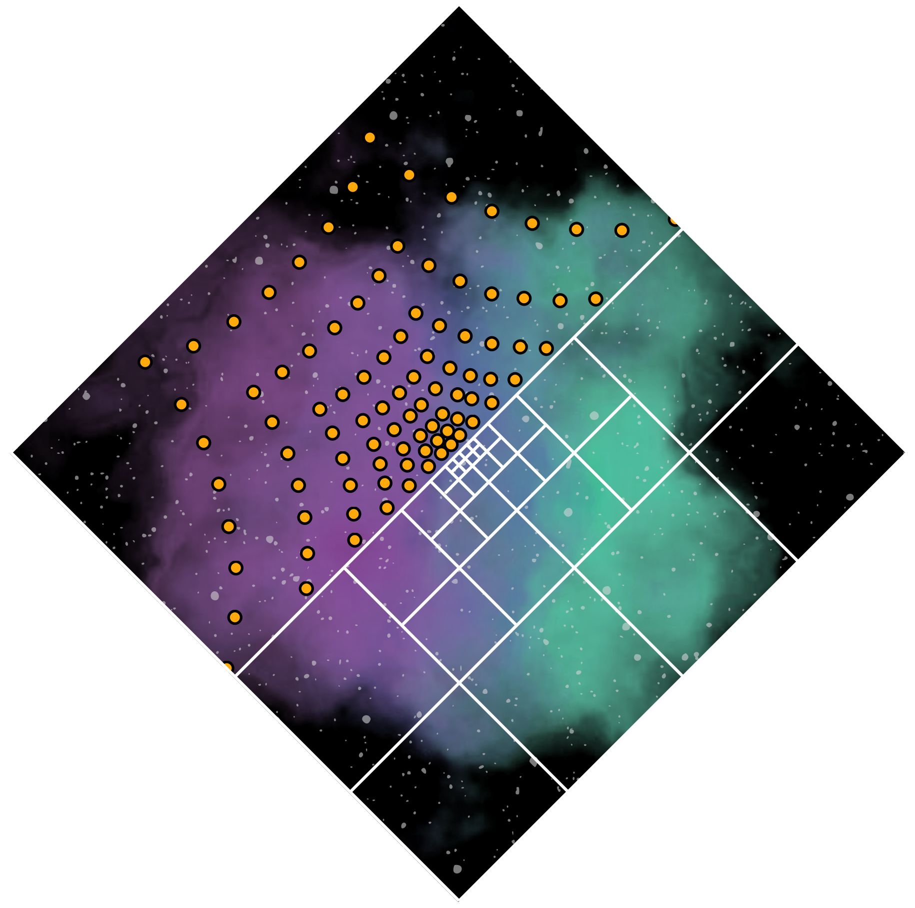

FRANCE 2030
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ORIGINES

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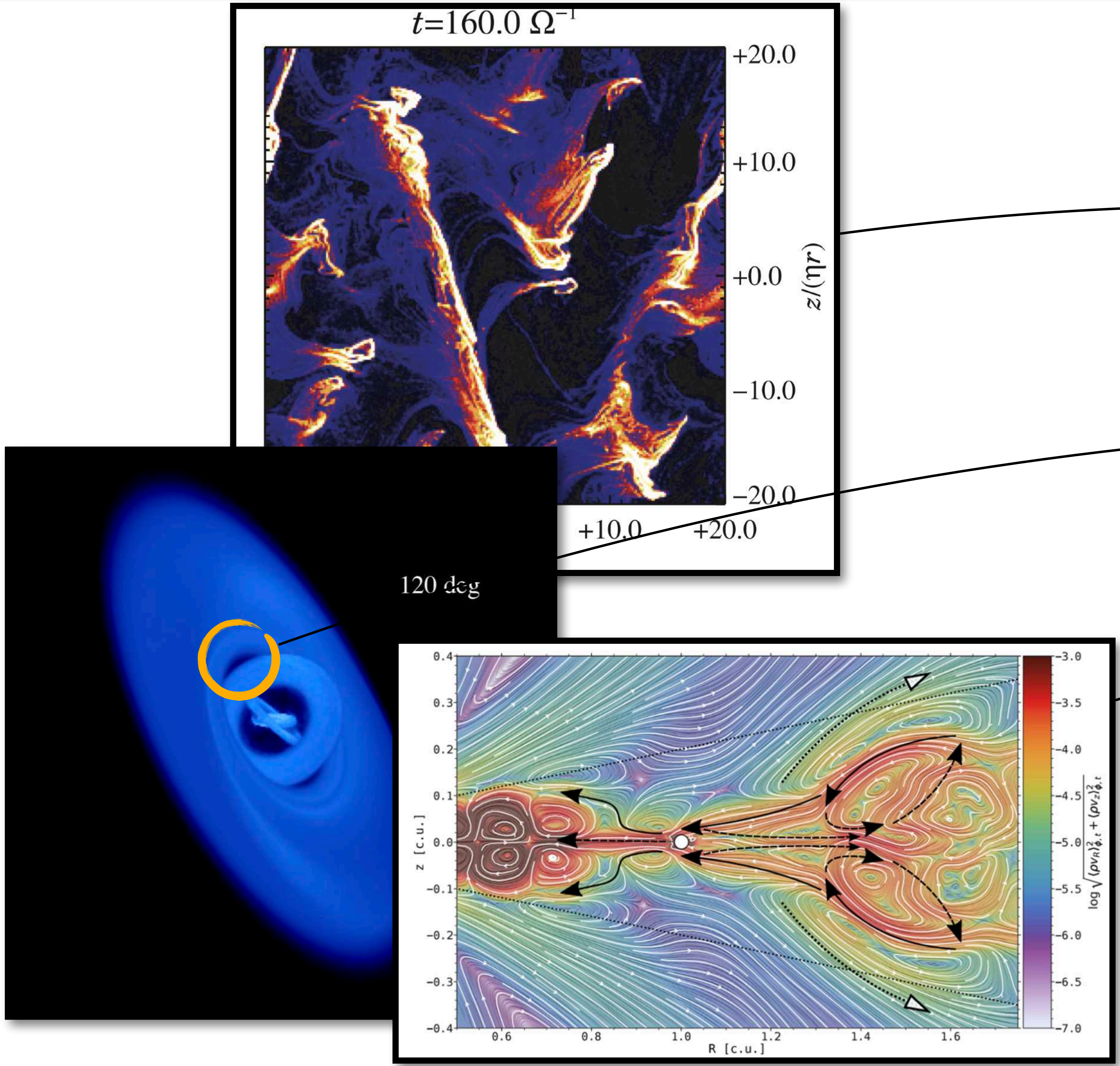
Why ???????????????????

Why a new code ?

Context & Aims



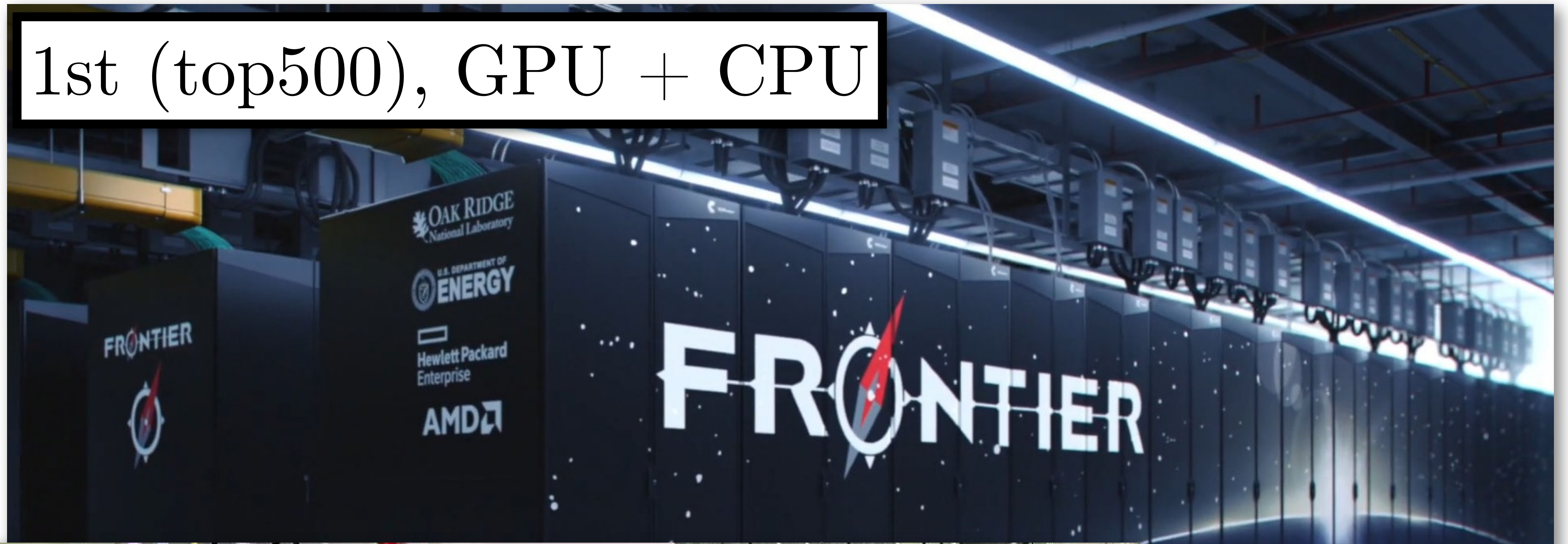
S.I. In global discs ?

What happens here ?

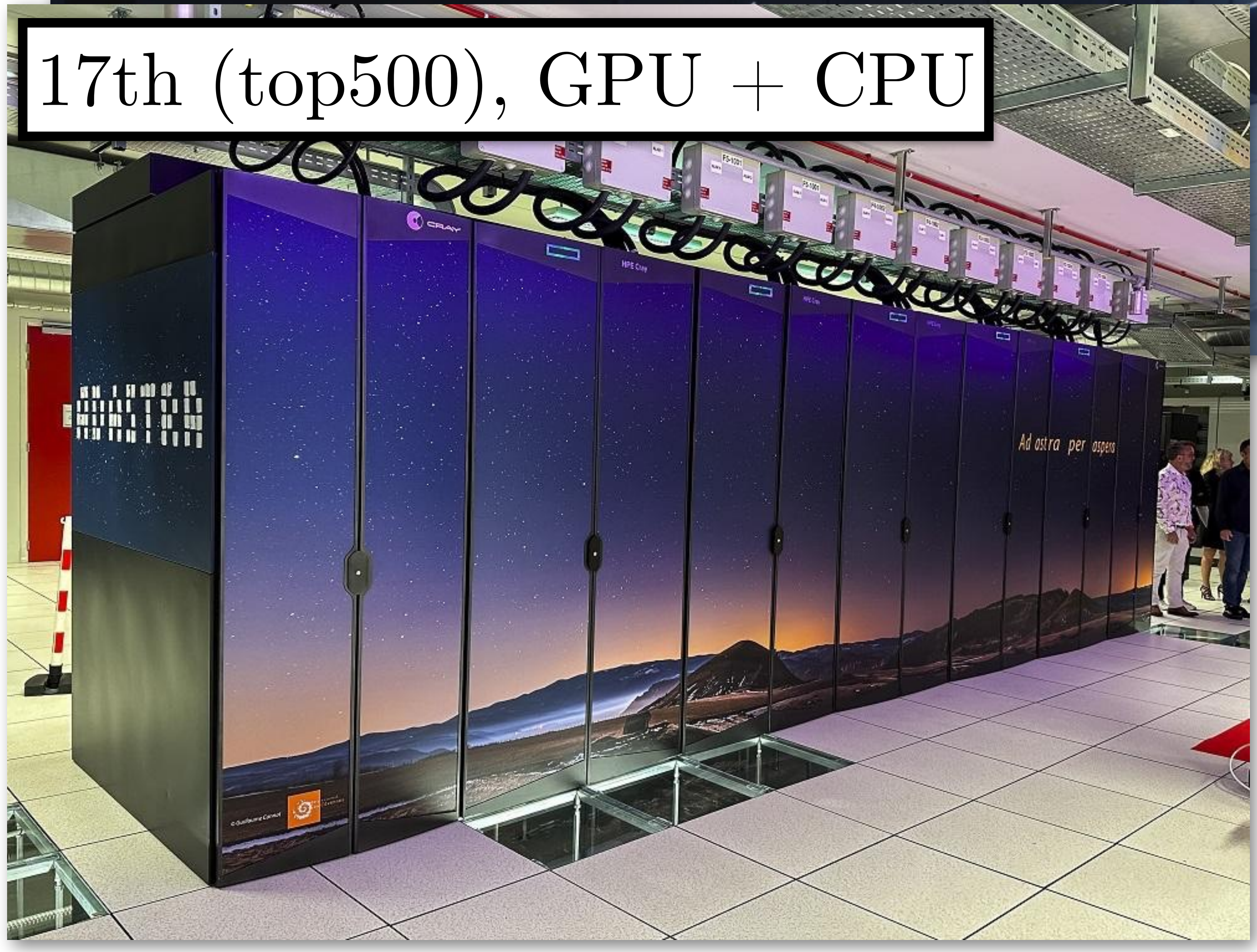
And close to a planet ?

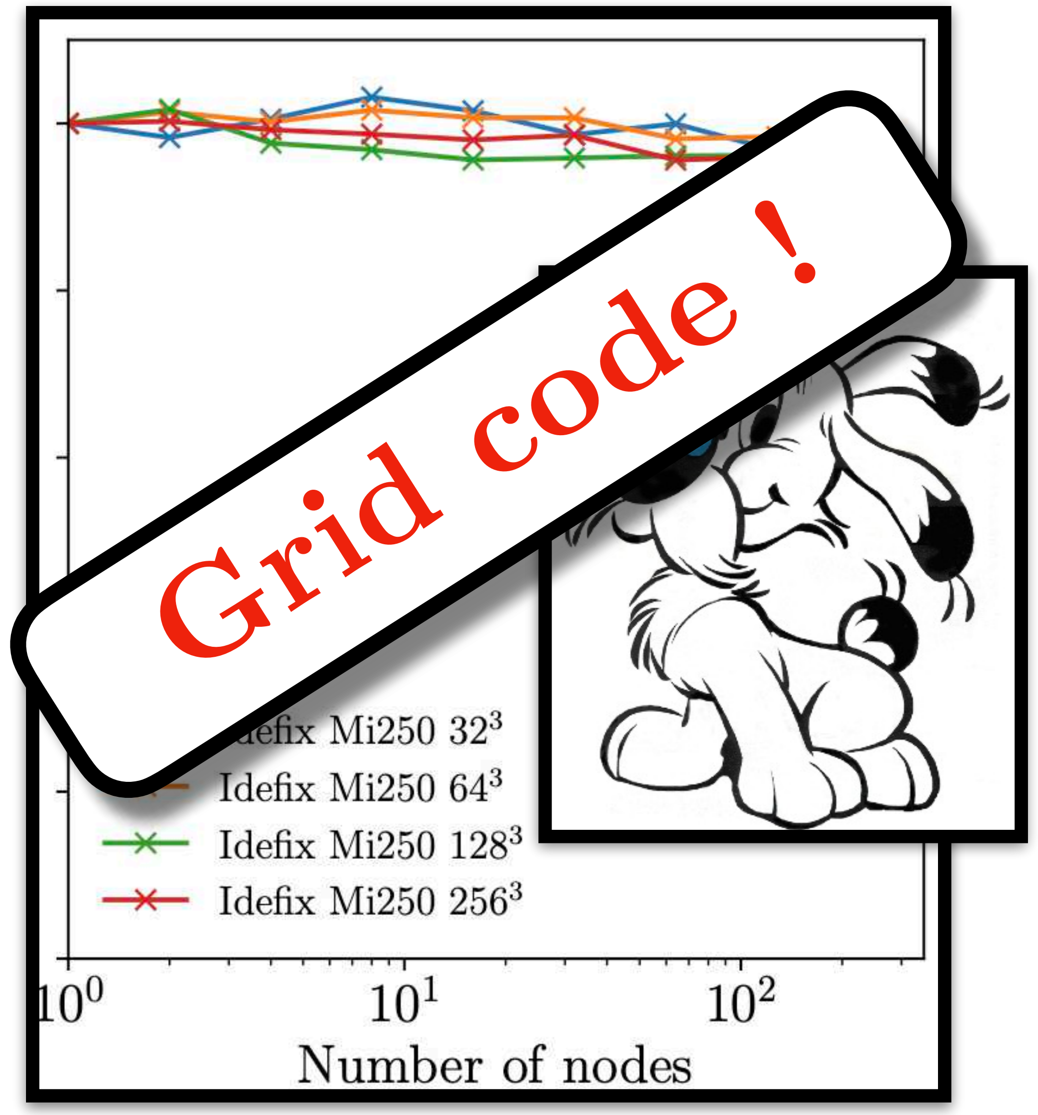
Resolution is mandatory !!!

