ACM/CS 114
Parallel algorithms for scientific applications

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Unstructured grids

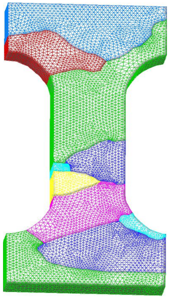
- when solving differential equations using structured grids
  - the grid itself is stationary
  - finite differences use the grid nodes as sampling points for a field
  - finite volumes consider the grid as a collection of matter containers and formulate problems in terms of fluxes across their boundaries
- finite elements take a different approach
  - subdivide the domain into elements
  - construct basis functions over each element to approximate the solution
  - allow the mesh nodes to move along with the object
  - use the elements to compute the material response to the induced deformations
  - apply this response to nodal fields in a linear manner
- a *simplicial mesh* is a decomposition of a region of space in terms of simplices
- what follows is an overview of very common but surprisingly hard problems that occur in simulations of physical systems

Meshing

- creating simplicial meshes is a surprisingly hard problem
- in two dimensions
  - there is a well posed mathematical problem with some guarantees that a triangulation can be generated for sufficiently well defined domains
    - given a set of vertices, one can always find a *Delaunay* triangulation where no vertex falls in the interior of the circumcircle of any triangle
    - the quality of the triangulation can be improved by adding extra vertices
  - for practical purposes, this is sufficient to handle most cases
  - the problem is rather challenging numerically, with high incidence of round-off errors, overflows and underflows
    - certain geometrical tests are so sensitive that robust packages employ exact arithmetic
- similar guarantees exist when triangulating surfaces embedded in three dimensional space
- in three dimensions the problem is theoretically intractable at this point
  - meshing packages are full of heuristics to avoid the known pathological cases
- no known parallel implementations

Parallelization

- typically, the finest grain task is the element update that models the response of the material to the deformation induced by the motion of the vertices
  - that's where all the physics is
  - computationally intensive for non-trivial responses
    - usually involves solving a complicated variational problem, such as energy minimization
  - little or no interaction with neighboring elements, although non-local updates are becoming more common
    - e.g. thin shells, fracture based on deformation energy in a neighborhood
- coarse grain tasks are defined through *graph partitioning* that decomposes the mesh into smaller subgraphs
  - with uniform element and node distributions
  - well characterized boundaries
- performance characteristics
  - computational cost grows with the number of elements
  - communication cost grows with the number of nodes on partition boundaries

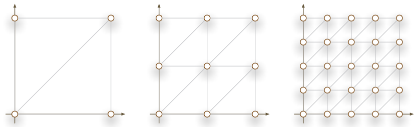


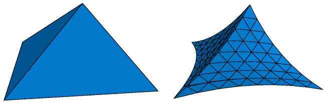
Graph partitioning

- mesh domain decomposition is mathematically identical to graph partitioning
  - a *hard* computational problem
  - with wide applicability to many practical problems
  - hence, there are many excellent algorithms – and software packages – that solve most problems of practical interest
- algorithms fall into two broad categories
  - those that use geometrical information, such as nodal coördinates
  - those that rely only on graph connectivity
    - breadth first search, spectral bisection, Kernighan/Lin
- comparison metrics
  - speed of partitioning: important since meshes tend to be large
  - number of cut edges
  - for finite elements: important to minimize the number of nodes on partition boundaries, since it is directly linked to the communication cost of the calculation
- METIS from George Karypis' lab at the University of Minnesota
  - multi-level Kernighan/Lin algorithms, other heuristics
  - ParMETIS is the parallel implementation

Uniform subdivision

- high fidelity simulations require high resolution
  - i.e. small elements, which implies large element counts
  - many interesting problems require tens or hundreds of millions of elements before they converge
  - creating input meshes of this size sequentially is impractical
- one possibility is *parallel uniform subdivision*
  - the input mesh is partitioned and distributed among processes
  - each process subdivides its simplices
    - edges get split in two, triangles in four, tetrahedra in eight
    - mesh quality is not affected significantly: only two new classes of simplices are introduced, regardless of the number of subdivision levels
    - the formation of new entities on partition boundaries implies the recalculation of the communications maps among processes





