Data Structures for Scientific Computing

Orion Sky Lawlor

charm.cs.uiuc.edu

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Overview

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

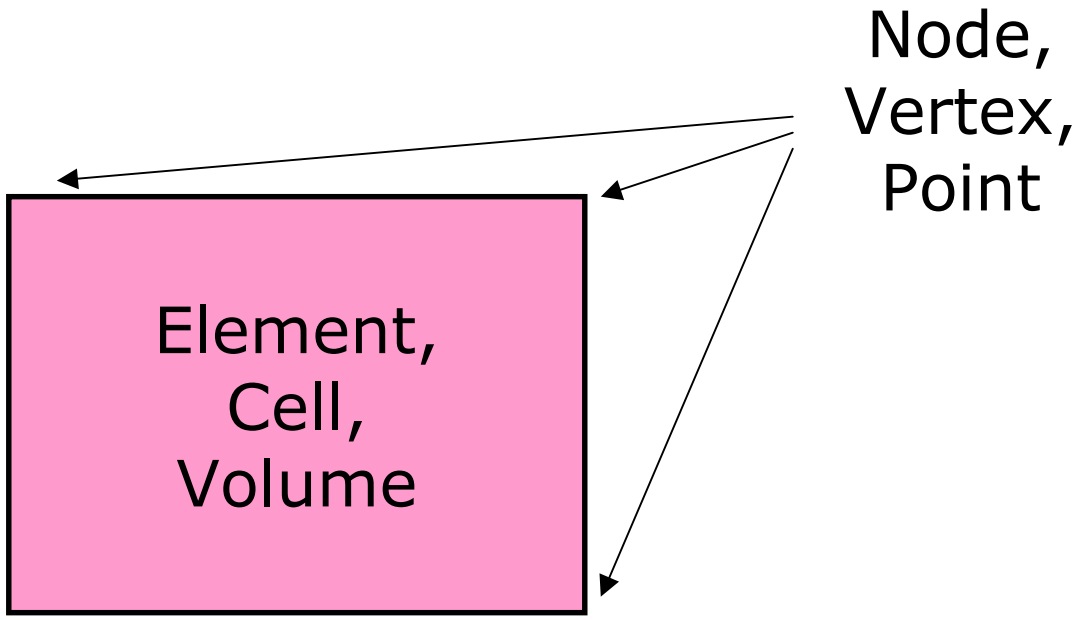
Introduction / Motivation

- There are only a few ways to represent the problem domain:
  - Structured Grids
  - Unstructured Grids
  - Particles
- This set covers all our grants!
- Knowing the basic terms helps you talk to application folks, and understand their stuff

