDev	Style	Range
41.0%	81,610 s	12288	6,641 ms	6,019 ms	4,330 ms	56,130 ms	3,064 ms	PushPop	godfine1
17.0%	34,130 s	12288	2,777 ms	1,873 ms	1,640 ms	50,349 ms	2,231 ms	PushPop	call unsplit
12.0%	23,957 s	12288	1,950 ms	1,870 ms	1,422 ms	38,178 ms	1,056 ms	PushPop	first unparallelized part
11.0%	23,118 s	12288	1,881 ms	1,010 ms	891,428 μs	49,242 ms	1,693 ms	PushPop	ctoprim
7.0%	14,299 s	12288	1,164 ms	1,005 ms	626,919 μs	38,482 ms	964,970 μs	PushPop	godunov_fine loops over inner
3.0%	6,851 s	12288	557,559 μs	549,591 μs	388,902 μs	26,238 ms	421,711 μs	PushPop	uslope
3.0%	6,847 s	12288	557,194 μs	259,935 μs	170,164 μs	37,794 ms	940,941 μs	PushPop	godunov_fine loops
0.0%	1,279 s	36864	34,704 μs	24,491 μs	22,274 μs	36,054 ms	521,073 μs	PushPop	cmpflxm
0.0%	1,239 s	12288	100,790 μs	73,305 μs	62,615 μs	36,000 ms	702,611 μs	PushPop	godunov_fine unlock all octs

full GPU



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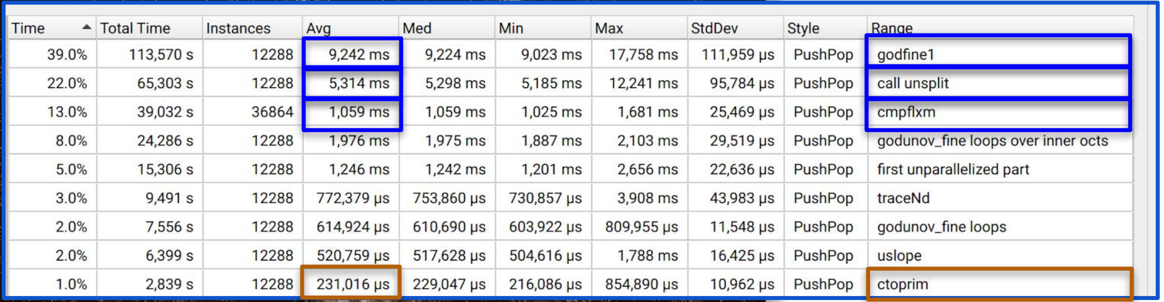
48.0%	80,413 s	12288	6,544 ms	6,052 ms	4,877 ms	53,906 ms	2,871 ms	PushPop	godfine1
21.0%	35,495 s	12288	2,889 ms	2,754 ms	2,241 ms	46,178 ms	1,471 ms	PushPop	first unparallelized part
8.0%	14,446 s	12288	1,176 ms	1,123 ms	919,285 μs	37,484 ms	1,140 ms	PushPop	call unsplit
8.0%	13,940 s	12288	1,134 ms	930,689 μs	610,382 μs	37,596 ms	1,315 ms	PushPop	godunov_fine loops over inner octs
6.0%	10,559 s	12288	859,311 μs	845,610 μs	657,483 μs	37,162 ms	629,059 μs	PushPop	ctoprim
3.0%	6,071 s	12288	494,035 μs	173,551 μs	153,833 μs	35,851 ms	1,067 ms	PushPop	godunov_fine loops
0.0%	1,396 s	12288	113,644 μs	72,332 μs	60,166 μs	34,240 ms	816,981 μs	PushPop	godunov_fine unlock all octs
0.0%	1,074 s	36864	29,131 μs	24,435 μs	21,840 μs	36,200 ms	295,540 μs	PushPop	cmpflxm
0.0%	603,318 ms	12288	49,098 μs	37,341 μs	34,819 μs	33,996 ms	563,886 μs	PushPop	save flux Y



