ARGONNE
ATPESC2023
EXTREME-SCALE COMPUTING

AMReX: Building a Block-Structured AMR Application (and more)

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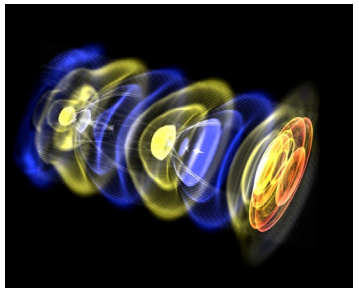
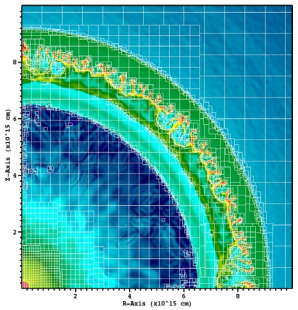
On behalf of the AMReX team

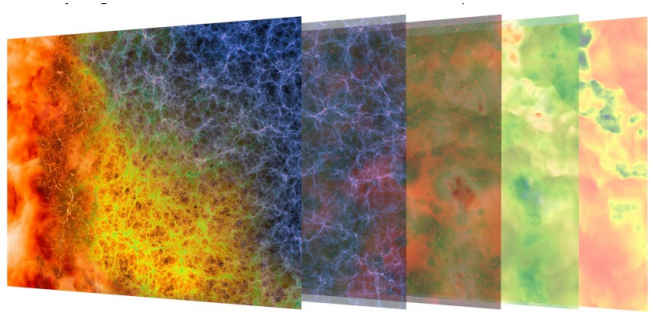
AMReX: software framework for block-structured AMR

Astrophysics:
- **Castro** (compressible)
- MaestroEx (low-Mach)
- SedonaEx (Monte Carlo radiation transport)
- Emu (neutrino transport)
- Quokka (radiation-hydrodynamics)





Cosmology:
- **Nyx**



Combustion:
- **PeleC (Compressible)**
- **PeleLM (Low Mach)**

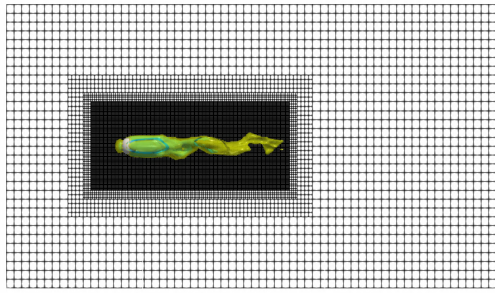
Accelerator Modelling:
- **WarpX**
- ImpactX
- Hipace++

Magnetically-confined fusion:
- GEMPIC

Ocean Modeling:
- ROMS-X

Incompressible Navier-Stokes:
- IAMR
- incflo

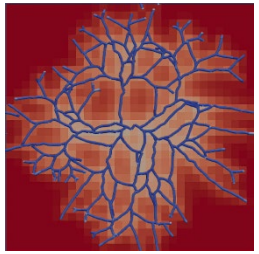
Atmospheric science:
- **AMR-wind**
- ERF



Multi-phase Flow:
- **MFIX-Exa**

Solid Mechanics:
- Alamo

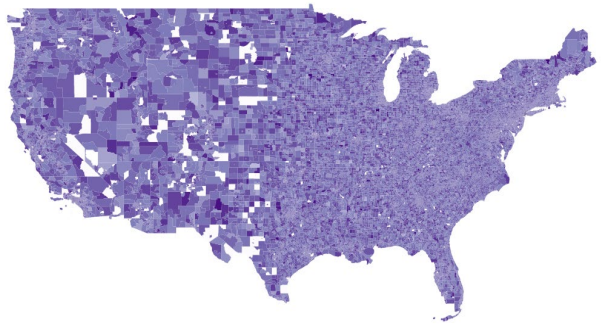
Biological cell modelling:
- BoltzmanMFX
- CCM

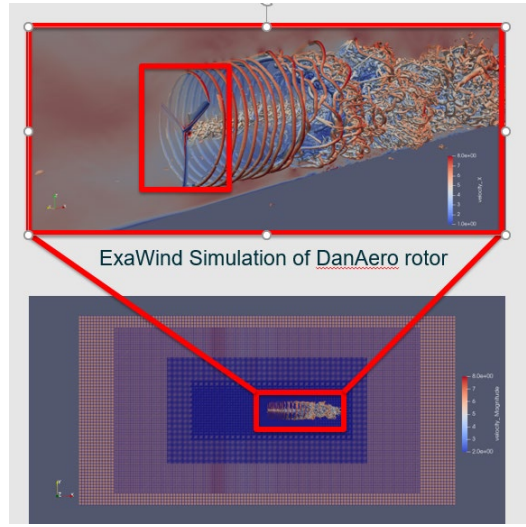


Multiscale Modelling and Stochastic Systems:
- FHDeX

Electromagnetics:
- ARTEMIS

Epidemiology:
- Exa-Epi





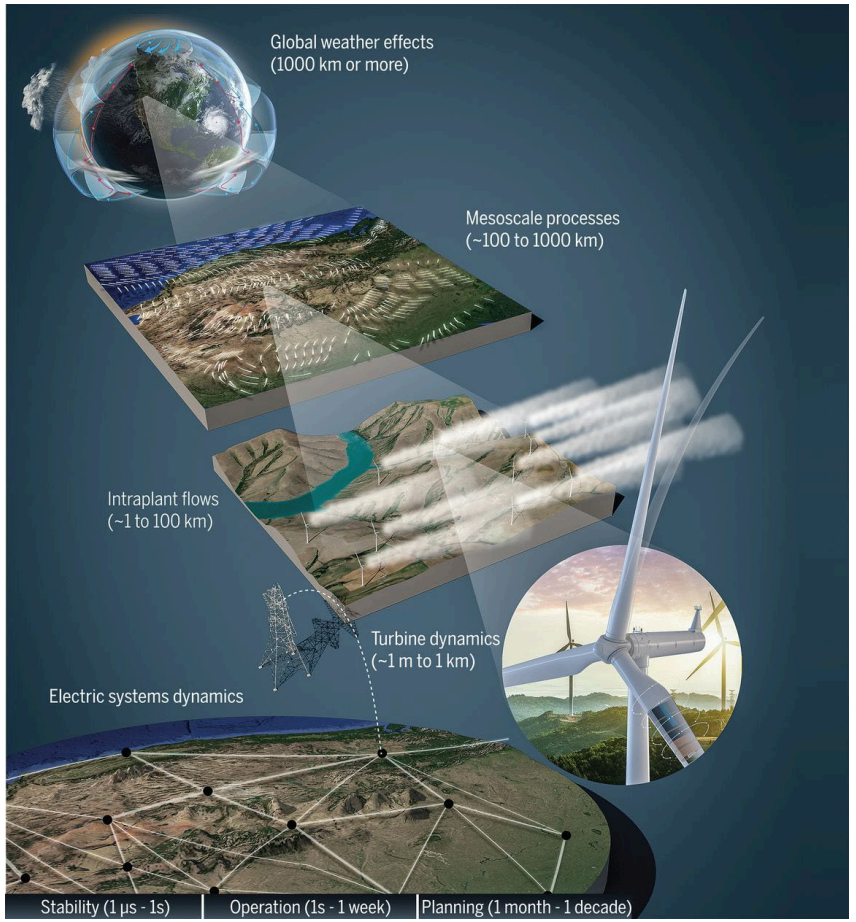
Setting the Stage

Most of the problems we solve today are hard.

Characteristics of these problems are
often that they couple multiple physical processes
across a range of spatial and temporal scales.

