Data Structures for Scientific Computing

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2011/04/14

Overview

- Introduction and Motivation
- Structured Grids
  - Adaptive structured grids
- Unstructured Grids
  - Adaptive unstructured grids
- Particles and Spatial Search
  - Regular grids
  - Trees

Introduction / Motivation

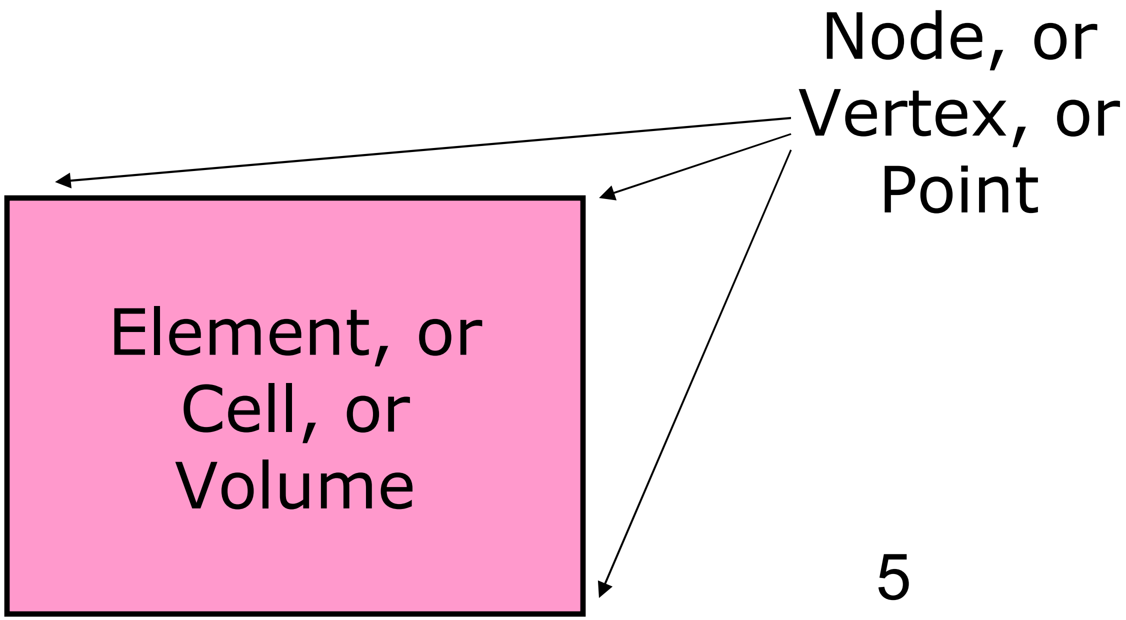
- There are only a few ways to represent the problem domain:
  - Structured Grids
  - Unstructured Grids
  - Particles

- Knowing the basic terms helps you talk to application folks, and understand their code

Grids in General

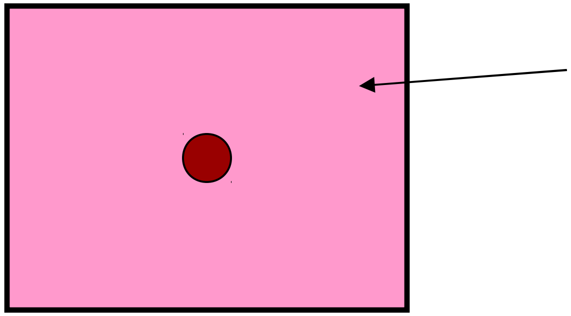
Grids: Introduction

- **So you're trying to represent some physical situation, like heat flow**
- **You decide to divide up space into a bunch of little pieces:**



