Dyablo

A new hardware-agnostic AMR code for Exascale using Kokkos

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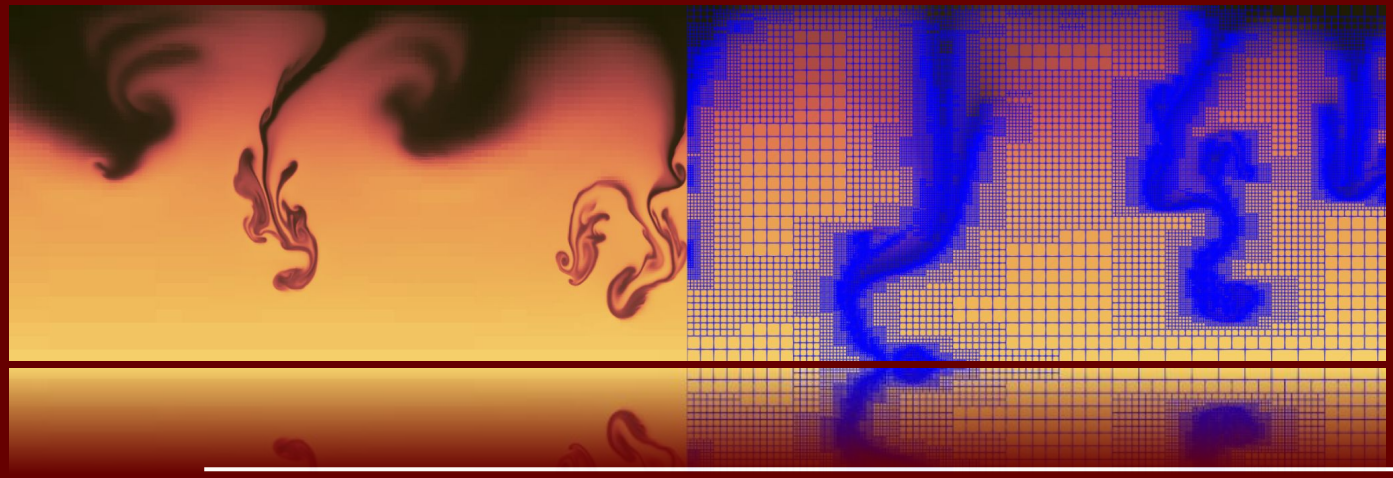
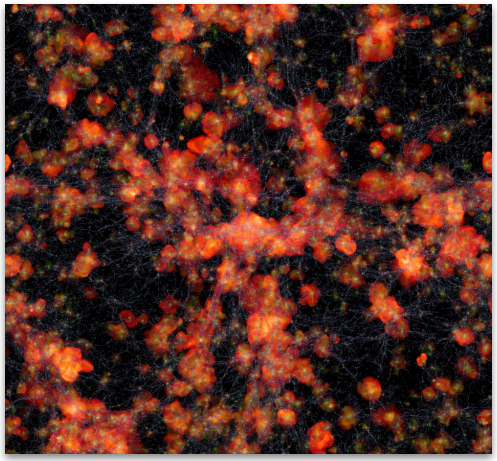
Workshop GPUs Numpex - 13/06/2024

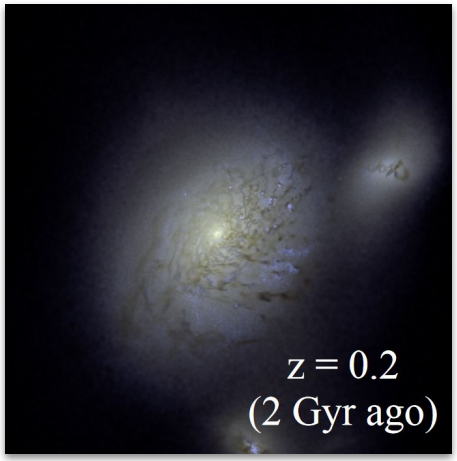


HPC needs for Astrophysics

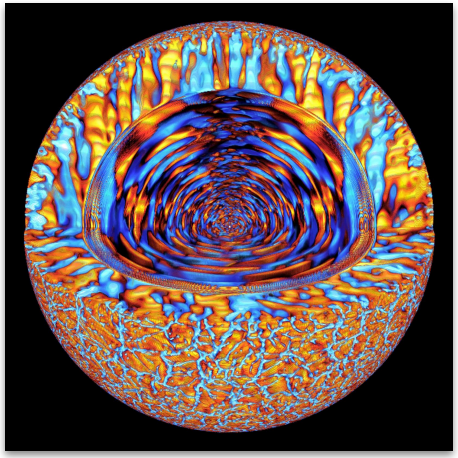
Simulate physical phenomena at every scale



Cosmology
Extreme Horizon
(RAMSES)



Galaxies
(RAMSES)



Solar/Stellar
(ASH)

An ever-growing need for computing power to better understand the universe

Towards Exascale

A diversity of new supercomputer architectures

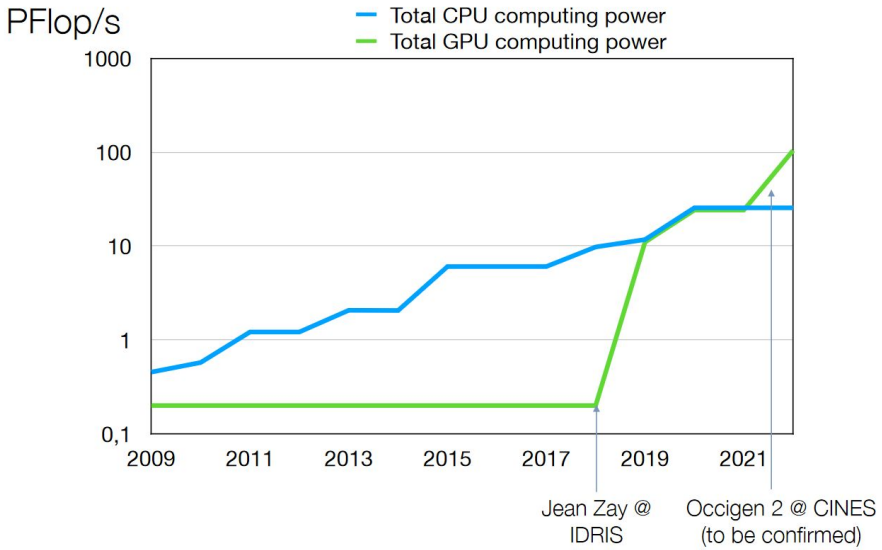
Older CPU architectures
x86, Intel, AMD, …
- Low energy efficiency, Low power density

➡ Need a lot of compute nodes

Newer GPU architectures (Exascale)
FR : *Jean-Zay*, *Irene* (Nvidia), *Ad-Astra* (AMD)
EU: *LUMI* (Finland, AMD), *Leonardo* (Italy, Nvidia)
US : *Frontier* (AMD), *Summit*, *Sierra* (Nvidia)
- Better energy efficiency, More power per node
- Massively parallel shared memory architectures