Grids in General

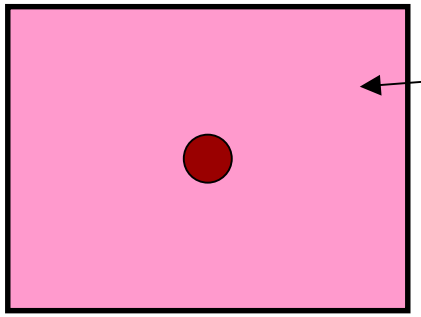
Grids: Introduction

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



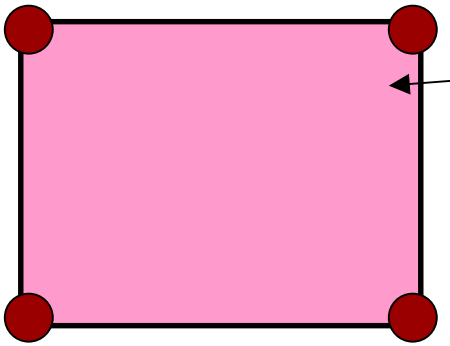
Grids: Location of Data

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



Data values constant (or simple) in a cell

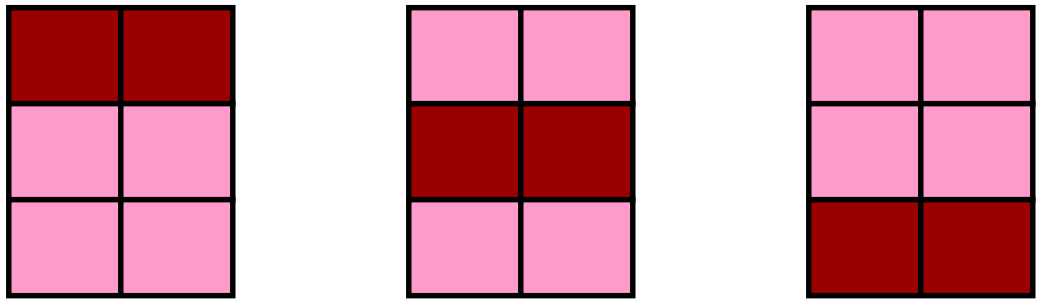
- **Node Centered Data**
  - **Structural dynamics/FEM**



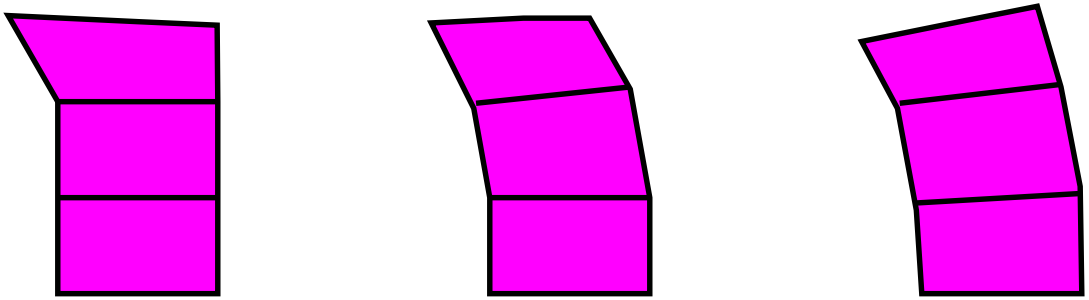
"Shape function" interpolates between nodes

Grids: Motion of Grid and Data

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



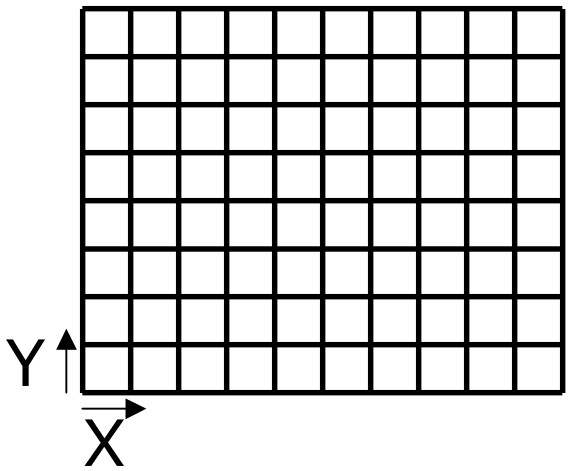
- **Lagrangian: moving grid**
  - **E.g., grid deformation follows the structure deformation in FEM**

