并行程序开发

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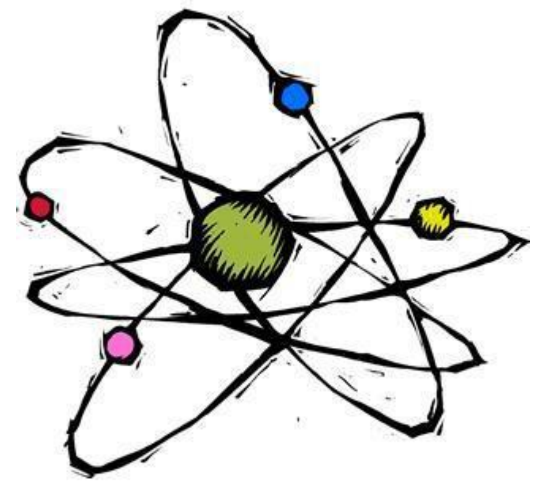
Roadmap

- Solving non-trivial problems.
- The n-body problem.
- The traveling salesman problem.
- Applying Foster's methodology.
- Starting from scratch on algorithms that have no serial analog.

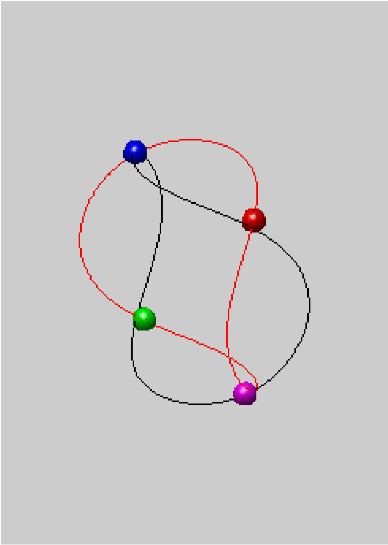
 

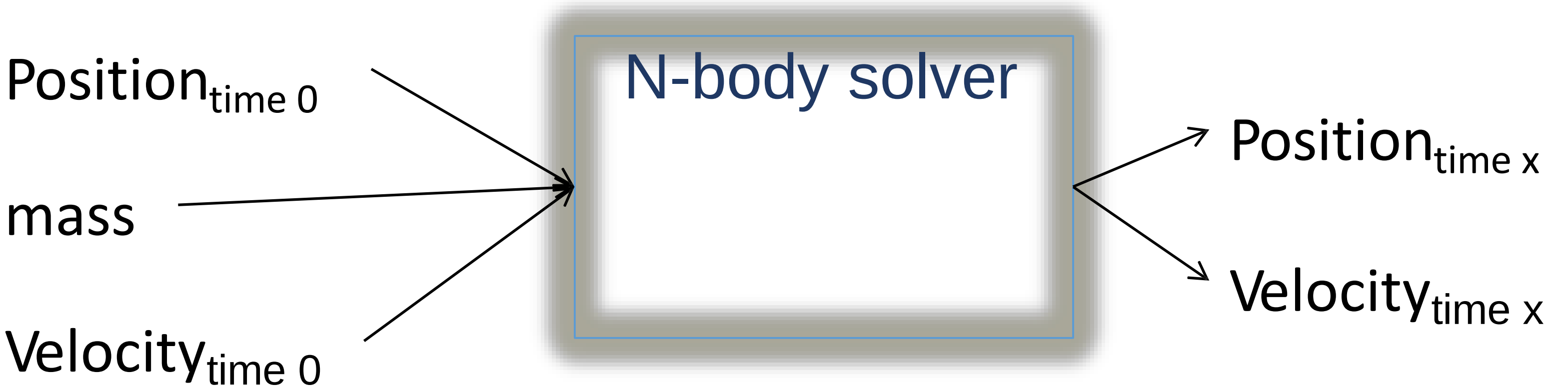
Two N-Body Solvers

The n-body problem

- Find the positions and velocities of a collection of interacting particles over a period of time.