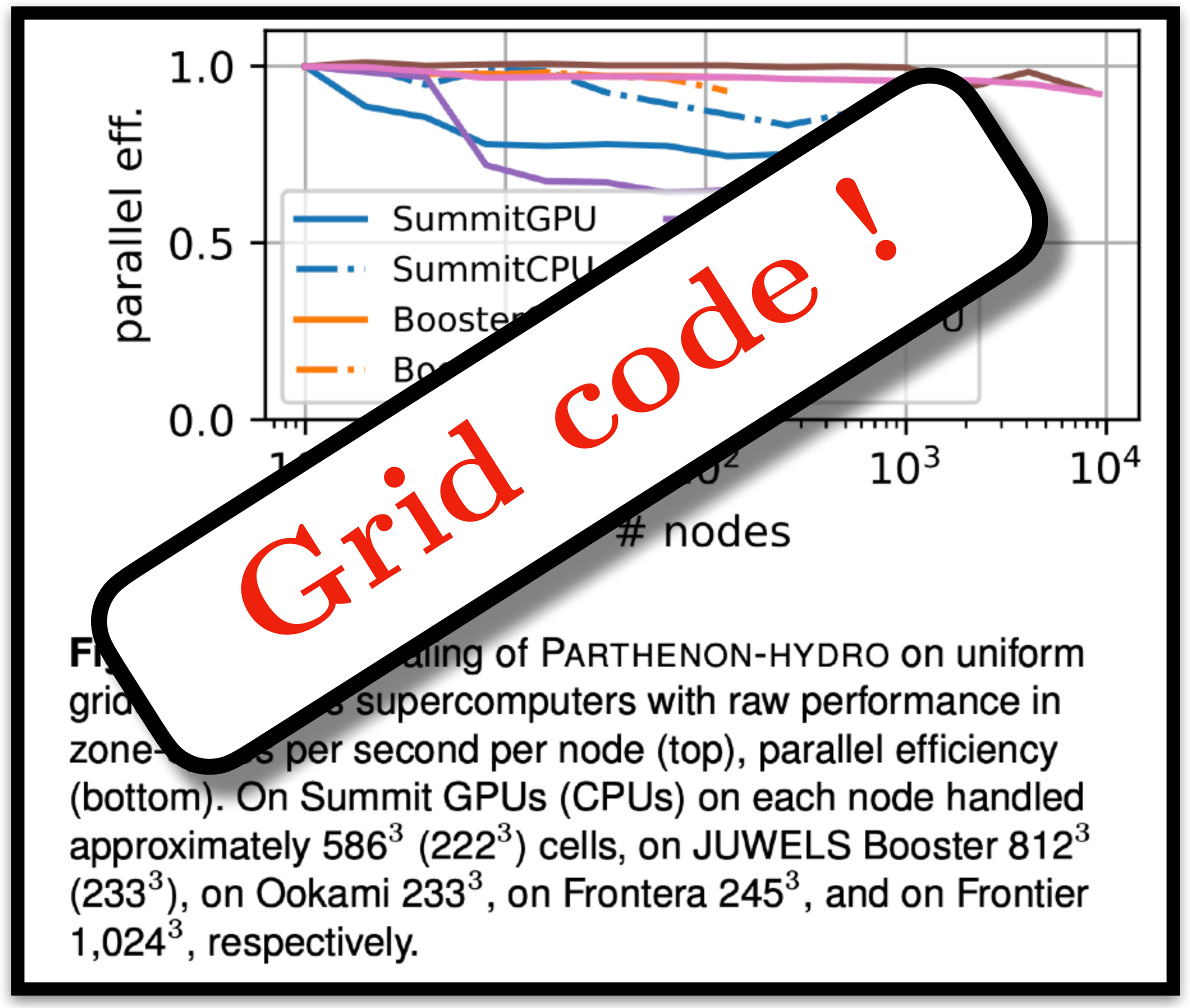
Context & Aims


1st (top500), GPU + CPU

FRONTIER
OAK RIDGE National Laboratory
U.S. DEPARTMENT OF ENERGY
Hewlett Packard Enterprise
AMD


17th (top500), GPU + CPU





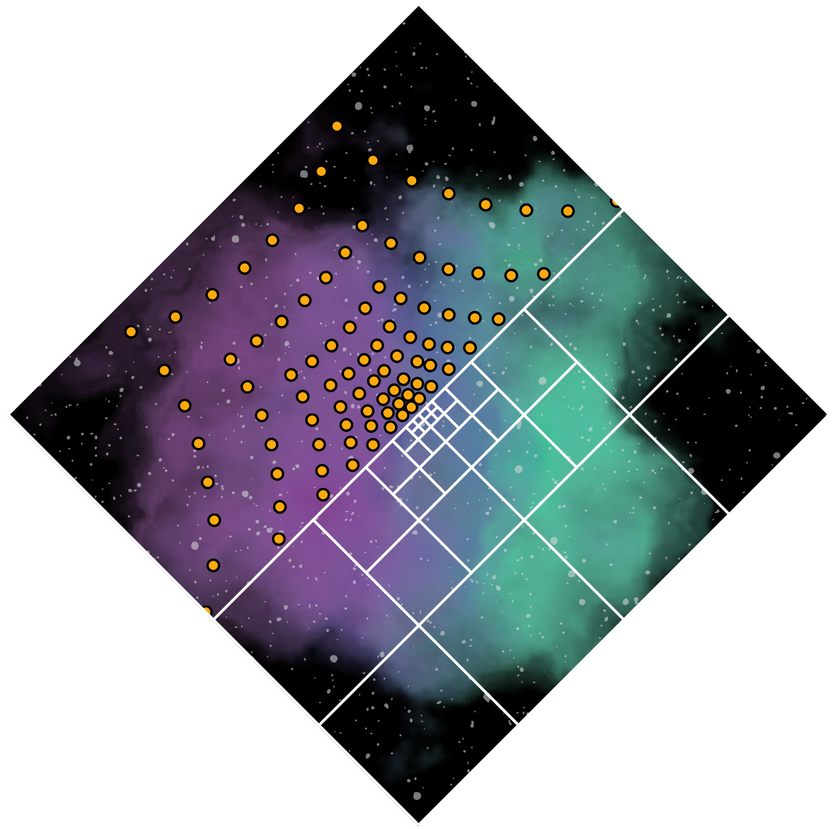
Fi... ...ling of PARTHENON-HYDRO on uniform grid... ...s supercomputers with raw performance in zone-... ...s per second per node (top), parallel efficiency (bottom). On Summit GPUs (CPUs) on each node handled approximately 586^3 (222^3) cells, on JUWELS Booster 812^3 (233^3), on Ookami 233^3, on Frontera 245^3, and on Frontier $1{,}024^3$, respectively.

A software framework for massively... ...ed adaptive mesh refinement (AMR) applications

Where is SPH ???

So we need something ....

Well you know where this is going ....



Technical Locks

- `>1G part` in a simulation

  How do you store a lot of particles on a cluster ?

- Fast on GPU

  Can you optimise SPH on GPU

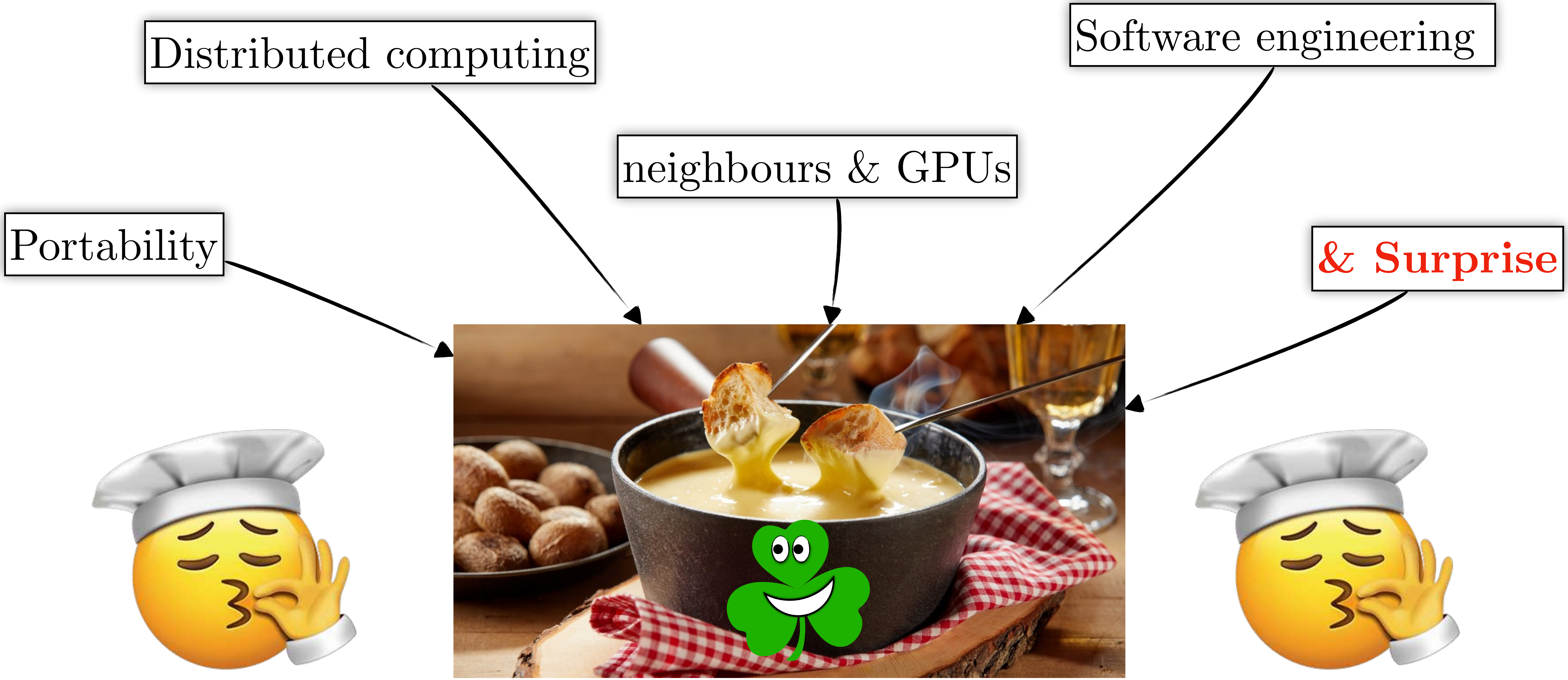
- Neighbours finding

  How do you work with neighbours on GPU

- Portability

  But you need also to run well on CPU

The plan !



Distributed computing

neighbours & GPUs

Software engineering

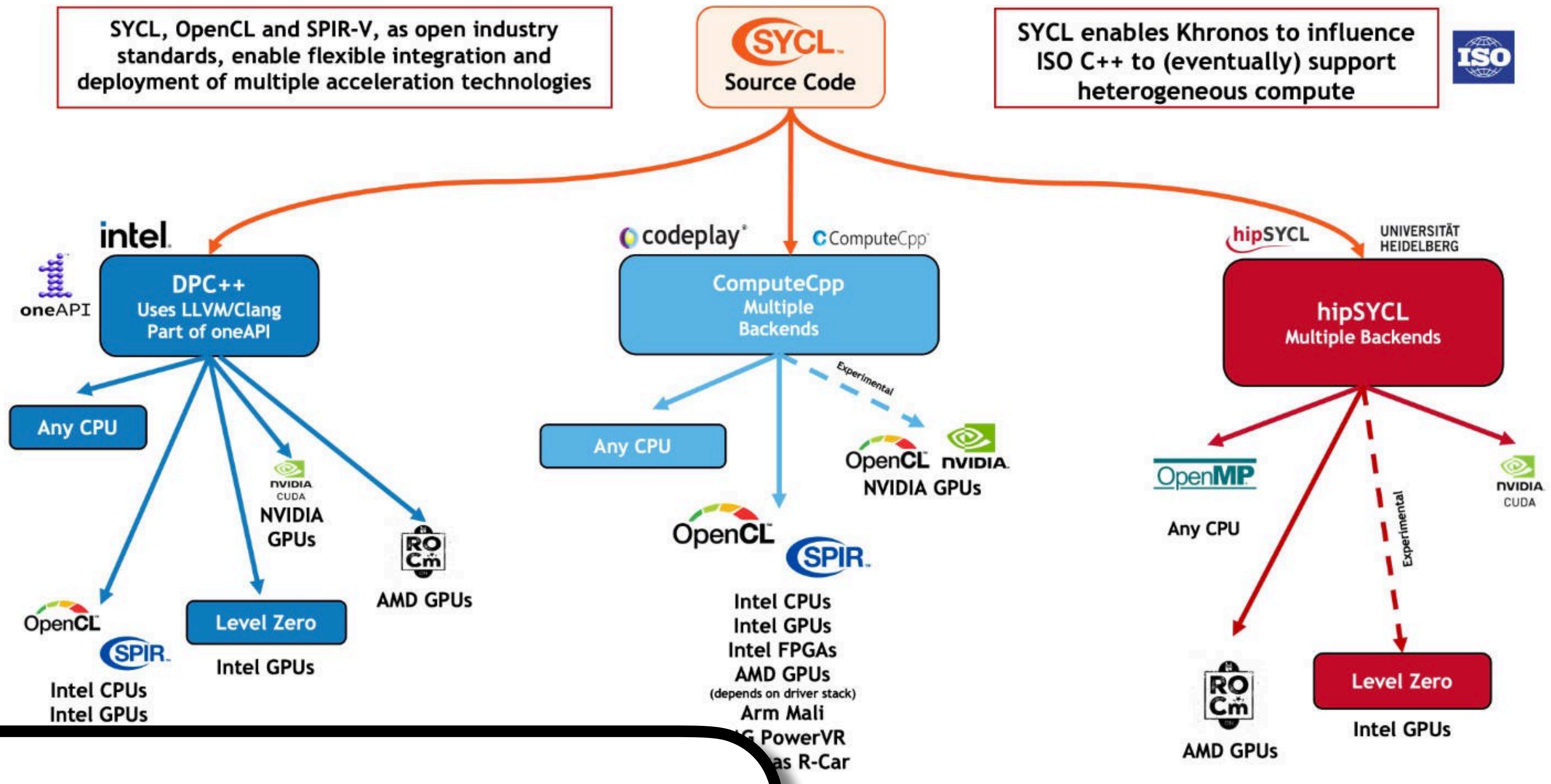
Portability

& Surprise

Source : passeportsante.net

Portability

Our choice : SYCL™



- C++17
- Can be compiled to native CUDA, hip, OpenMP, ...
- Support **<u>all</u>** CPU & GPUs

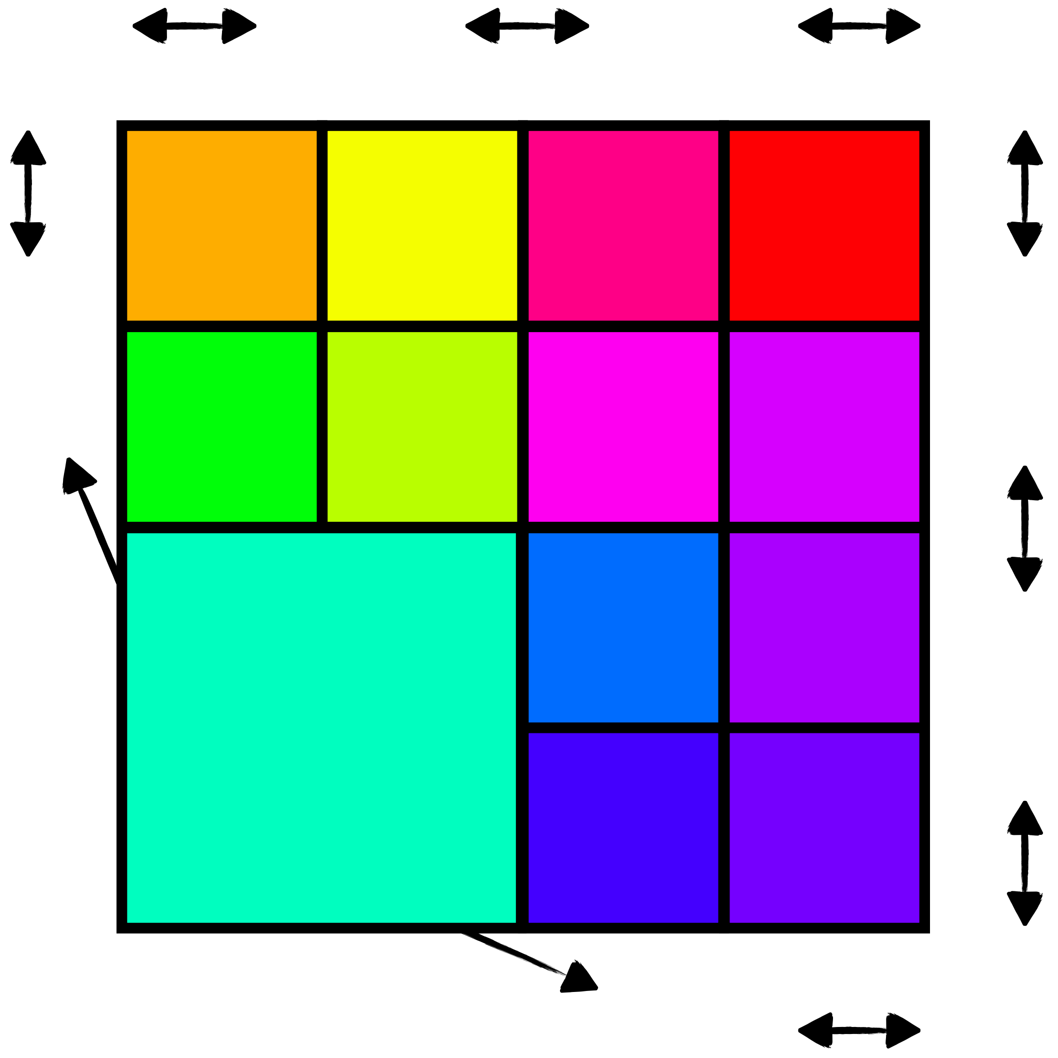
- Portability

  But you need also to run well on CPU

Domain decomposition

The global simulation is divided into multiple patches (**abstract decomposition**)