➡ ***More efficient but harder to code***

And other new vector architectures : ARM (A64FX, EPI), RISC-V, …



Computing power in French national centers (GENCI 2021)

New architecture for Exascale are harder to program and need new software stacks

Dyablo

Replacing the software stack for Exascale

Older applications and Exascale

Ex : RAMSES - Failed to port to GPU *(contrat de progres - Idris - 2019)*

- Older languages (Fortran) and prog. models
- No shared-memory parallelism (MPI only)
- Sequential algorithms

➡ **Need new software stack and algorithms**

Dyablo's software stack

- Written in *C++*, uses external libraries *(HDF5, PABLO, ...)*
- *Kokkos + MPI* parallelism
- New parallel algorithms

➡ **Supports Exascale Hardware**

Dyablo

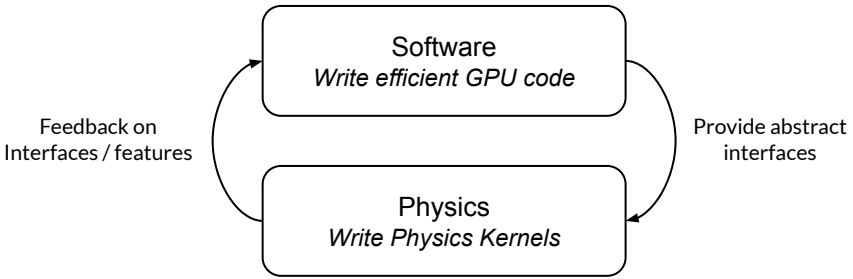
Leverage current software development methods

Development of older simulation codes

- One-man codes : physicists also optimize code
- Code from scratch : not leveraging libraries
- Physical model are becoming more complicated
- Code is harder to optimize (new architectures)

➡ **Need “separation of concerns”**

Code is written by code experts and physics kernels are written by physicists



Dyablo’s development organization

- *Modular* : plugins for kernels, IOs, …
- Uses *abstract interfaces* to separate optimization details from physics kernels

Encourage collaboration :

- *Software development / support* *(CEA DEDIP)*
  - Write abstract interfaces perform operations on the AMR mesh
  - Optimize behind the scene algorithms
- *Physics labs :* (ex: CEA DAp Whole-Sun, …)
  - Write physics kernels using this interface
  - Create applications based on dyablo
  - Provide feedback for the software dev. team

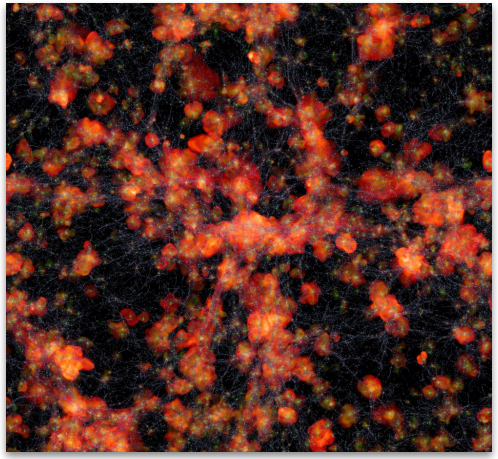
Features in Dyablo

Address simulation needs for the astrophysical community

Multi-physics simulations
- Hydrodynamics / MHD
- Self-Gravity
- Particles
- …

Adaptive Mesh Refinement (AMR)
- Wide range of time/space scales in same simulation

Massively parallel simulations :
- Shared-memory parallelism with *Kokkos* (CPU, GPU, …)
- Distributed parallelism with MPI



Extreme Horizon (RAMSES)

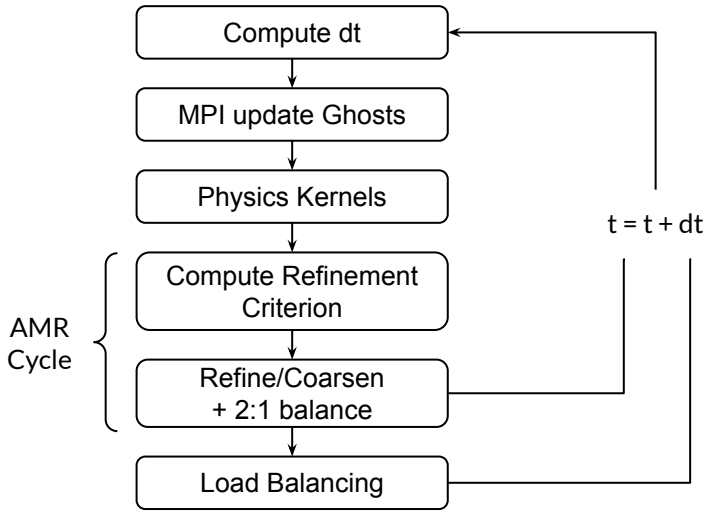
Features in Dyablo will evolve with the specific needs of the involved laboratories
- *RAMSES Community (DAp, …)* Same needs as RAMSES, but at Exascale : dark matter self-gravity, star or galaxy formation, …
- Whole Sun (DAp) - Solar simulation : Convection, radiative transfer, spherical geometry, …

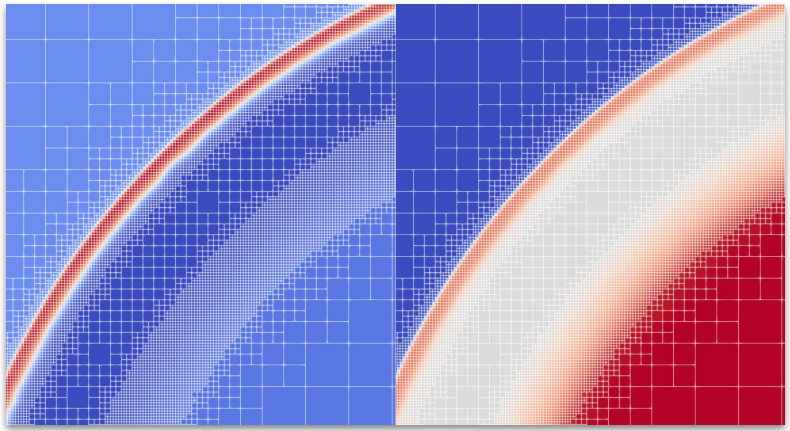
AMR in Dyablo

Adaptive Mesh Refinement (as in RAMSES)

- More resolution in regions of interest
- Octree-based AMR mesh *(cartesian AMR)*
- *Dynamic mesh* changing at every timestep

➡ *AMR cycle may be costly, access patterns are random*





Refined mesh for a Sedov Blast in Dyablo

AMR on GPU in Dyablo

GPU Data Structures for the AMR Octree

AMR mesh :

- How to store physical fields?