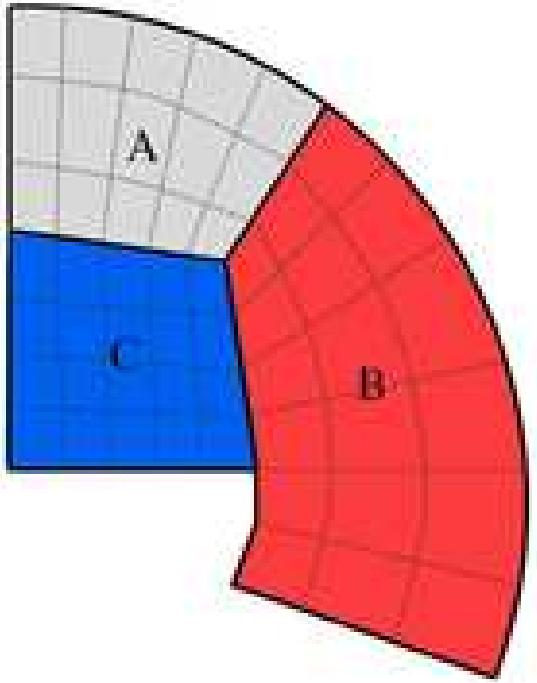


Structured Grids

Structured Grids: Introduction

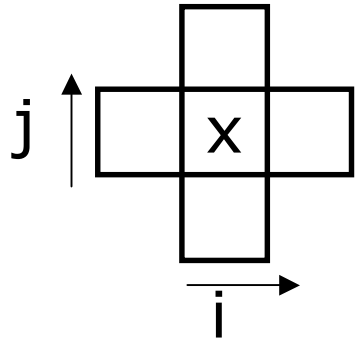
- AKA "Regular Grid", since grid cells lie in regular rows and columns
- Cells are stored in a 3D array
- Cells can lie along axes ("rectilinear grid"); or curve through space



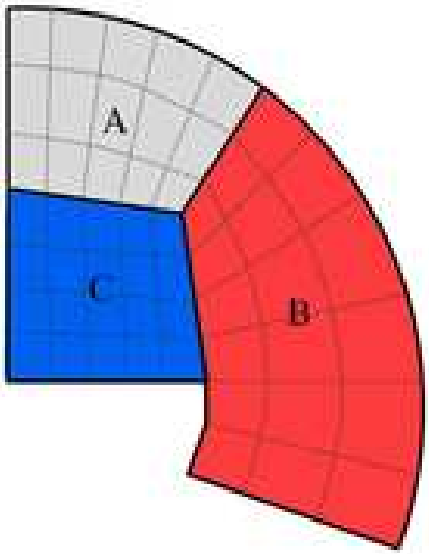


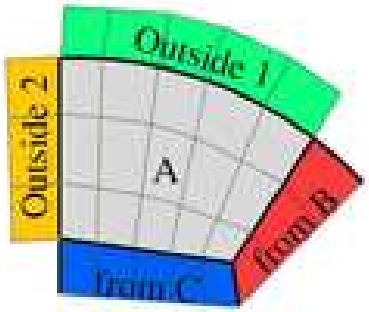
Structured Grids: Terminology

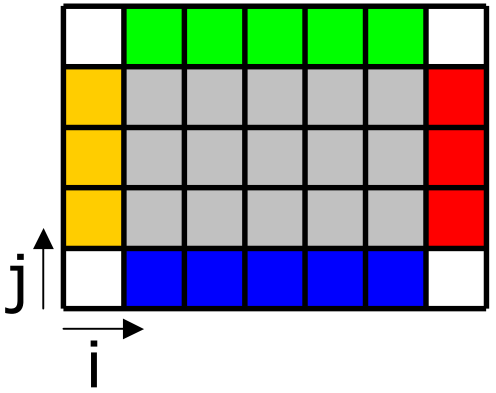
- "Stencil" of source cells to compute a destination cell
  - Common in fluid dynamics
  - Also found in PDE solvers



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







Structured Grids: Applications

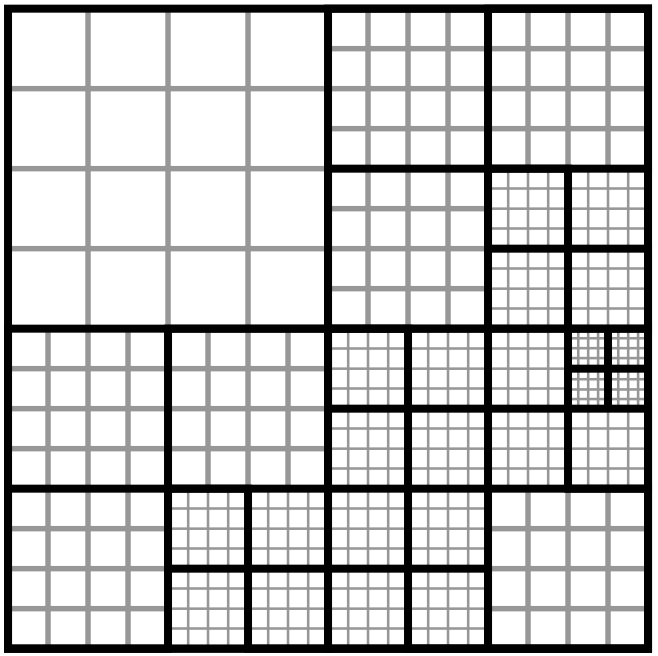
- Fluid Dynamics
  - CSAR's Rocflo (Jiri Blazek)
- Jacobi and other PDE solvers
  - "Finite Difference" formulation
- Level set methods
  - CPSD (Danzig)
- Image processing
  - Just a 2D pixel array!