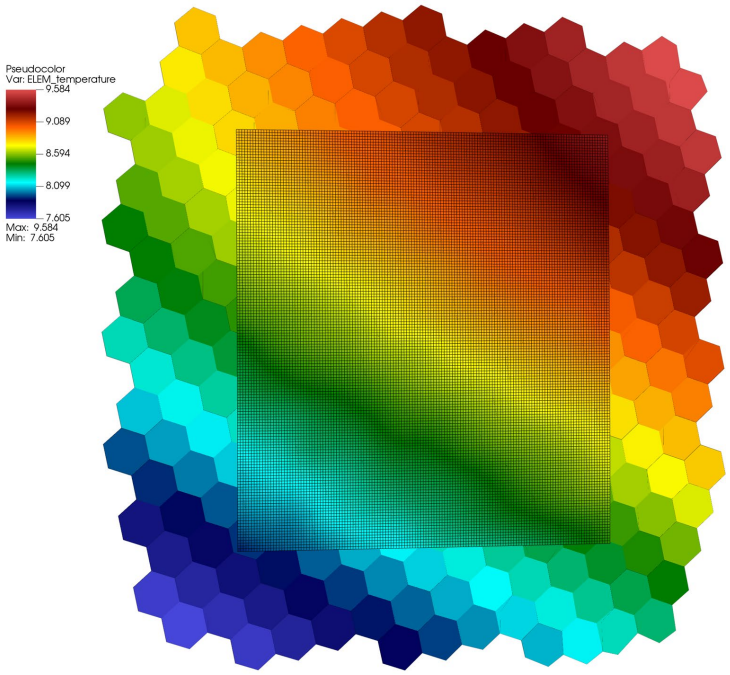
Gone are the days of simple physics, simple geometry, single algorithm, homogeneous architectures … ☹

So how do we build algorithms and software for hard multi-physics multi-scale multi-rate problems without starting over every time?



Grand challenges in the science of wind energy
Veers, P. et al., 2019 *Science,* Vol. 366, Issue 6464
https://science.sciencemag.org/content/366/6464/eaau2027

Setting the Stage (p2)



Not all simulations use a mesh

But for those that do, the choice is usually **structured** vs **unstructured.**

Structured:

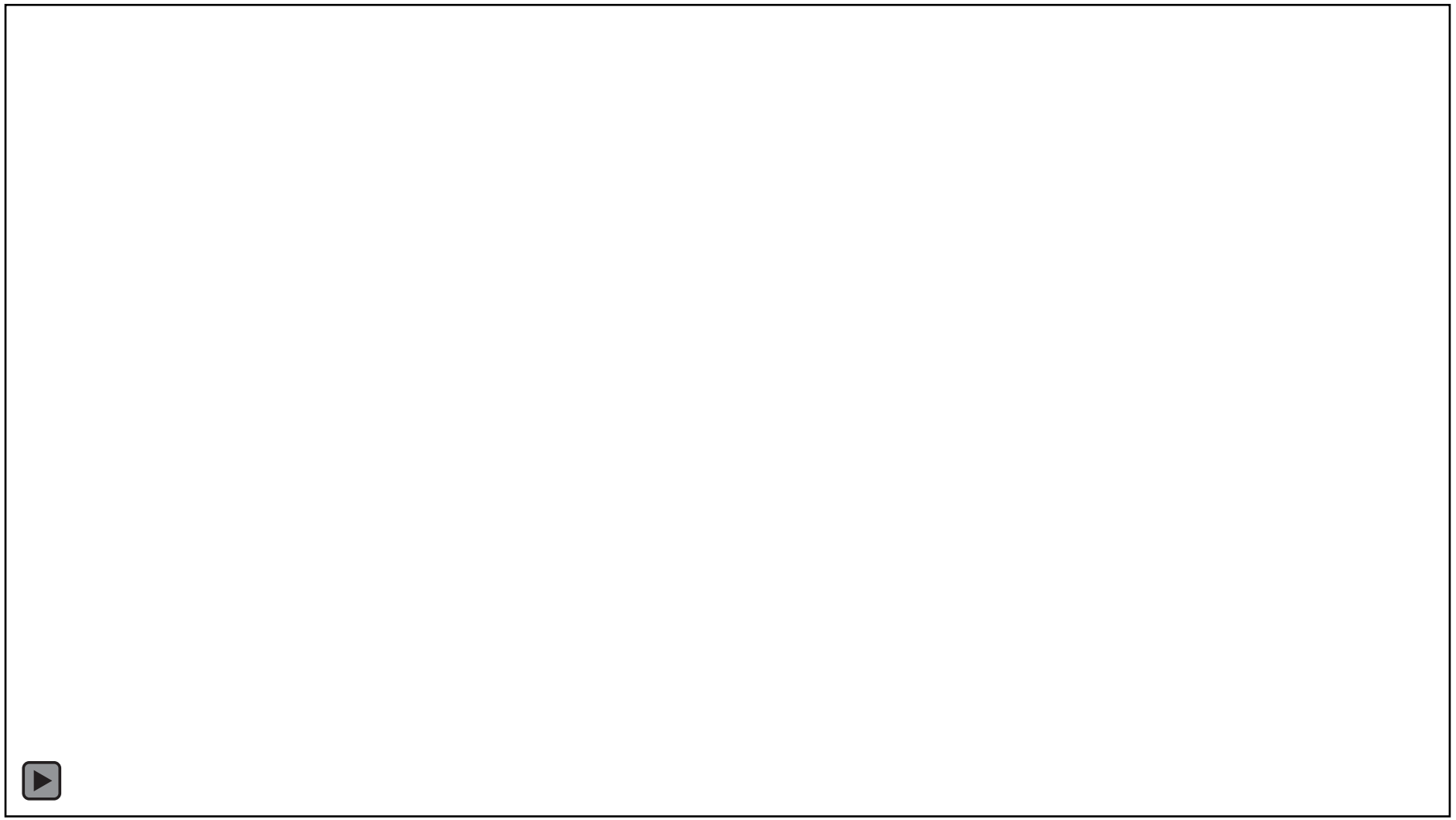
- Easier to write discretizations
- Simple data access patterns
- Extra order of accuracy due to cancellation of error
- Easy to generate complex boundaries through cut cells but hard to maintain accuracy at boundaries

Unstructured:

- Can fit the mesh to any geometry – much more generality
- No loss of accuracy at domain boundaries
- More “book-keeping” for connectivity information, etc
- Geometry generation becomes time-consuming

Both structured and unstructured meshes can be **dynamically adaptive**.

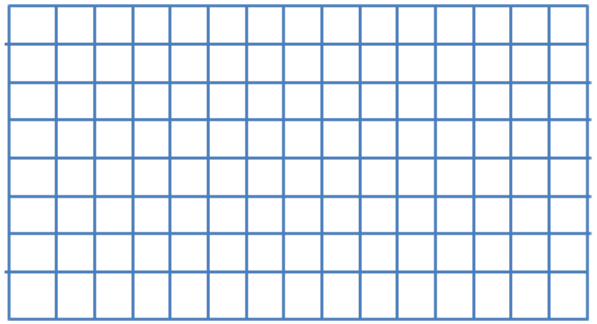
Structured vs Unstructured?



ExaWind simulation of two NREL 5-MW turbines in turbulent atmospheric flow.

Image credit: Brazell, Brunhart-Lupo, Henry de Frahan, Rood, Sharma, Vijayakumar, et al.

