ACM/CS 114
Parallel algorithms for scientific applications

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A more careful look at contact detection

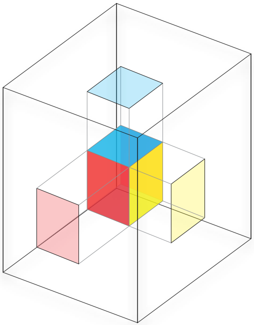
- consider a collection of tetrahedral meshes that model bodies in relative motion with triangular meshes as boundaries
- during the simulation, the bodies may come in contact
  - with each other or themselves
  - *contact events* consist of intersections among nodes, edges or faces
  - unless the mechanics is informed of the contact events, the objects will inter-penetrate
  - contact *detection* involves isolating the pairs of topological entities from each boundary that have intersected, whereas contact *resolution* refers to the calculation of appropriate restoring forces on the bodies
- the typical simulation update step proceeds along the following lines
  1. define the contact surfaces at time t
  2. predict the location of the nodes at a later time $t + \Delta t$ by integrating the equations of motion
  3. search for potential contact events among nodes, edges and faces to identify the entities that come in contact
  4. correct the future location of the nodes by applying forces that tend to remove the overlap

Contact search

- the contact event identification in Step 3 above has the potential to dominate the calculation
  - given a candidate pair, the intersection logic involves very expensive geometrical calculations
  - naïve algorithms are $\mathcal{O}(n^2)$ in the number of topological entities on the boundary, prohibitively expensive even for moderate size calculations
- hence, a more sensible strategy is to break up the contact search into two separate steps
  - use a specialized data structure that encodes the location of mesh nodes and build a relatively fast algorithm to narrow down the candidates to a small number
  - perform the detailed calculations on the reduced set
- typically, the fast searches are implemented using *orthogonal range queries* that identify points whose coördinates fall within a given box
  - build a bounding box that contains the initial and final position of a given surface element, perhaps in some reduced form
  - form the *capture box* by enlarging the bounding box to account for the motion of the nodes
  - query the data structure for nodes that fall within the capture box

Orthogonal range queries

- an orthogonal range query is a generalization of the interval test to higher dimensions
  - given a number p and an interval $[a, b)$, return `true` if the number falls within the interval, otherwise return `false`
  - extend by performing a test for each coördinate: does the point p fall within a given box?
- there is a variety of data structures that are *a priori* well suited to this problem
  - however, the problem context establishes some crucial constraints



- we will classify algorithms according to the following metrics
  - $b(N)$: the time it takes to initially populate the data structure with N points
  - $r(N)$: the complexity of rebuilding or update the data structure
  - $s(N)$: the amount of storage required
  - $q(N, n)$ and $\bar{q}(N, n)$: the (average) time required to perform a query if there are n points in the given range
- also, we'll start out in one dimension and generalize

Sequential scan

- the simplest approach is to look at each record and determine whether it falls in the range
  - this algorithm is trivial to implement and requires no extra storage
  - the performance is acceptable for sufficiently small N, or if most of the records fall in the query interval

$$\begin{aligned} b_{\mathtt{SCAN}} &= \mathcal{O}(N) \quad , \quad r_{\mathtt{SCAN}} = 0 \\ s_{\mathtt{SCAN}} &= \mathcal{O}(N) \quad , \quad q_{\mathtt{SCAN}} = \mathcal{O}(N) \end{aligned}$$

Algorithm 1: RQ.SCAN(points, interval)

```
candidates ← ∅
for point in points do
    if point ∈ interval then
        candidates.insert(point)
return candidates
```

Binary search

- if the records are sorted, a binary search can locate any record with cost $\mathcal{O}(\log N)$, so in order to find all $p \in [a, b)$
  - find the first point that satisfies $p >= a$
  - and collect points in sequence while $p < b$
  - simple analysis yields

$$\begin{array}{lclclcl} b_{\mathtt{BS}} & = & \mathcal{O}(N \log N) & , & r_{\mathtt{BS}} & = & \mathcal{O}(N) \\ s_{\mathtt{BS}} & = & \mathcal{O}(N) & , & q_{\mathtt{BS}} & = & \mathcal{O}(\log N + n) \end{array}$$

  since the records must be sorted initially, while rebuilding the data structure can be done in linear time since it is almost sorted