We only have to communicate the interface to itera

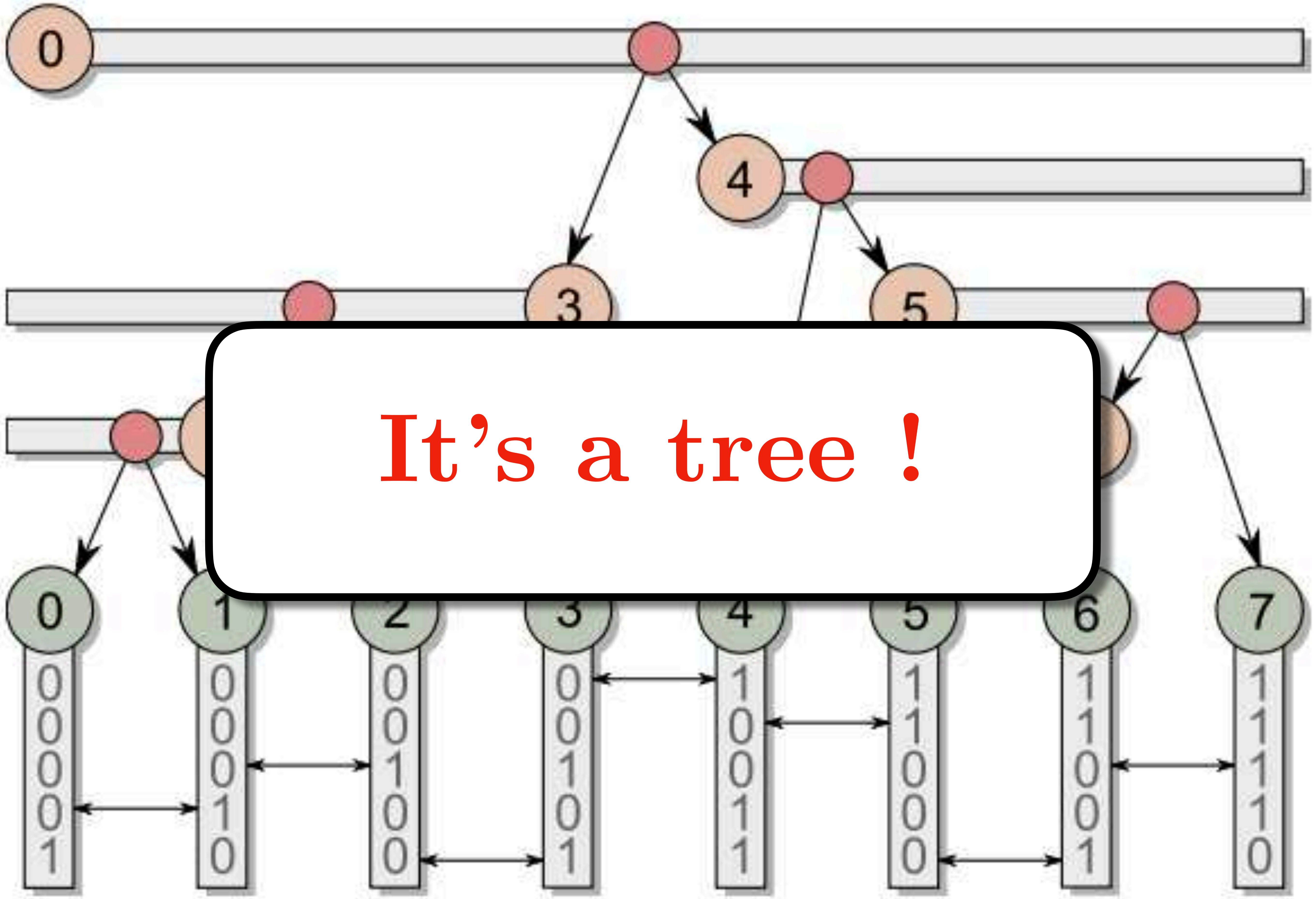


- >1G part in a simulation

Patches are scattered across the nodes

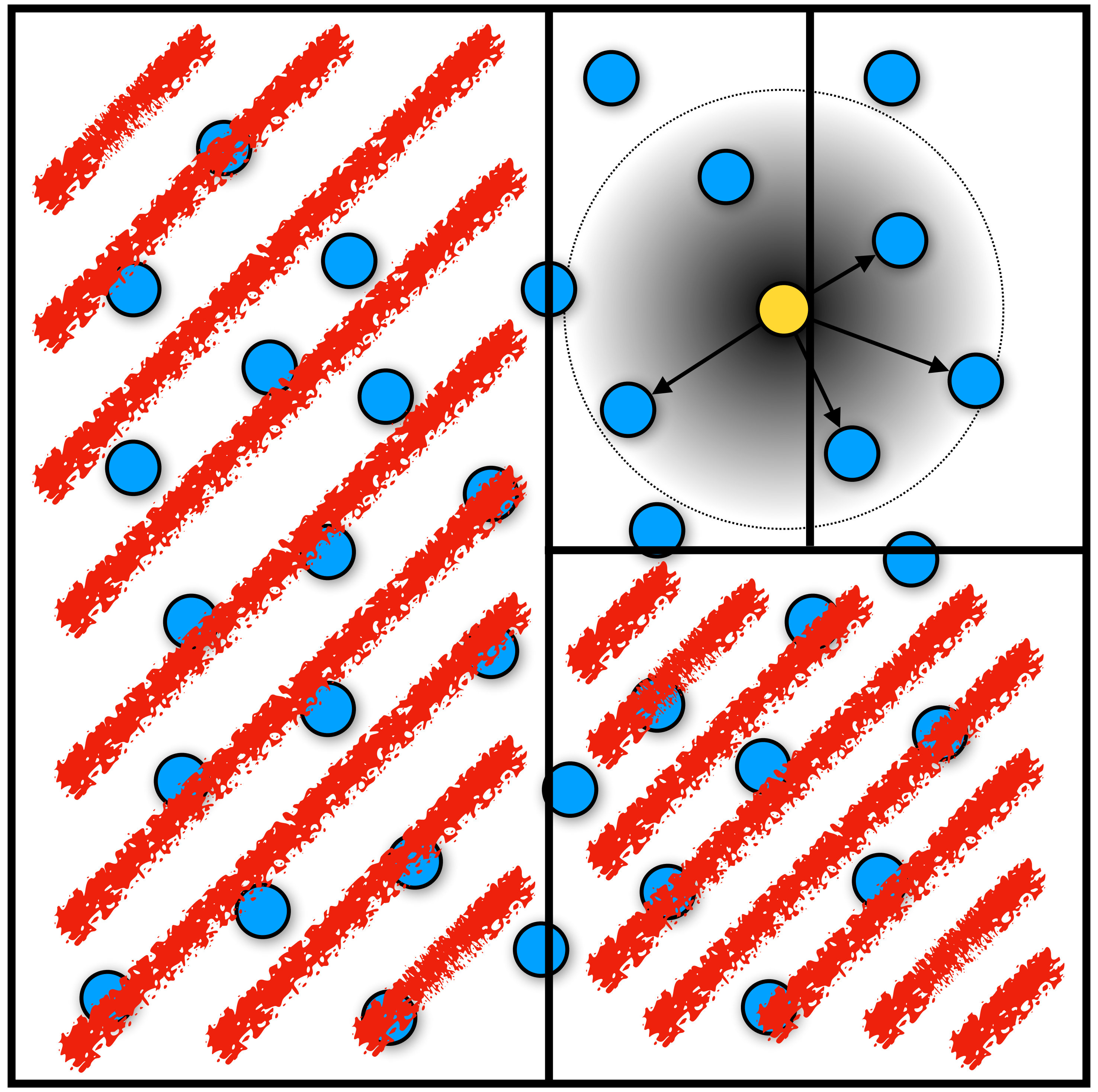
If patches are too large they split
If they are too small they merge

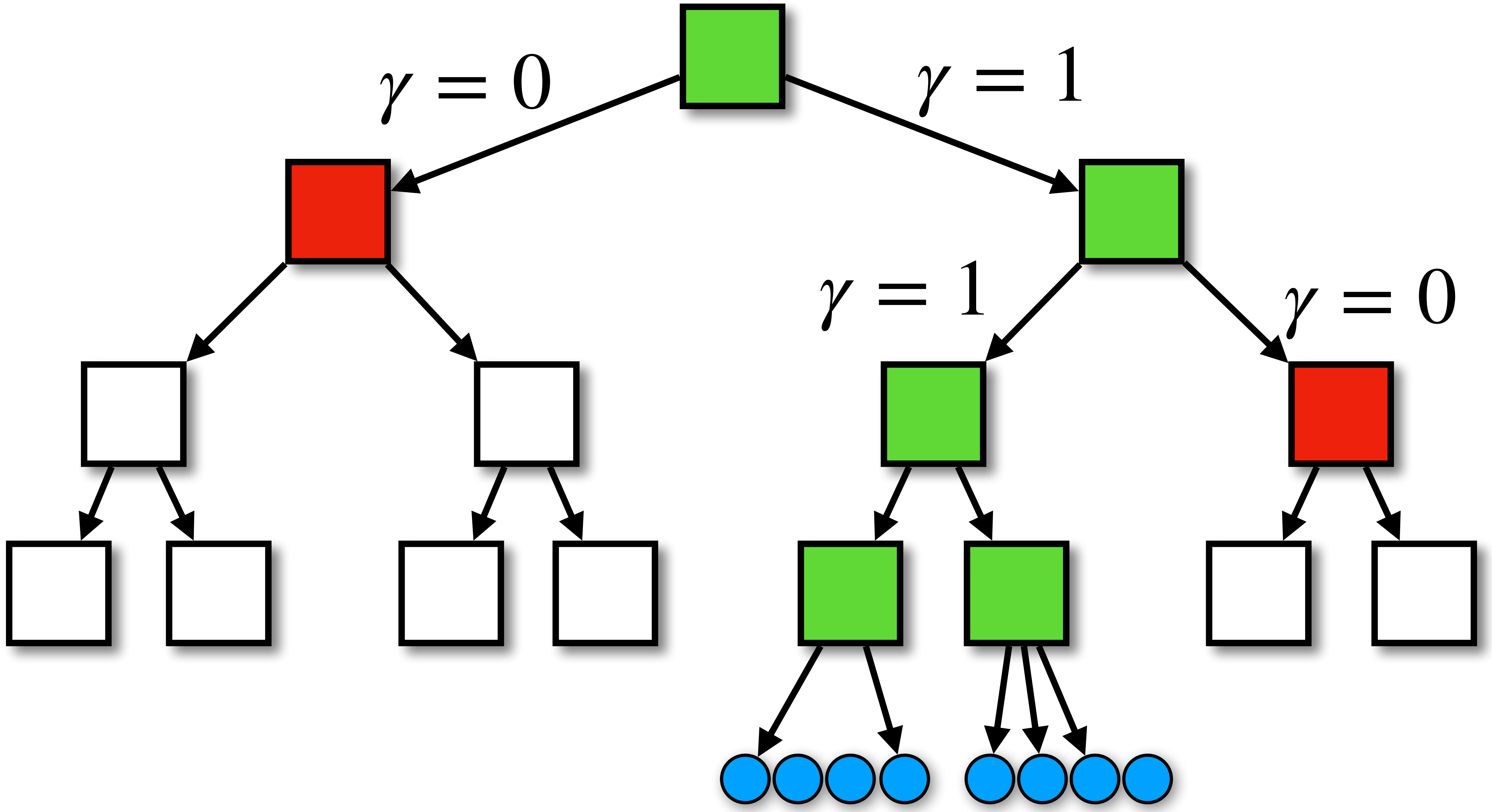
What is that ?



It's a tree !

Neighbour finding





Tree based version :

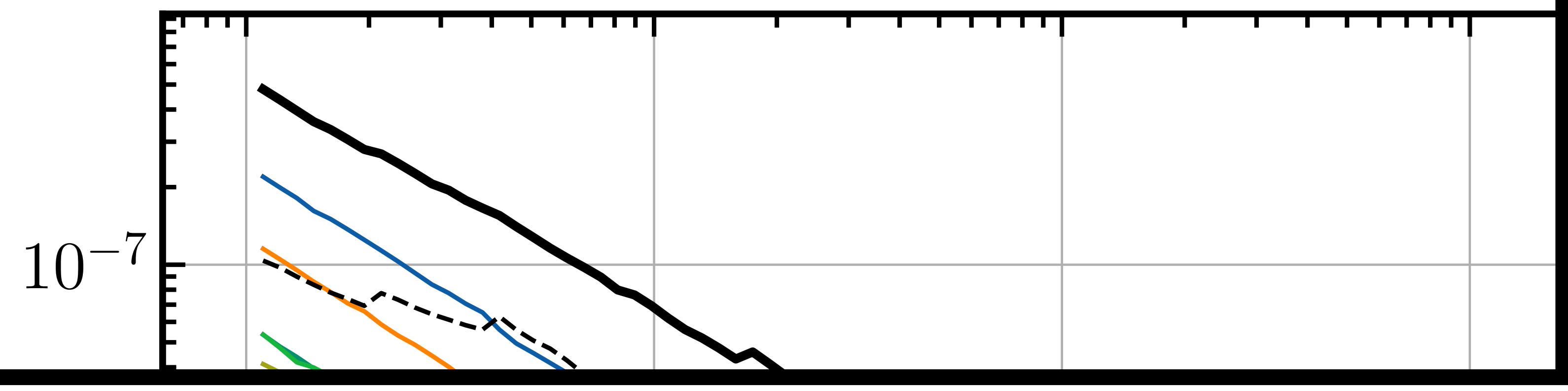
Complexity :$\mathcal{O}(n\log(n))$

- Exclude half of the space every steps
- The remaining particles are likely to interact

It took a year ....

Tree algorithm :

- Using binary arithmetics (fast)
- Morton code to convert position to binary
- Internal layout using binary tree
- just rebuild it !



🔓

- Fast on GPU

  Can you optimise SPH on GPU

🔓

- Neighbours finding

  How do you work with neighbours on GPU

Shamrock paper 1 (in prep)

y **faster than a timestep !**

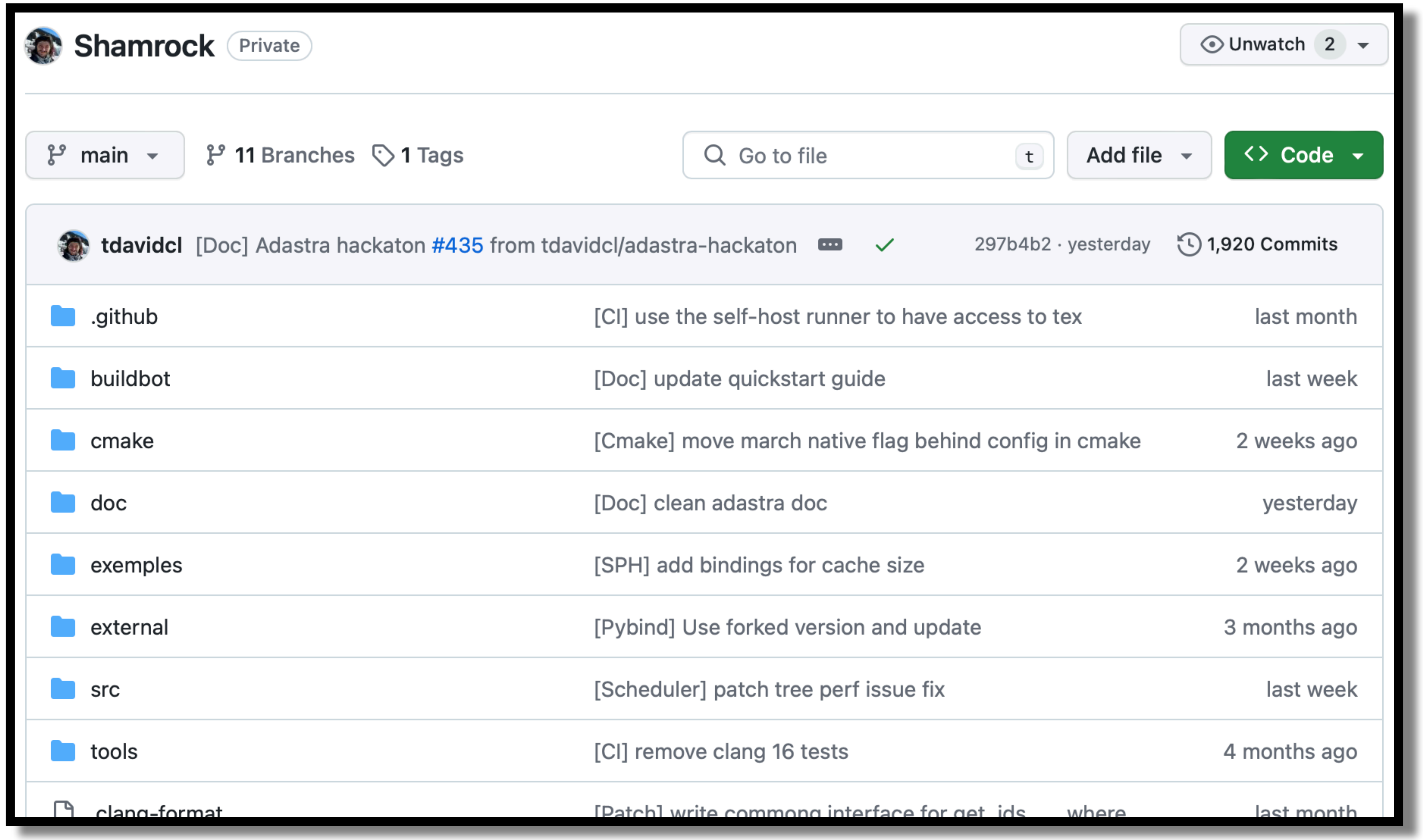
A100 SXM4 : >400.000.000 objects/ 1 sec

But .....

A lot of code → Software engineering ....