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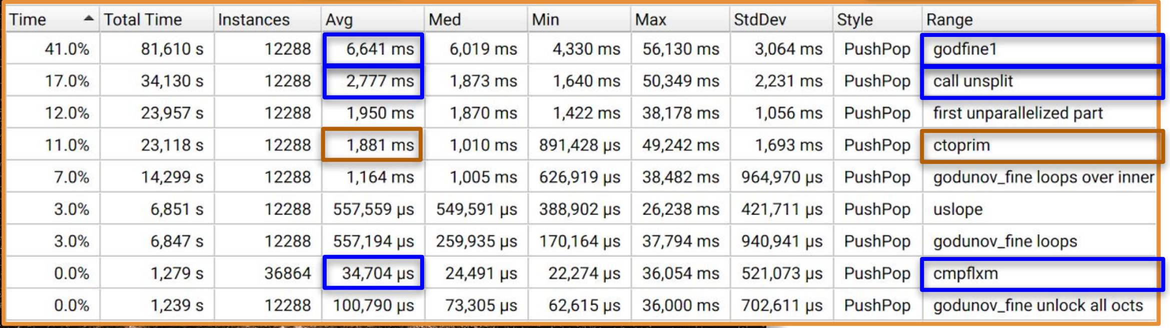

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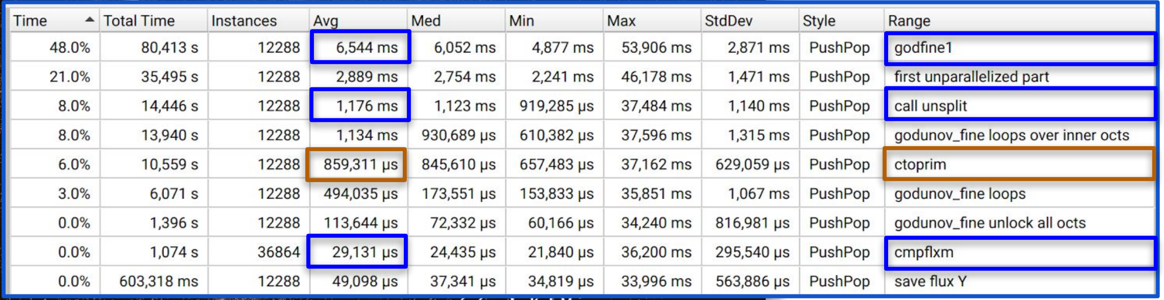

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8.0%	14,446 s	12288	1,176 ms	1,123 ms	919,285 µs	37,484 ms	1,140 ms	PushPop	call unsplit
8.0%	13,940 s	12288	1,134 ms	930,689 µs	610,382 µs	37,596 ms	1,315 ms	PushPop	godunov_fine loops over inner octs
6.0%	10,559 s	12288	859,311 µs	845,610 µs	657,483 µs	37,162 ms	629,059 µs	PushPop	ctoprim
3.0%	6,071 s	12288	494,035 µs	173,551 µs	153,833 µs	35,851 ms	1,067 ms	PushPop	godunov_fine loops
0.0%	1,396 s	12288	113,644 µs	72,332 µs	60,166 µs	34,240 ms	816,981 µs	PushPop	godunov_fine unlock all octs
0.0%	1,074 s	36864	29,131 µs	24,435 µs	21,840 µs	36,200 ms	295,540 µs	PushPop	cmpflxm
0.0%	603,318 ms	12288	49,098 µs	37,341 µs	34,819 µs	33,996 ms	563,886 µs	PushPop	save flux Y

Improvements?