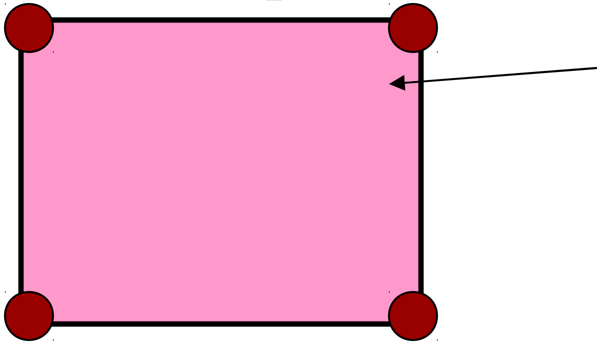
Grids: Location of Data

- **Element Centered Data**
  - **Fluid Dynamics, most PDEs**



Data values constant (or simple) in a cell

- **Node Centered Data**
  - **Structural dynamics/FEM**



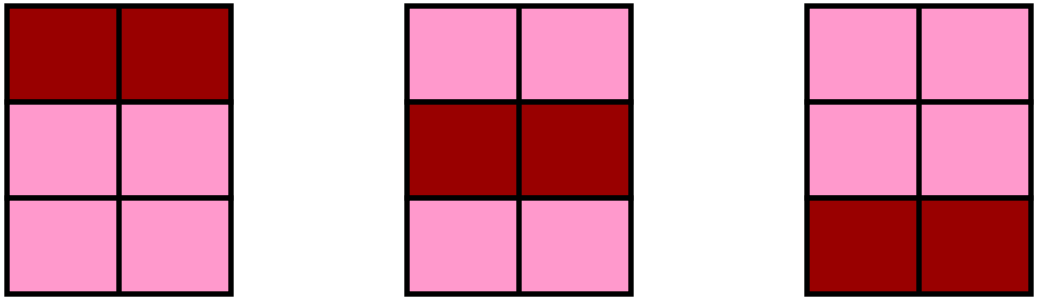
"Shape function" interpolates between nodes

Hybrids too,like

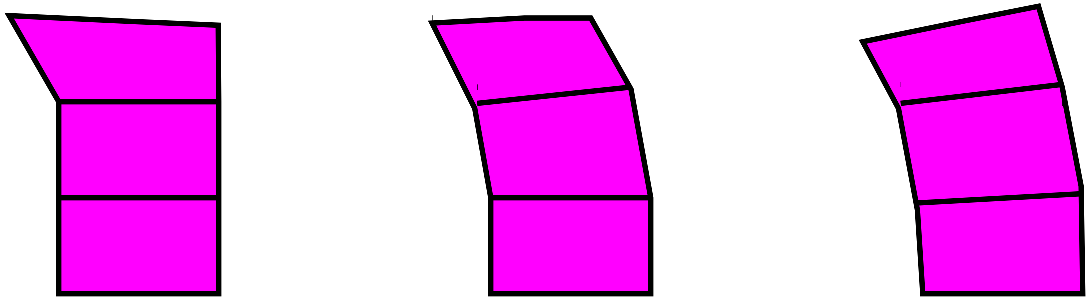
Arakawa C-grid

Grids: Motion of Grid and Data

- **Eulerian: non-moving grid**
  - **E.g., pressure waves move through the grid in CFD**



- **Lagrangian: moving grid**
  - **E.g., grid deformation follows the structure deformation in FEM**

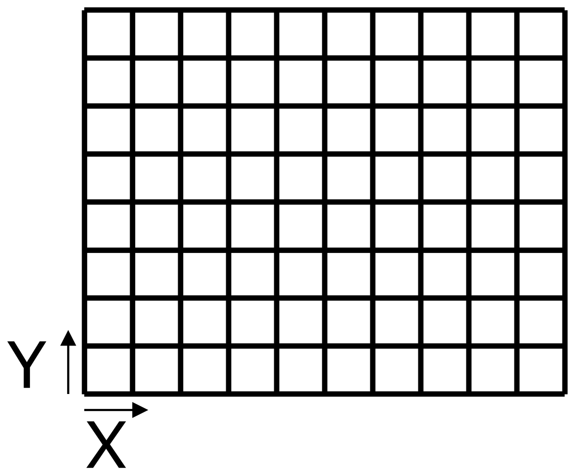


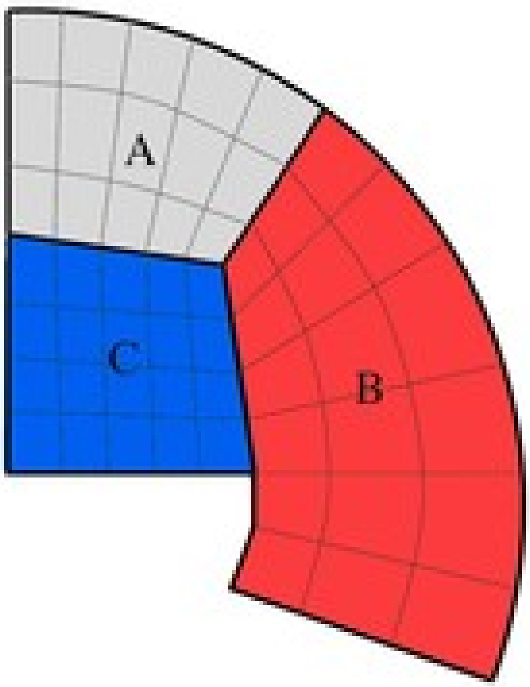
Or hybrid, e.g. "ALE"