Octree associated with mesh :

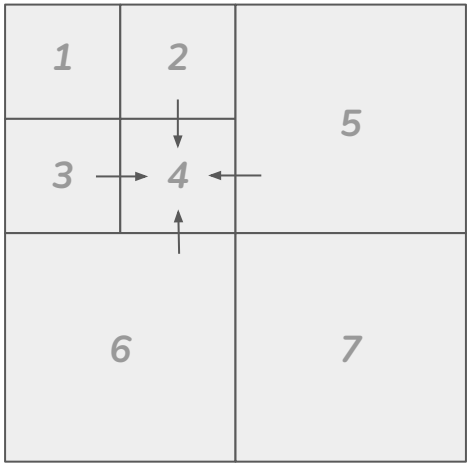
- How to iterate on cells?
- How to get neighbors?

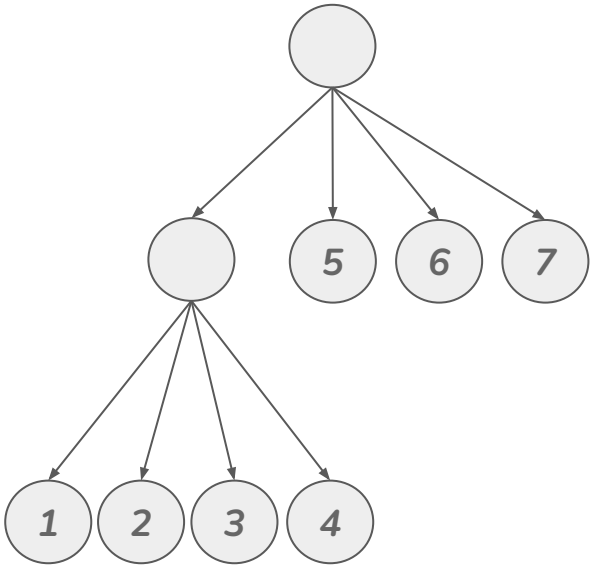
Finite Volume Scheme

For each cell :

1. Compute Gradients/Reconstruction
2. Flux computation *(Riemann solver)*
3. Update Cell

=> Need neighborhood (*stencil*)





AMR on GPU in Dyablo

GPU Data Structures for the AMR Octree

Storing and updating the AMR Octree

- Chained structures not efficient on GPU
- Neighbors must be close in memory

➡ Fields are stored in arrays (`Kokkos::View`)

➡ Cells are stored in Morton Order (Z-curve)

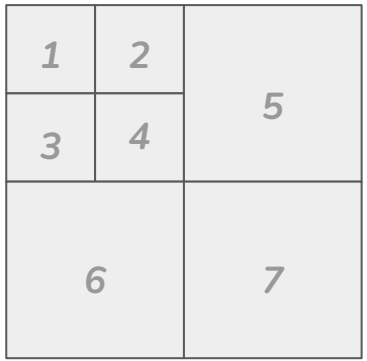
Accessing neighborhood

- “Linear octree”
- Using hashmap to find neighbors (`Kokkos::UnorderedMap`)

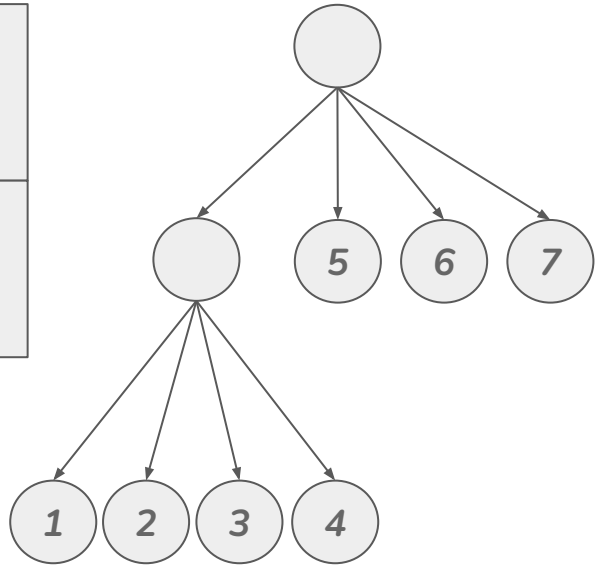
Modularity : 2 AMR backends

- PABLO : 3rd party CPU only library
  - 2 Octree representations for CPU/GPU (+translations)
- Dyablo : our own backend based on Kokkos
  - GPU compatible, more flexibility

AMR mesh



Associated Octree

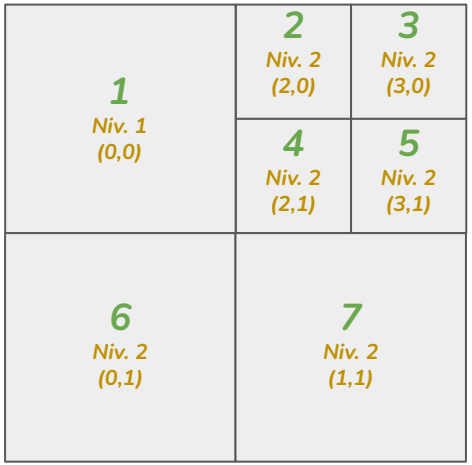


AMR on GPU in Dyablo

Finding neighbors

Unstructured linear tree

- **index** : of the cell in **Morton** order (Z-curve)
- **position** : refinement level and position on the regular grid at this level
- **Convert : index -> position** : array of positions
- **Convert : position** -> **index** : hashmap



Maillage AMR

Hashmap

*Key/value container that able to "quickly" (O(1)) a value (**index**) associated to the key (**position**)*

- `Kokkos::UnorderedMap`
- Key : **position**; Value : **index**

Request a neighbor from an index:

1. **index -> position** (Array)
2. Arithmetics on **position**
   (neighbor could be at a different level)
3. Neighbor's **position** -> Neighbor's **index**

À gauche de *4* :

1. *4* **->** ***Niv. 2 : (2,1)***
2. À droite : ***Niv. 2 : (2-1,1)***
3. ***Niv. 2 : (1,1)*** ***n'existe pas :***
   On cherche au niveau 1 : ***Niv. 1 : (0,0)***
4. ***Niv. 1 : (0,0)*** -> **1**

AMR on GPU in Dyablo

Write AMR Kernels

Kernels are written using abstract interfaces :

- User friendly and readable by *normal* humans
- Optimization possible without changing kernel code

Apply function on each cell :

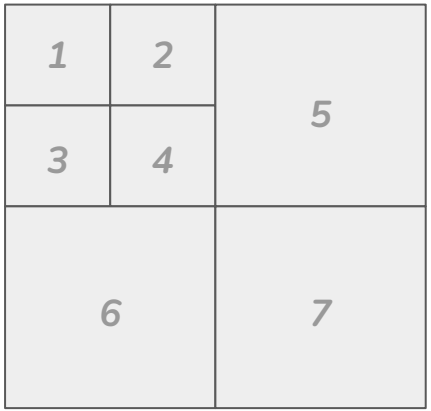
`foreach_cell()`

- Lambda-based loop
- Hide Kokkos

Access data :