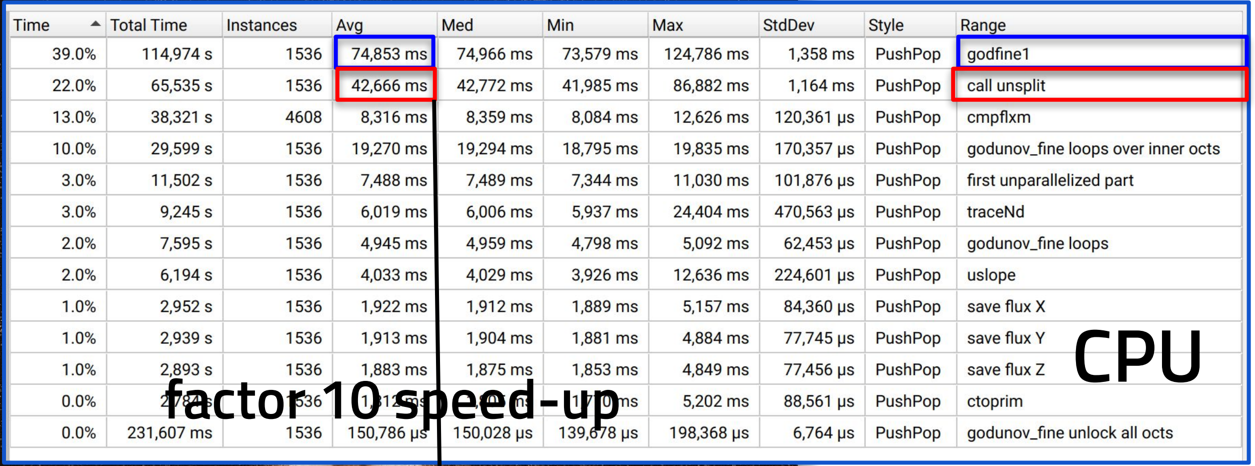
Each call to the godfine1 subroutine results in a speedup of approximately **1.5 times (low).**

The primary reason for the limited gain is the **overhead associated with memory management and communication** between the CPU and GPU.

These tasks consume a significant portion of the processing time, offsetting the potential performance improvements.