- An n-body solver is a program that finds the solution to an n-body problem by simulating the behavior of the particles.



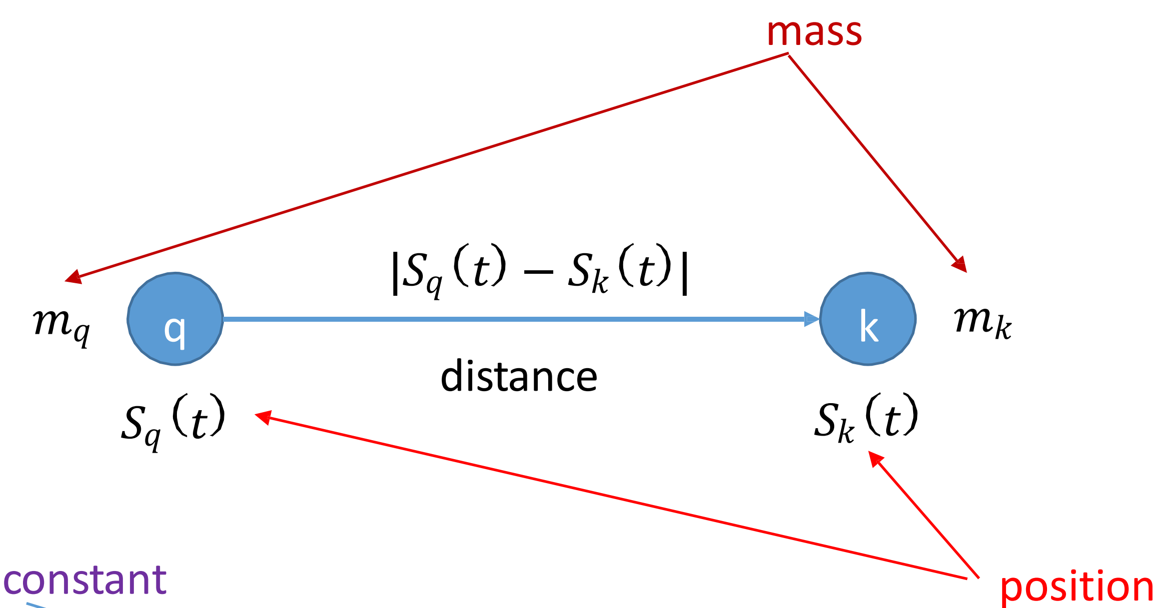


Position$_{time\ 0}$
mass
Velocity$_{time\ 0}$
N-body solver
Position$_{time\ x}$
Velocity$_{time\ x}$

Simulating motion of planets

- Determine the positions and velocities:
  - Newton’s second law of motion.牛顿第二定理
  - Newton’s law of universal gravitation. 万有引力定理