Algorithm 2: RQ.BS(points, interval=(a,b))

$candidates \leftarrow \emptyset$
$iterator \leftarrow$ BINARY-SEARCH-LOWER-BOUND$(points, a)$
while $\star iterator \leq b$ **do**
    if $point \in interval$ **then**
        $candidates.insert(point)$
return $candidates$

Tricks with trees

- alternatively, we can store the points at the leaves of a binary tree data structure
  - each internal tree node acts has a *discriminator* that splits the data set into two subsets
  - numbers less than the discriminator go to the left branch, the rest to the right
  - once the population drops below some threshold, create a leaf node to hold the points
- two sensible choices for the discriminator are
  - the midpoint of the interval: yields a recursive subdivision of the interval
    - also known as interval trees or *orthotrees*
    - quadtrees in two dimensions, octrees in three
  - the median of the data set: partitions the data in subsets of equal size
    - *kd* trees

Creating a binary tree

Algorithm 3: TREE.MAKE(points)

if $length[points] < tree.leafSize$ **then**
  $leaf \leftarrow tree.newLeaf()$
  $leaf.insert(points)$
  return $leaf$
else
  $branch \leftarrow tree.newBranch()$
  select branch $discriminator$
  $left \leftarrow \{x \in points : x < discriminator\}$
  $branch.left \leftarrow tree.make(left)$
  $right \leftarrow \{x \in points : x >= discriminator\}$
  $branch.right \leftarrow tree.make(right)$
  return $branch$

Algorithm 4: RQ.TREE(tree, interval=(a,b))

```
if tree is leaf then
    return RQ.SCAN(tree.points, interval)
else
    candidates ← ∅
    if tree.discriminator ≥ a then
        candidates ← candidates + RQ.TREE(tree.left, interval)
    if tree.discriminator < b then
        candidates ← candidates + RQ.TREE(tree.right, interval)
    return candidates
```

Performance of binary trees

- for midpoint splitting, the depth D of the tree depends on the point distribution

$$
\begin{array}{lll}
b_{\texttt{ORTHO}} = \mathcal{O}((D+1)N) & r_{\texttt{ORTHO}} = \mathcal{O}((D+1)N) & \\
s_{\texttt{ORTHO}} = \mathcal{O}((D+1)N) & q_{\texttt{ORTHO}} = \mathcal{O}(N) & \bar{q}_{\texttt{ORTHO}} = \mathcal{O}(D+n)
\end{array}
$$

- for median splitting the depth of the tree depends only on the number of records

$$
\begin{array}{ll}
b_{\texttt{KD}} = \mathcal{O}(N \log N) & r_{\texttt{KD}} = \mathcal{O}(N) \\
s_{\texttt{KD}} = \mathcal{O}(N) & q_{\texttt{KD}} = \mathcal{O}(n + \log N)
\end{array}
$$

Binning

- another strategy is to partition the interval $[a, b)$ into M cells of width

$$\delta := x_{m+1} - x_m = \frac{b-a}{M}$$

  - the m^{th} cell C_m holds points in the interval $[x_m, x_{m+1})$
  - the point container then becomes an array of M point containers
  - and the array index for a point p is obtained through

$$i = \lfloor \frac{p-a}{\delta} \rfloor$$

- the process of putting the points in the container is known as a *cell sort*
- they are optimal when properly tuned

$$\begin{array}{lll} b_{\texttt{CELL}} = \mathcal{O}(N+M) & r_{\texttt{CELL}} = \mathcal{O}(N+M) & \\ s_{\texttt{CELL}} = \mathcal{O}(N+M) & q_{\texttt{CELL}} = \mathcal{O}(J+n) & \bar{q}_{\texttt{CELL}} = \mathcal{O}(n) \end{array}$$

where J is the number of cells that overlap the query interval

Querying a cell array

Algorithm 5: RQ.CELL(cells, interval=(a,b))