Structured Grid Options

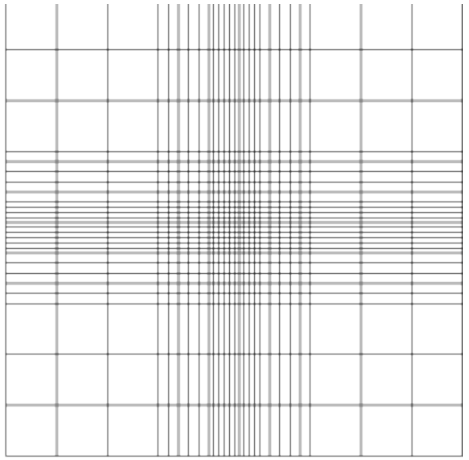


https://commons.wikimedia.org/wiki

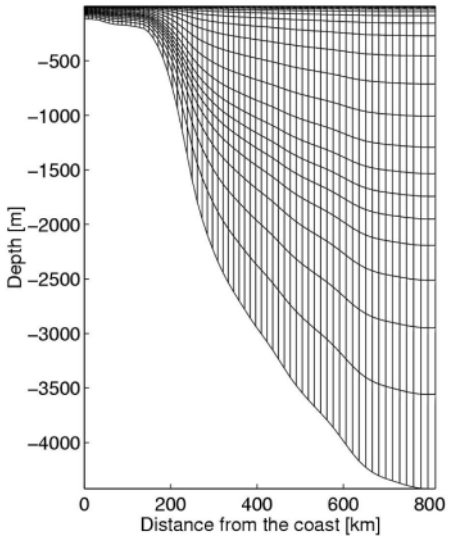
Logically rectangular doesn't mean physically rectangular

Structured with non-constant cells split pros and cons of structured vs unstructured:

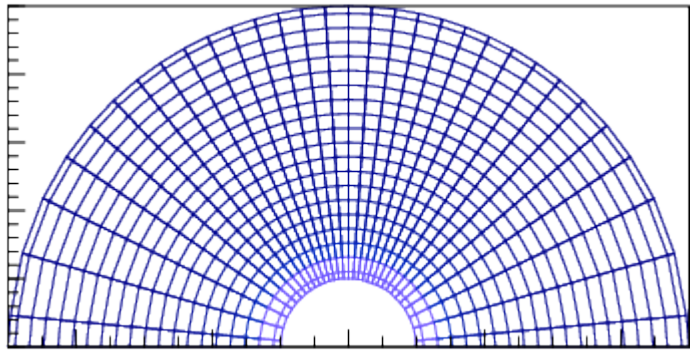
- Can fit (simple) non-rectangular boundaries while still having known connectivity
- Finer in certain regions (mesh refinement)
- Harder to maintain accuracy



http://silas.psfc.mit.edu/22.15/lectures/chap4.xml

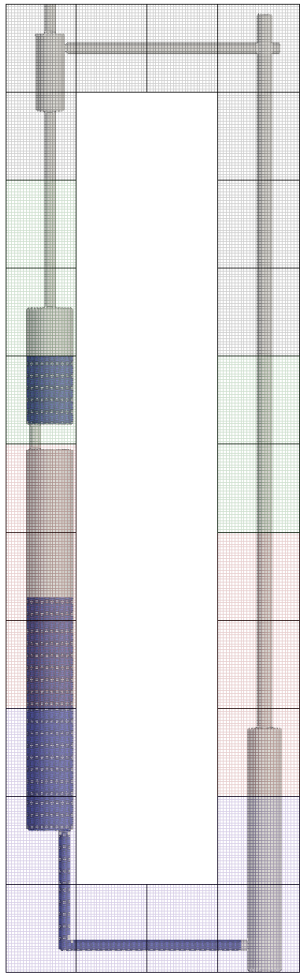


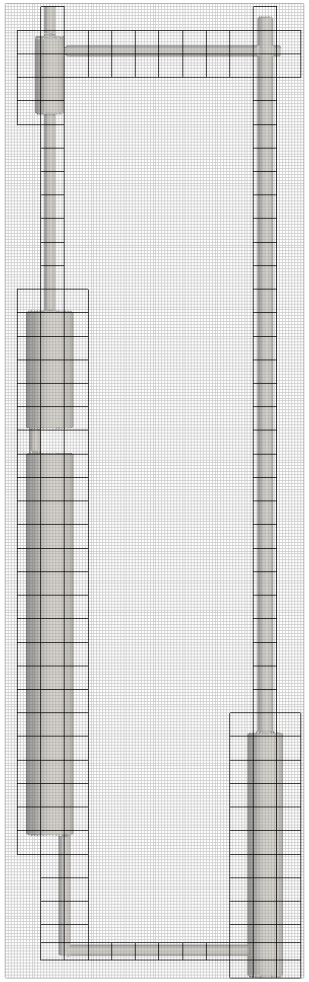
http://www.cfoo.co.za/simocean/modelsroms.php



http://silas.psfc.mit.edu/22.15/lectures/chap4.xml

More Structured Grid Options





Structured grid does not have to mean the entire domain is logically rectangular either.

One can also “prune” the grids so as to not waste memory or MPI ranks – can still use rectangular cells in non-rectangular domain.

Grid pruning can save both memory and work.

Why Is Uniform Cell Size Good?

Numerical Analysis 101:

$$\phi_{i+1} = \phi(x_i) + \Delta x_r \phi_x + \tfrac{1}{2}(\Delta x_r)^2 \phi_{xx} + O(\Delta x_r{}^3)$$
$$\phi_{i-1} = \phi(x_i) - \Delta x_l \phi_x + \tfrac{1}{2}(\Delta x_l)^2 \phi_{xx} + O(\Delta x_l{}^3)$$

We often use a centered difference as an approximation for a gradient,

$$\frac{\phi_{i+1} - \phi_{i-1}}{\Delta x_l + \Delta x_r} = \phi_x + \tfrac{1}{2}(\Delta x_r - \Delta x_l)\phi_{xx} + O(\Delta x^2)$$

Note we only get second-order accuracy if we use constant cell spacing.

Can we confine this error?

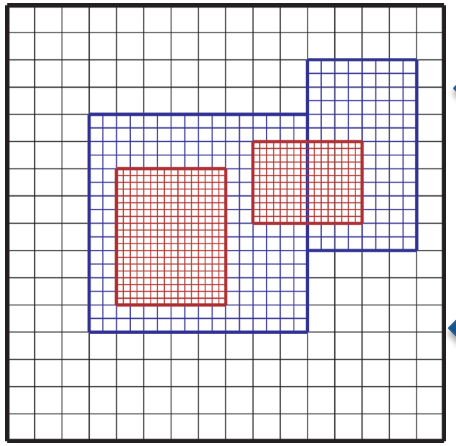
Can We Have the Best Of Both Worlds?

Distorting the mesh is not ideal, but we can't afford uniformly fine grid.

Adaptive Mesh Refinement:

- refines mesh in regions of interest
- allows local regularity – accuracy, ease of discretization, easy data access
- naturally allows hierarchical parallelism
- uses special discretizations only at coarse/fine interfaces (co-dimension 1)
- requires only a small fraction of the book-keeping cost of unstructured grids

Example:
AMReX



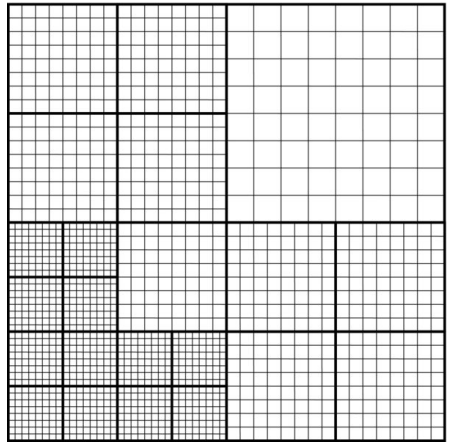
Grid sizes

May differ ← → Same

Child grid have unique parent?