`CellArray, CellIndex`

- Hide mem. Layout
- Hide index computation
- AMR neighbor access




```
double dt;
ForeachCell foreach_cell(...);
FieldManager field_manager({IP,IDPDX});
CellArray_ghosted U = foreach_cell.allocate_ghosted_array(
foreach_cell.foreach_cell(
    "compute_pressure_gradient",
    U,
    CELL_LAMBDA(const CellIndex& iCell_U)
{
    double P_left = 0;
    CellIndex iCell_Uleft = iCell_U.getNeighbor({-1,0,0});
    if( iCell_Uleft.level_diff() >= 0 )
        double P_left = U.at(iCell_Uleft, IP);
    else
    {
        int nbCells = foreach_sibling<ndim>(
          iCell_Uleft, U,
          [&](const CellIndex& iCell_subcell)
        {
          P_left += U.at(iCell_subcell, IP);
        });
        P_left = P_left/nbCells;
    }
    double P_right;
    [...]
    U.at(iCell_Uout, IDPDX) = (P_right - P_left) / h;
});
```

AMR on GPU in Dyablo

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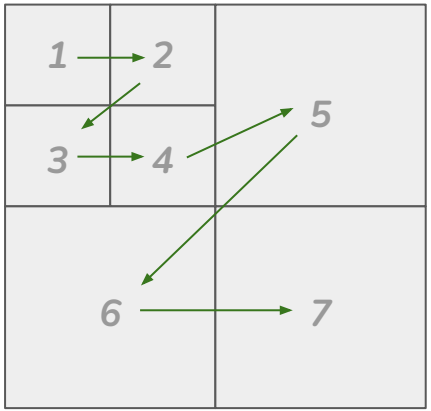


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AMR on GPU in Dyablo

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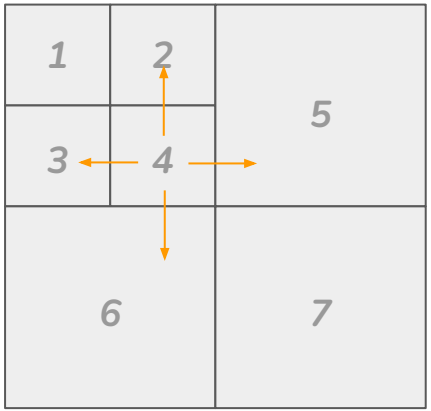


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AMR on GPU in Dyablo

Other differences compared to RAMSES

Block-based AMR

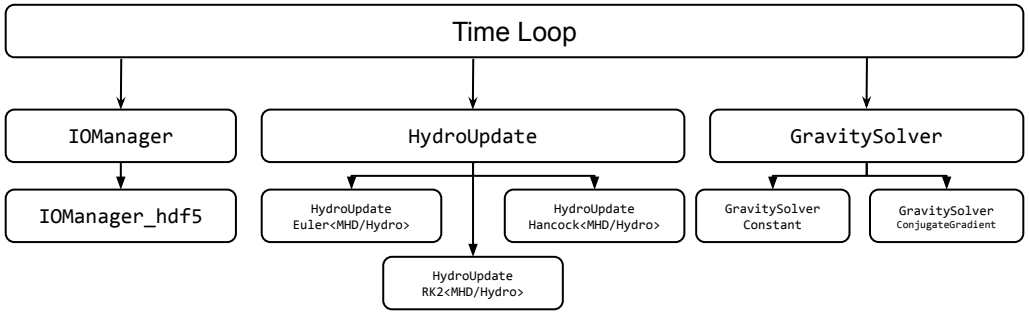
- Store cartesian blocs of cells at leaves of the Octree

➡ Cartesian grids better for GPU

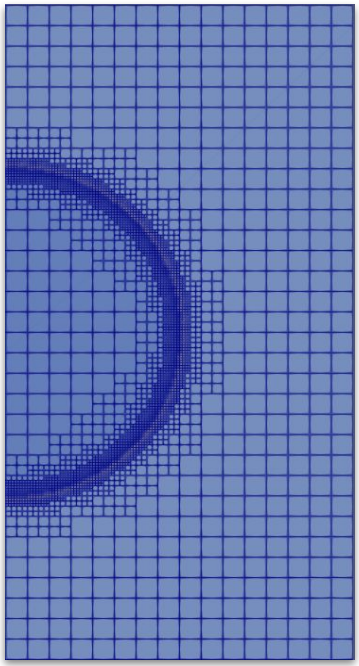
➡ Octree is smaller : AMR cycle is faster

Modularity : plug-ins

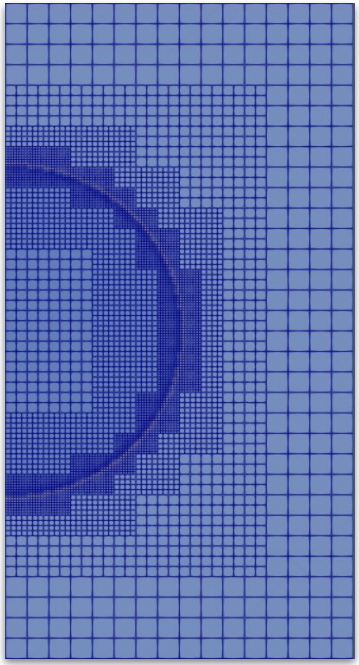
- Modern software architecture and patterns
- New Kernels can be added as plug-ins
- Choose at execution time : 2D/3D, numerical scheme, IOs, …