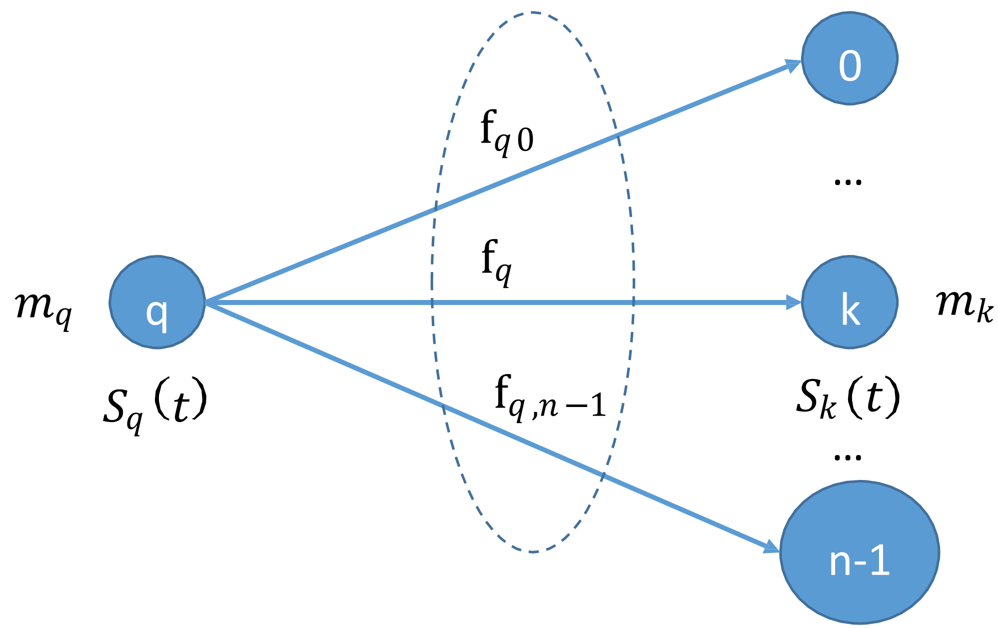
Force on particle q exerted by k



G: gravitational constant

$$\mathbf{f}_{qk}(t) = -\frac{\boxed{G} m_q m_k}{\left|\mathbf{s}_q(t) - \mathbf{s}_k(t)\right|^3}\left[\mathbf{s}_q(t) - \mathbf{s}_k(t)\right] \qquad (6.1)$$

Total force on particle q



$$\mathbf{F}_q(t) = \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \mathbf{f}_{qk} = -Gm_q \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \frac{m_k}{\left|\mathbf{s}_q(t) - \mathbf{s}_k(t)\right|^3} \left[\mathbf{s}_q(t) - \mathbf{s}_k(t)\right] \qquad (6.2)$$

Acceleration of particle q

- According to Newton's second law of motion:

$$F_q(t) = m_q a_q(t) = m_q S_q''(t)$$

$$\Downarrow$$

$$a_q(t) = S_q''(t) = \frac{F_q(t)}{m_q}$$

$$\Downarrow$$

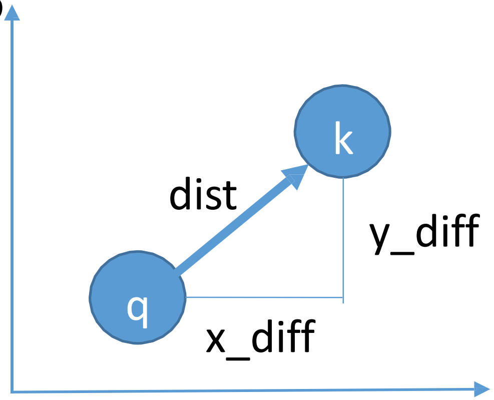
$$\mathbf{s}_q''(t) = -G \sum_{\substack{j=0 \\ j \neq q}}^{n-1} \frac{m_j}{\left|\mathbf{s}_q(t) - \mathbf{s}_j(t)\right|^3} \left[\mathbf{s}_q(t) - \mathbf{s}_j(t)\right] \qquad (6.3)$$

$$t = 0, \Delta t, 2\Delta t, \ldots, T\Delta t$$

Serial pseudo-code

```
Get input data;
for each timestep {
   if (timestep output) Print positions and velocities of particles;
   for each particle q
      Compute total force on q;
   for each particle q
      Compute position and velocity of q;
}
Print positions and velocities of particles;
```

Computation of the forces




```
for each particle q {
   for each particle k != q {
      x_diff = pos[q][X] − pos[k][X];
      y_diff = pos[q][Y] − pos[k][Y];
      dist = sqrt(x_diff*x_diff + y_diff*y_diff);
      dist_cubed = dist*dist*dist;
      forces[q][X] −= G*masses[q]*masses[k]/dist_cubed * x_diff;
      forces[q][Y] −= G*masses[q]*masses[k]/dist_cubed * y_diff;
   }
}
```