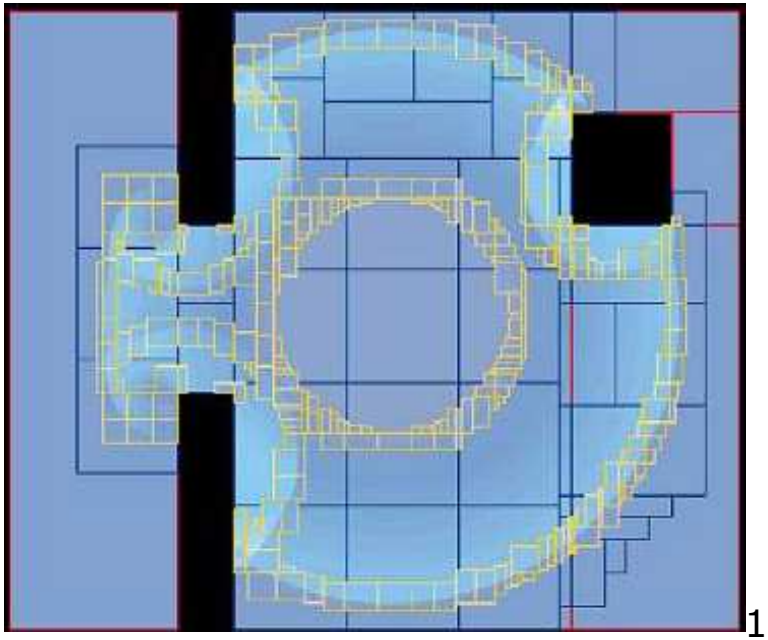
- Charm++ Multiblock Framework

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"