full CPU

superoct level 5

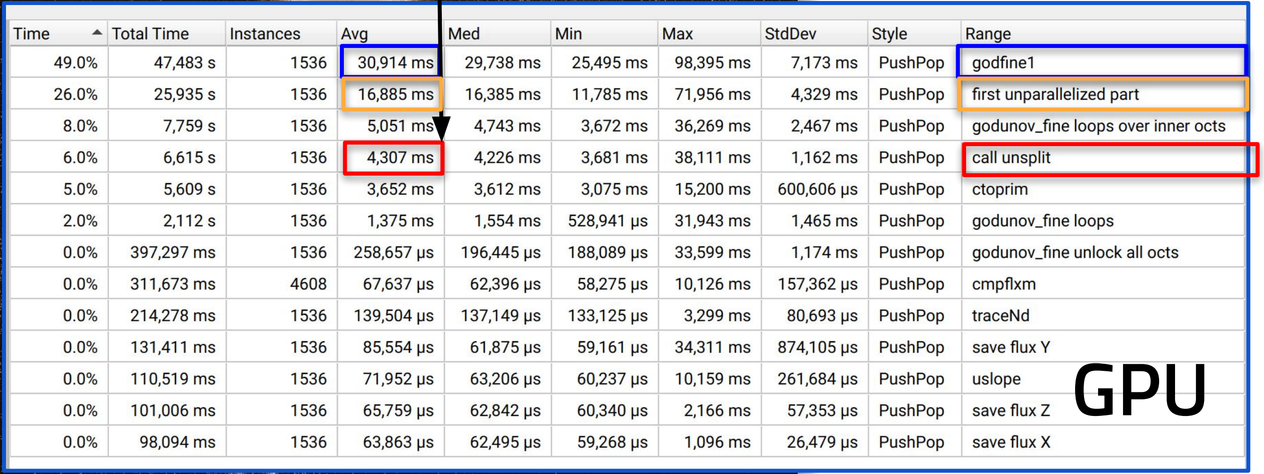


Time	Total Time	Instances	Avg	Med	Min	Max	StdDev	Style	Range
39.0%	114,974 s	1536	74,853 ms	74,966 ms	73,579 ms	124,786 ms	1,358 ms	PushPop	godfine1
22.0%	65,535 s	1536	42,666 ms	42,772 ms	41,985 ms	86,882 ms	1,164 ms	PushPop	call unsplit
13.0%	38,321 s	4608	8,316 ms	8,359 ms	8,084 ms	12,626 ms	120,361 μs	PushPop	cmpflxm
10.0%	29,599 s	1536	19,270 ms	19,294 ms	18,795 ms	19,835 ms	170,357 μs	PushPop	godunov_fine loops over inner octs
3.0%	11,502 s	1536	7,488 ms	7,489 ms	7,344 ms	11,030 ms	101,876 μs	PushPop	first unparallelized part
3.0%	9,245 s	1536	6,019 ms	6,006 ms	5,937 ms	24,404 ms	470,563 μs	PushPop	traceNd
2.0%	7,595 s	1536	4,945 ms	4,959 ms	4,798 ms	5,092 ms	62,453 μs	PushPop	godunov_fine loops
2.0%	6,194 s	1536	4,033 ms	4,029 ms	3,926 ms	12,636 ms	224,601 μs	PushPop	uslope
1.0%	2,952 s	1536	1,922 ms	1,912 ms	1,889 ms	5,157 ms	84,360 μs	PushPop	save flux X
1.0%	2,939 s	1536	1,913 ms	1,904 ms	1,881 ms	4,884 ms	77,745 μs	PushPop	save flux Y
1.0%	2,893 s	1536	1,883 ms	1,875 ms	1,853 ms	4,849 ms	77,456 μs	PushPop	save flux Z
0.0%	2,784 s	1536	1,812 ms	1,805 ms	1,710 ms	5,202 ms	88,561 μs	PushPop	ctoprim
0.0%	231,607 ms	1536	150,786 μs	150,028 μs	139,678 μs	198,368 μs	6,764 μs	PushPop	godunov_fine unlock all octs