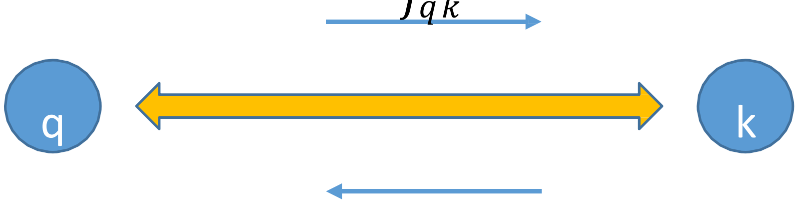
$$\mathbf{F}_q(t) = \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \mathbf{f}_{qk} = -Gm_q \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \frac{m_k}{\left|\mathbf{s}_q(t) - \mathbf{s}_k(t)\right|^3} \left[\mathbf{s}_q(t) - \mathbf{s}_k(t)\right]$$

Newton’s third law of motion

- For every action, there is an equal and opposite reaction.

The force on q due to k

f_{qk}

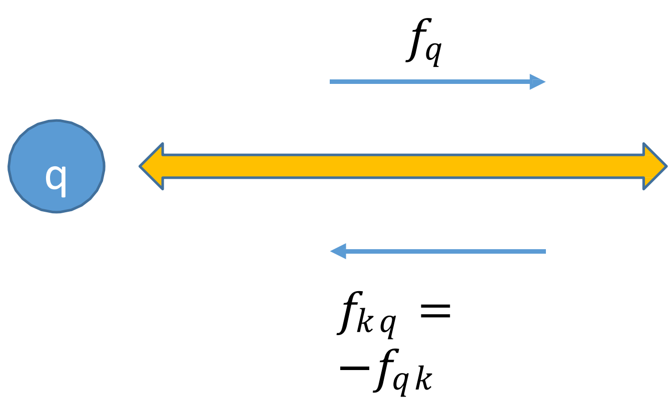


$$f_{kq} = -f_{qk}$$

The force on k due to q

The individual forces

$$\begin{array}{cc} & \begin{array}{ccccc} \phantom{-\mathbf{f}_{0,n-1}} & f_{qk} & \phantom{-\mathbf{f}_{2,n-1}} & & \phantom{\mathbf{f}_{0,n-1}} \end{array} \\ f_{kq} = -f_{qk} & \begin{bmatrix} 0 & & \mathbf{f}_{02} & \cdots & \mathbf{f}_{0,n-1} \\ & 0 & \mathbf{f}_{12} & \cdots & \mathbf{f}_{1,n-1} \\ -\mathbf{f}_{02} & -\mathbf{f}_{12} & 0 & \cdots & \mathbf{f}_{2,n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mathbf{f}_{0,n-1} & -\mathbf{f}_{1,n-1} & -\mathbf{f}_{2,n-1} & \cdots & 0 \end{bmatrix} \end{array}$$