CI

Github test pipeline + regression ✅



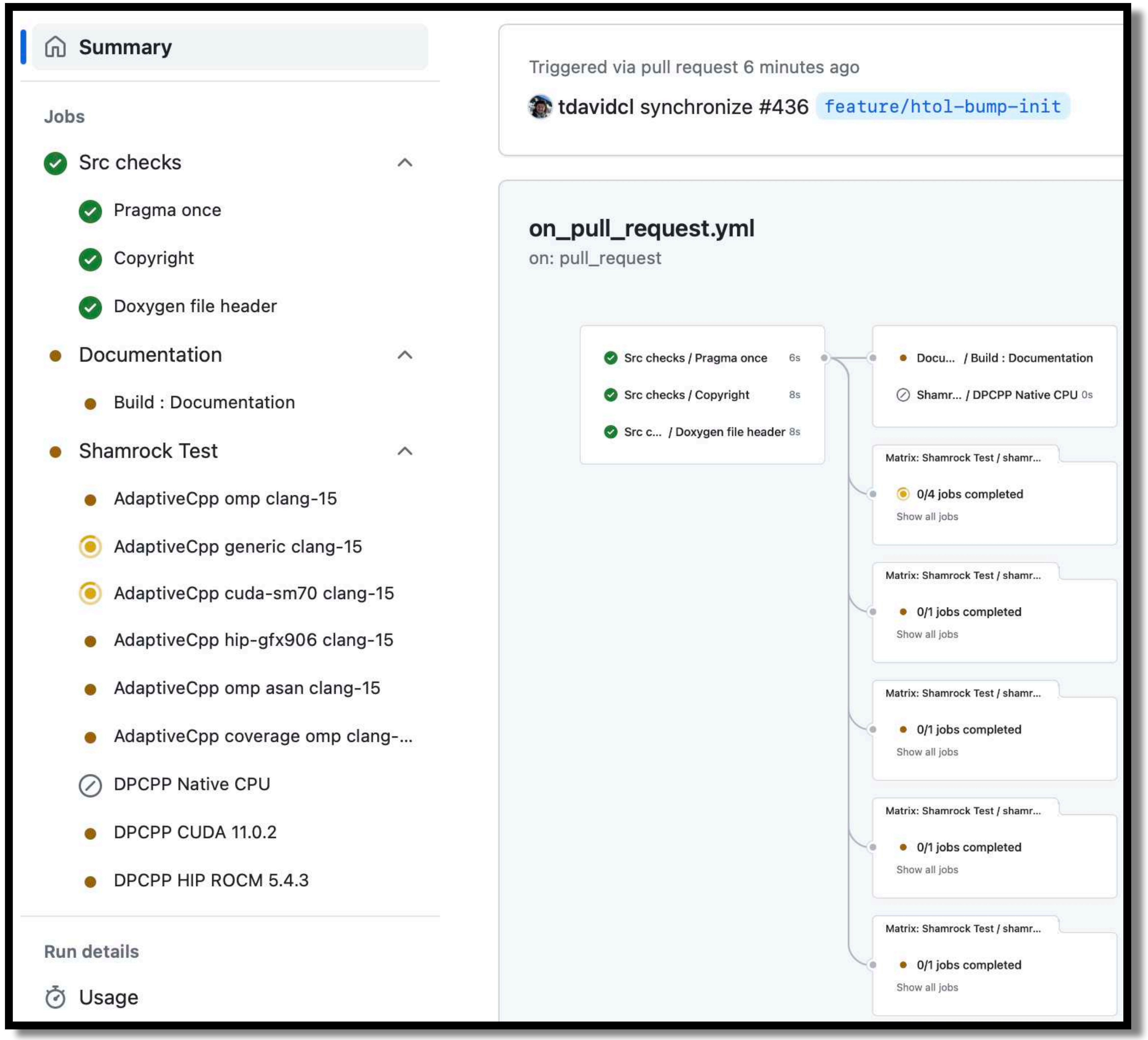
Shamrock Private

Unwatch 2

main · 11 Branches · 1 Tags · Go to file t · Add file · Code

tdavidcl [Doc] Adastra hackaton #435 from tdavidcl/adastra-hackaton ✓ 297b4b2 · yesterday · 1,920 Commits

.github	[CI] use the self-host runner to have access to tex	last month
buildbot	[Doc] update quickstart guide	last week
cmake	[Cmake] move march native flag behind config in cmake	2 weeks ago
doc	[Doc] clean adastra doc	yesterday
exemples	[SPH] add bindings for cache size	2 weeks ago
external	[Pybind] Use forked version and update	3 months ago
src	[Scheduler] patch tree perf issue fix	last week
tools	[CI] remove clang 16 tests	4 months ago
.clang-format	[Patch] write commong interface for get_ids_where	last month



Summary

Jobs

- ✓ Src checks
  - ✓ Pragma once
  - ✓ Copyright
  - ✓ Doxygen file header
- ● Documentation
  - ● Build : Documentation
- ● Shamrock Test
  - ● AdaptiveCpp omp clang-15
  - ◉ AdaptiveCpp generic clang-15
  - ◉ AdaptiveCpp cuda-sm70 clang-15
  - ● AdaptiveCpp hip-gfx906 clang-15
  - ● AdaptiveCpp omp asan clang-15
  - ● AdaptiveCpp coverage omp clang-...
  - ⊘ DPCPP Native CPU
  - ● DPCPP CUDA 11.0.2
  - ● DPCPP HIP ROCM 5.4.3

Run details

Usage

Triggered via pull request 6 minutes ago

tdavidcl synchronize #436 `feature/htol-bump-init`

on_pull_request.yml

on: pull_request

✓ Src checks / Pragma once 6s

✓ Src checks / Copyright 8s

✓ Src c... / Doxygen file header 8s

● Docu... / Build : Documentation

⊘ Shamr... / DPCPP Native CPU 0s

Matrix: Shamrock Test / shamr...
◉ 0/4 jobs completed
Show all jobs

Matrix: Shamrock Test / shamr...
● 0/1 jobs completed
Show all jobs

Matrix: Shamrock Test / shamr...
● 0/1 jobs completed
Show all jobs

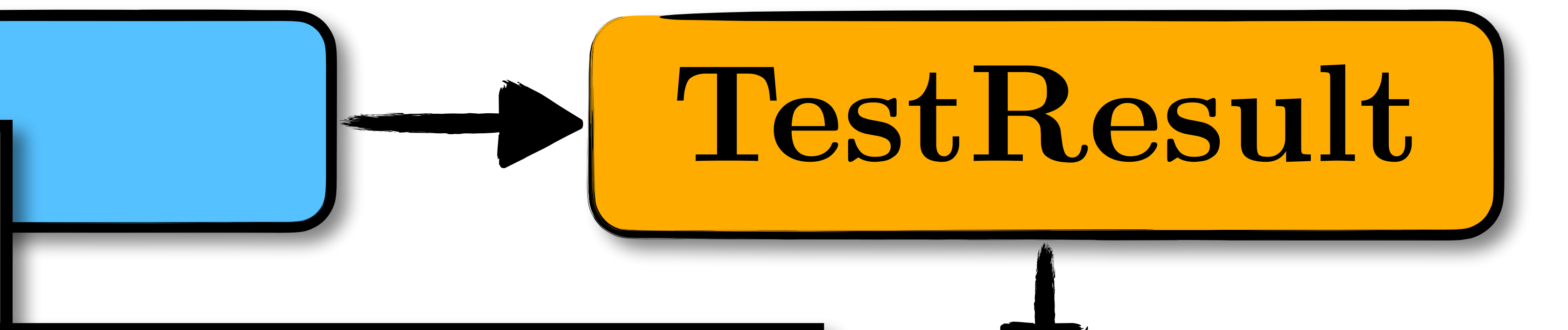
Matrix: Shamrock Test / shamr...
● 0/1 jobs completed
Show all jobs

Matrix: Shamrock Test / shamr...
● 0/1 jobs completed
Show all jobs

Testing library

Testing :

- Integrated
- Can outp
- Can run
- Can run

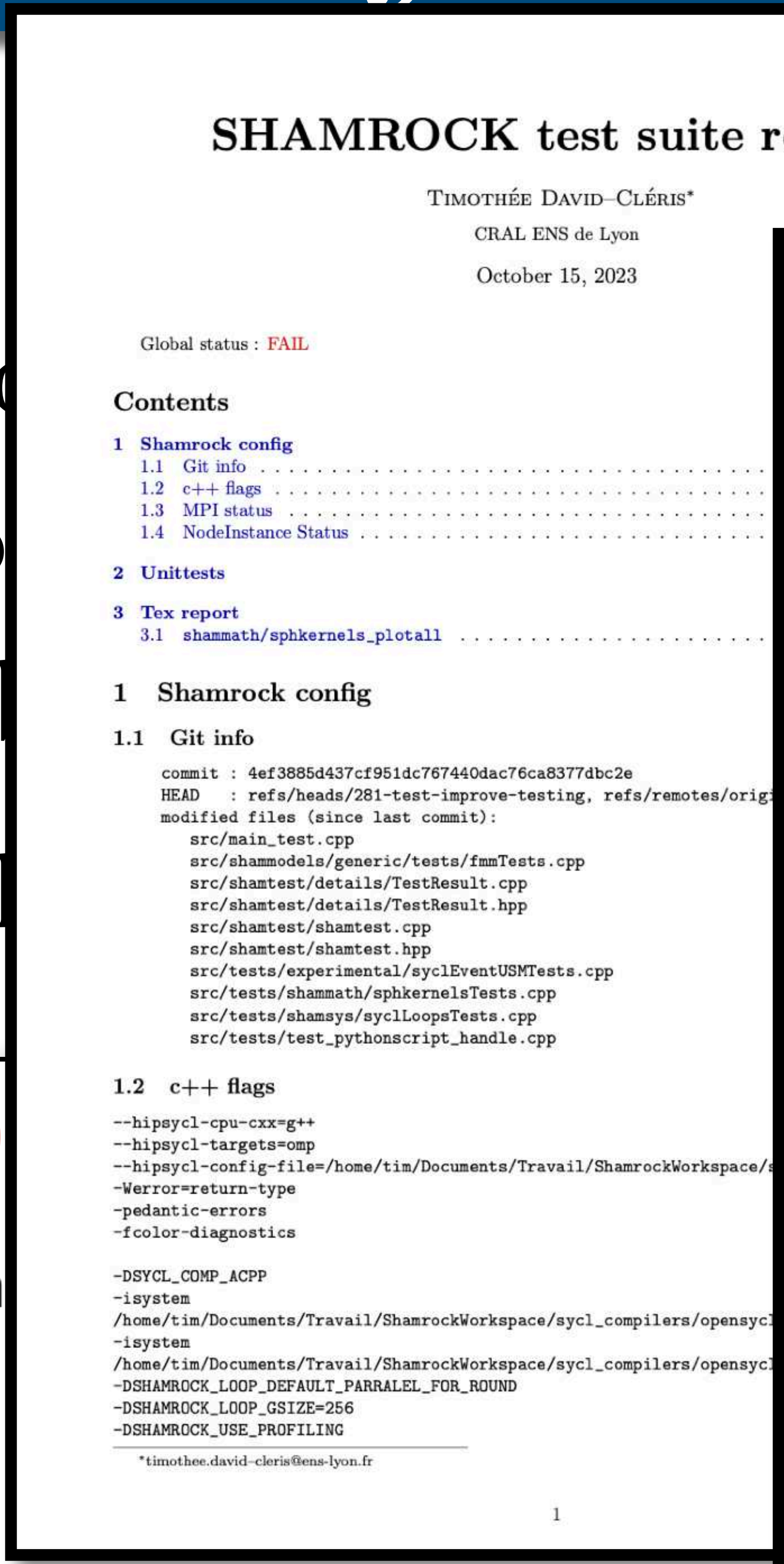

Test

TestResult

exReport

```
TestStart(Unittest, "coo

    using namespace sham

    auto & dataset = tes

    dataset.add_data("X", {0,1,2,3,4});
    dataset.add_data("Y", {0,1,2,3,4});

    asserts().assert_bool("why not", true);
}
```

```
) {

)

    )"
}
```



SHAMROCK test suite report

Timothée David–Cléris*

CRAL ENS de Lyon

October 15, 2023

Global status : FAIL

Contents

1 Shamrock config

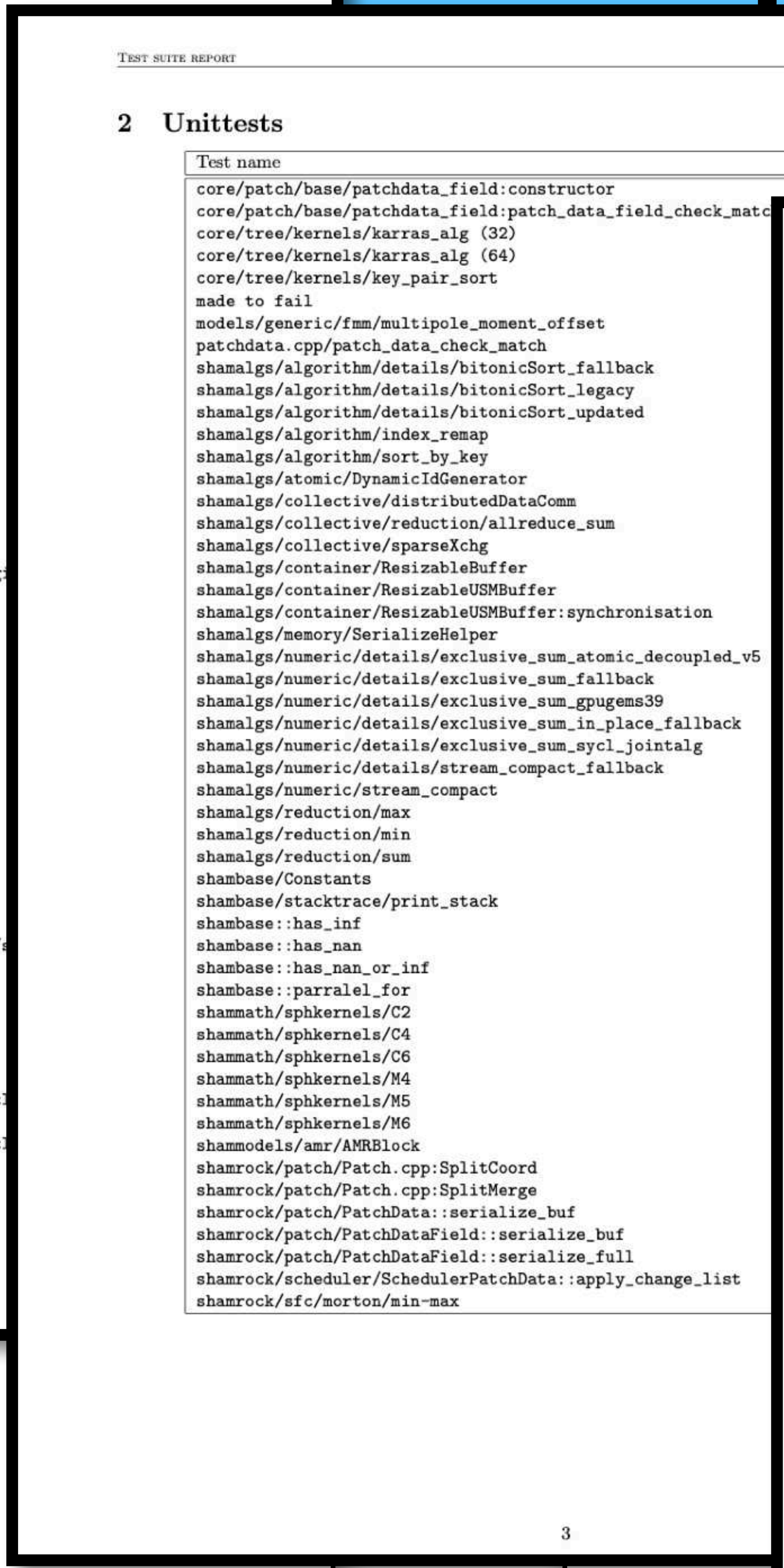
1.1 Git info

```
    commit : 4ef3885d437cf951dc767440dac76ca8377dbc2e
    HEAD   : refs/heads/281-test-improve-testing, refs/remotes/orig
    modified files (since last commit):
       src/main_test.cpp
       src/shammodels/generic/tests/fmmTests.cpp
       src/shamtest/details/TestResult.cpp
       src/shamtest/details/TestResult.hpp
       src/shamtest/shamtest.cpp
       src/shamtest/shamtest.hpp
       src/tests/experimental/syclEventUSMTests.cpp
       src/tests/shammath/sphkernelsTests.cpp
       src/tests/shamsys/syclLoopsTests.cpp
       src/tests/test_pythonscript_handle.cpp
```