CPU

factor 10 speed-up

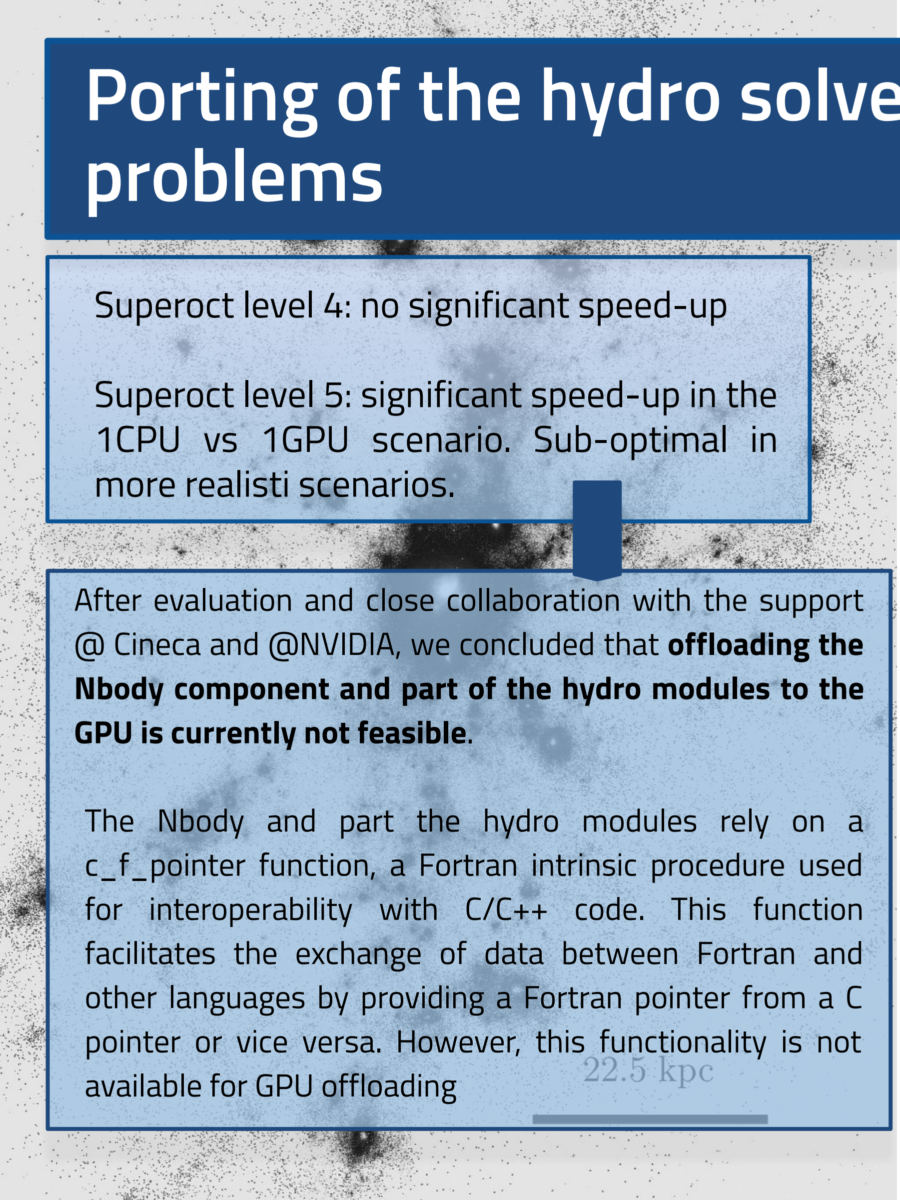
full GPU



Time	Total Time	Instances	Avg	Med	Min	Max	StdDev	Style	Range
49.0%	47,483 s	1536	30,914 ms	29,738 ms	25,495 ms	98,395 ms	7,173 ms	PushPop	godfine1
26.0%	25,935 s	1536	16,885 ms	16,385 ms	11,785 ms	71,956 ms	4,329 ms	PushPop	first unparallelized part
8.0%	7,759 s	1536	5,051 ms	4,743 ms	3,672 ms	36,269 ms	2,467 ms	PushPop	godunov_fine loops over inner octs
6.0%	6,615 s	1536	4,307 ms	4,226 ms	3,681 ms	38,111 ms	1,162 ms	PushPop	call unsplit
5.0%	5,609 s	1536	3,652 ms	3,612 ms	3,075 ms	15,200 ms	600,606 μs	PushPop	ctoprim
2.0%	2,112 s	1536	1,375 ms	1,554 ms	528,941 μs	31,943 ms	1,465 ms	PushPop	godunov_fine loops
0.0%	397,297 ms	1536	258,657 μs	196,445 μs	188,089 μs	33,599 ms	1,174 ms	PushPop	godunov_fine unlock all octs
0.0%	311,673 ms	4608	67,637 μs	62,396 μs	58,275 μs	10,126 ms	157,362 μs	PushPop	cmpflxm
0.0%	214,278 ms	1536	139,504 μs	137,149 μs	133,125 μs	3,299 ms	80,693 μs	PushPop	traceNd
0.0%	131,411 ms	1536	85,554 μs	61,875 μs	59,161 μs	34,311 ms	874,105 μs	PushPop	save flux Y
0.0%	110,519 ms	1536	71,952 μs	63,206 μs	60,237 μs	10,159 ms	261,684 μs	PushPop	uslope
0.0%	101,006 ms	1536	65,759 μs	62,842 μs	60,340 μs	2,166 ms	57,353 μs	PushPop	save flux Z
0.0%	98,094 ms	1536	63,863 μs	62,495 μs	59,268 μs	1,096 ms	26,479 μs	PushPop	save flux X

GPU

Porting of the hydro solver: problems



Superoct level 4: no significant speed-up

Superoct level 5: significant speed-up in the 1CPU vs 1GPU scenario. Sub-optimal in more realisti scenarios.

After evaluation and close collaboration with the support @ Cineca and @NVIDIA, we concluded that **offloading the Nbody component and part of the hydro modules to the GPU is currently not feasible**.

The Nbody and part the hydro modules rely on a c_f_pointer function, a Fortran intrinsic procedure used for interoperability with C/C++ code. This function facilitates the exchange of data between Fortran and other languages by providing a Fortran pointer from a C pointer or vice versa. However, this functionality is not available for GPU offloading

Hydro:

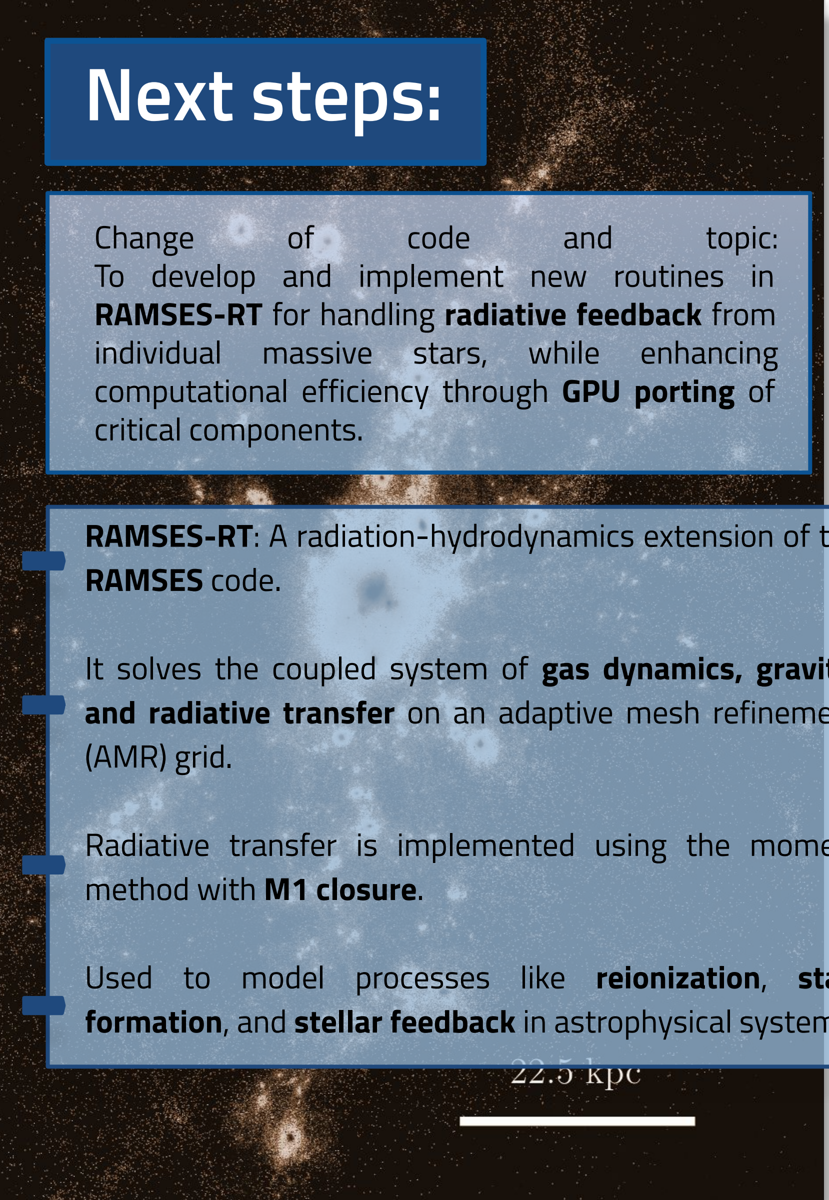
The hydrodynamic equations describing the fluid motion are solved

N-body:

~~the trajectories of collisionless particles (e.g., dark matter) are evolved using the leapfrog algorithm.~~

Completing the GPU porting of these components would require a complete rewrite of the memory management routines in MiniRAMSES, making the code significantly different from the public version and essentially turning it into a separate codebase from the original project.

Next steps:



Change of code and topic: To develop and implement new routines in **RAMSES-RT** for handling **radiative feedback** from individual massive stars, while enhancing computational efficiency through **GPU porting** of critical components.

RAMSES-RT: A radiation-hydrodynamics extension of the **RAMSES** code.

It solves the coupled system of **gas dynamics, gravity, and radiative transfer** on an adaptive mesh refinement (AMR) grid.

Radiative transfer is implemented using the moment method with **M1 closure**.

Used to model processes like **reionization**, **star formation**, and **stellar feedback** in astrophysical systems.