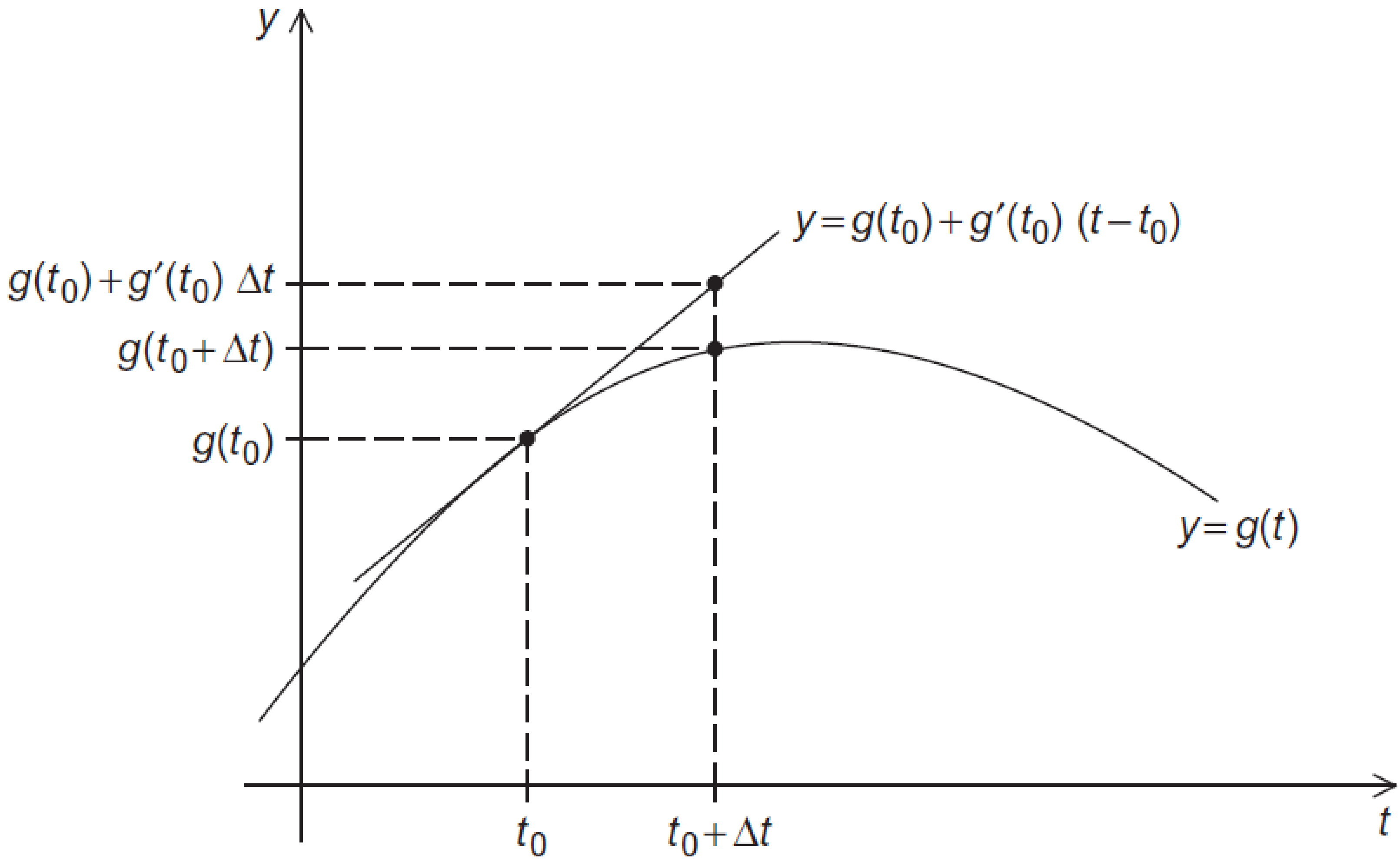


A Reduced Algorithm for Computing N-Body Forces

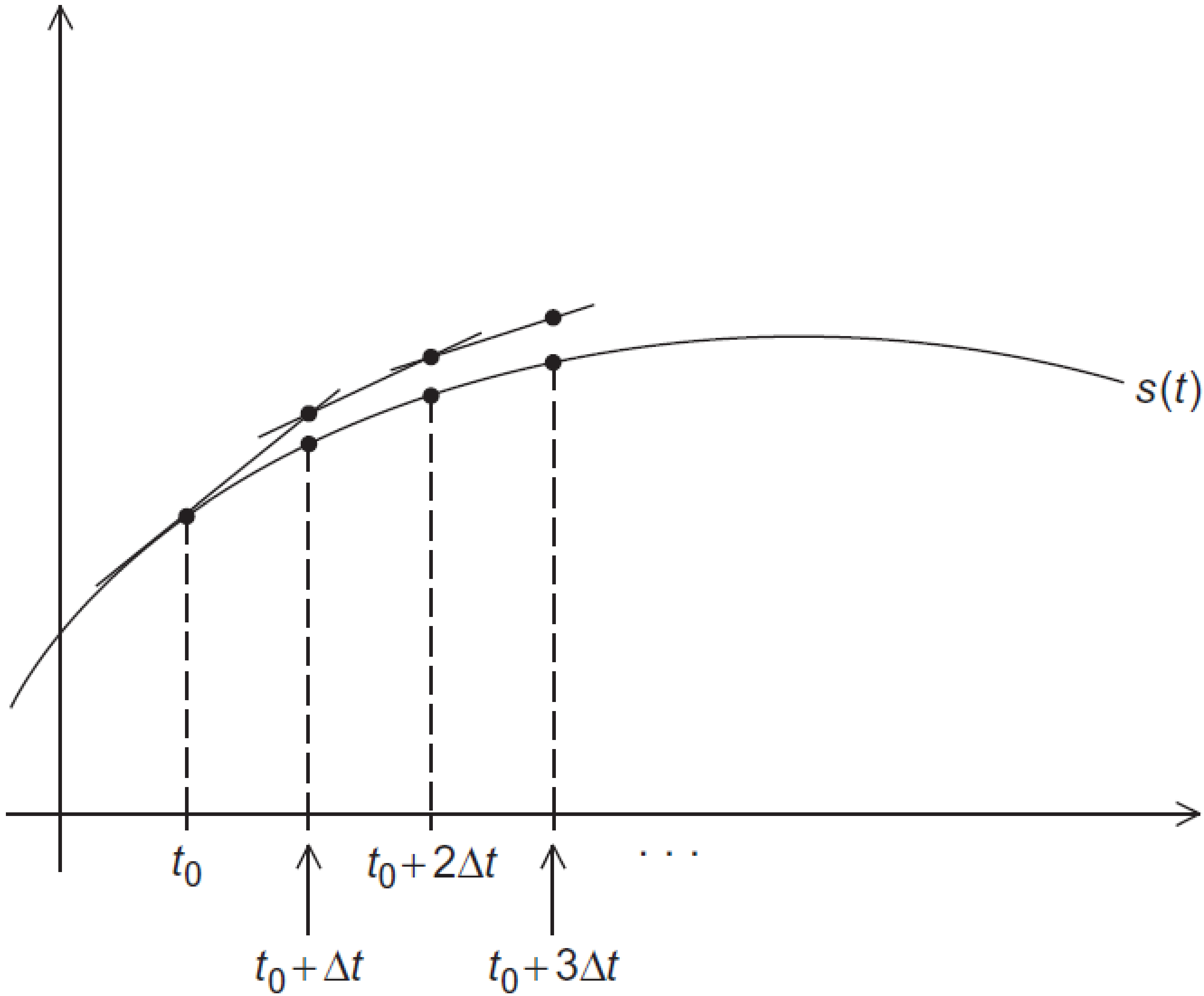
```
for each particle q
   forces[q] = 0;
for each particle q {
   for each particle k > q {
      x_diff = pos[q][X] − pos[k][X];
      y_diff = pos[q][Y] − pos[k][Y];
      dist = sqrt(x_diff*x_diff + y_diff*y_diff);
      dist_cubed = dist*dist*dist;
      force_qk[X] = G*masses[q]*masses[k]/dist_cubed * x_diff;
      force_qk[Y] = G*masses[q]*masses[k]/dist_cubed * y_diff

      forces[q][X] += force_qk[X];
      forces[q][Y] += force_qk[Y];
      forces[k][X] −= force_qk[X];
      forces[k][Y] −= force_qk[Y];
   }
}
```