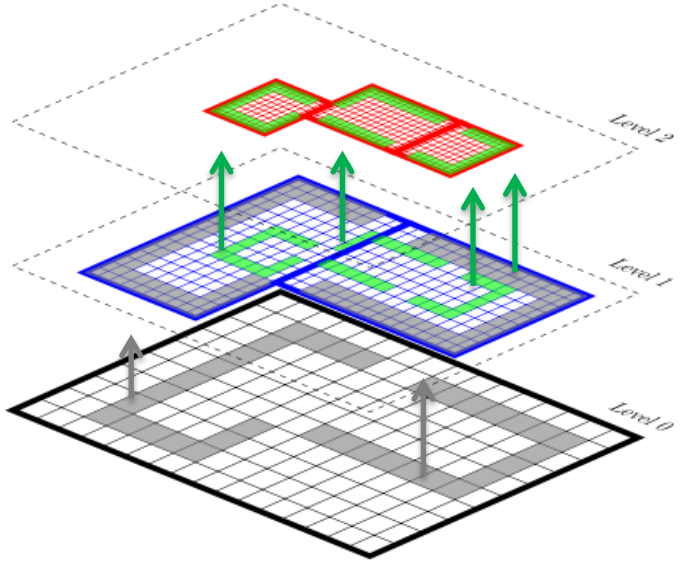
No ← → Yes

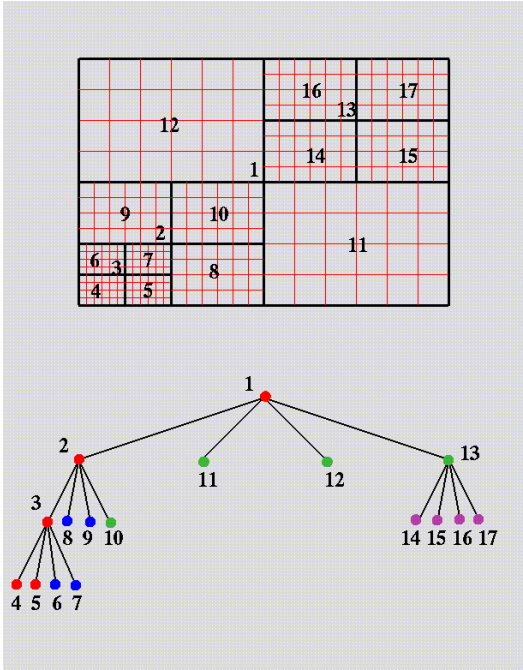
Example:
FLASH



https://iopscience.iop.org/article/10.1088/0067-0049/186/2/457)

Patch-Based vs OctTree





http://cucis.ece.northwestern.edu/projects/DAMSEL/

Both styles of block-structured AMR break the domain into logically rectangular grids/patches. Level-based AMR organizes the grids by levels; quadtree/octree organizes the grids as leaves on the tree.

What is an “AMR algorithm”?

Key things you need to know if you want to use AMR:

- How to advance the solution one patch at a time
- What the right matching conditions are at coarse/fine interfaces
    - This depends very much on the type of equation, e.g. hyperbolic vs elliptic, and what features of the solution are important (e.g., is conservation important?)
    - How you solve on the patch (e.g. with implicit vs explicit update) affects how you synchronize between levels

What about Time-Stepping?

AMR doesn't dictate the spatial or temporal discretization on a single patch, but we need to make sure the data at all levels gets to the same time.

The main question is:

To subcycle or not to subcycle?

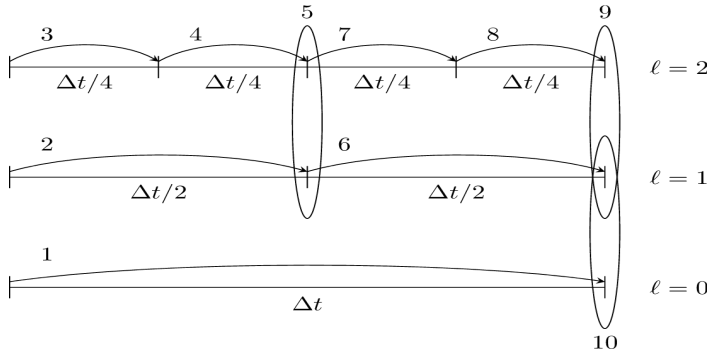
Subcycling in time means taking multiple time steps on finer levels relative to coarser levels.

Non-subcycling:

- Same dt on every grid at every level
- Every operation can be done as a multi-level operation before proceeding to the next operation, e.g. if solving advection-diffusion-reaction system, we can complete the advection step on all grids at all levels before computing diffusion

Subycling:

- dt / dx usually kept constant
- Requires separation of "level advance" from "synchronization operations" – but this can often feel more intuitive
- Can make algorithms substantially more complicated



AMReX Hands-On Examples

Let's do a few hands-on exercises that demonstrate AMReX capabilities

"**AMR 101**": AMR for scalar advection

- Multilevel mesh data – fluid velocity on faces and tracer on cell centers
- Dynamic AMR
- Strong scaling behavior
- Performance portability (CPU vs GPU)

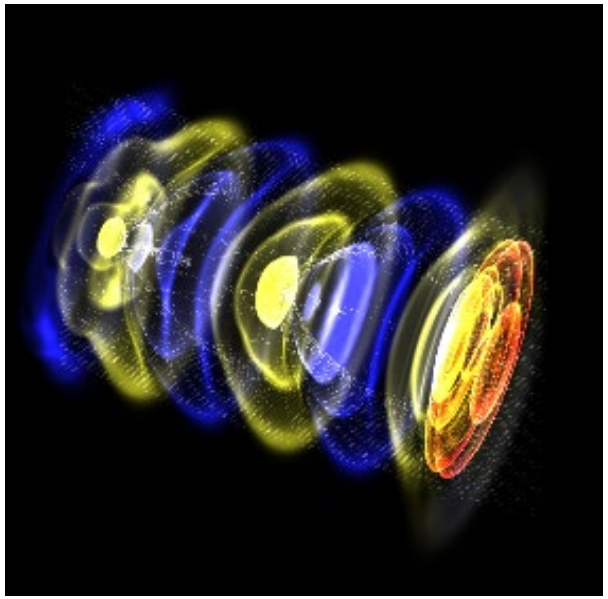
Instructions for how to access and run the code are on the web page:

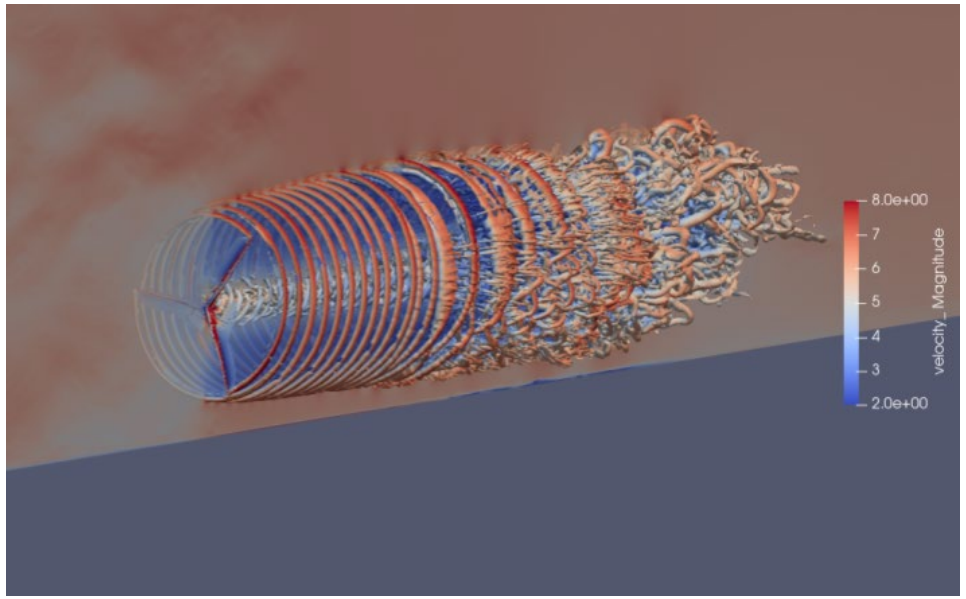
https://xsdk-project.github.io/MathPackagesTraining2023/lessons/amrex/

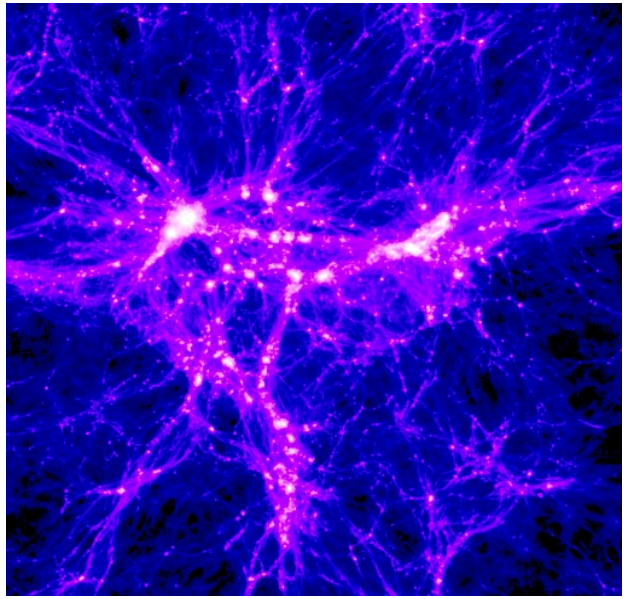
Let's all move to the slack channel to ask questions and share results!