Structured Grids

Structured Grids: Introduction

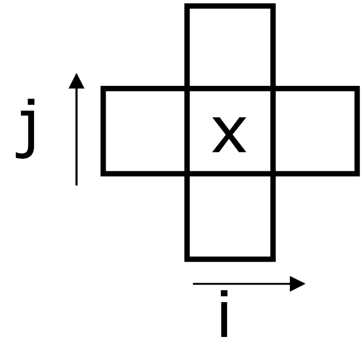
- **AKA "Regular Grid", since grid cells lie in regular rows and columns**
- **Cells are stored in a 3D array**
- **Cells can lie along axes ("rectilinear grid"); or curve through space**



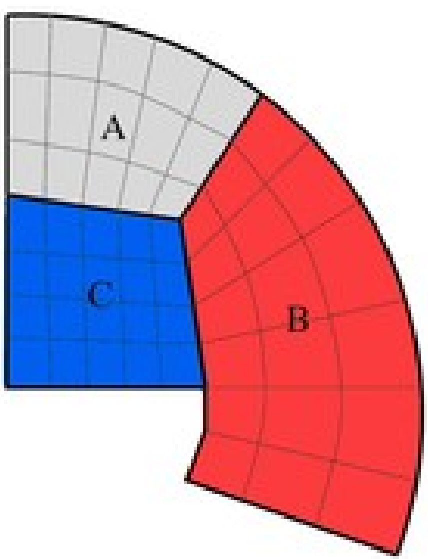


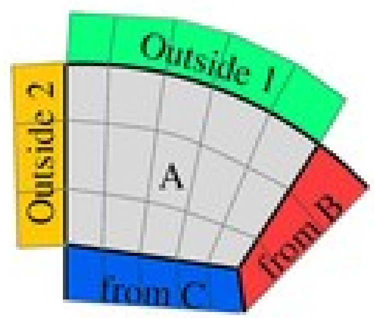
Structured Grids: Terminology

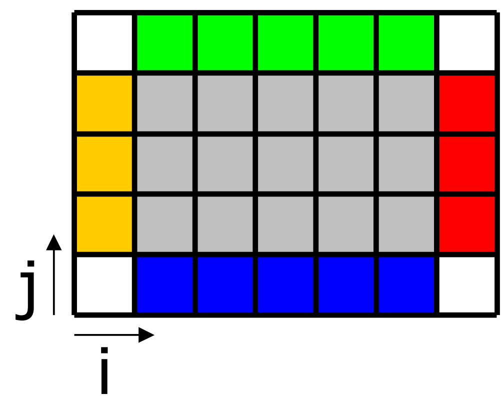
- "Stencil" of source cells to compute a destination cell
  - Classic GPU algorithm
  - Common in fluid dynamics
  - Also found in PDE solvers