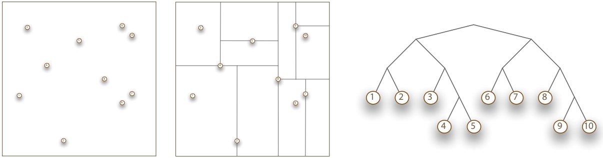
$candidates \leftarrow \emptyset$
$i \leftarrow index(cells, a)$
$j \leftarrow index(cells, b)$
for $point$ **in** $cells[i]$ **do**
    if $point \geq a$ **then**
        $candidates.insert(point)$
for k **in** $[i+1..j-1]$ **do**
    if $point$ **in** $cells[k]$ **then**
        $candidates.insert(point)$
for $point$ **in** $cells[j]$ **do**
    if $point < b$ **then**
        $candidates.insert(point)$
return $candidates$

Generalizing to higher dimensions

- the sequential scan algorithm has trivial generalizations
  - its performance is only acceptable for very small numbers of points
  - frequently used by the other algorithms to manage small size point sets
- binary search generalizes to the *projection* method in d dimensions
  - sort the points according to their k^{th} coördinate and build a reference set for this ordering
  - for example, one can number the points, sort them according to each coördinate, and build arrays of the point indices, or arrays of pointers to the actual data
  - a range query along any dimension yields all the points that lie within a slice of the domain
  - to perform an orthogonal range query
    - perform a range query along each dimension using binary searches
    - identify the coördinate slice with the fewest records
    - perform a sequential scan

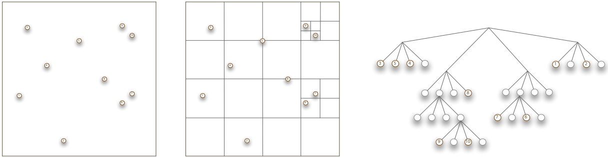
kd trees

- in d dimensions, there is a median point for each coördinate
  - split the tree using the coördinate with the largest spread
  - repeat this process at each level of the tree until the number of points to insert into the tree drops below some threshold
  - every internal node of the tree has to record at least
    - the direction that was chosen for the split
    - the value of the discriminant
    - references to the left and right branches of the node
  - leaf nodes are just point containers
- the orthogonal range query is defined recursively
  - at each internal node, check whether the left and right subdomains intersect the query interval by examining the discriminator
  - recurse into the branches that intersect the range
  - leaf nodes are examined using a sequential search



Orthotrees

- orthotrees are the generalization of interval trees in d dimensions
  - commonly known as *quadtrees* in two dimensions, and *octrees* in three
  - recursively split the d-dimensional domain into 2^d equal size hyperboxes
  - each internal node has 2^d branches
  - some of the branches lead to leaf nodes that contain the actual data
- the depth of the tree depends on the actual distribution of points in the input set
  - points that are very close to each other could lead to some very deep trees
- orthogonal range queries are implemented similarly to *kd* trees



Binning in higher dimensions

- cell sort extends naturally to d dimensions
  - form a regular grid of spacing δ_i along the i^{th} dimension
  - convert the point coordinates into cell indices along each dimension using the same formula as in one dimension
- the orthogonal range query consists of accessing cells that
  - entirely interior to the query box
  - partially overlap the boundary of the query box
  - the former are unconditionally included in the candidate list, while point in the latter must be checked individually
- tuning is crucial to the performance of this method
  - cells that are too large can lead to many false positives
  - cells that are too small have higher access times
  - it is best to know the size of the query boxes so that the cell spacing can be optimized
- can be easily combined with any of the other methods to speed up access to the points in each cell
  - most combinations do not offer significant advantages
  - but using binary searches is an exception

Parallelization

- minimization of the communication cost
  - best to avoid communication altogether if possible
  - any type of globally distributed data structure would eventually dominate the calculation
  - so would global data exchanges to maintain locally consistent information
- load balancing
  - the parallel characteristics of contact are different from the solver update
  - it is probably unavoidable that a few processors will be responsible for detecting and resolving the bulk of contact
- utilize point-to-point communications as much as possible
  - build/exchange bounding boxes for the geometry kept by each processor
  - use it to build point-to-point communication maps
  - exchange boundary elements so contact resolution can happen locally
  - exchange the resulting forces
- a research problem
  - we know that processing multiple queries has better parallel characteristics than a single one
  - we need a self-balancing, dynamically repartitioning data structure