- can be done in linear time
  - scales well and can create enormous meshes (billions of elements)

Non-uniform subdivision and adaptive remeshing

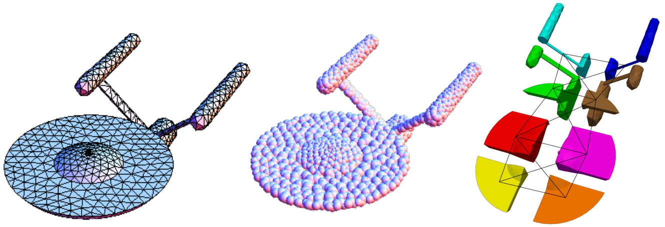
- there are many good non-uniform subdivision algorithms
  - e.g. longest edge subdivision: each tetrahedron that has an edge longer than some threshold gets subdivided by splitting that edge in two and connecting the new node to the two non-adjacent vertices
- they tend to be difficult to parallelize because they induce *one-sided* topological changes on the partition boundaries that must be communicated to the neighboring process
  - hence they are rarely used in large scale calculations
  - this is an *architectural* limitation, not an *algorithmic* one!
  - it requires restructuring the solver to support non-trivial communication with its neighbors
- similar considerations apply to adaptive remeshing
  - where a process discovers that it requires a higher element density to satisfy some correctness criterion
  - but difficult to implement when the refinement reaches the partition boundary

Contact detection

- modeling impact requires detecting when bodies come into contact and computing appropriate forces
  - both are difficult problems, especially for non-smooth, distributed meshes
  - the computations involve only elements on the free boundary
- the element updates and contact search have very different communication patterns
  - contact is *global*, since any two surface triangles can collide
  - and it is expensive, since it involves geometrical queries
  - it is best solved as an auxiliary parallel problem with its own partitioning
    - boundary partitioned using geometric criteria, such as axis-aligned cutting planes
    - requires frequent re-balancing as mesh geometry and topology change
- in *surface driven* contact detection
  - the boundary is partitioned and the centers of all the faces are inserted in some kind of spatial data structure
    - so that coarse calculations about contact candidates can be made efficiently
    - typically bucket or sparse-bucket arrays that support *orthogonal range queries* (ORQ)
  - candidates can be checked pairwise for actual contact using ray-triangle and edge-triangle intersection algorithms

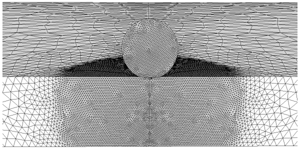
Volume based contact detection

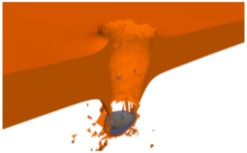
- volume based approaches replace the elements on the boundary with equivalent spheres
- a variety of geometrical criteria can be used:
  - equivalent volume
  - diameter determined by the longest edge
- contact detection can take place very efficiently using ORQ algorithms
- simple spring models resolve the contact forces
  - based on simple potentials that take into account the sphere inter-penetration



Fracture and fragmentation

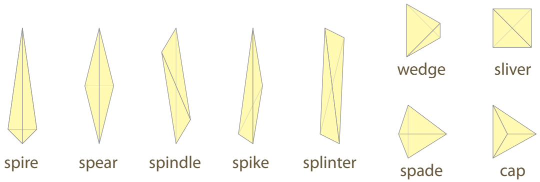
- when the material is under sufficient tension, modeling the physics correctly requires topological changes to the mesh
  - the material *fractures* when it is energetically favorable for an opening to form between two elements that are being pulled apart
- modeling this typically involves *cohesive elements*
  - prismatic elements that are inserted in the place of what used to be the common face of two tetrahedra and absorb excess energy
- when some threshold is exceeded, the cohesive element fractures and becomes free surface
- cohesive element insertion involves node, edge and face splitting
- difficulties arise as cracks run up to process boundaries and must be propagated across
- eventually, fragments form as cracks disconnect portions of the mesh