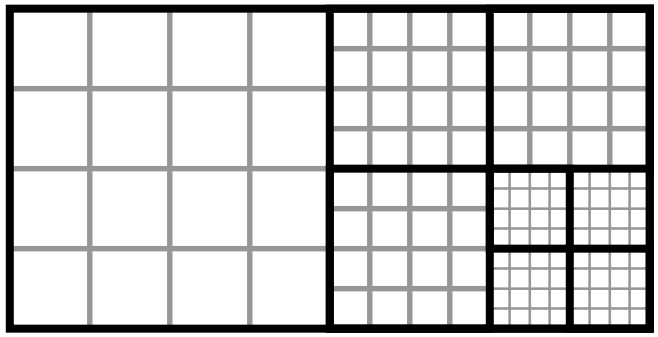


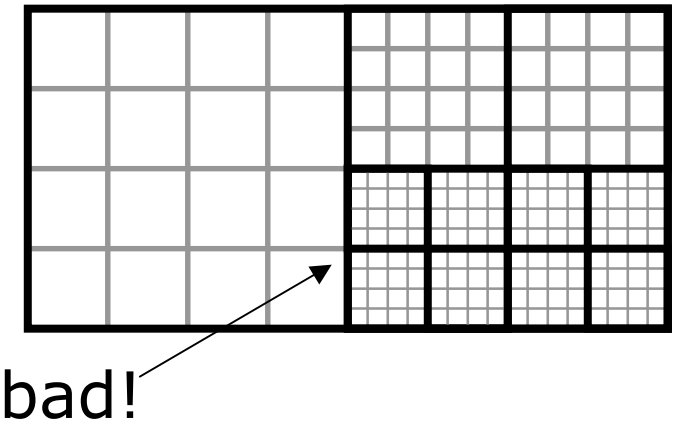
from LLNL SC98 SAMRAI flier

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**





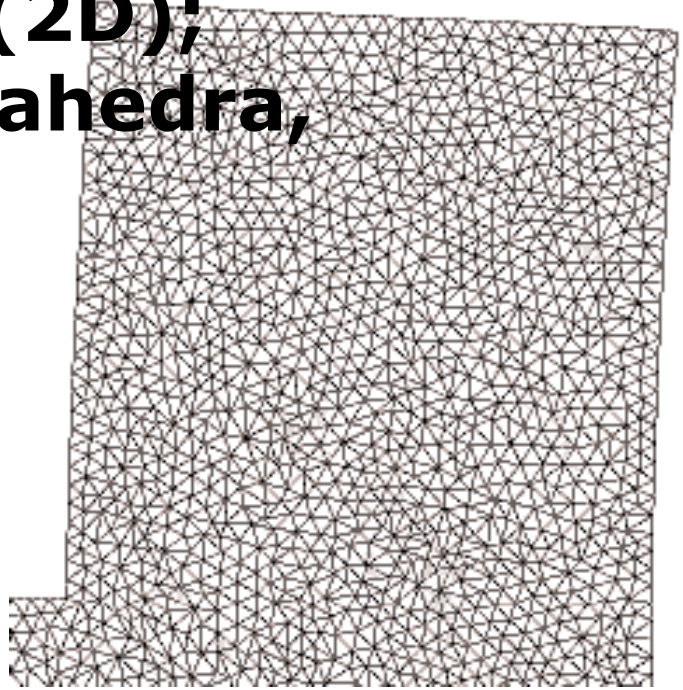
Adaptive Structured Grids: Apps

- Adaptive physics solvers
  - CPSD Dendritic Growth (Danzig)
    - Octree-based 3D fluids code
- LLNL SAMRAI C++ Framework
- NASA GSFC PARAMESH
- AMRITA (James Quirk)
- Charm++ AMR Framework (Narula, Jyothi)

Unstructured Grids

Unstructured Grids: Introduction

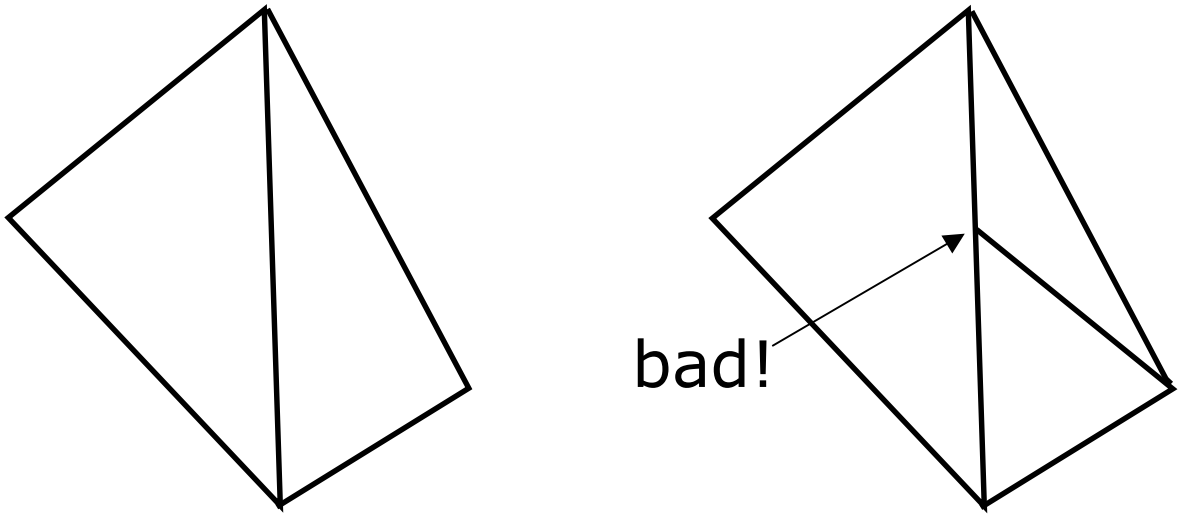
- AKA "Mesh"
- Cells are stored in 1D array
- Vertices ("nodes") of cells ("elements") listed explicitly
- Mesh consists of triangles and/or quadrilaterals (2D); tetrahedra, cubes/hexahedra, prisms, pyramids (3D)