Cell Based
600k Octants
600k Cells

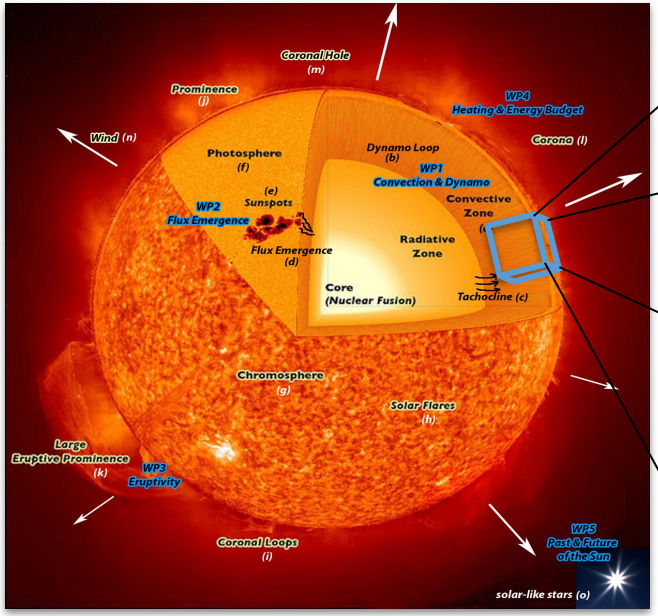


Block Based
18k Octants
1100k Cells

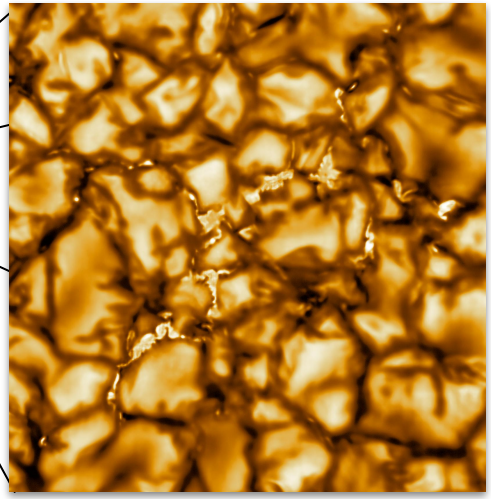


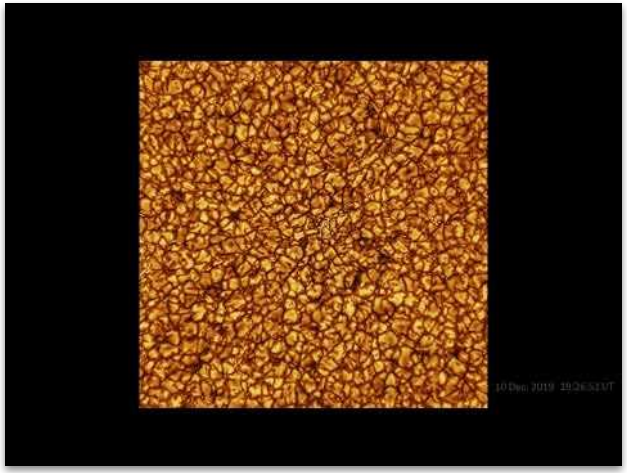
Application #1

Solar convection benchmark towards whole sun simulations *(DAp ERC-Synergy Whole Sun)*



Credit: [Whole Sun website]





Credit: NSO/NSF/AURA/DKIST

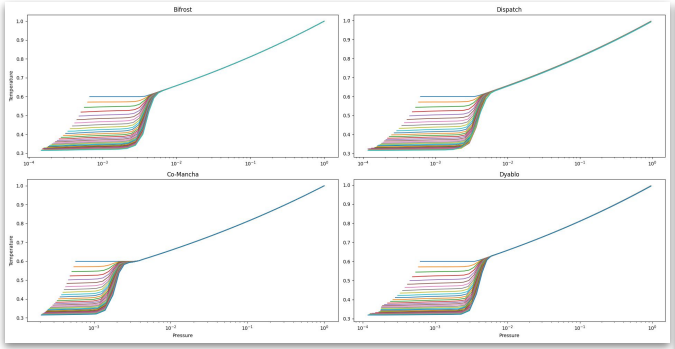
Solar convection

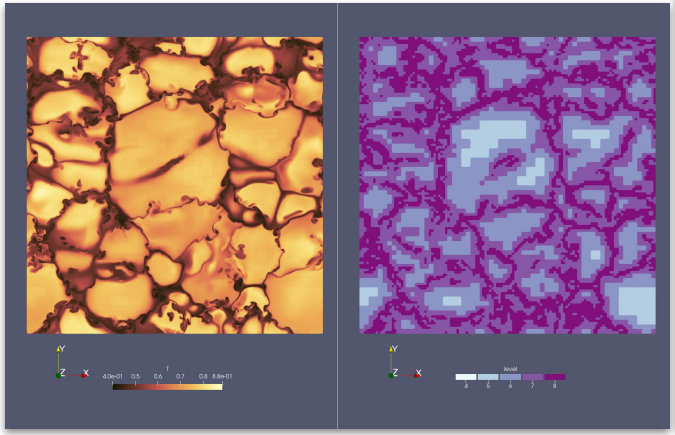
Two convection benchmarks

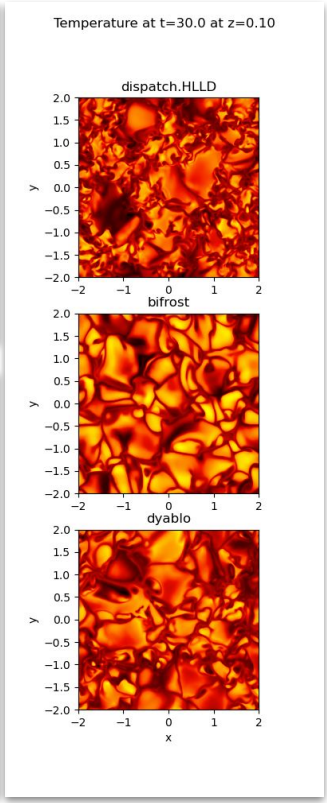
Setup #1

- Open boundary setup
- Surface cooling to simulate Solar atmosphere
- Code comparison with state of the art
  - Bifrost
  - Dispatch
  - Mancha
- Solving for :
  - Hydro
  - Gravity
  - Thermal conduction
  - Viscosity
  - Newtonian cooling

Code has been validated wrt to state of the art





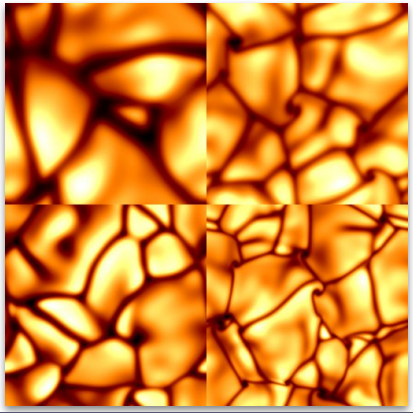


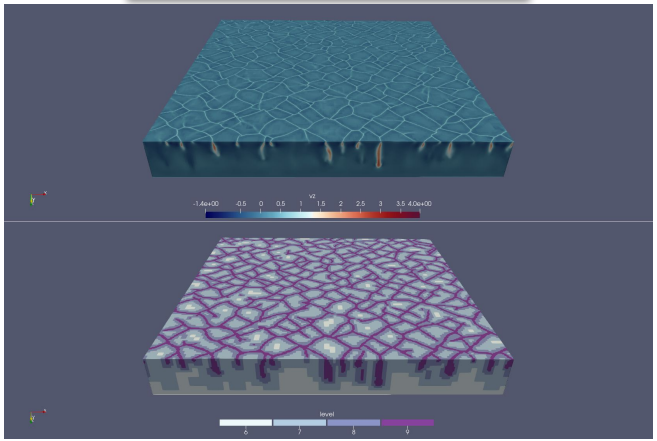
Solar convection

Two convection benchmarks

Setup #2

- Closed boundary setup
- Based on 90's and 00's classical setups
- Better control on the experiment
- Parameter study on Prandlt number and stratification
- Solving for :
  - Hydro
  - Gravity
  - Thermal conduction
  - Viscosity
  - (MHD)