- Read-only "Ghost" or "Dummy" cells around boundary







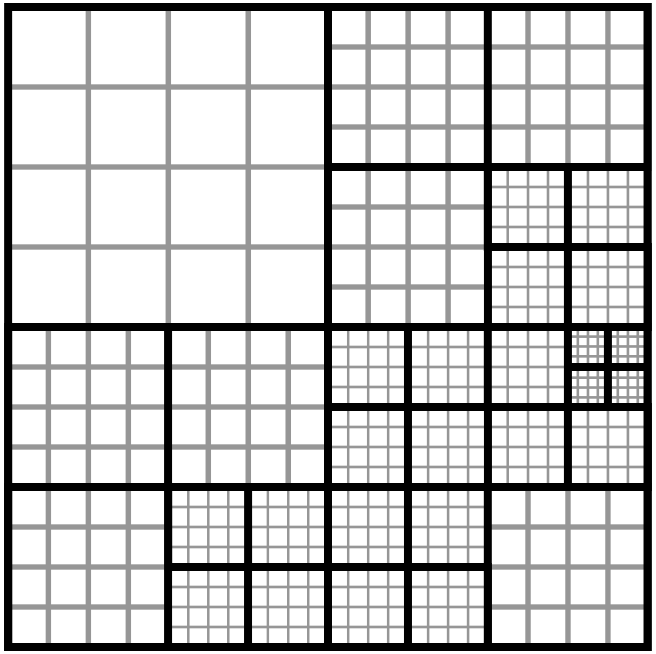
Structured Grids: Applications

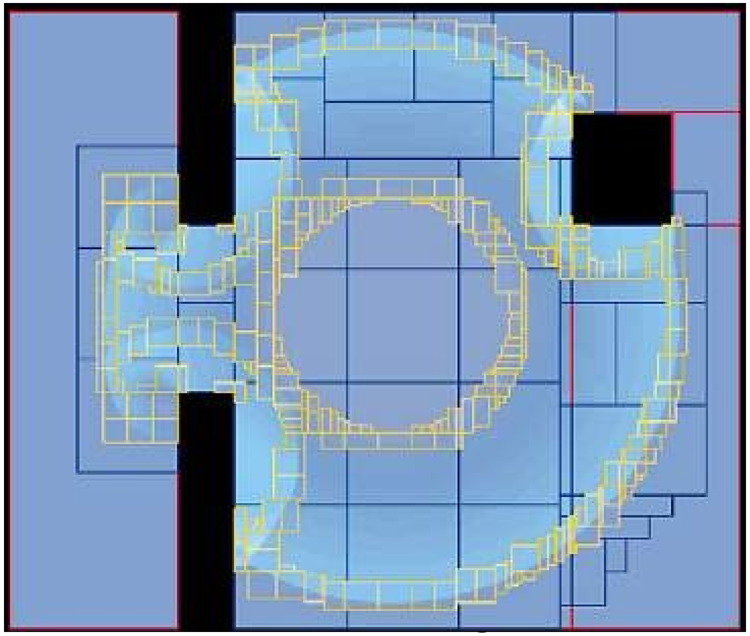
- Fluid Dynamics
  - Classical fluid dynamics grid
- Jacobi and other PDE solvers
  - "Finite Difference" formulation
- Level set methods
  - E.g., fluid solidification phase field
- Image processing
  - Just a 2D pixel array!

Adaptive Structured Grids

Adaptive Structured Grids: Intro

- "Adaptive Mesh Refinement"/AMR
- Cells are stored in small 3D arrays, linked together with pointers
- For regular refinement, use quadtree (2D) or octree (3D); can be irregular "block structured AMR"



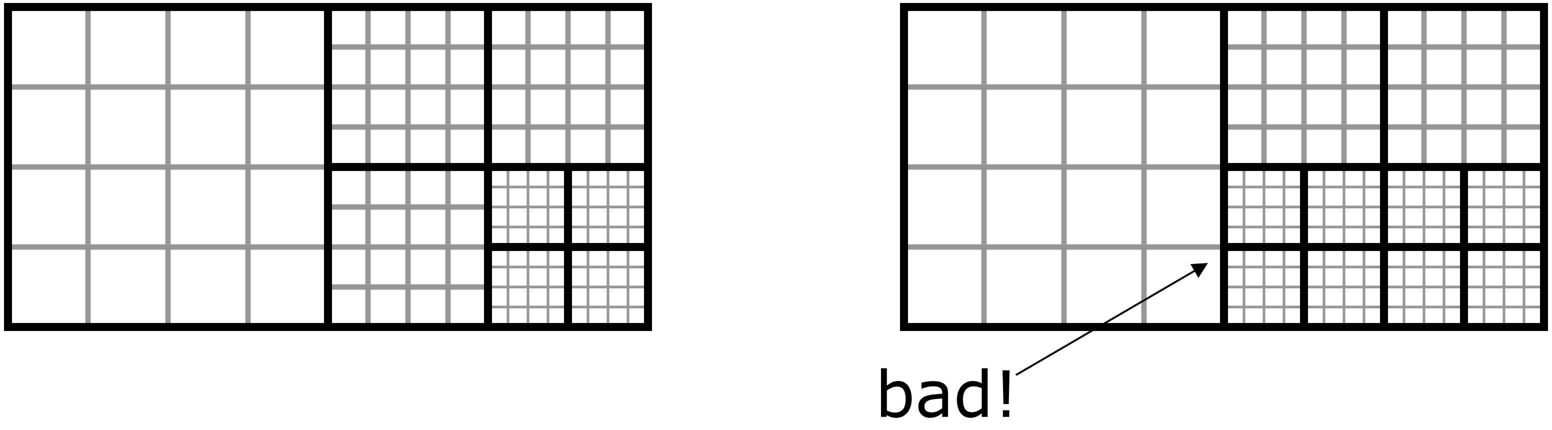


from LLNL SC98 SAMRAI flier

Adaptive Structured Grids: Terms

- "Refinement" and "Coarsening" criteria control evolution of mesh
  - Basically simulation error estimates

- "Hanging Node Constraint"
  - Neighbors must have similar (±1) refinement level