Unstructured Grids: Terms

- "Ghosts", like structured grids
- "Shared nodes" along partition boundaries--see FEM manual

- "Conformality"
  - Nodes never land in middle of element



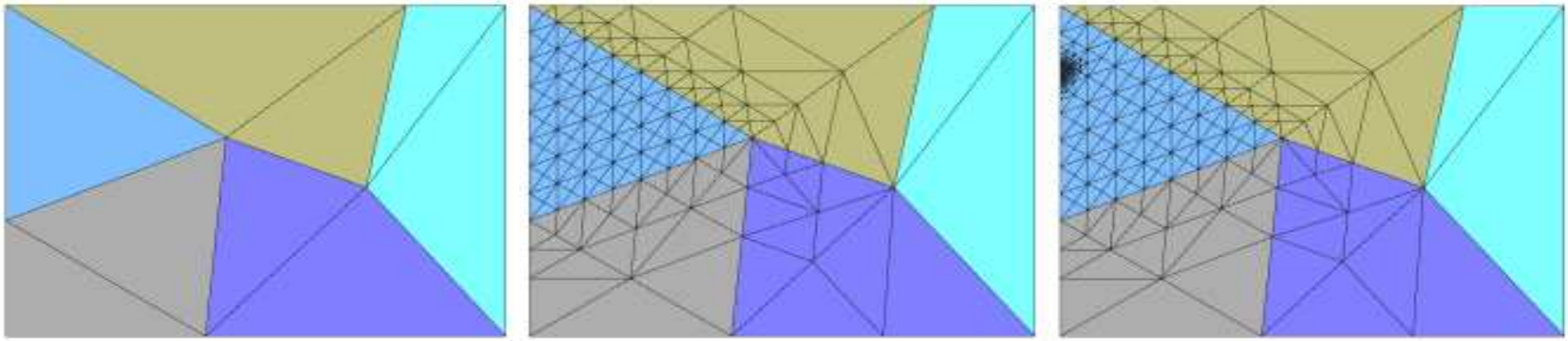
Unstructured Grids: Applications

- Structural Mechanics
  - CSAR's Fractography (Geubelle)
- Fluid Dynamics
  - CSAR's Rocflu (Haselbacher)
- Even Adaptive Meshes!
  - CPSD Dendritic Growth (Danzig)
- Charm++ FEM Framework (Lawlor)

