Parallel Algorithms: Adaptive Mesh Refinement (AMR) method and its implementation

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• Solving Partial Differential Equations (PDEs)
  • PDEs solved using discrete domain
  • Algebraic equations estimate values of unknowns at the mesh points
  • Resolution/Spacing of mesh points determines error

• Goal of grid adaptivity:
  • tracking features much smaller than overall scale of the problem providing adequate higher spatial and temporal resolution where needed.
AMR - Introduction

**Uniform meshes**
- High resolution required for handling difficult regions (discontinuities, steep gradients, shocks, etc.)
- Computationally extremely costly

**Adaptive Mesh Refinement**
- Start with a coarse grid
- Identify regions that need finer resolution
- Superimpose finer subgrids only on those regions
- Increased computational savings over a static grid approach.
- Increased storage savings over a static grid approach.
- Complete control of grid resolution, compared to the fixed resolution of a static grid approach.

AMR makes it feasible to solve problems that are intractable on uniform grid
Demo of a Shock wave passing over a step function (wind tunnel with a step), rendered using the FLASH code. Courtesy of the Univ. of Chicago, Flash Code group

- CFD
- Astrophysics
- Climate Modeling
- Turbulence
- Mantle Convection Modeling
- Combustion
- Biophysics
- and many more
AMR Techniques

- mesh distortion

Courtesy of Dr. Andrea Mignone, University of Turin
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• mesh distortion
• point-wise structured (tree-based) refinement

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AMR Techniques

- mesh distortion
- point-wise structured (tree-based) refinement
- block structured:

- data blocks are created so that the same stencil can be used for all points and no special treatment is required.
- High level objects that encapsulate the functionality for AMR and its parallelization are independent of the details of the physics algorithms and the problem being solved.
- Simplifies the process of adding/replacing physics modules as long as they adhere to the interface requirements.

Courtesy of Dr. Andrea Mignone, University of Turin
Existing Frameworks

- PARAMESH - [http://www.physics.drexel.edu/~olson/paramesh](http://www.physics.drexel.edu/~olson/paramesh)
- SAMRAI - [https://computation.llnl.gov/casc/SAMRAI/](https://computation.llnl.gov/casc/SAMRAI/)
- Chombo - [https://commons.lbl.gov/display/chombo/Chombo](https://commons.lbl.gov/display/chombo/Chombo)
- and many more
Typical grid hierarchy

- Each block has a fixed number of grid points
- Each block can be divided into $2^{\text{ndim}}$ sub-blocks
- Blocks are distributed between processes minimizing communications (see next slides)

An Example:
- 6 x 4 grid is created on each block
- The numbers assigned to each block designate the blocks location in the quad-tree
- The numbers assigned to each block designate the blocks location in the quad-tree

From Paramesh User Guide
• All the grid blocks are related to one another as the nodes of a tree.
• The starting block is called root block, and the blocks with an higher resolution are called leaf blocks.
• When a leaf block is designated for refinement, it spawns 2 child blocks in 1D, 4 child blocks in 2D or 8 child blocks in 3D, and the original block is called mother (or parent) block.
• These child blocks cover the same physical line, area or volume as their parent but with twice the spatial resolution.
• Usually it is helpful to use a particular numbering algorithm (see next slides).

From Paramesh User Guide
Usually, the most used block ordering algorithm is Morton (or Z) ordering. It is particularly useful in order to:
- Optimize the usage of cache memory;
- Optimize ghost cells communications between process (see next slide);
Usually, each block is composed by:
- standard cells
- ghost cells

In Fortran, the indexes starts with 1 and ends with $N_{(X \text{ or } Y \text{ or } Z)} + 2 \times (\text{number of ghost cells})$

In C, the indexes starts with 0 and ends $N_{(X \text{ or } Y \text{ or } Z)} + 2 \times (\text{number of ghost cells}) - 1$

Indexing scheme for a 2D grid block with 2 guard cells $(\text{nguard}=2)$ at each block boundary. Interior cells are colored red, guard cells are colored blue.

From Paramesh User Guide
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- ghost zones values need to be filled before integration;
- Patches at the same level are synchronized;
- Physical boundaries are imposed externally;
- Fine-Coarse and Coarse-Fine interface need interpolation / averaging
- Integration proceeds as for the single-grid case
When we pass the ghost cells to the adjoining blocks, if these blocks have different resolutions we must modify the data.

The most simple (and used) method is the interpolation method:
• If we must pass the ghost cells to a block with higher resolution we can use the linear interpolation to artificially increase the resolution.
• If we must pass the ghost cells to a block with lower resolution we can average the data in order to have the same resolution.