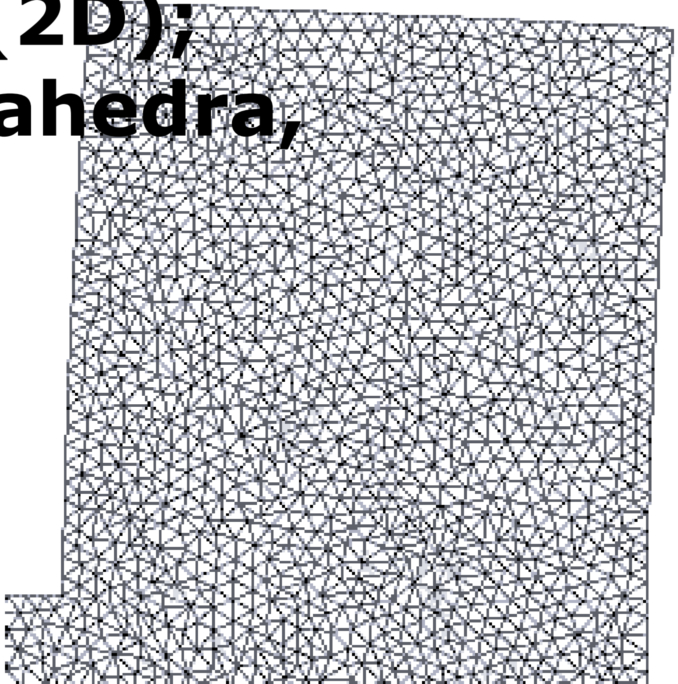
Adaptive Structured Grids: Apps

- Adaptive physics solvers
- LLNL SAMRAI C++ Framework
- NASA GSFC PARAMESH
- AMRITA (James Quirk)
- INRIA GPU Gems 3:5

Unstructured Grids

Unstructured Grids: Introduction

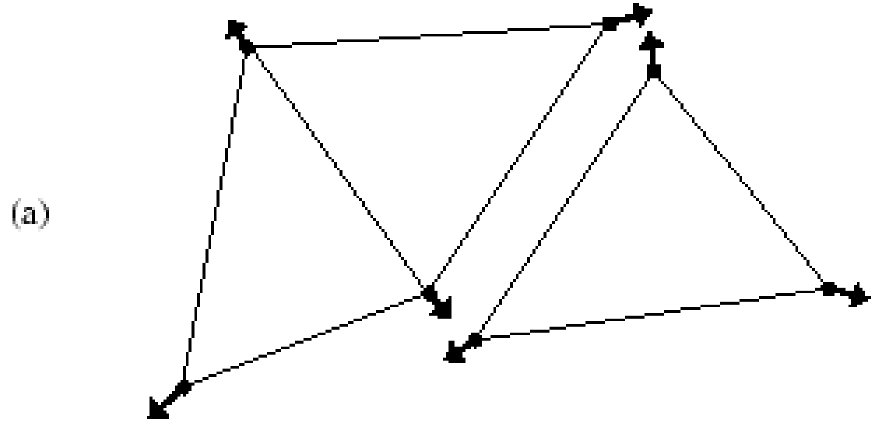
- **AKA "Mesh"**
- **Cells are stored in 1D array**
- **Vertices ("nodes") of each cell ("element") are listed explicitly**
- **Mesh consists of triangles and/or quadrilaterals (2D); tetrahedra, cubes/hexahedra, prisms, pyramids (3D)**



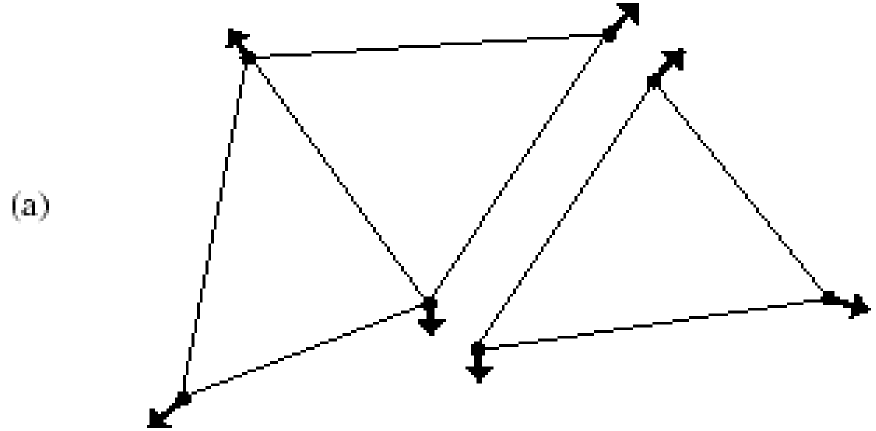
Unstructured Grids: Terms

- "Ghost regions", like structured grids
- "Shared nodes" along partition boundaries:

- Run computation on separate pieces

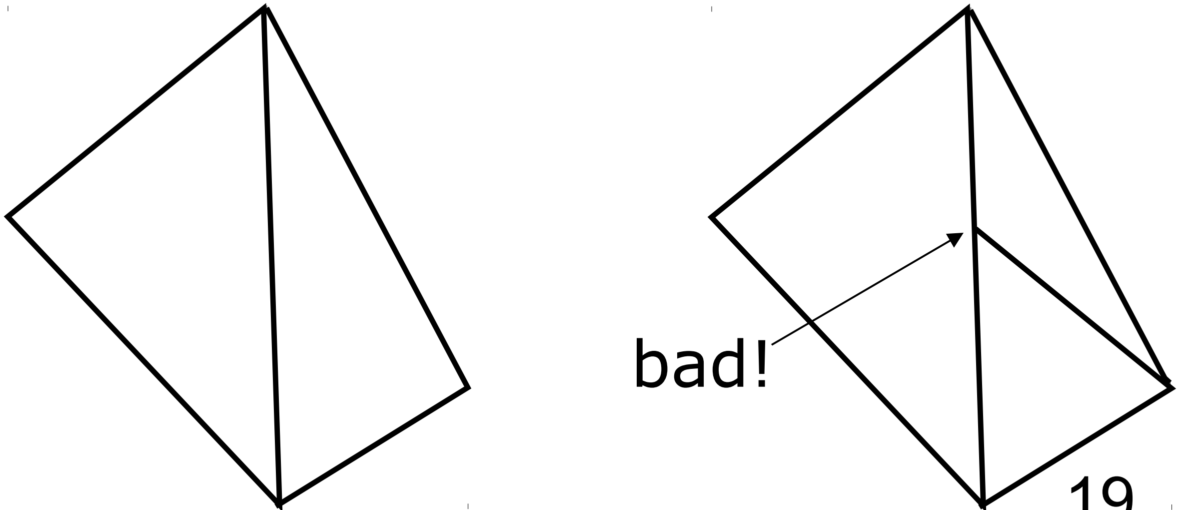


- Add up node forces along boundaries



Unstructured Grids: Terms

- "Conformality"
  - Nodes never land in middle of element
  - Enforced during mesh generation/modification



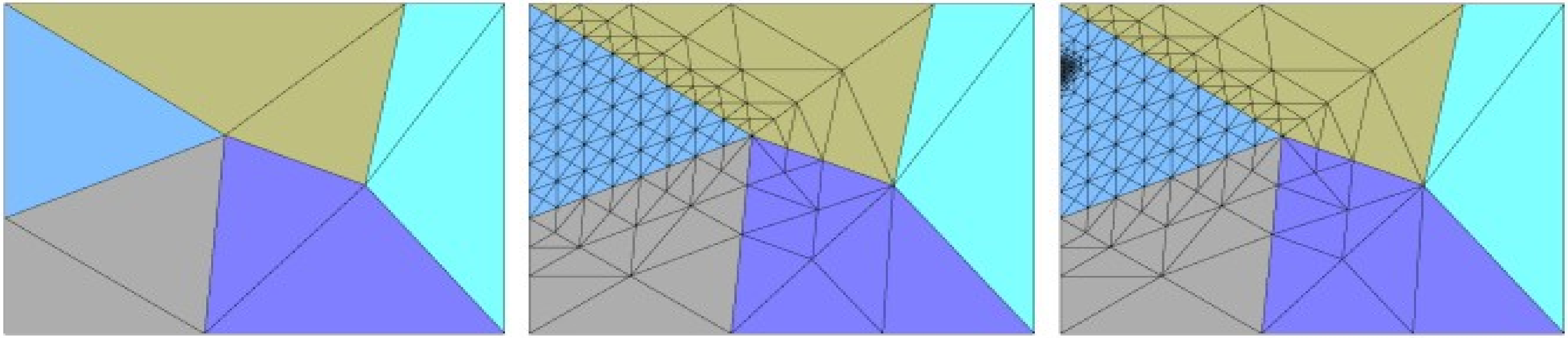
Unstructured Grids: Applications

- Structural Mechanics
  - This is the classic finite element mesh
- Fluid Dynamics
  - In strange domains, where structured grids are tough to automatically generate
- Can be extended to Adaptive Meshes!