Beyond Linear Advection

This tutorial wasn't actually very complicated, but hopefully it suggests that if you don't want to write a parallel GPU-ready AMR code from scratch, something like this might be a good starting point…

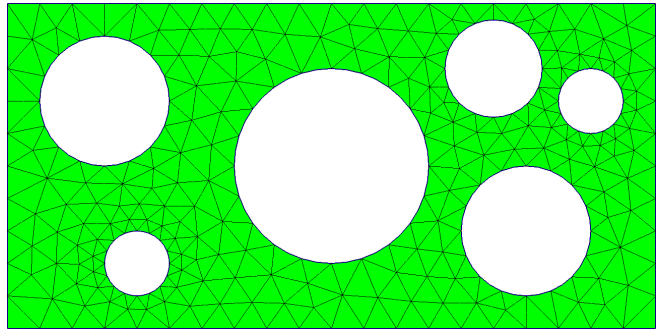






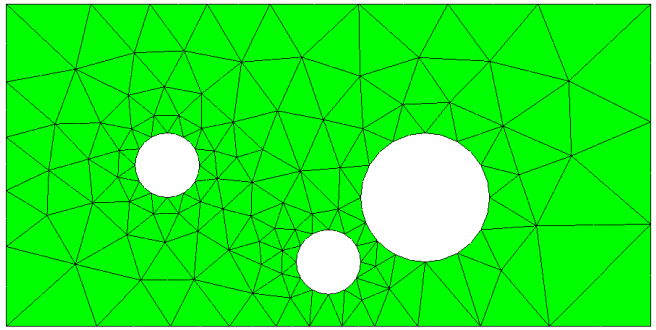
Let’s model the dye a different way …

Let’s imagine instead that we model the dye as a collection of particles. And let’s make the flow more interesting by inserting an obstacle in the flow.



Unstructured meshes change with the geometry

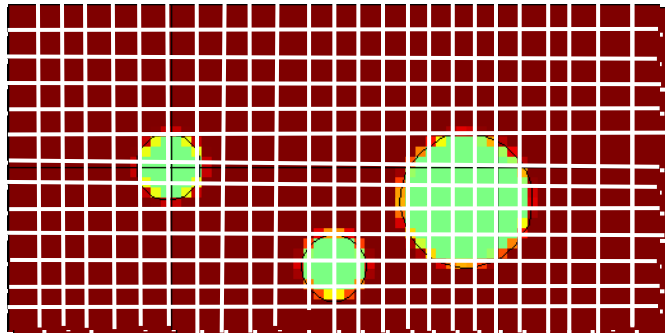
In addition to mesh and particle data, AMReX supports geometric data for solid obstacles/boundaries in the form of “cut cell” quantities (EB = embedded boundary representation)



Structured meshes don’t … but we need to compute new intersections

Note that the cut cell / embedded boundary approach in a structured mesh is very different than an unstructured mesh:

- In a structured mesh, “creating” the geometry means locally intersecting the object with the mesh
- In an unstructured mesh, “creating” the geometry means defining the entire mesh in a way that aligns with the object



AMReX Hands-On Examples

Let's do another hands-on exercise

"**AMR 102**": Particles and Linear Solvers and EB, Oh My!

- Fluid velocity initialized on cell faces
- Obstacle placed in the flow using EB approach
- Velocity field "projected" to ensure divergence-free flow around the object
- Passive particles move with the velocity field, mimicking the presence of the dye

Instructions for how to access and run the code are on the web page:

https://xsdk-project.github.io/MathPackagesTraining2023/lessons/amrex/

Let's all move to the slack channel to ask questions and share results!

Software Support for AMR

There are a number of AMR software packages available –

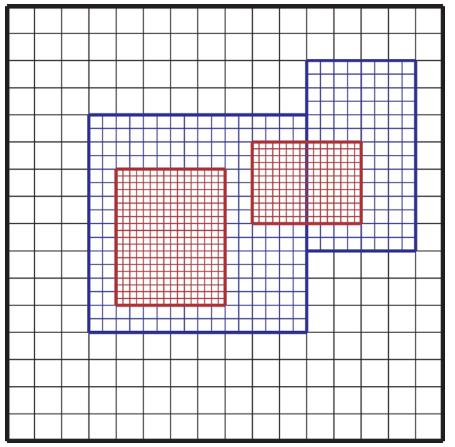
They all
- Provide data containers for blocks of data at different resolutions
- manage the metadata – same-level and coarse-fine box intersections
- manage re-gridding (creation of new grids based on user-specified refinement criteria)

They differ on:

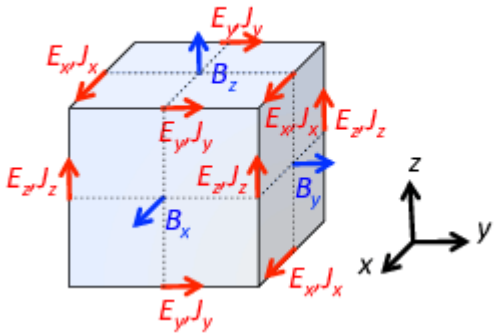
- what types of data they support – e.g. mesh data on cell-centers vs nodes, particles, …?
- what types of time-stepping they support (many are no-subcycling only)
- whether they support separate a “dual grid” approach
- what degree of parallelism do they support? (If MPI+X what X?)
- what task iteration support – asynchronous, fork-join, kernel launching…?
- how flexible is the load balancing?
- what additional “native” features – e.g. AMG/GMG solvers?
- how many flavors of GPUs they can use?

Mesh Data Structures

- Most AMReX applications involve mesh data of some kind
- AMReX provides tools for storing distributed mesh data (i.e. multidimensional arrays associated with each patch in the AMR hierarchy).
- Mesh data can be cell, face, edge, or node centered. Useful for, e.g.
  - staggered “Yee” grid for electromagnetics / Arakawa C-grid
  - MAC projection in fluid simulation
  - etc…
- Also provide tools for parallel communication (gpu-aware):
  - Ghost cell exchange (Fillboundary - copy valid to ghost, SumBoundary - add ghost to valid), Nodal Syncing
  - General ParallelCopy - copy / add from one layout to another