Pros:
• Easy to implement
• It is possible to use many different kind of interpolation (linear, quadratic, and so on) increasing precision

Cons:
• Non-conservative
Flux conservation:
It is possible to ensure flux conservation after the interpolation checking the equation:
\[ f_1 A_1 + f_2 A_2 + f_3 A_3 + f_4 A_4 = F_{\text{Tot}} A_{\text{Tot}} \]

Summation of fluxes at shared cell faces on adjoining grid blocks at different refinement levels. Flux densities are denoted by \( f \) and cell face areas by \( A \).

From Paramesh User Guide
Passing ghost cells to neighbors blocks

Circulation integral control:
It is possible also to check the value of some physical quantity at the edges of the cells

NOTE: Both these three methods are usable in order to change the resolution of the blocks.

From Paramesh User Guide

Edge based data on the shared cell face of adjoining grid blocks of different refinement level.
When we have a non symmetric computational domain many different approach can be used. For a rectangular domain:

• We can have different number of points per block on x and y directions ($dx = dy$)

• We can have different number of points on x and y directions ($dx \neq dy$)

• We can use more blocks on the x directions, and 1 block on x direction (same resolution on x and y, and more parallelizable)

If we have more complicate computational domains, we can always use more blocks in order to fully cover the whole domain.

From Paramesh User Guide
• fill data, level 0

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How to refine

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- find where refinement is needed;

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efficiency = 0.5
efficiency = 0.9
efficiency = 0.7

Courtesy of Dr. Andrea Mignone, University of Turin
Little more background on AMR

Refinement structure can be represented using a quad-tree (2D)/oct-tree (3D)

An important condition in AMR
Refinement levels of neighboring blocks differ by ±1
Note: This is generally true, but Chombo library allow more than 1 refinement level discrepancy.
A set of blocks assigned to a process
Use space-filling curves for load balancing
Traditional Approach - Disadvantages

- Adaptive mesh restructuring:
  - Tree metadata replicated on each process
    - Required memory increases with # of cores
    - Memory can became a problem if we use more than $10^5$ cores (and more than $10^6$ boxes)
  - Level-by-level restructuring
    - Ripple propagation
    - Step needed to propagate restructuring $\propto$ level of refinement ($d$)

- Load Balancing
  - Memory needed $\propto$ Number of blocks used
  - Time needed $\propto$ Number of blocks used

- Currently for 3D problems with less than $10^6$ boxes standard AMR library scales up to few tens of thousands of cores
- This is a serious problem considering that next generation supercomputers will require the use of many hundreds of thousands of cores
1. Compress tree metadata
   • Already implemented in the last versions of CHOMBO, PARAMESH and SAMRAI libraries

2. Rewrite the algorithm for coarse-fine interpolation in order to minimize communications
   • Already implemented in the last versions of CHOMBO, PARAMESH libraries
   • Using these first two methods it is possible to scale up to $2 \times 10^5$ cores using $10^7$ grid cells

3. Use a distributed memory version for tree metadata
   • Currently Langer at al are working on the implementation of this algorithm on CHARM++
Some additional information about PARAMESH

- Written in Fortran 90
- Easy to implement on an existing code
- Support many geometries (Cartesian, cylindrical, spherical, from 1D to 3D)
- Refinement levels of neighboring blocks differ by ±1
- Compatible with hdf5 format
- Some simple routine are already written by the authors of the library in order to save the data and the grid structure into Fortran binary format, and hdf5 format.
- Easy visualization of the results using many external programs (e.g. visit)
Some additional information about CHOMBO

• Written in C
• Easy to implement on an existing code
• Support many geometries (Cartesian, cylindrical, spherical, from 2D to 3D)
• Compatible with hdf5 format
• Easy visualization of the results using many external programs (e.g. visit)
**Problem:** Blast Wave – Cloud Interaction

**Base Grid:** 128x128

**Levels of Refinement:** 5 (eq. 4096x4096)

**Method:** Unsplit PPM

**Code:** PLUTO + Chombo Lib

Example: 2D Blast Wave

Courtesy of Dr. Andrea Mignone, University of Turin
Example: 3D Rayleigh-Taylor

**Problem:**
Rayleigh Taylor

**Base Grid:**
32x64x32

**Levels of Refinement:**
2 (eq. 128x256x128)

**Method:**
Unsplit PPM

**Code:**
PLUTO + Chombo Lib

Courtesy of Dr. Andrea Mignone, University of Turin
Thank you for attention

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