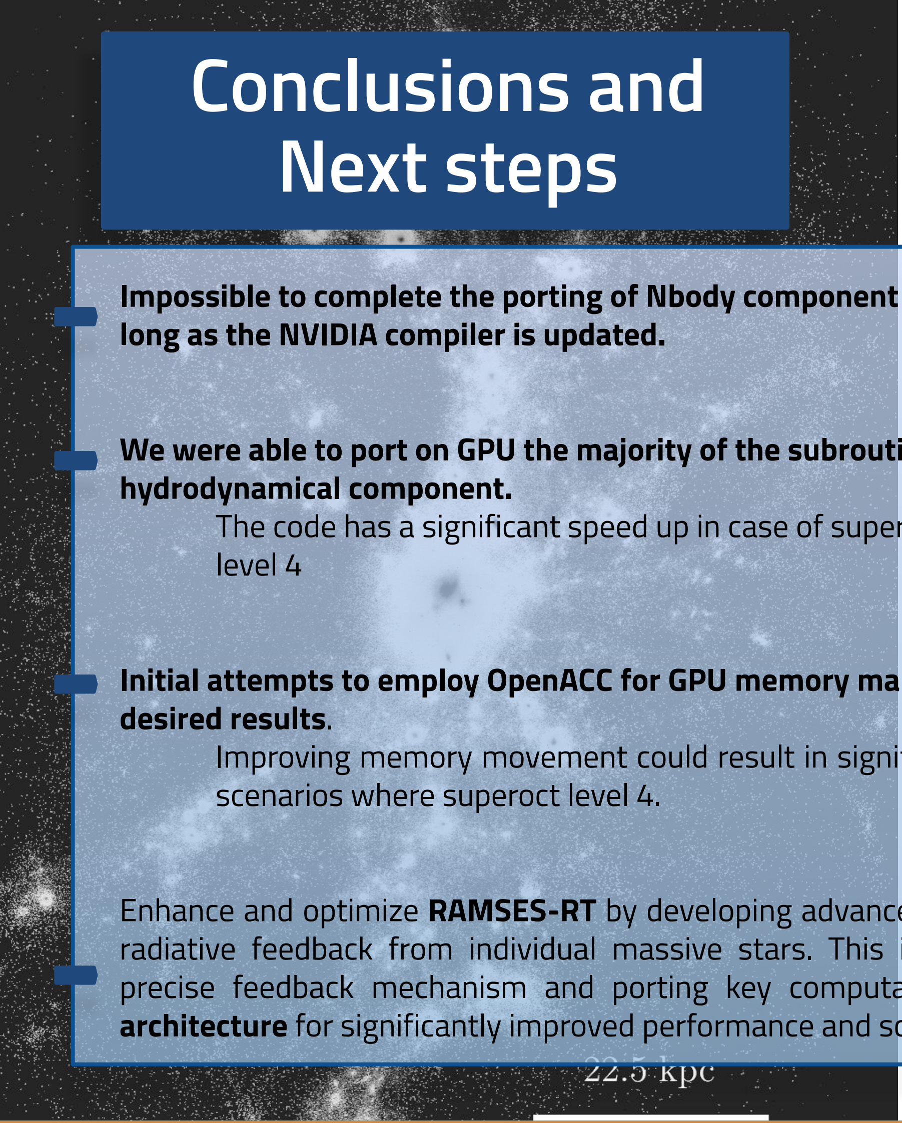
New Radiative Feedback Routine

- **Individual star tracking**: Implement feedback from single massive stars instead of bulk populations.
- **Accurate photoionization**: Direct coupling between stellar radiation and surrounding gas.
- **Time-dependent flux**: Account for star luminosity evolution in time.

Porting to GPU

- Offloading key routines from CPU to **GPU** to achieve higher parallelization.
- Reducing computational bottlenecks in **radiative transfer and flux updates**.
- Achieving significant speedup for **large-scale simulations**.

Conclusions and Next steps



- **Impossible to complete the porting of Nbody component and Hydrodynamic solver as long as the NVIDIA compiler is updated.**

- **We were able to port on GPU the majority of the subroutines associated with hydrodynamical component.**
  The code has a significant speed up in case of superoct level 5, but not superoct level 4

- **Initial attempts to employ OpenACC for GPU memory management have not yielded the desired results**.
  Improving memory movement could result in significant speed-ups, particularly in scenarios where superoct level 4.

- Enhance and optimize **RAMSES-RT** by developing advanced routines to accurately model radiative feedback from individual massive stars. This includes implementing a more precise feedback mechanism and porting key computational components to a **GPU architecture** for significantly improved performance and scalability.