Adaptive Unstructured Grids

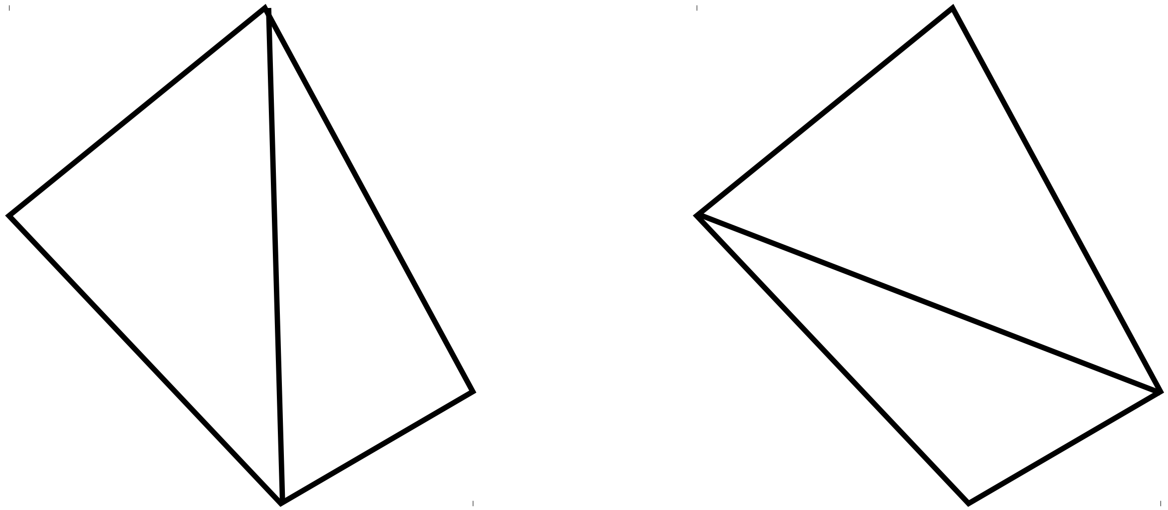
Adaptive Unstructured Grids: Intro

- AKA "Mesh Refinement", shades into from-scratch "Mesh Generation"
- Cells still stored in 1D arrays, but the cells can now change
- Must respect conformality
- Must ensure element "quality"
- Must work in parallel

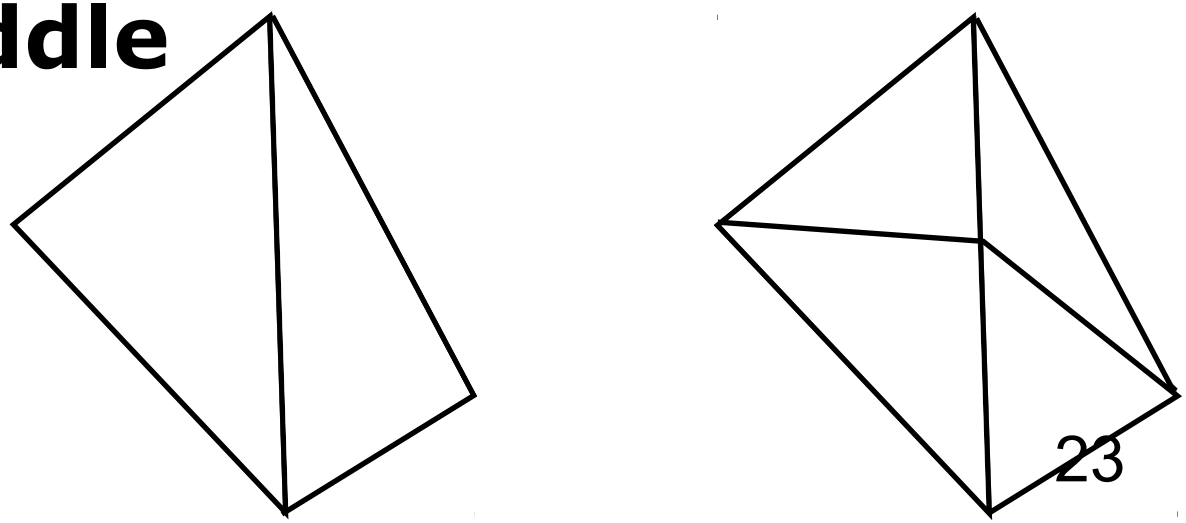


Adaptive Meshes: Terminology

- **"Delaunay" mesh and "flip"**



- **"Edge bisection": cut edge in middle**



Adaptive Meshes: Applications

- **Almost every unstructured mesh program wants to be adaptive.**

- **Charm++ Triangle Mesh Refinement (Wilmarth)**
- **Charm++ PMAF3D (Wilmarth)**
- **Charm++ Tet Data Transfer Library (Lawlor)**