Element erosion

- mesh distortions induced by large deformations
  - degrade the numerical accuracy of the calculation
  - force the timestep sizes to impractical values
  - eventually cause the simulation to fail



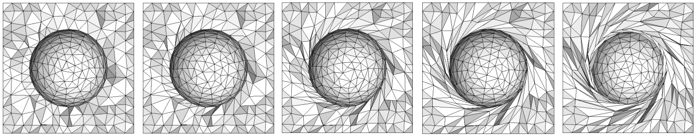
- a strategy in wide use is to *erode* badly distorted elements
  - using physically motivated erosion criteria that model fracture mechanics
  - trivial to implement sequentially
  - less so in parallel, as it involves geometrical and topological changes to the mesh
- candidates are selected based on some element quality metric
- erosion takes place when the deformation energy in a suitable neighborhood exceeds the fracture energy

Mesh optimization

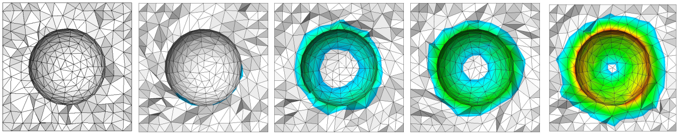
- the numerical accuracy of finite element calculations is determined in part by the quality of the mesh
    - the initial triangulation generated by the mesher
    - distortions induced by large deformations
- element quality is intuitively related to its deviation from an equilateral tetrahedron
    - there are a dozen or so pathological cases that involve either extremely small or extremely large internal angles
- optimizing mesh quality requires
    - an element quality metric that places a high penalty on the pathological cases
    - geometrical optimization: redistributing the mesh nodes so that it is possible to construct a defect-free triangulation
    - topological optimization: adjusting the way nodes are connected to form simplices
    - control over the element size, which is linked directly to both the numerical accuracy and the computational cost of the simulation
    - a sufficiently well characterized description of the boundary so that when new nodes are inserted near the boundary they do not induce distortions

Mesh optimization examples

- consider a mesh with an embedded sphere that is undergoing rigid rotation
- a quarter of a turn is sufficient to distort the mesh



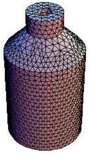
- continuous remeshing maintains good mesh quality; after three whole revolutions

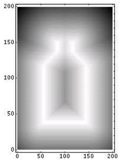


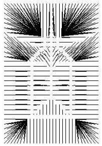
- challenges:
  - keep numerical diffusion under control
  - implement in parallel

Implicit representations of surfaces

- simulating phenomena that involve the interaction of solids and fluids has its own challenges
  - fluid solvers are typically Eulerian, with structured grid that is fixed in space while the fluid flows through it
  - whereas solid solvers are typically Lagrangian, with an unstructured grid that moves along with the body it describes
- coupling requires some form of information exchange that enables
  - the solid solver to inform the fluid about the position and velocity of its evolving boundary
  - the fluid solver to exert a force on the solid through its pressure field on the boundary
- the solution involves constructing *level sets*, and computing the distance to the solid, the closest node and the closest face for each point on the grid







Summary of open problems

- many interesting physics problems require making topological changes to the simplicial meshes, and propagating them across process boundaries
  - good sequential algorithms exist, but they are difficult to parallelize
  - naïve parallelization is almost always prohibitively expensive
    - because maintaining coherence and consistency of the global information requires a lot of communication
- changing the solver architecture may be key to efficient parallel implementations
  - evolving mesh topology requires complicated interactions among processes
  - *event based* solutions enable such interactions
  - and improve simulation control by external agents
    - better monitoring through probes and sensors
    - *instrumentation* for virtual experiments