1.2 c++ flags

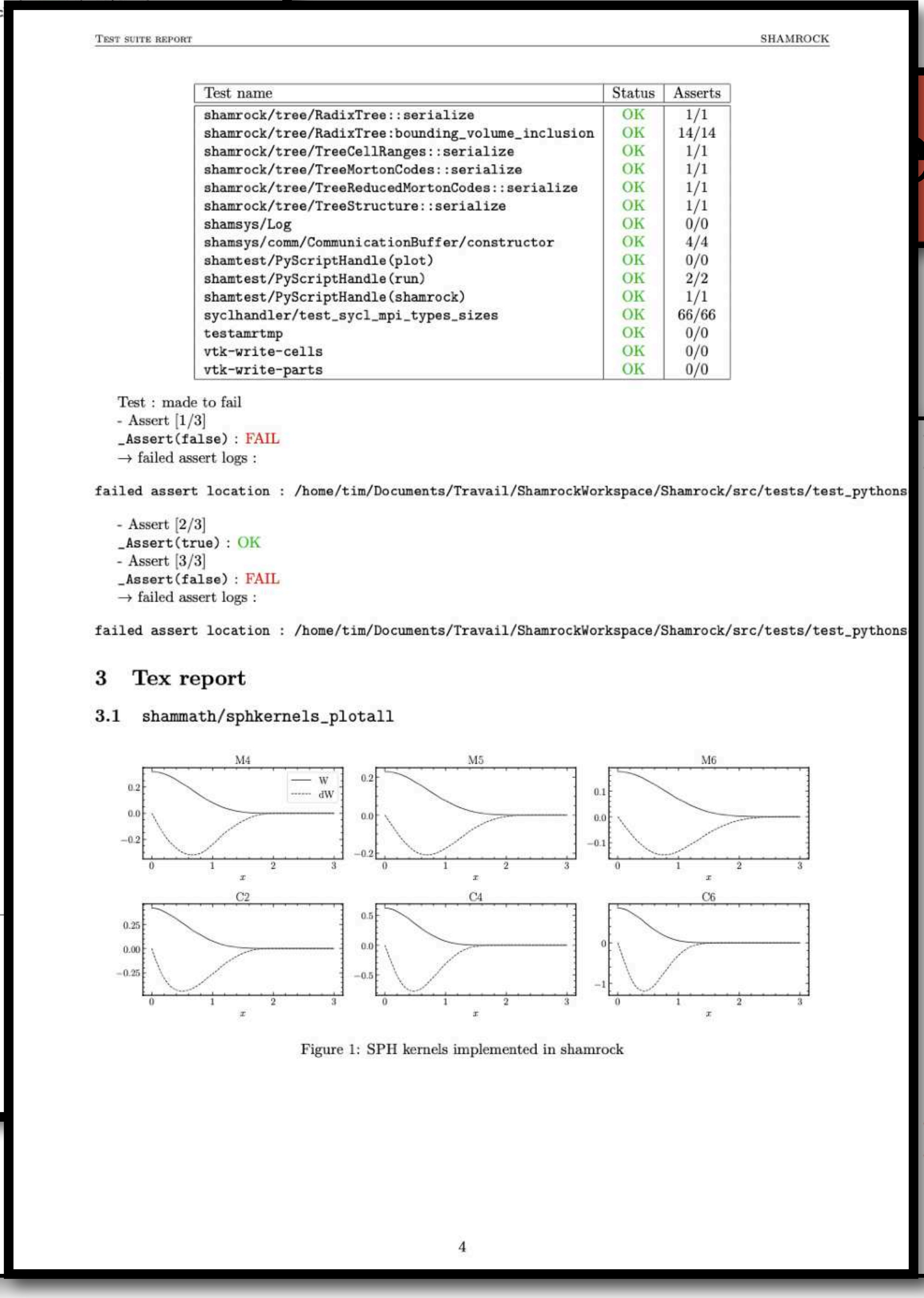
```
--hipsycl-cpu-cxx=g++
--hipsycl-targets=omp
--hipsycl-config-file=/home/tim/Documents/Travail/ShamrockWorkspace/s
-Werror=return-type
-pedantic-errors
-fcolor-diagnostics

-DSYCL_COMP_ACPP
-isystem
/home/tim/Documents/Travail/ShamrockWorkspace/sycl_compilers/opensycl
-isystem
/home/tim/Documents/Travail/ShamrockWorkspace/sycl_compilers/opensycl
-DSHAMROCK_LOOP_DEFAULT_PARRALEL_FOR_ROUND
-DSHAMROCK_LOOP_GSIZE=256
-DSHAMROCK_USE_PROFILING
```

[*] timothee.david-cleris@ens-lyon.fr



2 Unittests

Test name	Status	Asserts
core/patch/base/patchdata_field:constructor	OK	5/5
core/patch/base/patchdata_field:patch_data_field_check_matc		
core/tree/kernels/karras_alg (32)		
core/tree/kernels/karras_alg (64)		
core/tree/kernels/key_pair_sort		
made to fail		
models/generic/fmm/multipole_moment_offset		
patchdata.cpp/patch_data_check_match		
shamalgs/algorithm/details/bitonicSort_fallback		
shamalgs/algorithm/details/bitonicSort_legacy		
shamalgs/algorithm/details/bitonicSort_updated		
shamalgs/algorithm/index_remap		
shamalgs/algorithm/sort_by_key		
shamalgs/atomic/DynamicIdGenerator		
shamalgs/collective/distributedDataComm		
shamalgs/collective/reduction/allreduce_sum		
shamalgs/collective/sparseXchg		
shamalgs/container/ResizableBuffer		
shamalgs/container/ResizableUSMBuffer		
shamalgs/container/ResizableUSMBuffer:synchronisation		
shamalgs/memory/SerializeHelper		
shamalgs/numeric/details/exclusive_sum_atomic_decoupled_v5		
shamalgs/numeric/details/exclusive_sum_fallback		
shamalgs/numeric/details/exclusive_sum_gpugems39		
shamalgs/numeric/details/exclusive_sum_in_place_fallback		
shamalgs/numeric/details/exclusive_sum_sycl_jointalg		
shamalgs/numeric/details/stream_compact_fallback		
shamalgs/numeric/stream_compact		
shamalgs/reduction/max		
shamalgs/reduction/min		
shamalgs/reduction/sum		
shambase/Constants		
shambase/stacktrace/print_stack		
shambase::has_inf		
shambase::has_nan		
shambase::has_nan_or_inf		
shambase::parralel_for		
shammath/sphkernels/C2		
shammath/sphkernels/C4		
shammath/sphkernels/C6		
shammath/sphkernels/M4		
shammath/sphkernels/M5		
shammath/sphkernels/M6		
shammodels/amr/AMRBlock		
shamrock/patch/Patch.cpp:SplitCoord		
shamrock/patch/Patch.cpp:SplitMerge		
shamrock/patch/PatchData::serialize_buf		
shamrock/patch/PatchDataField::serialize_buf		
shamrock/patch/PatchDataField::serialize_full		
shamrock/scheduler/SchedulerPatchData::apply_change_list		
shamrock/sfc/morton/min-max		



Test name	Status	Asserts
shamrock/tree/RadixTree::serialize	OK	1/1
shamrock/tree/RadixTree:bounding_volume_inclusion	OK	14/14
shamrock/tree/TreeCellRanges::serialize	OK	1/1
shamrock/tree/TreeMortonCodes::serialize	OK	1/1
shamrock/tree/TreeReducedMortonCodes::serialize	OK	1/1
shamrock/tree/TreeStructure::serialize	OK	1/1
shamsys/Log	OK	0/0
shamsys/comm/CommunicationBuffer/constructor	OK	4/4
shamtest/PyScriptHandle(plot)	OK	0/0
shamtest/PyScriptHandle(run)	OK	2/2
shamtest/PyScriptHandle(shamrock)	OK	1/1
syclhandler/test_sycl_mpi_types_sizes	OK	66/66
testamrtmp	OK	0/0
vtk-write-cells	OK	0/0
vtk-write-parts	OK	0/0

Test : made to fail
- Assert [1/3]
_Assert(false) : FAIL
→ failed assert logs :

```
failed assert location : /home/tim/Documents/Travail/ShamrockWorkspace/Shamrock/src/tests/test_pythons
```

- Assert [2/3]
_Assert(true) : OK
- Assert [3/3]
_Assert(false) : FAIL
→ failed assert logs :

```
failed assert location : /home/tim/Documents/Travail/ShamrockWorkspace/Shamrock/src/tests/test_pythons
```

3 Tex report

3.1 shammath/sphkernels_plotall

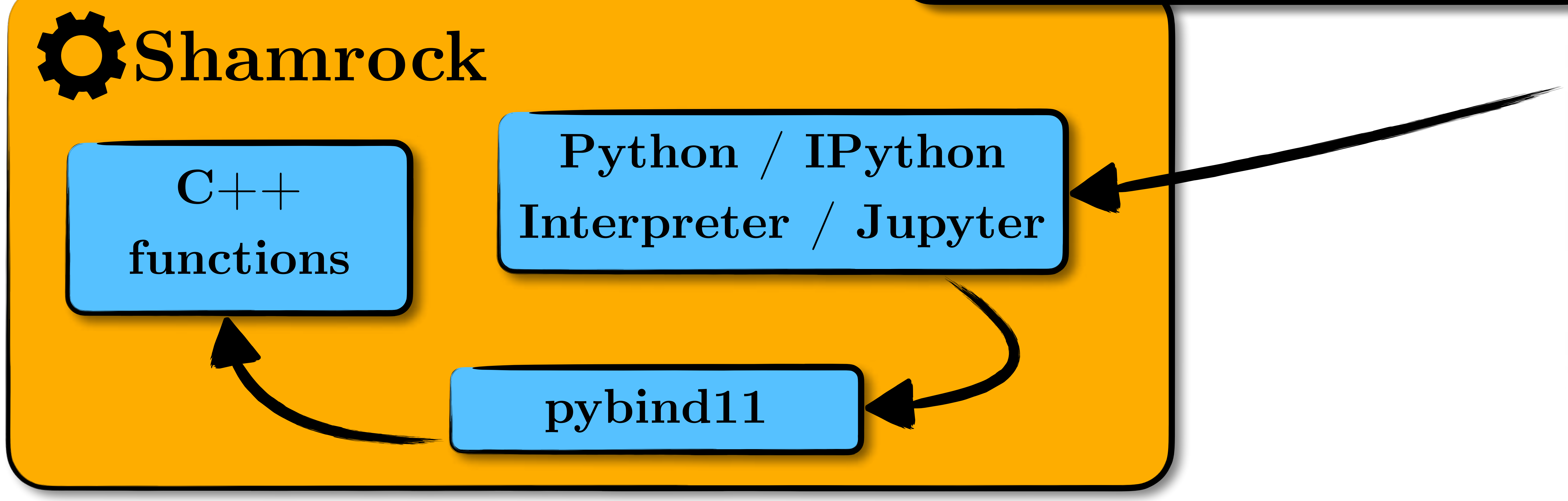
Figure 1: SPH kernels implemented in shamrock

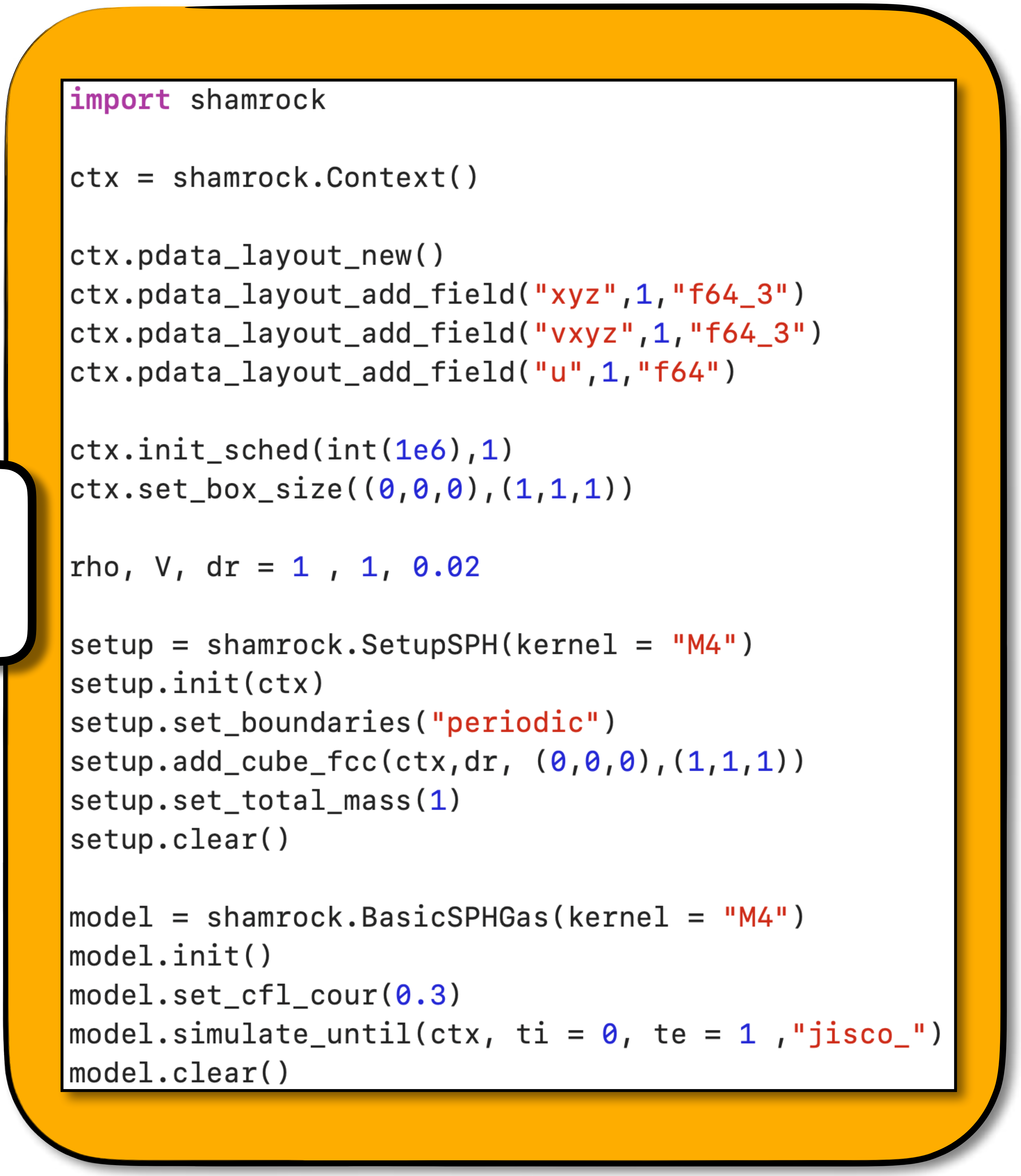
Python interop

Runscripts :

- Flexible for simulation inputs
- No C++ for the user
- Compatible with restarts
- One job multiple simulation
- Can be run interactively (IPytho

Quick exemple ...





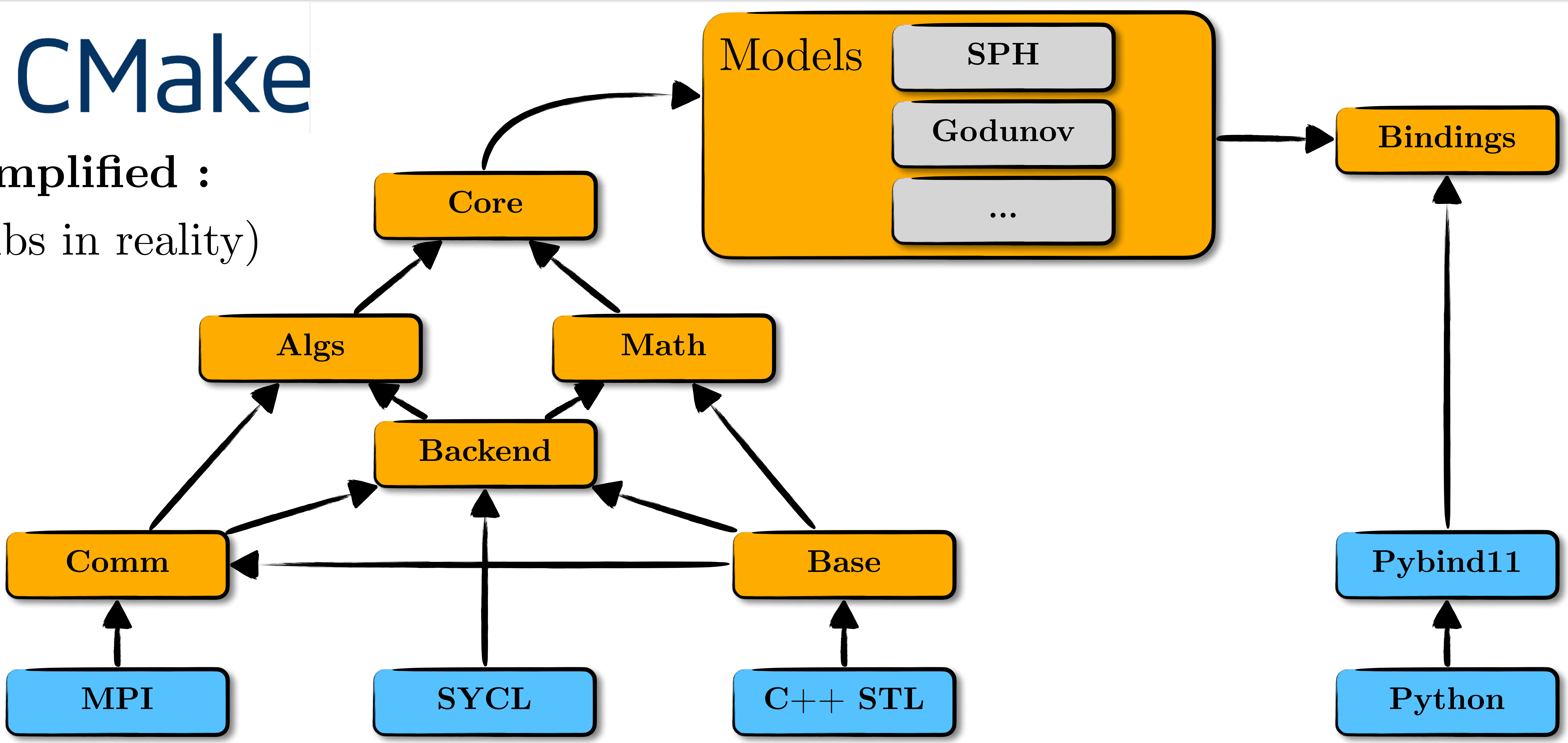
```
import shamrock

ctx = shamrock.Context()

ctx.pdata_layout_new()
ctx.pdata_layout_add_field("xyz",1,"f64_3")
ctx.pdata_layout_add_field("vxyz",1,"f64_3")
ctx.pdata_layout_add_field("u",1,"f64")

ctx.init_sched(int(1e6),1)
ctx.set_box_size((0,0,0),(1,1,1))

rho, V, dr = 1 , 1, 0.02

setup = shamrock.SetupSPH(kernel = "M4")
setup.init(ctx)
setup.set_boundaries("periodic")
setup.add_cube_fcc(ctx,dr, (0,0,0),(1,1,1))
setup.set_total_mass(1)
setup.clear()

model = shamrock.BasicSPHGas(kernel = "M4")
model.init()
model.set_cfl_cour(0.3)
model.simulate_until(ctx, ti = 0, te = 1 ,"jisco_")
model.clear()
```