Adaptive Unstructured Grids

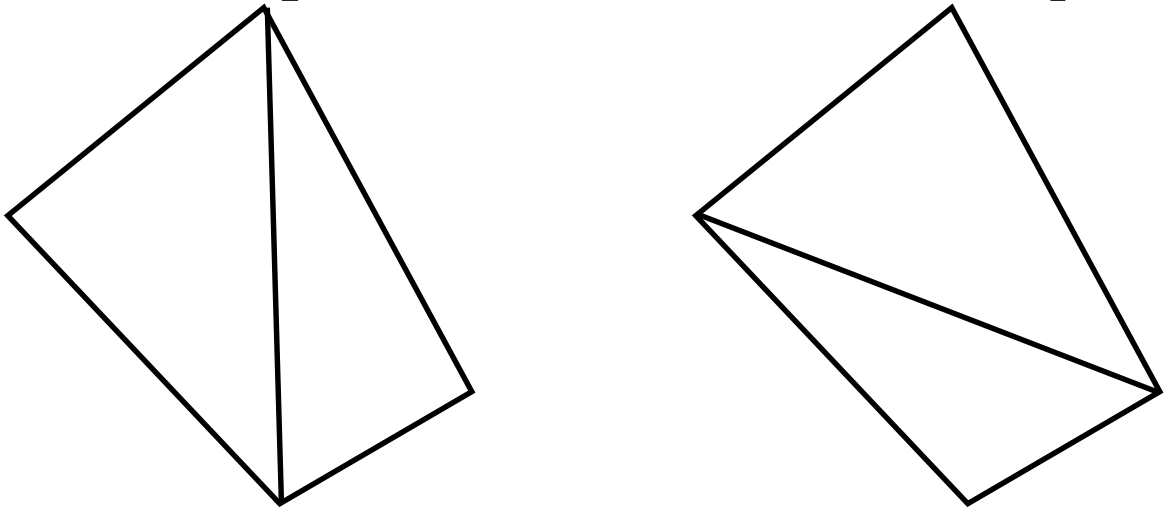
Adaptive Unstructured Grids: Intro

- 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

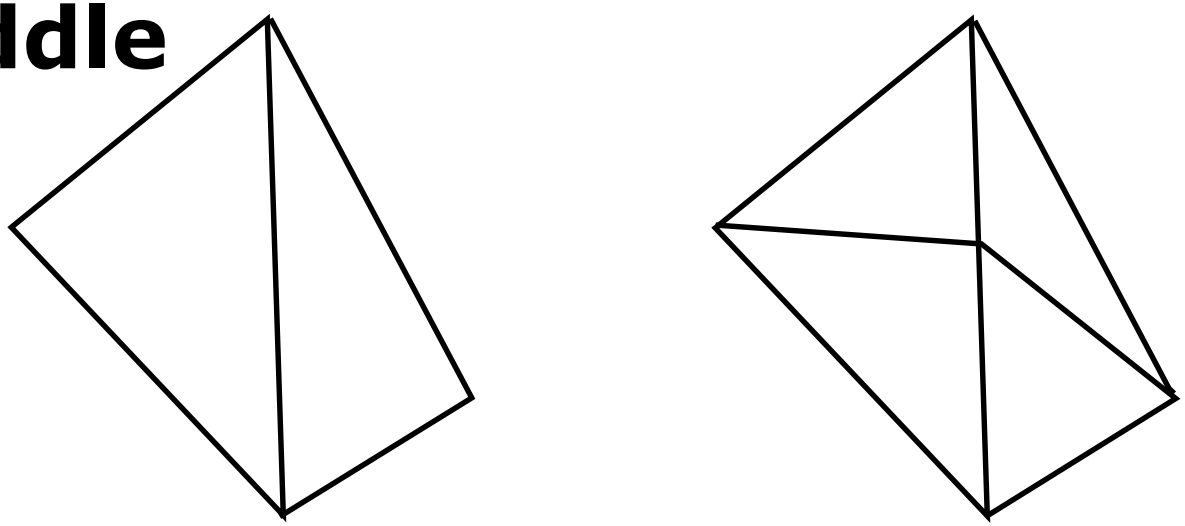


Adaptive Meshes: Terminology

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



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



Adaptive Meshes: Applications

- Every unstructured mesh program wants to be adaptive
  - CSAR, CPSD, etc…
- Charm++ Triangle Mesh Refinement (Wilmarth)
- Charm++ PMAF3D (Wilmarth)
- Charm++ Tet Data Transfer Library (Lawlor)