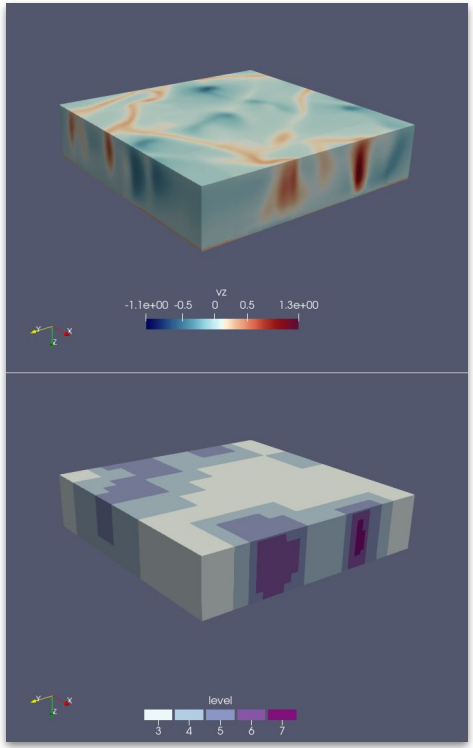
Works on CPUs and GPUs
Works with AMR

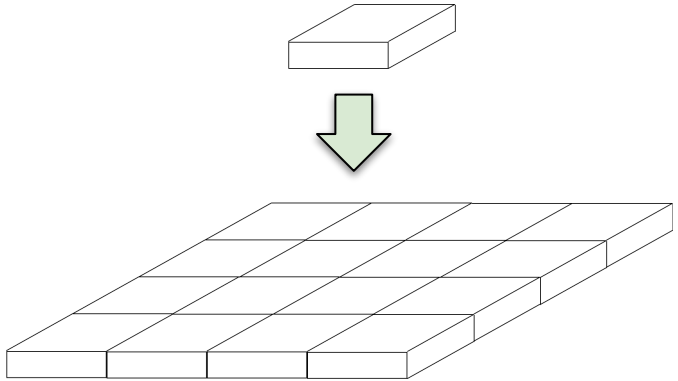
Weak scaling benchmarks

Use case

Solar convection slab :

- Convection slab:
  - Hydro + TC + viscosity + cooling
- 3-7 refinement levels
  - Base resolution 128x128x32
  - Max resolution 2048x2048x512
  - 30.6M cells per domain
- Horizontal tiling per MPI process
  - Load-balancing is ensured
- 100 iterations, 1 AMR cycle per iteration
- Scalability tested on Jean-Zay and Ad-Astra
  - CPU : CSL (JZ), Genoa (AA)
  - GPU : v100 (JZ), a100 (JZ), MI250X (AA)
  - Tested up to 2048 GPUs ~62 billion cells