Organisation

CMake

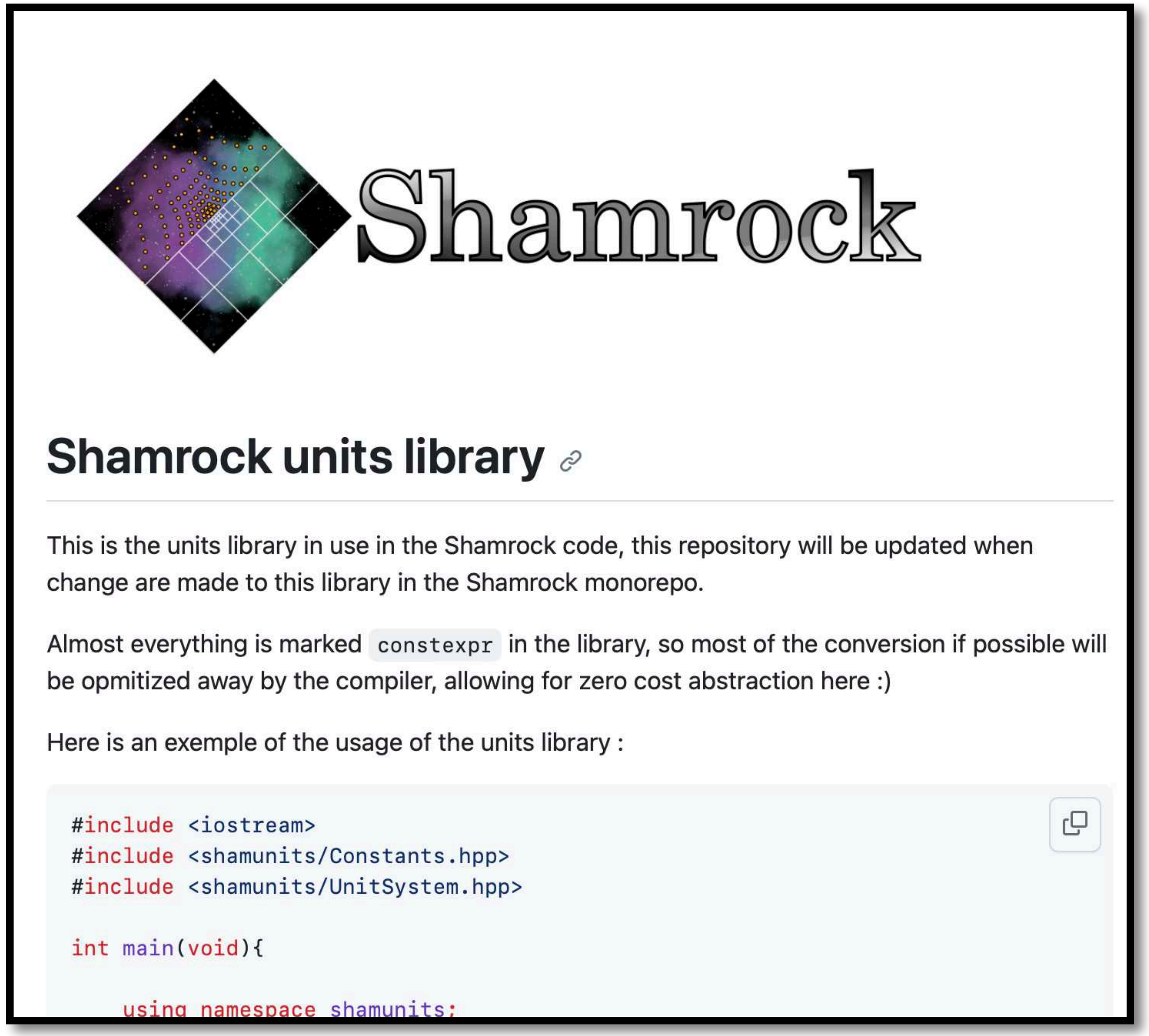
Simplified :

(12 libs in reality)



Units library (Public)

https://github.com/Shamrock-code/Shamrock-units



Shamrock units library

This is the units library in use in the Shamrock code, this repository will be updated when change are made to this library in the Shamrock monorepo.

Almost everything is marked `constexpr` in the library, so most of the conversion if possible will be opmitized away by the compiler, allowing for zero cost abstraction here :)

Here is an exemple of the usage of the units library :

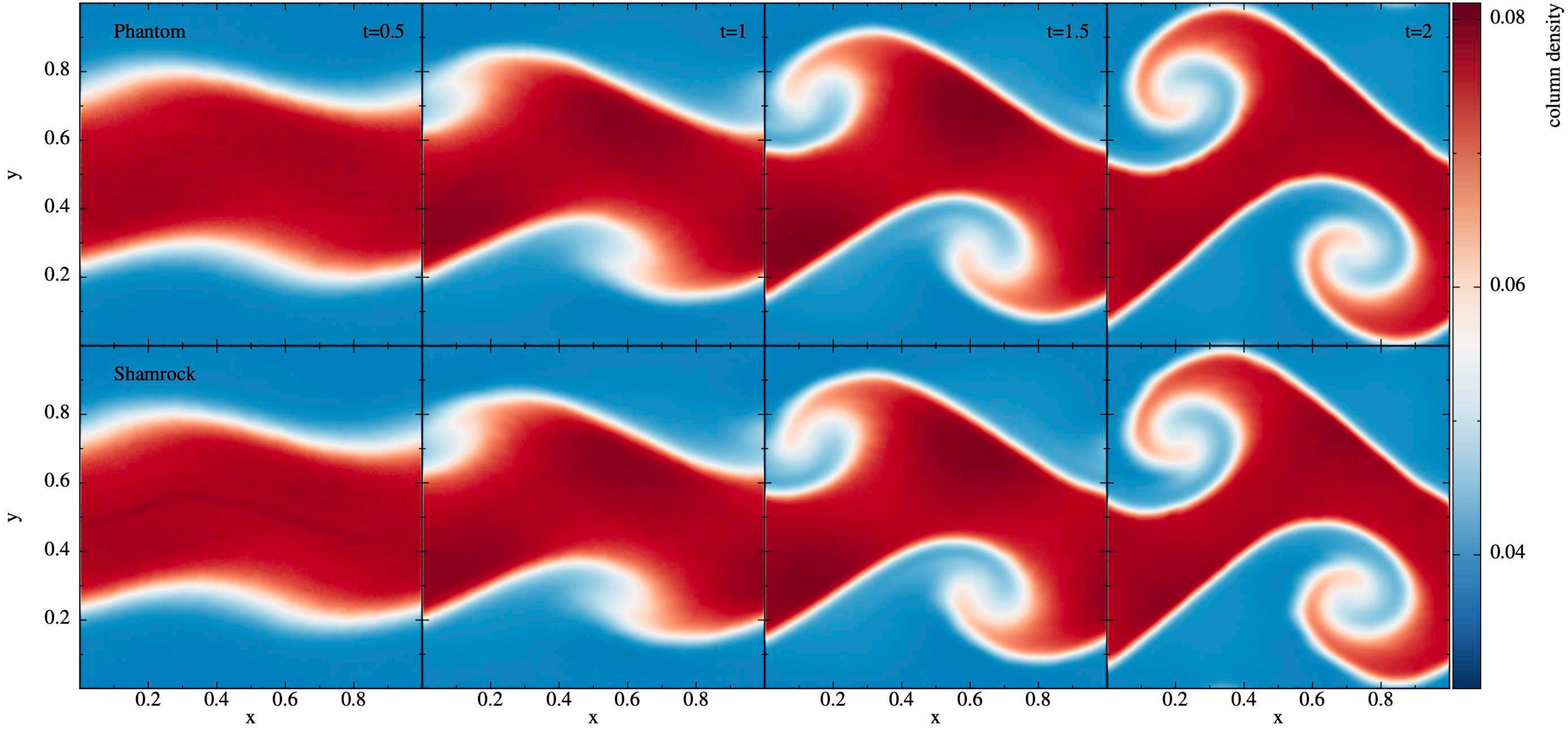
```
#include <iostream>
#include <shamunits/Constants.hpp>
#include <shamunits/UnitSystem.hpp>

int main(void){

    using namespace shamunits;
```

- Constexpr
- Simple
- Header only
- Can be used in GPU kernels
- Python bindings

Try it : https://godbolt.org/z/5zjGMea57

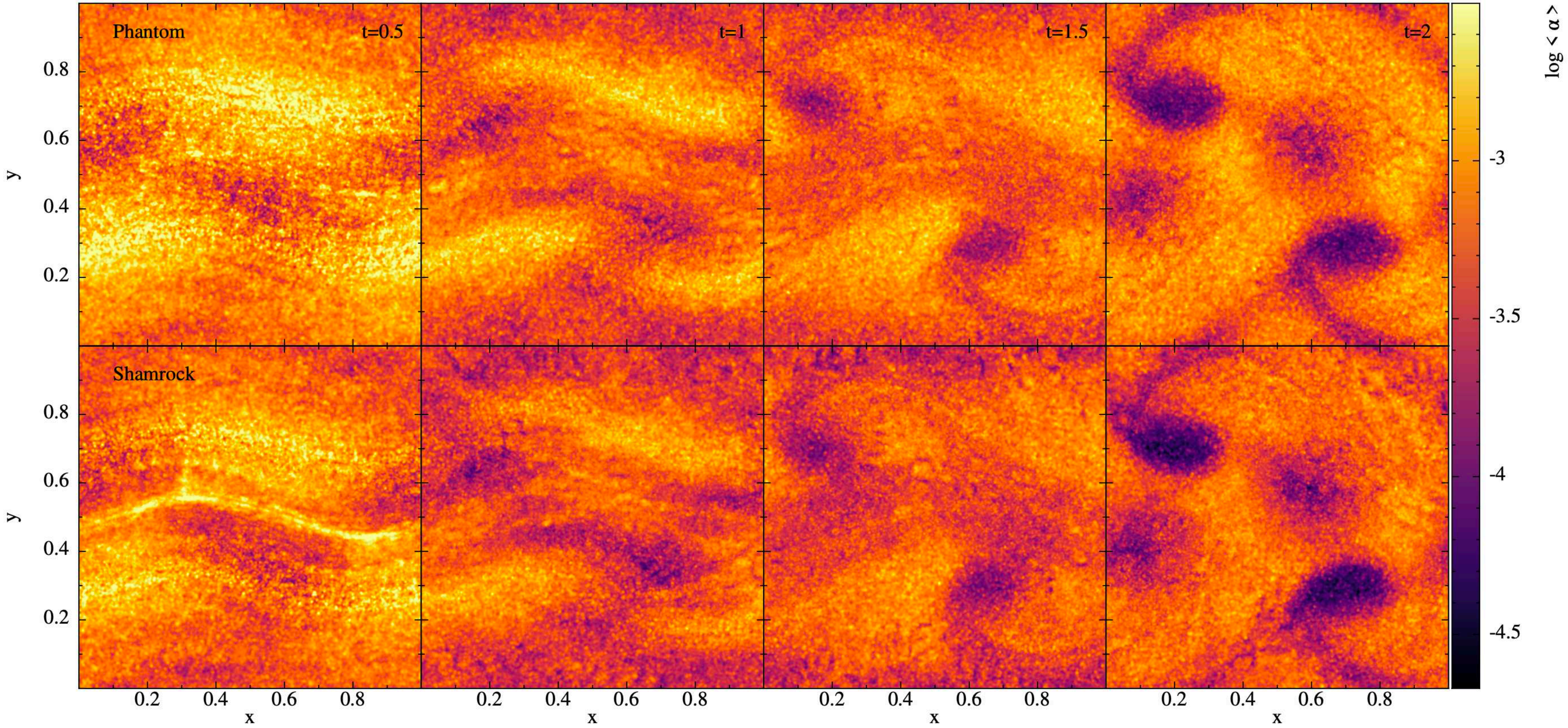
Results

Kelvin Helmotz



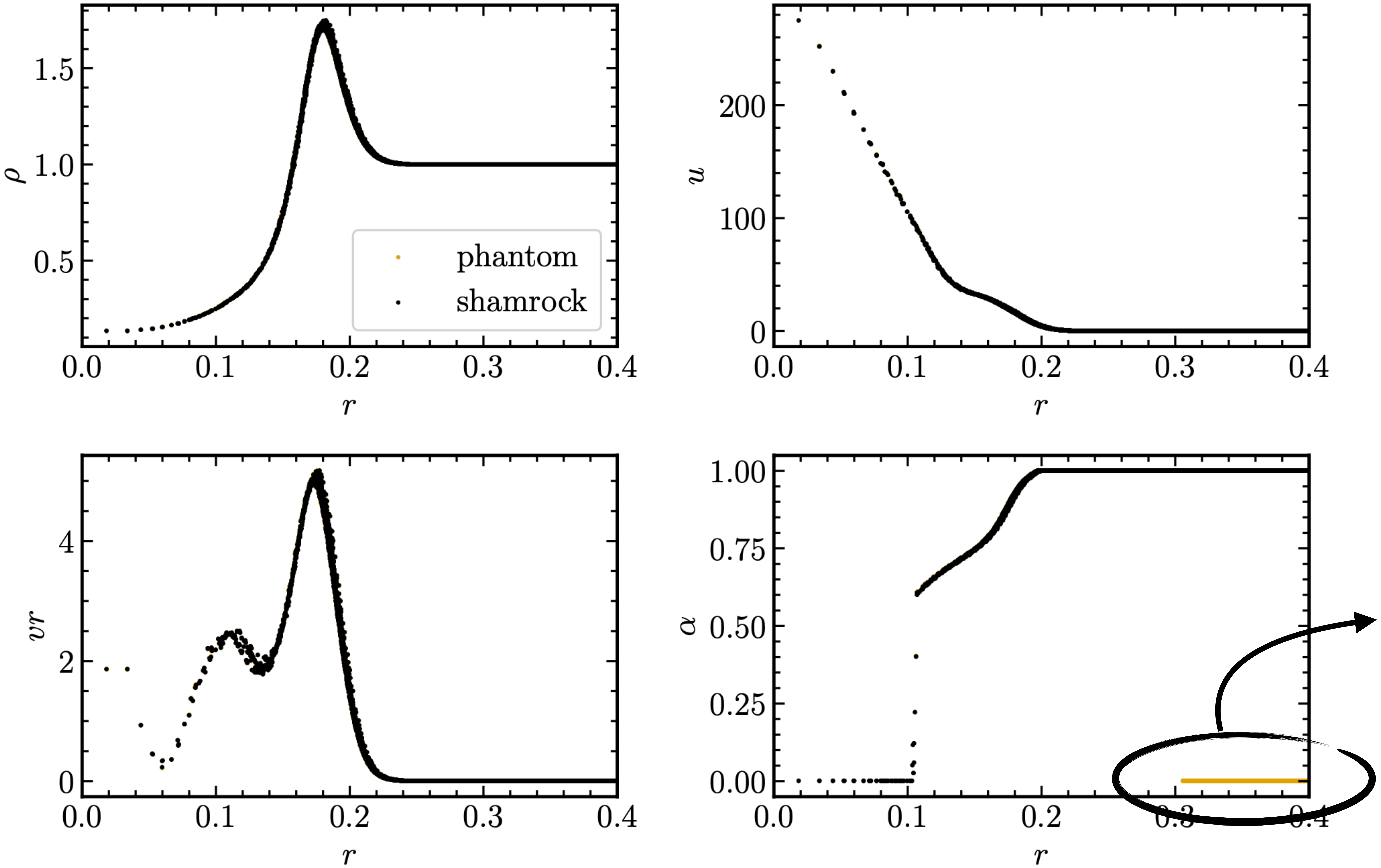
Looks similar : is the viscosity the same ?