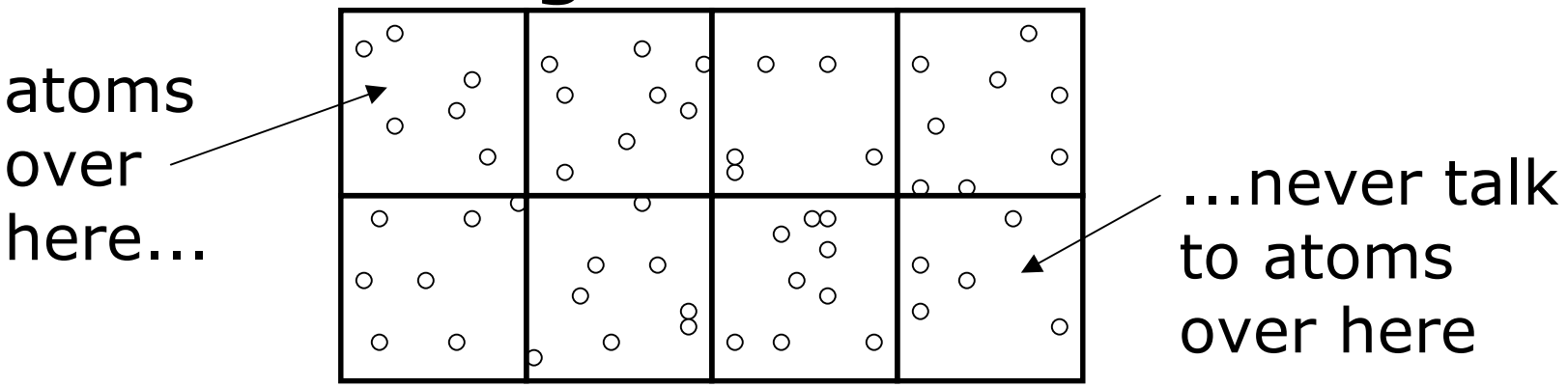
Particle Methods and Spatial Search

Particles and Spatial Search

- To work on a particle, you need nearby particles
  - E.g., all particles within cutoff *r*
    - Used by NAMD
  - or, all *k* nearest particles
    - Used by 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

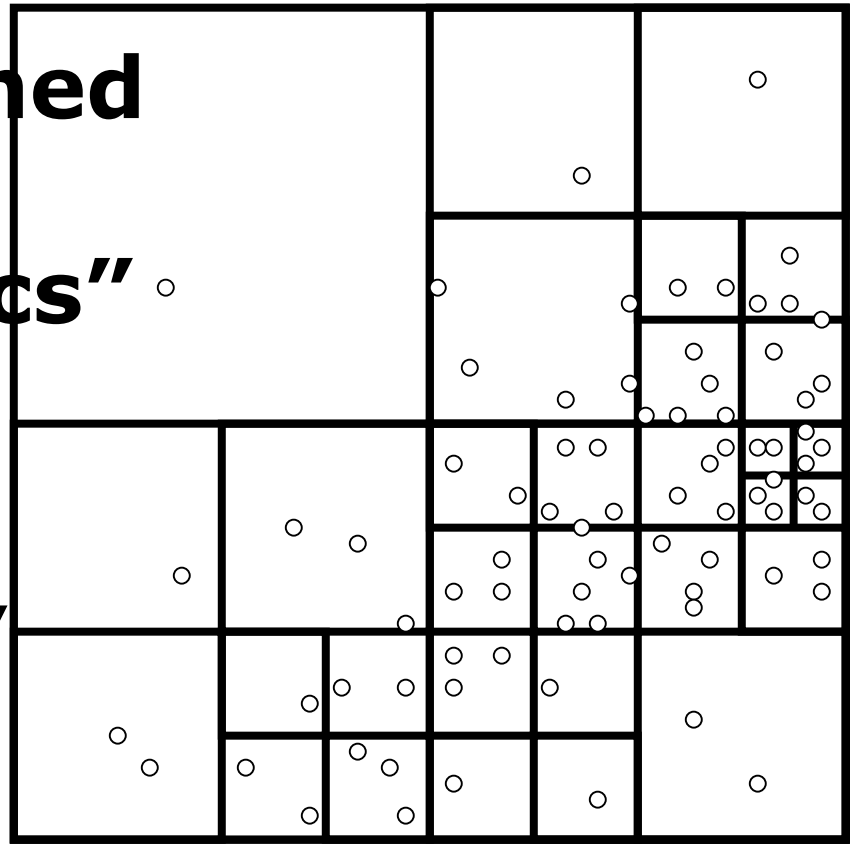
- **E.g., NAMD molecular dynamics**
  - **Particles are Atoms**
  - **Search structure is based on "Patches" of space in regular, rectilinear grid**



- **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 terms, but very few concepts**