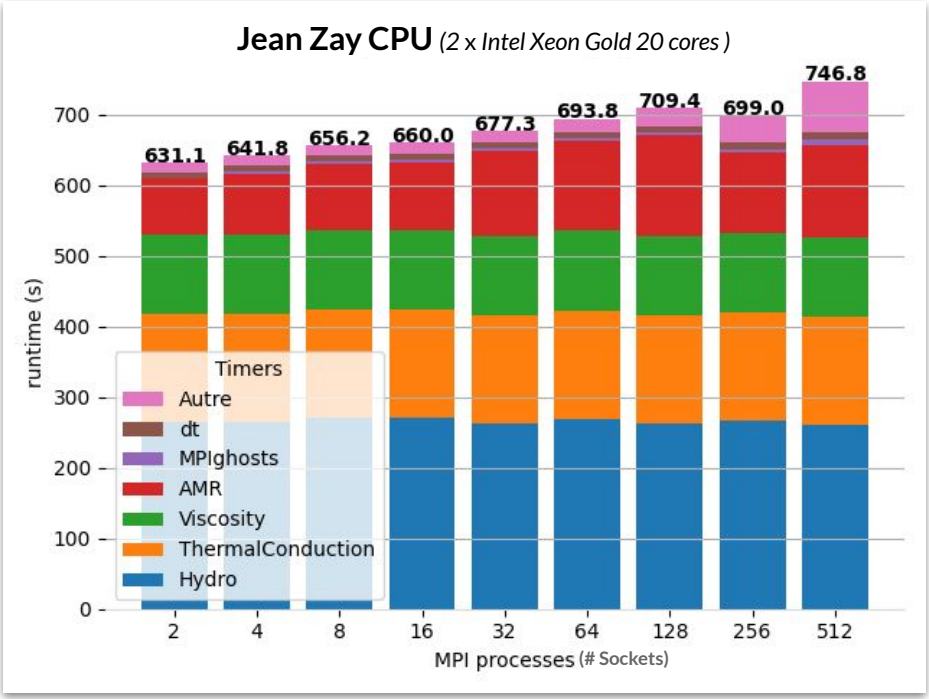


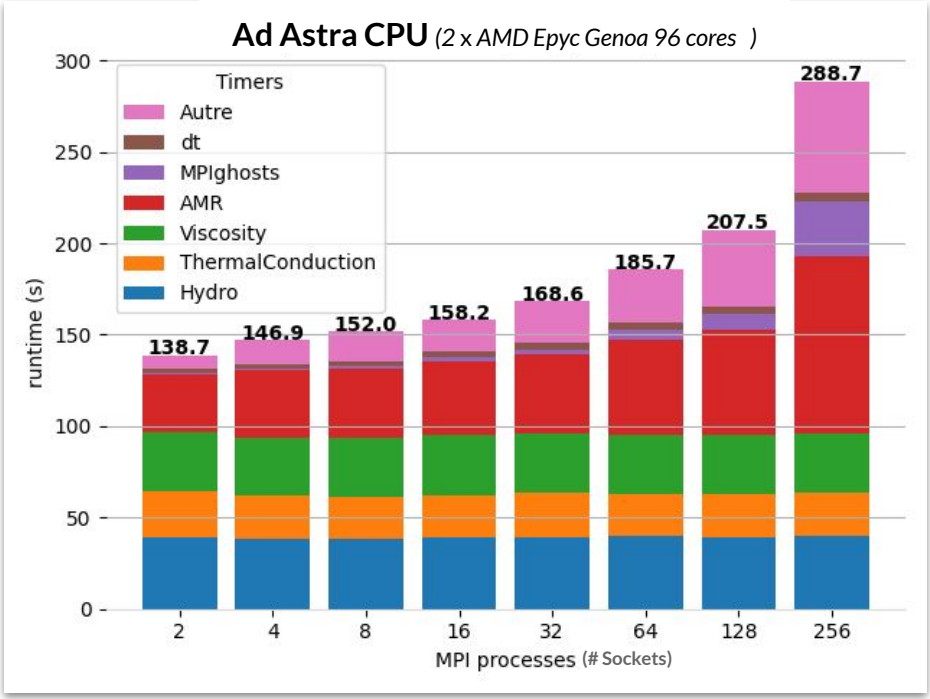


Replication on N MPI processes

Weak scaling benchmarks

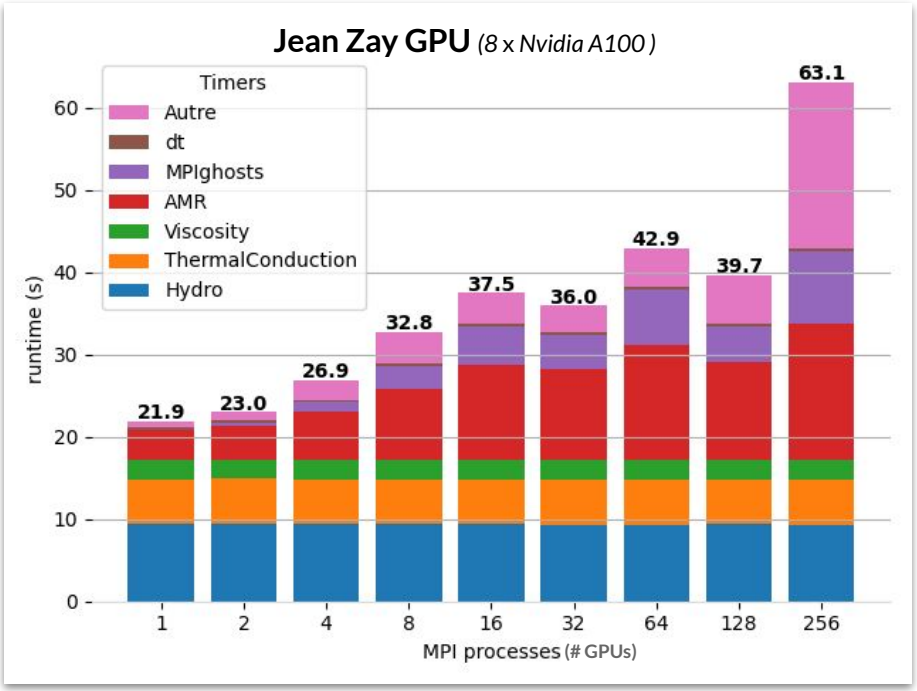
CPU results

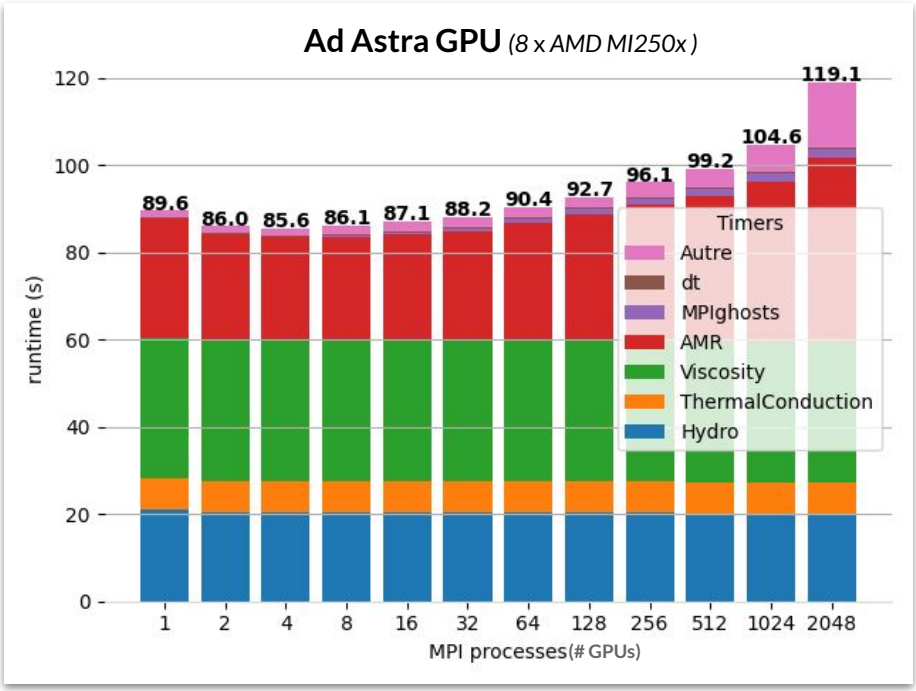




Weak scaling benchmarks

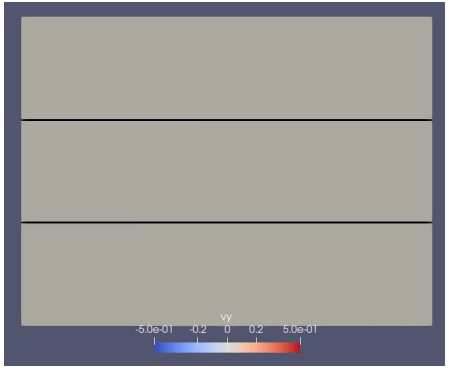
GPU results

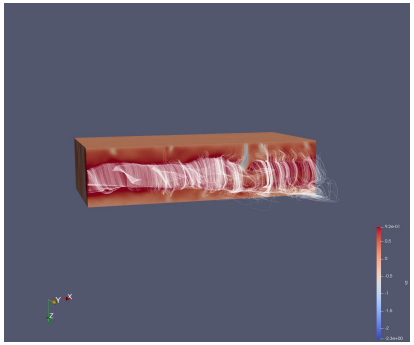




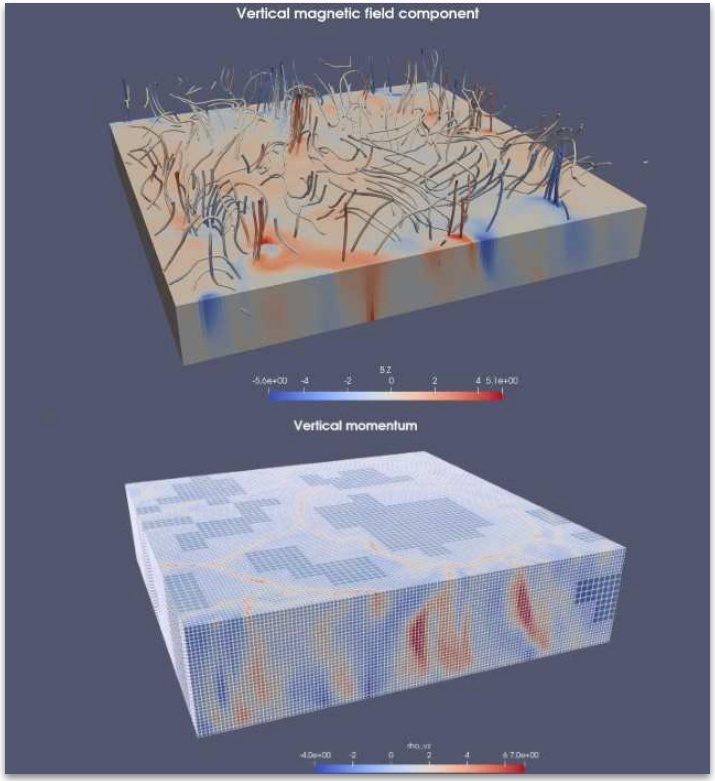
Ongoing work - Whole Sun project

Tri-layer setup (A. Finley)