Kelvin Helmotz



Yes ! (Differences due to difference in optimisation) **Is the solver the same ?**

Sedov-Taylor Blast



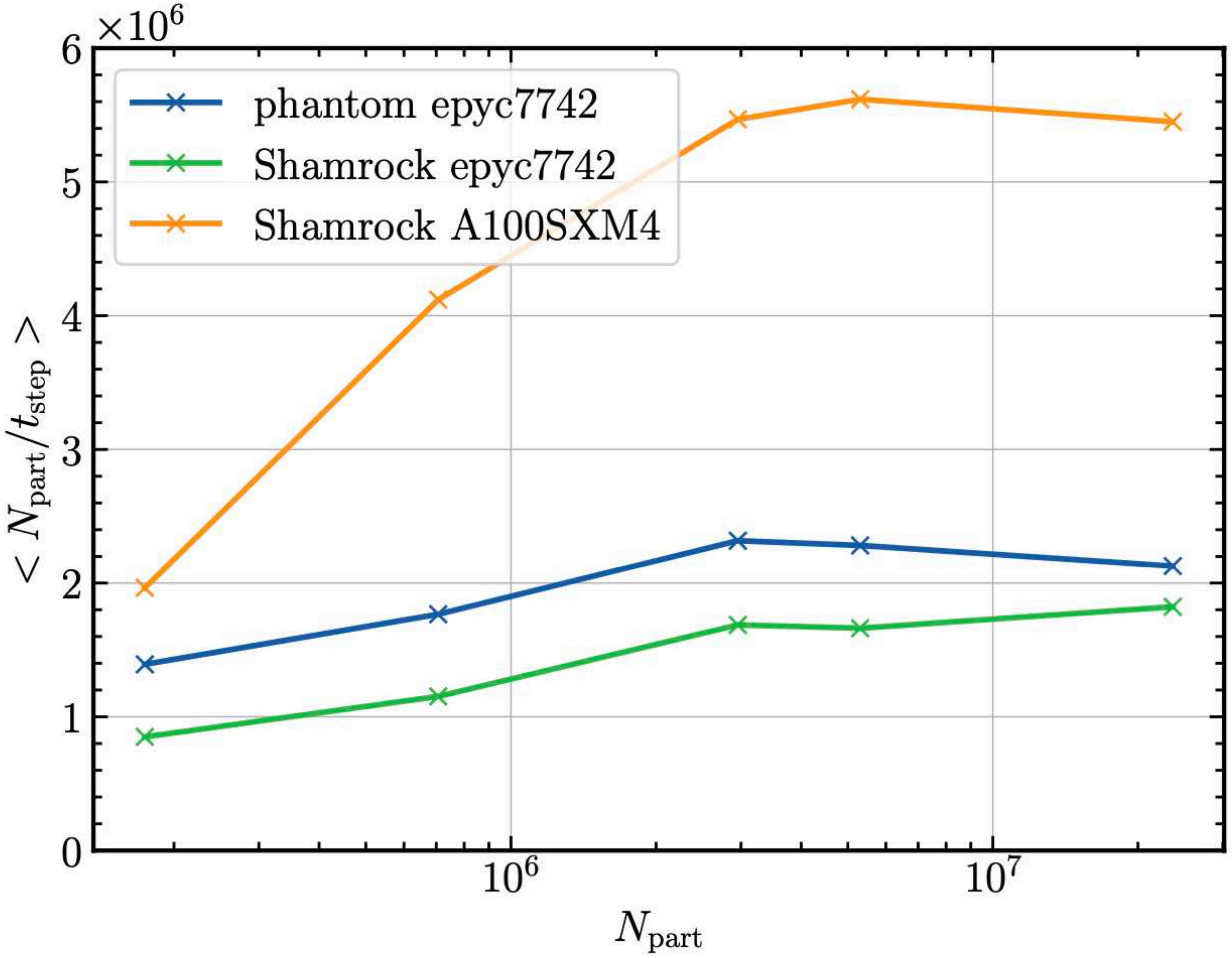
Rounding off when $c_s = 0$

Marginal differences :

- L2 distance r : 1.323e-05
- L2 distance h : 7.687e-06
- L2 distance vr : 0.0133
- L2 distance u : 0.03803

Yes !

Performance

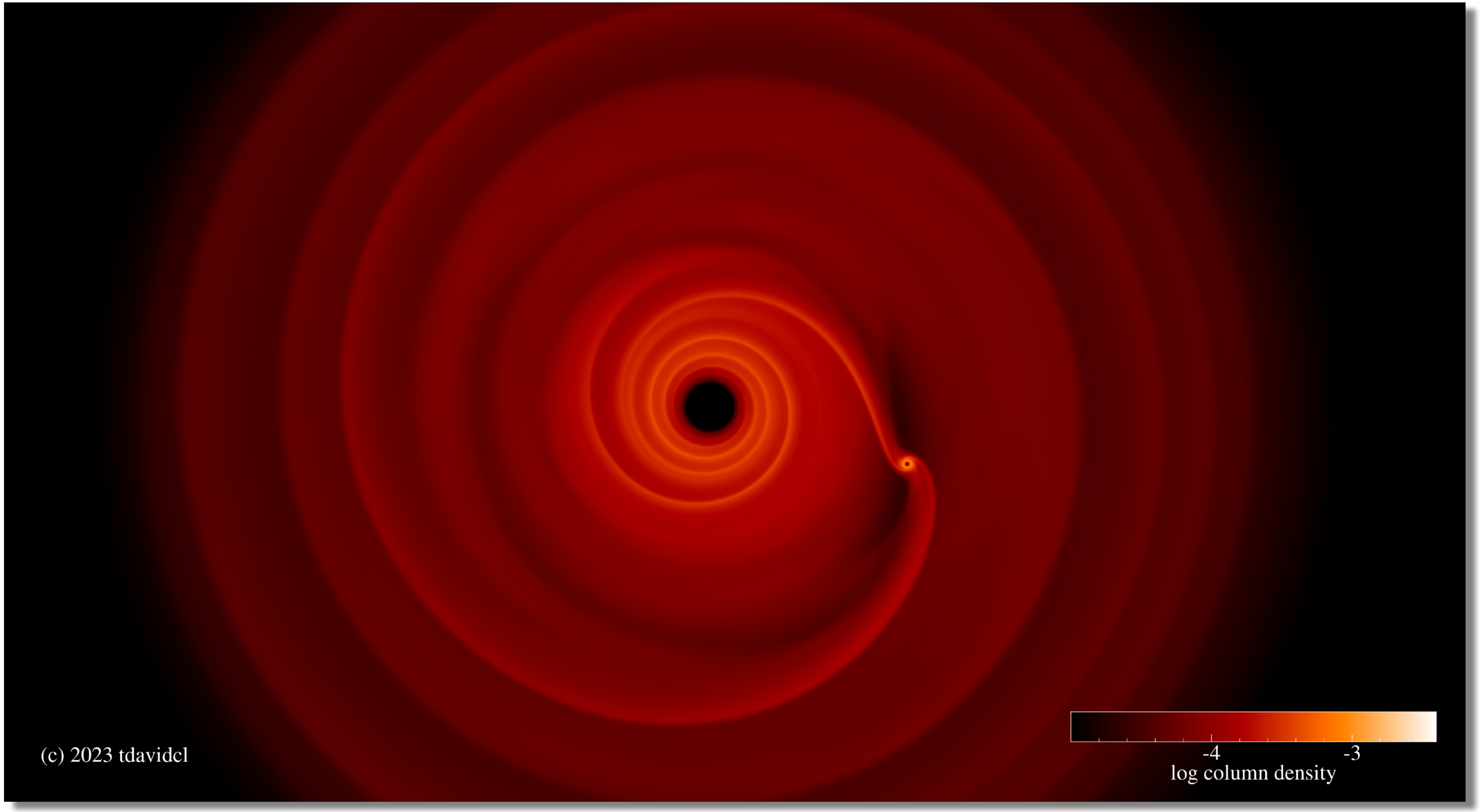


Sedov taylor blast :

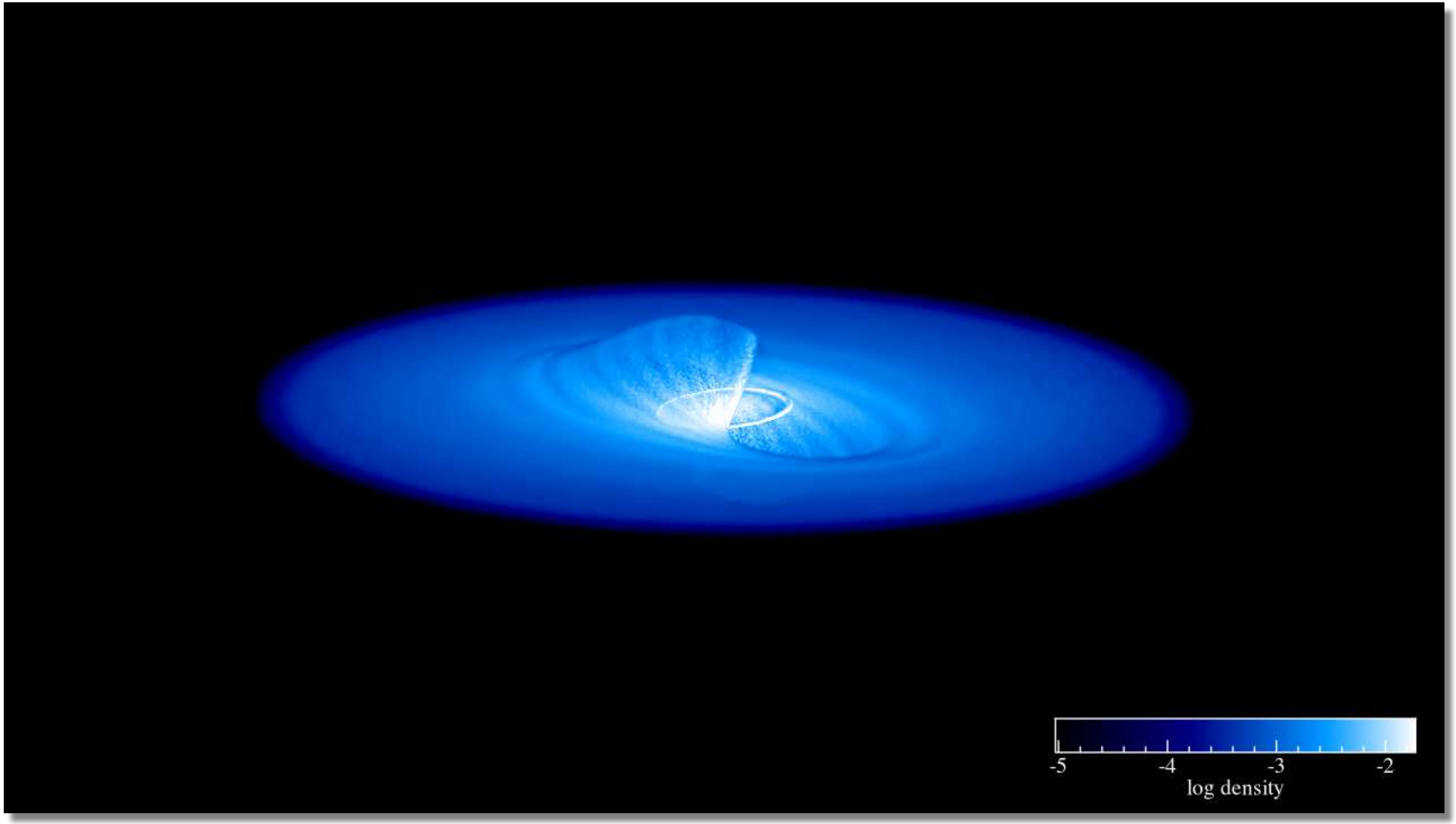
- Sightly slower on CPU
- Way faster with GPU

Discs

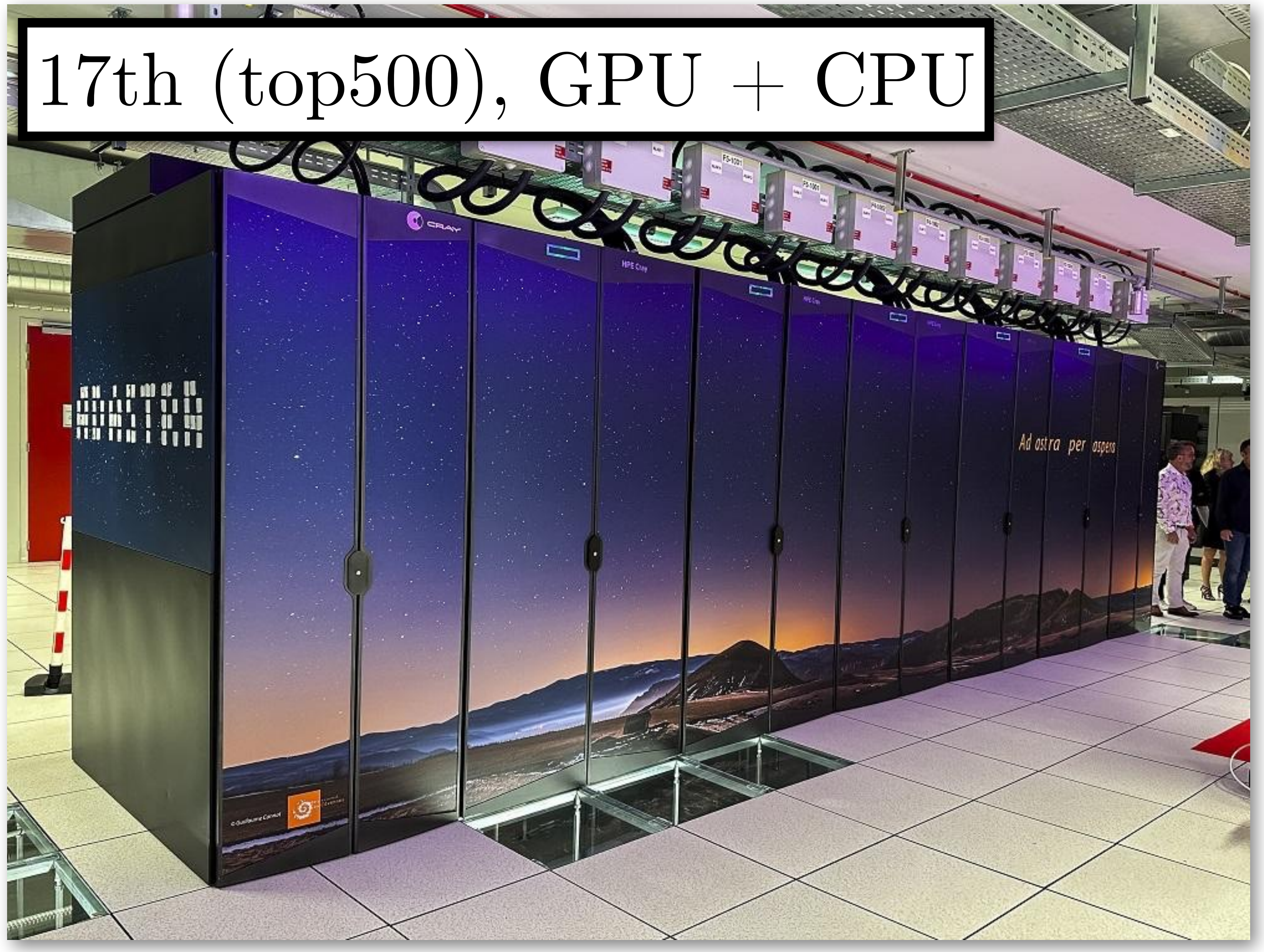
Same performance in discs !



Discs (also black holes ones)



Now if you take a big cluster

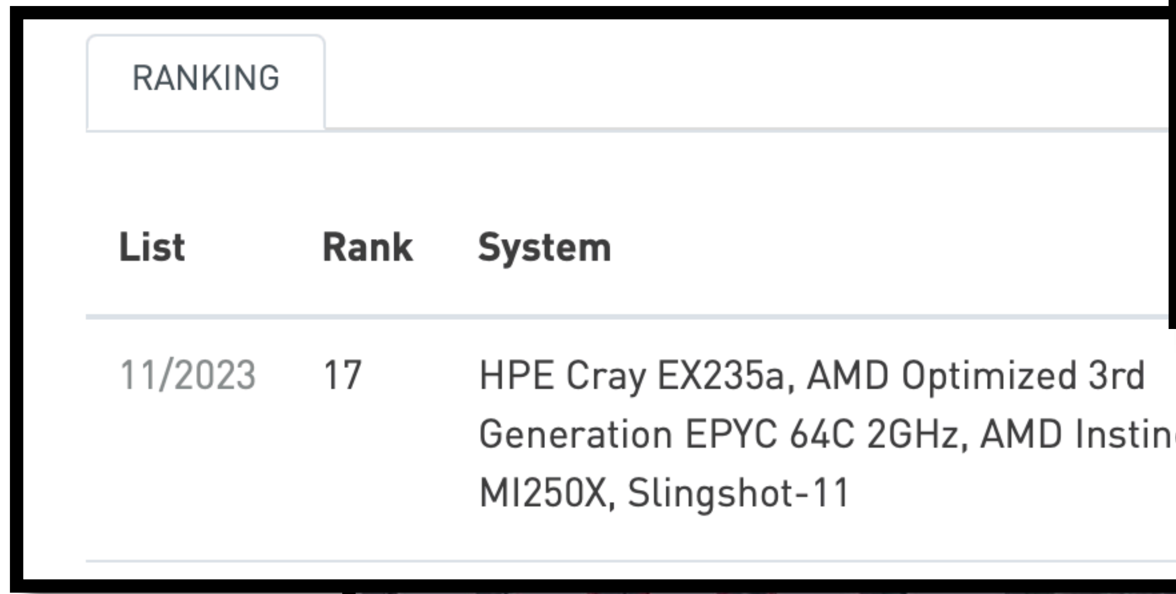


17th (top500), GPU + CPU

338 nodes, 4 MI250x / Nodes

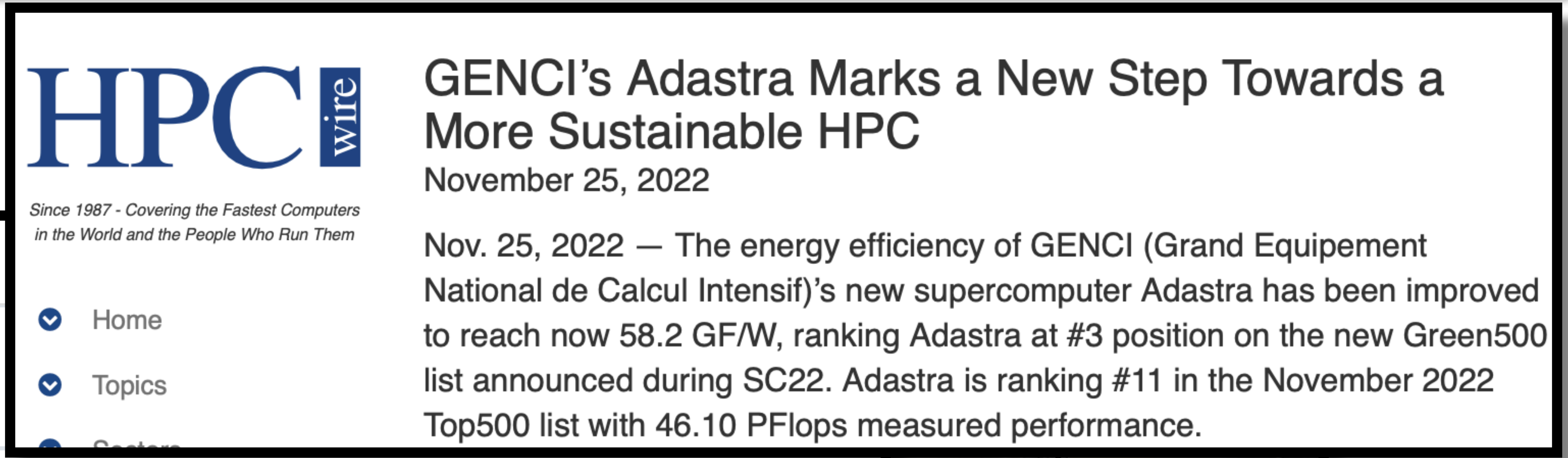
921kW (max)