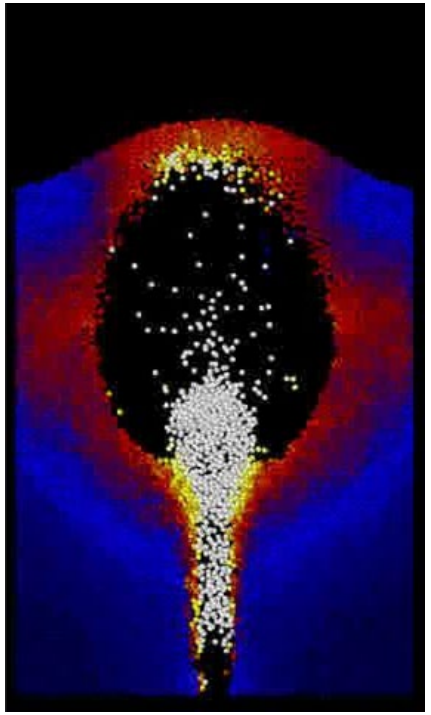


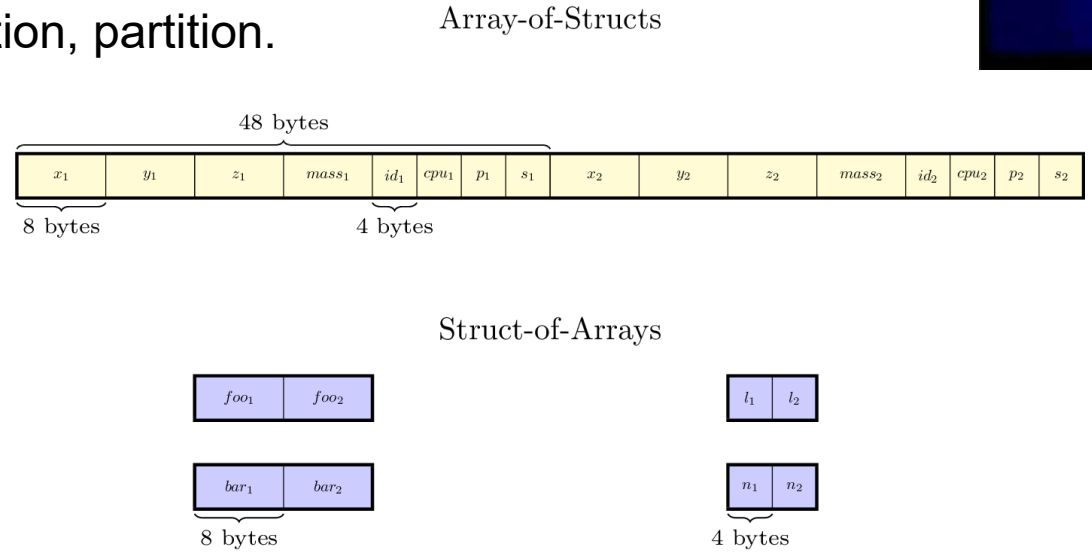
Staggered “Yee” mesh



Particle Data Structures

- Most AMReX applications also have particles - usually these live on / interact with an AMR hierarchy of mesh data.
- These could be passive, tracers, charged particles interacting through self-forces, fluid-particle drag, particle-particle collisions.
- Users can specify combination of AoS / SoA data layout.
- Tools for particle mesh interpolation, neighbor list construction + iteration.
- Tools for binning, sorting, stream compaction, partition.
- Parallel Communication patterns:
  - Both local and global redistribution
  - Halo exchange





Multi-Level Operations:

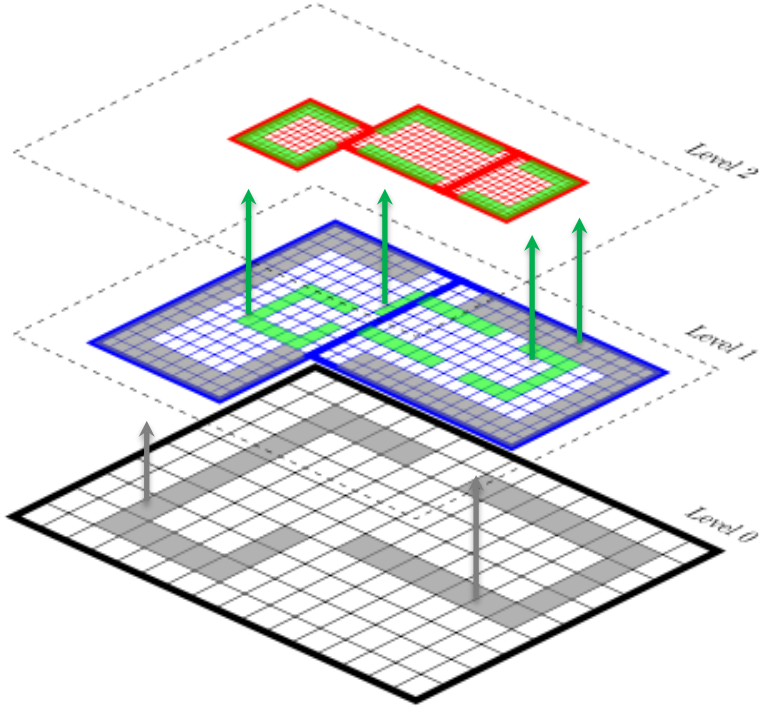
Regridding
- Tagging, grid construction, data filling ...

Interpolation:
- Ghost cell filling and regridding

Restriction:
- Average fine onto coarse for synchronization

Flux registers:
- Available in AmrCore/AmrLevel based applications – stores fluxes at coarse-fine interfaces for easy refluxing

Virtual and Ghost Particle Construction
- For representing effect of particles at coarser / finer levels



Embedded Boundary (Cut Cell) Support:

Use a cut cell approach for complex geometries

- Special stencils at/near cut cells
- Regular stencils elsewhere
- Connectivity information stored in a single integer.

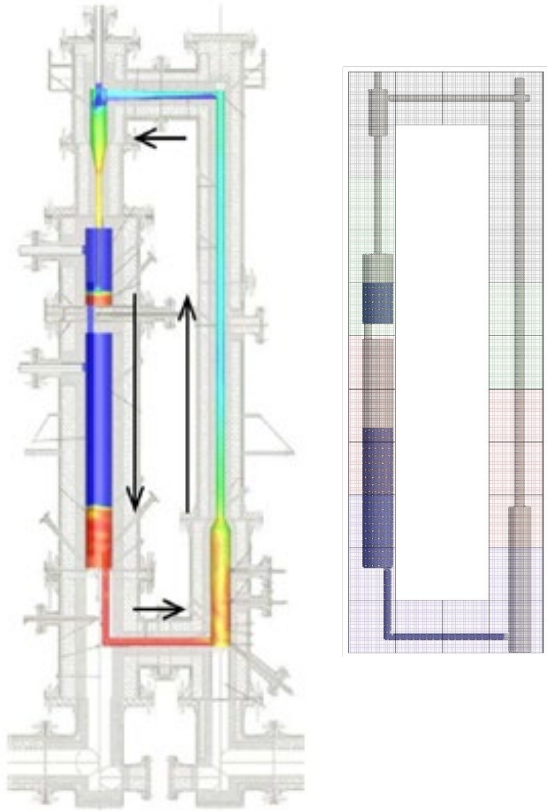
Grids/tiles can be queried as to whether they contain irregular cells

Support for EB-aware

- interpolation, e.g. from cell centers to face centroids
- restriction
- slopes
- linear solvers (cell-centered and nodal)

Option for mesh pruning (for memory savings)

Particles can see boundary through level set function



(L) Prototype of Chemical Looping Reactor (CLR) from MFIX-Exa project

(R) Grid generation using mesh pruning

Geometric Multigrid (GMG) Solvers:

Support for multi-AMR level GMG solvers

- cell vs nodal data
- variable coefficient Poisson or Helmholtz equation
- tensor solve for Navier-Stokes
- single- vs multi-component

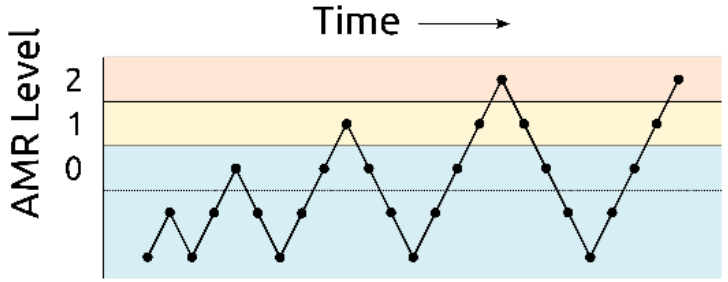
EB-aware options

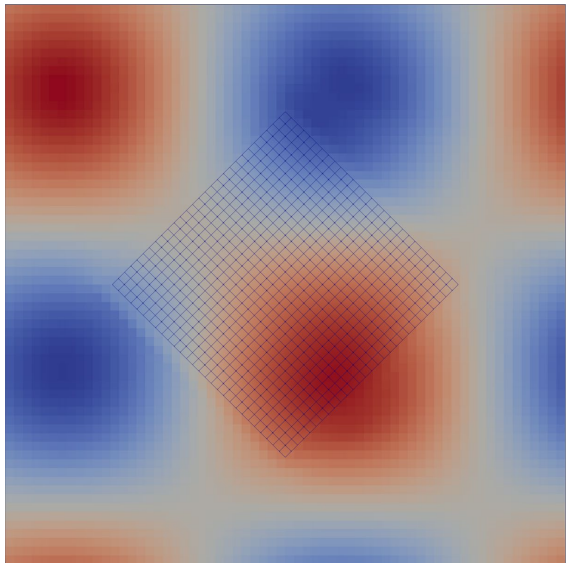
Option for masking to enable overset mesh algorithms