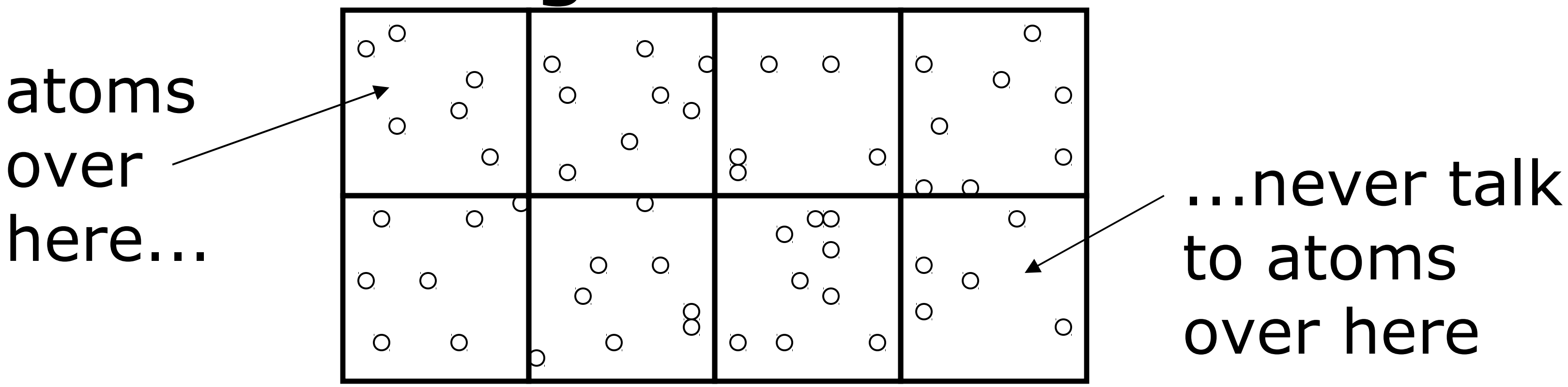
Particle Methods and Spatial Search

Particles and Spatial Search

- **To work on a particle, you need nearby particles**
  - **E.g., all particles within cutoff *r***
    - **Used for molecular dynamics (NAMD)**
  - **or, all *k* nearest particles**
    - **Used by Smoothed Particle Hydrodynamics (SPH) methods**
- **Search for neighboring particles is spatial, so need a "spatial search structure"**
  - **Can use: structured grid, adaptive search tree, unstructured grid, ...**

… using Structured Grids

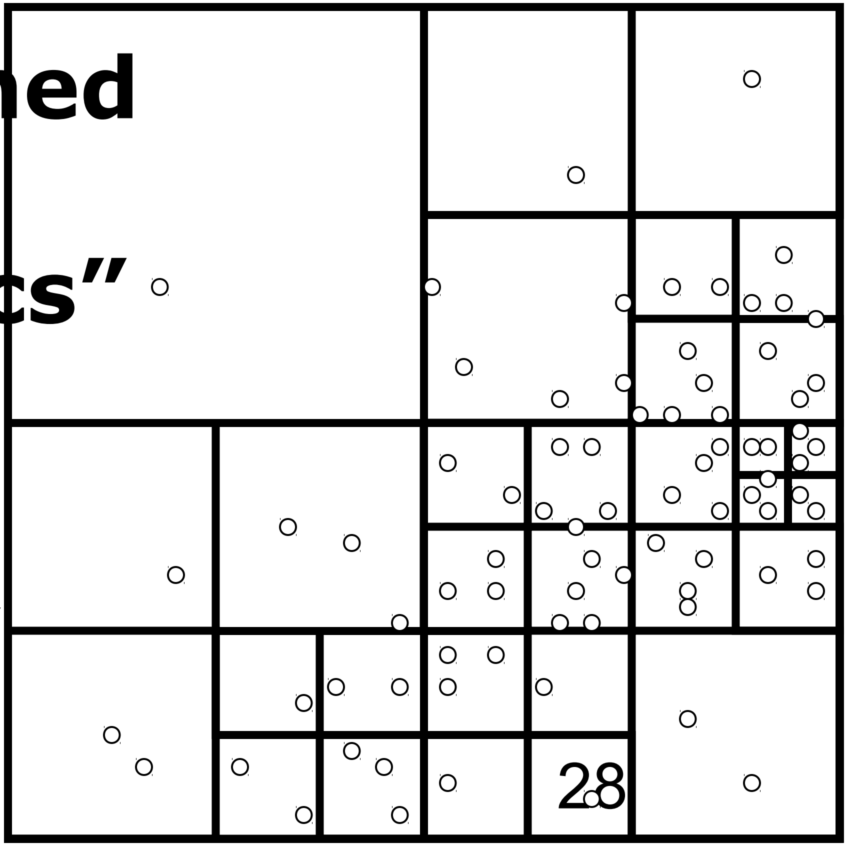
- **E.g., NAMD molecular dynamics**
  - **Particles are Atoms**
  - **Search structure is based on "Patches" of space in regular, rectilinear grid**



- **E.g., Charm++ Collision Library**
  - **Search structure is based on regular rectilinear voxel grid**

… using Search Trees

- E.g., Cosmology simulations
  - Particles are stars, galaxies
  - Search structure is a spatial octree
- SPH: “Smoothed particle hydrodynamics”
- Barnes-Hut gravity
  - “Tree walk”



Conclusions

Conclusions

- **There are only a few ways to represent the problem domain:**
  - **Structured Grids**
  - **Unstructured Grids**
  - **Particles**
- **There are a lot of specialized <u>terms</u>, but very few concepts**