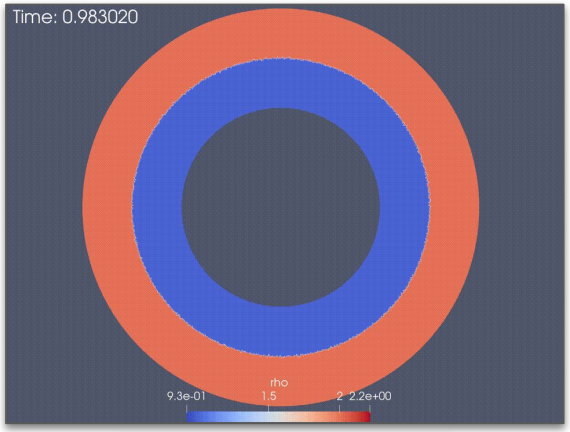


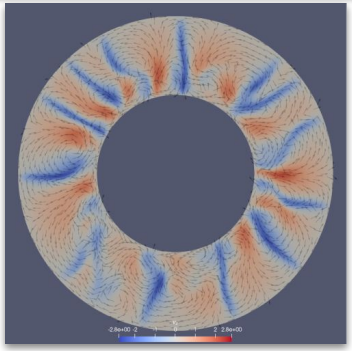
Flux tube experiment (C. Blume)



Convective Dynamo (A. S. Brun)

Geometry module (G. Doebele)



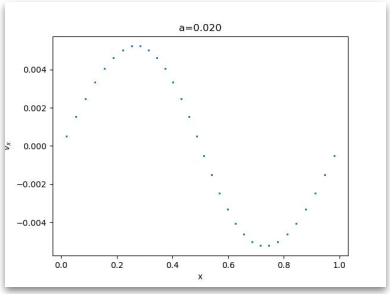


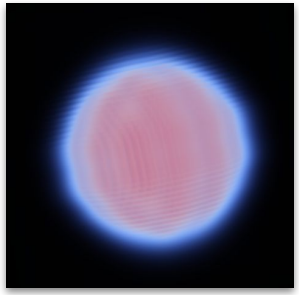
Application #2

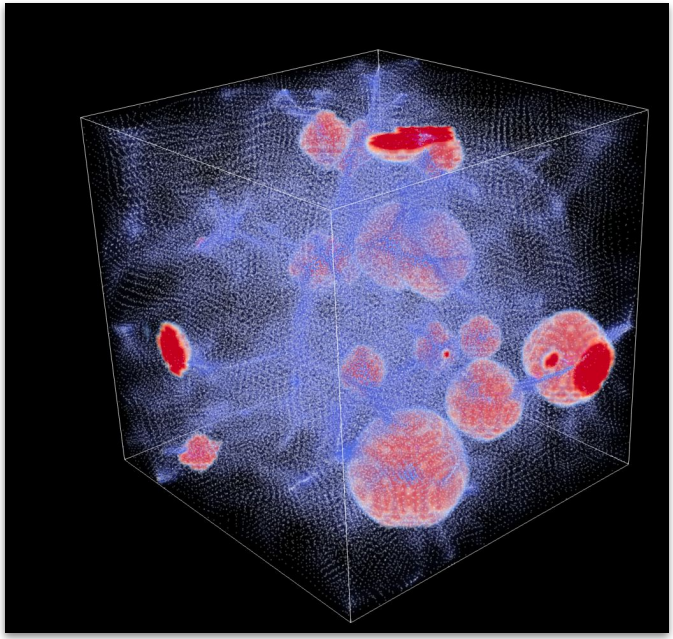
Cosmological radiative transfer

Setup :

- Collaboration with Observatoire de Strasbourg (D. Aubert, O. Marchal)
- Periodic expanding box (super-comoving coordinates)
- Solving for :
  - Hydro (mesh + particles)
  - Self-Gravity
  - Radiative transfer (M1)
- Allows for the simulation of large structure formation and ionization
- Validation tests :
  - Zeldovitch pancake
  - Stromgren sphere







A box of 64^3 points of width 4 Mpc
In blue : DM particles
In red: Ionized regions

Leveraging Exascale architectures with Kokkos

Performance Portability with Kokkos

- Dyablo runs on CPUs (Intel, AMD, ARM*) and GPUs (Nvidia, AMD*, Intel**) with one codebase
- Performance and Scalability
- Hide *some* of the GPU code complexity

Adapted AMR algorithms for GPUs

- Hashmap AMR Octree
- Block-based AMR
- Hide complexity behind abstract interfaces

➡ *Proof that Separation of concerns works for AMR at Exascale in Dyablo*

Two applications showcased

Solar physics

- Cartesian slabs over a few AMR levels
- MHD + diffusion operators
- Comparison with state of the art codes
- Weak scaling benchmark up to 2048 GPUs and ~50k CPU cores

Cosmology

- Expanding coordinates
- Particle-Mesh integration
- Hydro + Gravity + Radiation

More to come from collaborations at CEA, CNRS and the various partnerships in astrophysics labs : dust, stellar formation, galaxy formation, star-planet interaction, stellar physics, etc.

Dyablo - Projects, community and collaborations

Physics/Applicative projects :

- **Whole Sun :** ERC Synergy on solar physics
- **GINEA :** Groupement d'Instrumentation Numérique pour l'Exascale en Astrophysique (GT CNRS) -> Cosmology, Galaxy formation
- **PEPR Origins :** "From the formation of planets to life" -> 3 postdocs/PhD students potentially working on dyablo for the implementation of new physics.
    - Two confirmed working on dust and gravitational solvers.

HPC/Computer science projects

- **EUPEX :** European Pilot for Exascale -> Porting the code to ARM architectures
- **CExA :** Exascale at CEA -> ***PTC submitted to build optimization tools***
- **PEPR Numpex** *(Demonstrator PC5 Exa-DI)*
    - IO / Visualization tools for AMR *(1 post-doc PC3 Exa-Dost)*
    - Implicit methods / linear solvers on AMR grids
    - Load balancing
    - ...

Roadmap 2024

Core developments :

- Local time-stepping
- Units
- Geometry
- Logging

Post-treatment and analysis

- Python back-end

Publication and dissemination

- Method paper
- Solar convection paper
- Open sourcing the code
- Documentation

Performances

- Small grain CPU and GPU profiling
- Kernel optimization
- Tuning

PEPR Origins :

- Dust
- *Non ideal MHD*
- Constrained transport
- Gravitation

EUPEX :

- Profiling SVE and HBM
- Profiling on Grace Hopper
- Porting to Rhea [if available in 2024]

CExA :

- PTC-SN on tuning, automatic kernel extraction and optimization

PEPR NumPEX (PC3) :

- IO formats for AMR
- Data compression
- *PDI/DASK/DEISA integration*

PEPR NumPEX (PC5) - Propositions

- IOs and visualization formats and tools
- Implicit methods for diffusion operators
- Load balancing
- Kernel performance for all architectures