Native “bottom solver” is BiCG (or CG or both)

Interface to call hypre or PETSc as “bottom solver” --
which can be at any multigrid level, including the top

Options for agglomeration and consolidation on coarsening





Over set mesh coupling

In addition to what you've seen, AMReX supports:

- a "dual grid" approach – particles can live on different grid layout than fluid does
- MPI + OpenMP on multicore; MPI + CUDA/HIP/DPC++) on GPUs
  - support using lambdas for kernel launching on CPU vs GPU
  - (Can also use OpenMP / OpenACC)
  - Kernels can be C++ or Fortran
  - Performance portability – e.g., set USE_CUDA = TRUE or FALSE at compile-time
- task iteration – asynchronous, fork-join, kernel launching, kernel fusing…
- flexible load balancing
- "native" AMR/GMG solvers
- "native" async I/O along with support for HDF5 (some applications also use NetCDF)
  - format supported by Visit, Paraview, yt

Other things AMReX takes care of “under the hood”

Memory allocation

Memory “Arenas” for handling expense of frequent memory allocation, host/device transfers

Kernel fusing for working around launch latency

AMReX also provides ParallelFor routines that operate on multiple boxes at once

Optimized parallel communication

Takes advantage of kernel fusion for buffer packing / unpacking, GPU-aware MPI

Load balancing

Several different strategies: knapsack, space-filling curve, dual-grid approaches possible

Compile-time ParallelFor

For optimizing out expensive operations that aren’t used at runtime

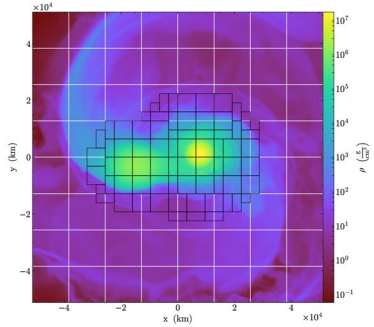
Efficient and portable prefix sum operation

(especially useful for particle methods)

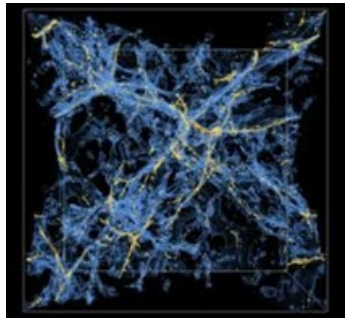
Visualization and I/O

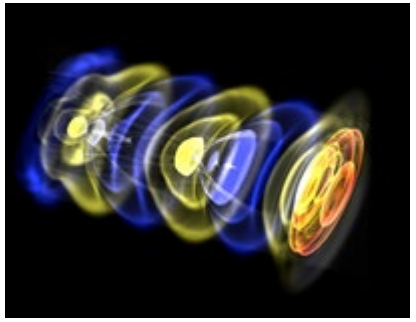
Native I/O format for plotfiles and checkpoint/restart

- multi-level mesh and particle data
- additional app-specific data may be included
- no restriction on number of ranks



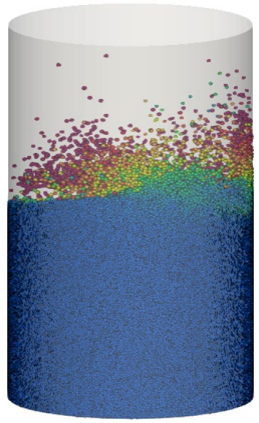
Plotfile format supported by Paraview, Visit, yt, AmrVis





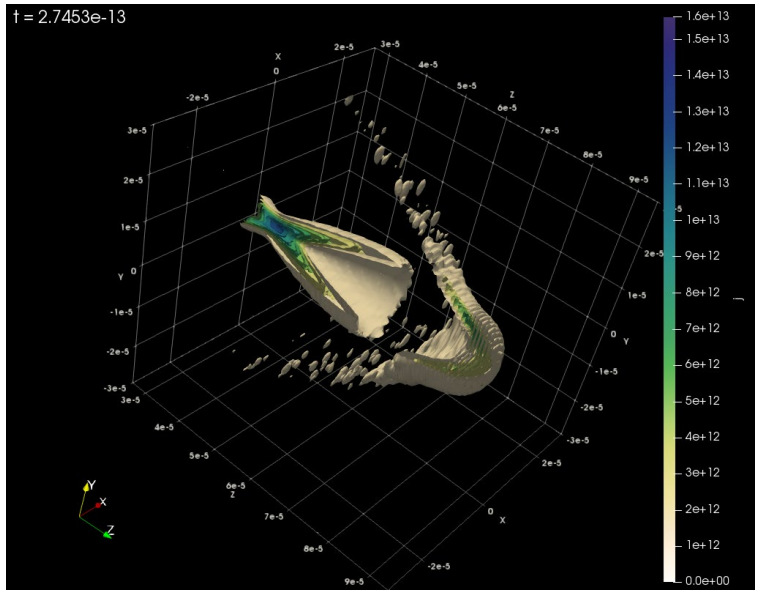
Optional HDF5 output format also supported (has compression)