61.6 PFlop/s



RANKING

List	Rank	System					
11/2023	17	HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11	HPE	319,072	46.10	61.61	921.48



HPC wire
Since 1987 - Covering the Fastest Computers in the World and the People Who Run Them
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Topics

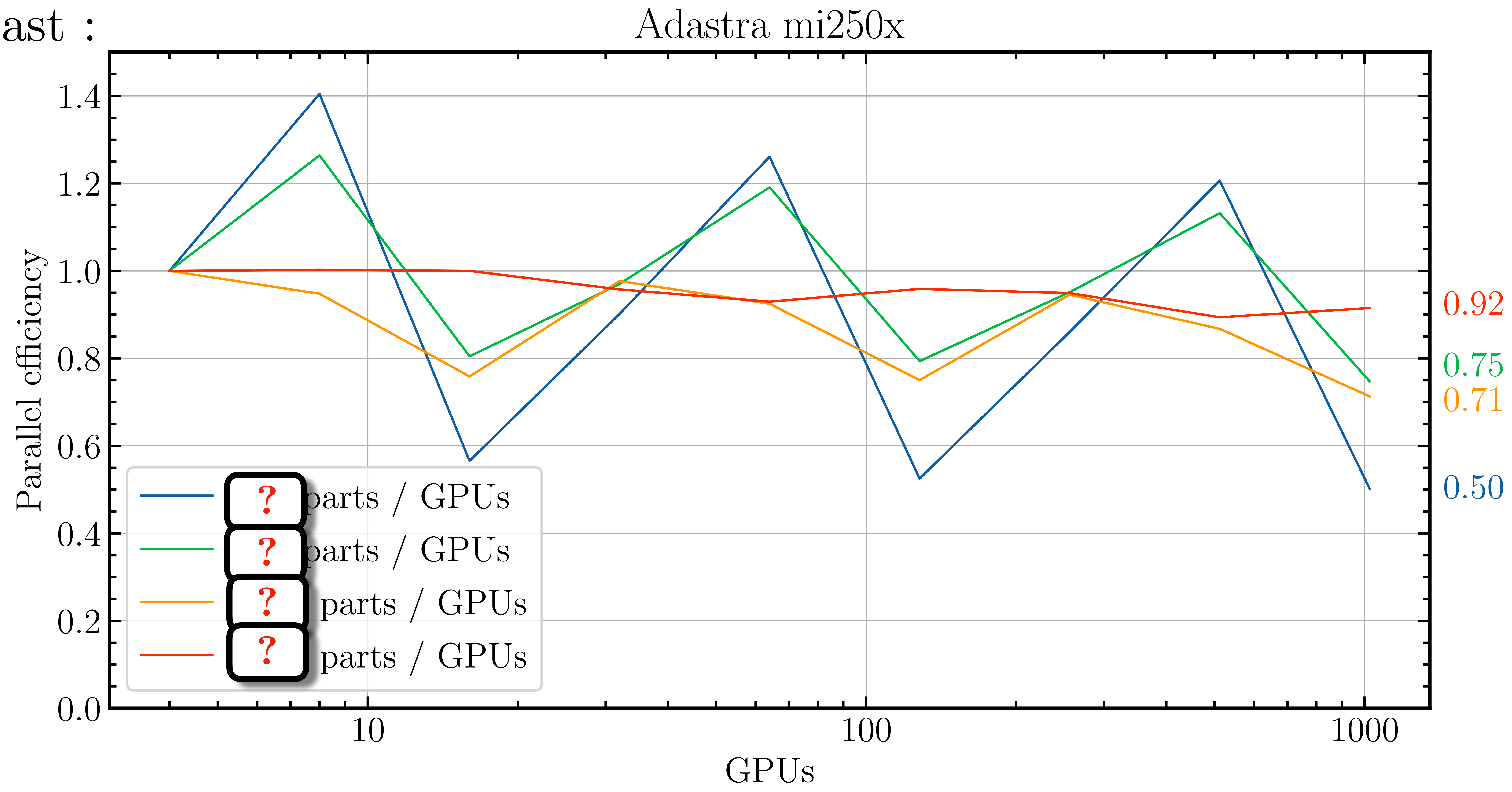
GENCI's Adastra Marks a New Step Towards a More Sustainable HPC

November 25, 2022

Nov. 25, 2022 — The energy efficiency of GENCI (Grand Equipement National de Calcul Intensif)'s new supercomputer Adastra has been improved to reach now 58.2 GF/W, ranking Adastra at #3 position on the new Green500 list announced during SC22. Adastra is ranking #11 in the November 2022 Top500 list with 46.10 PFlops measured performance.

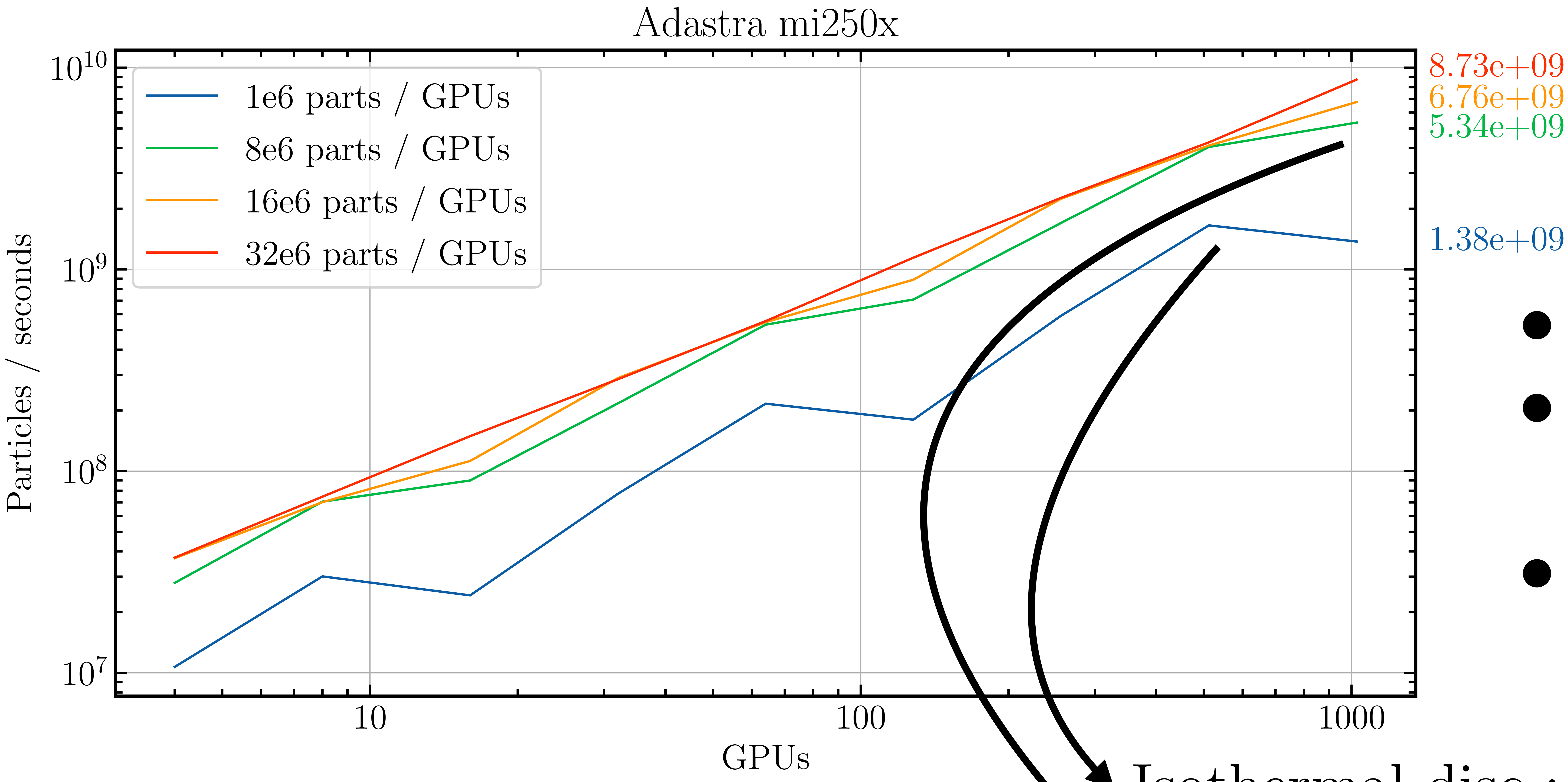
It scales !!! (Weak calling)

Sedov Blast :



0.92 efficiency !!!

Now if you take a big cluster



- 9G part / seconds
- 65.000.000.000 particles (4000^3)
- 7 sec / iterations

Global time steps :

(Estimate 10k steps at 1M part)

Isothermal disc : 1G part = 1 orbit/16h

Isothermal disc : 16G part = 1 orbit/4day

But it is also efficient

Adastra MI250 :

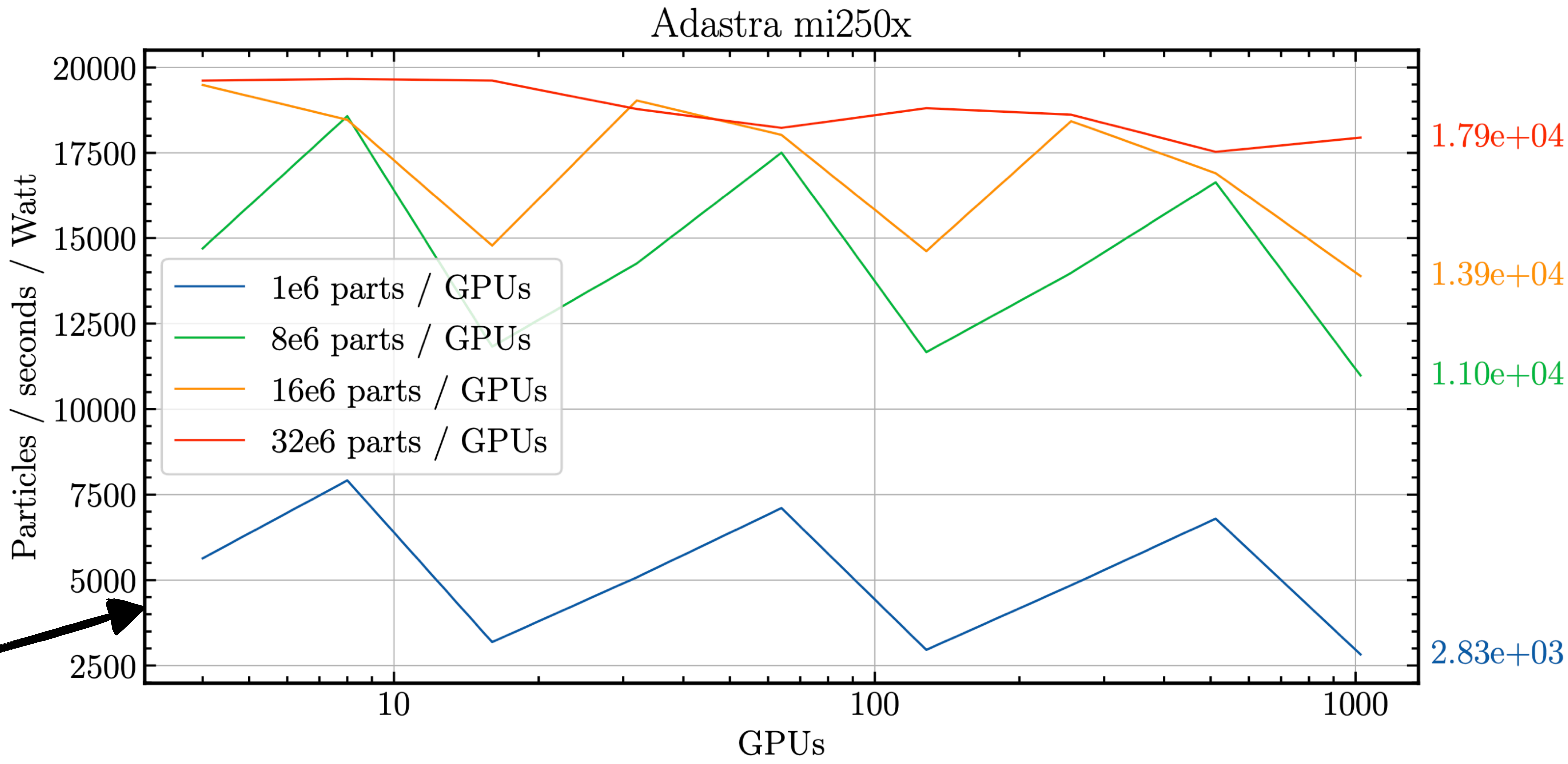
- 350W / GPU
- 90W CPU
- 80W Memory
- 1900W / Node (70% max power)

256 nodes tests : 486kW

(2/3 Adastra mi250)

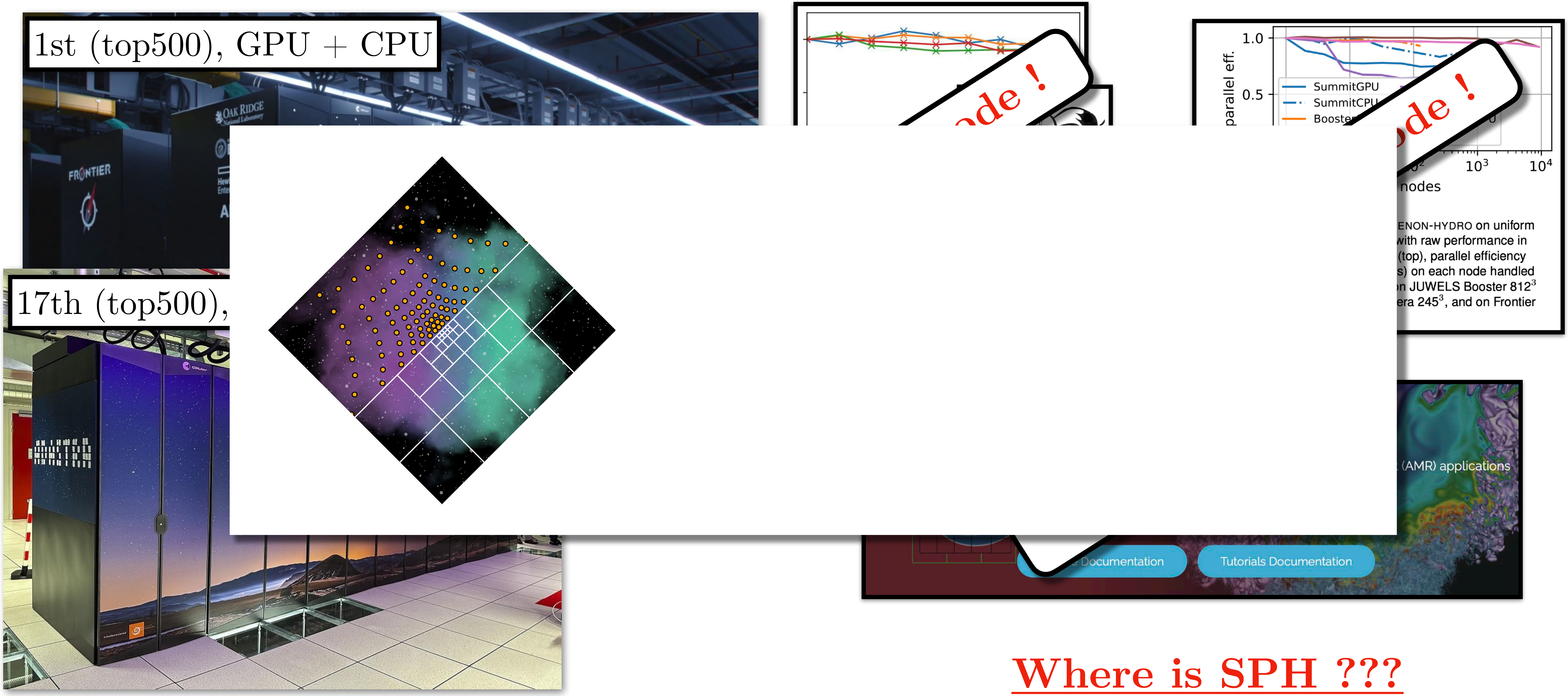
Epyc 7742 (Rome) Rack

4700 part/s/W



Large simulations required !

Context & Aims



Where is SPH ???

HPE Cray
HPE Cray
Ad astra per a

Thanks !