Async capability developed for CPU/GPU systems

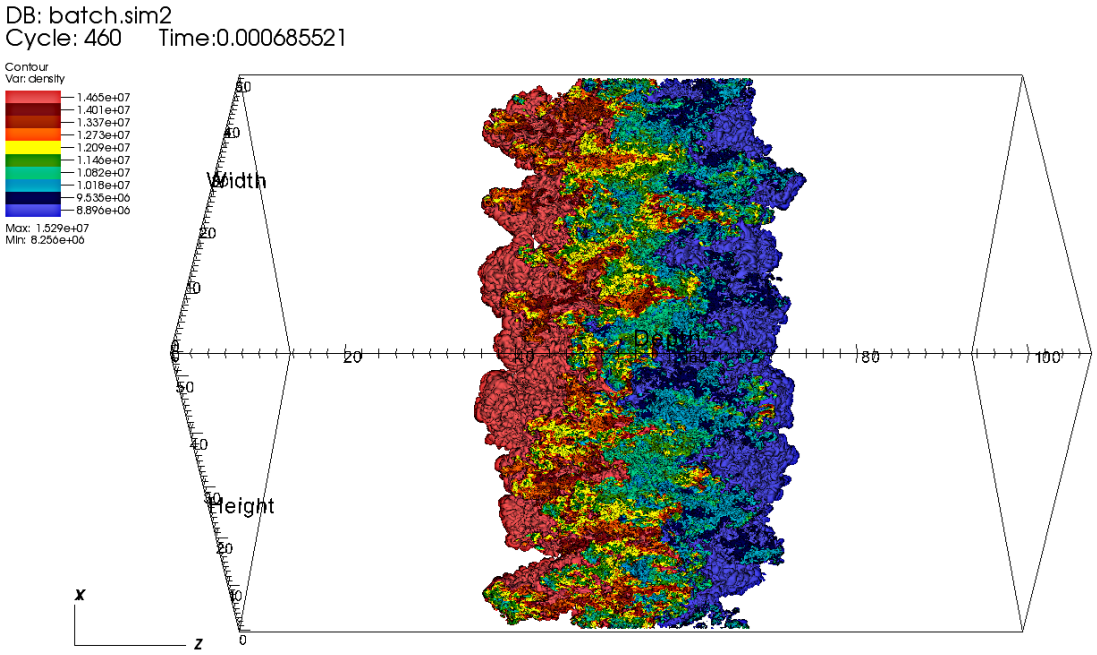


Some applications also interface with ADIOS

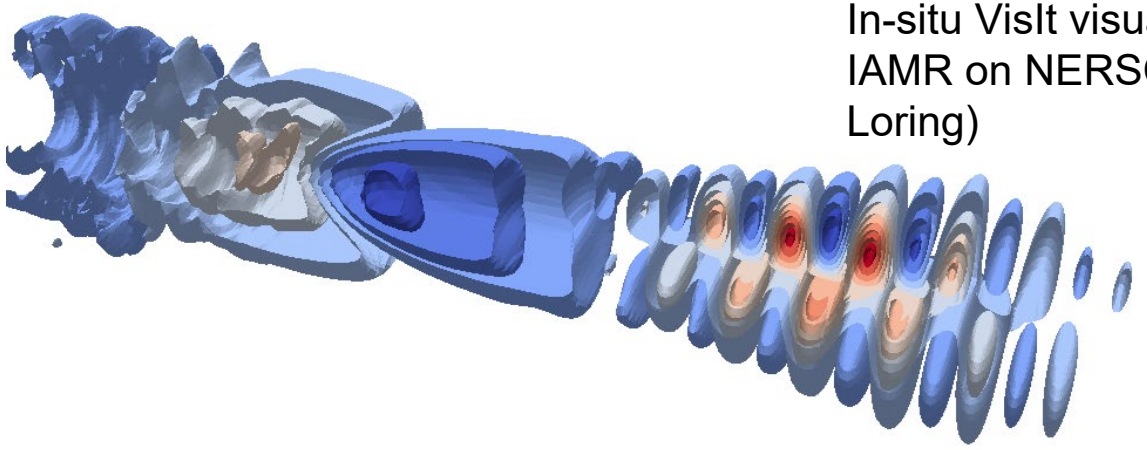
In-situ visualization with Ascent and SENSEI



In-situ visualization of an isocontour of j from WarpX using Paraview



In-situ VisIt visualization of a RT instability computing using IAMR on NERSC Cori with 2048 cores (courtesy of Burlen Loring)



Wakefield acceleration rendering using Ascent / VTKm

You shouldn’t have to use just one package:

Suppose your linear systems are too “hard” for geometric multigrid?

- Call **hypre/petsc** – as a solver for the full equation, or as a “bottom solver” in the GMG hierarchy

Suppose you want to experiment with different time-stepping schemes?

- AMReX is interoperable with **SUNDIALS** (see Time Integration section) – SUNDIALS time integrators understand MultiFABs …

Suppose your equations are too painful to type out in stencil form?

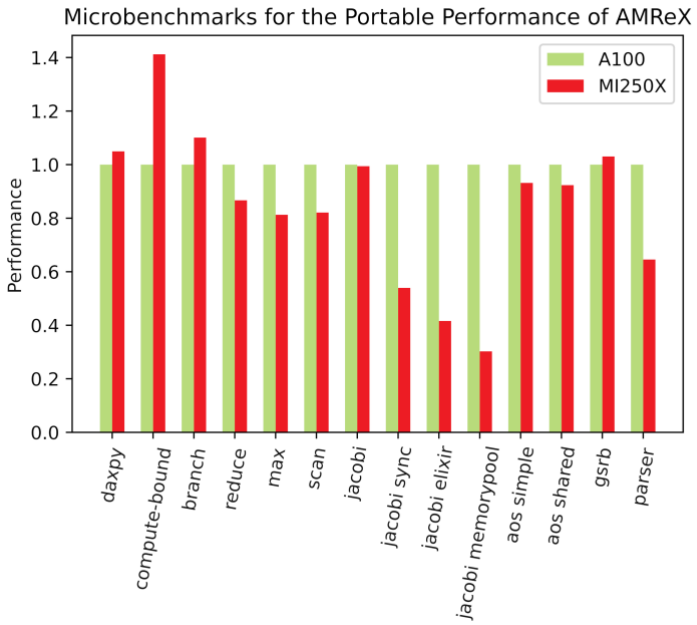
- Use the new “**CodeGen**” python/sympy → AMReX translator to express – in ready-to-compile code – the initial data and right hand side for your time evolution equation

Performance portability - ParallelFor looping construct

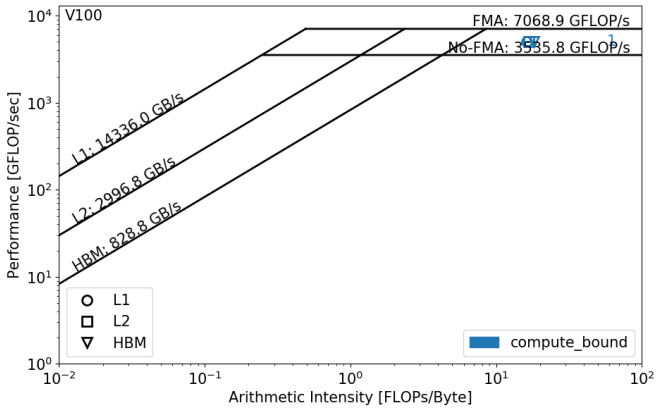
AMReX provides a ParallelFor looping construct based on C++ lambda functions (ported kernels from Fortran)

Similar to performance portability layers like Kokkos / Raja, but tailored to structured grid applications

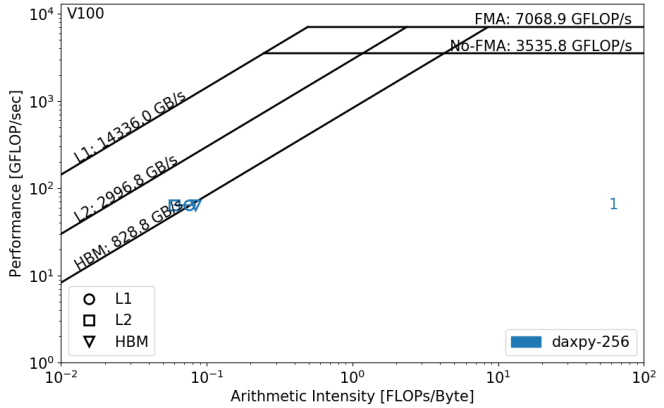
Translates to either a GPU kernel launch (CUDA / HIP / SYCL) or a normal for loop.




```
amrex::ParallelFor(bx,
[=] AMREX_GPU_DEVICE (int i, int j, int k) noexcept
{
    Real y = a(i,j,k);
    Real x = 1.0;
    for (int n = 0; n < 20; ++n) {
        Real dx = -(x*x-y) / (2.*x);
        x += dx;
    }
    a(i,j,k) = x;
});
```




```
amrex::ParallelFor(bx,
[=] AMREX_GPU_DEVICE (int i, int j, int k) noexcept
{
    a(i,j,k) = a(i,j,k) + 0.5*b(i,j,k);
});
```



In summary …

Recall what we've seen in our examples…

- "**AMR 101**": AMR for scalar advection
  - Multilevel mesh data – fluid velocity defined on faces and scalar ("ink") defined on cell centers
  - Dynamic AMR
  - Strong scaling behavior and CPU vs GPU ("performance portability")

- "**AMR 102**" : use a Poisson solve to compute incompressible flow around an obstacles and advect the particles in that flow field
  - Single-level mesh data – fluid velocity on faces, EB obstacles defined by volume and area fractions
  - Linear solver (geometric multigrid)
  - Particle advection

We didn't have time for this one, but "**AMReX-Pachinko**" is an example of particles falling under gravity through an obstacle course, bouncing off the solid obstacles – here we see an example of particle-obstacle and particle-wall collisions

https://xsdk-project.github.io/MathPackagesTraining2023/lessons/amrex/

Take Away Messages

- Different problems require different spatial discretizations and different data structures – the most common are
  - Structured mesh
  - Unstructured mesh
  - Particles (which can be combined with structured and/or unstructured meshes)

- Structured mesh doesn't equal "just" flow in a box

- There are quite a few AMR software packages – they have several commonalities and a large number of differences, both in what functionality they support and on what architectures they are performant

- Interoperability is important! See the next few sessions for how different packages can be used together.

If you're interested in learning more about AMREX:

- the software: https://www.github.com/AMReX-Codes/amrex
- the documentation: https://amrex-codes.github.io/amrex
- the tutorials: https://amrex-codes.github.io/amrex/tutorials_html/
- some movies based on AMReX: https://amrex-codes.github.io/amrex/gallery.html

A final takeaway …