Using the Tangent Line to Approximate a Function



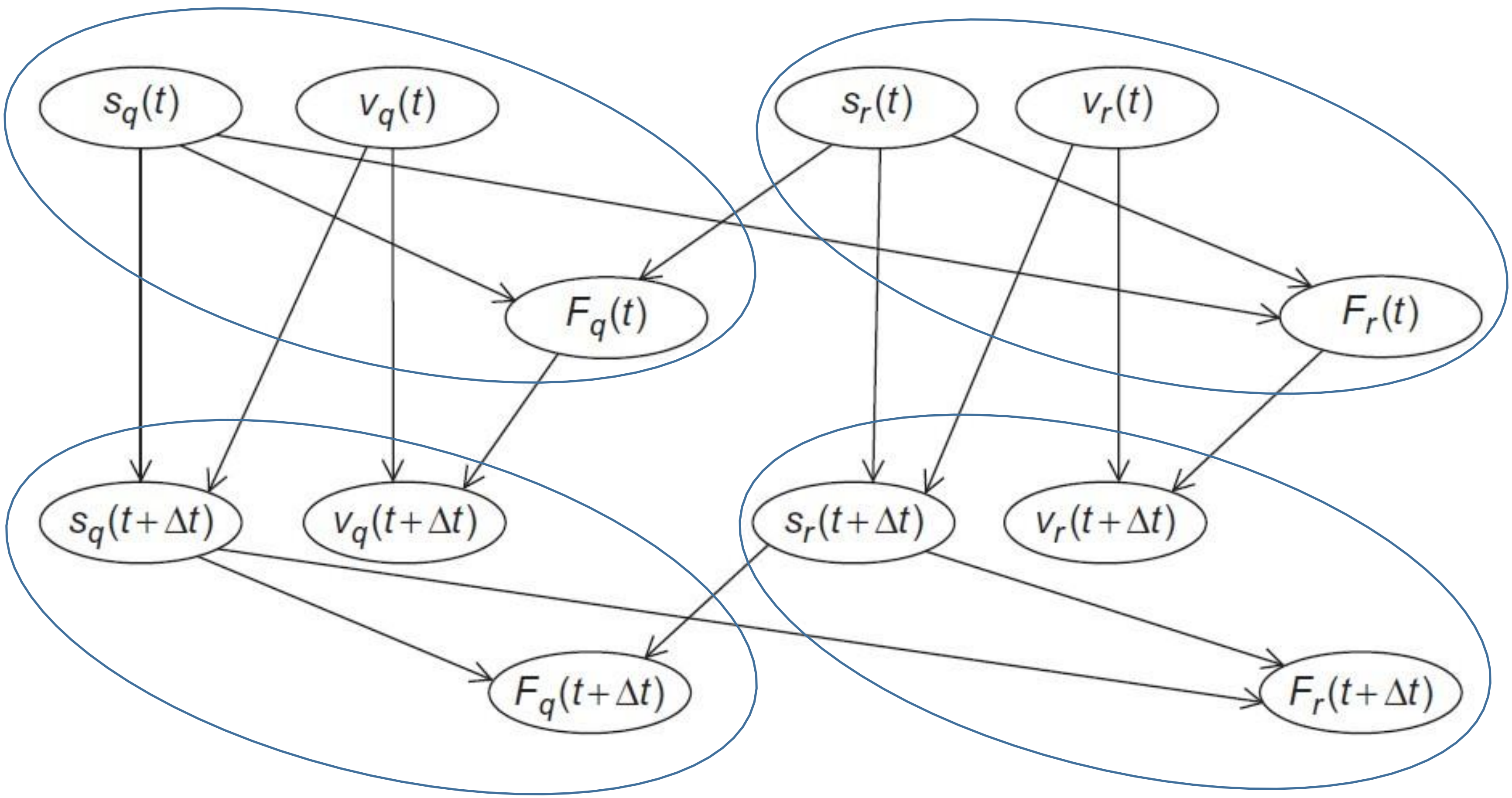
Euler’s Method



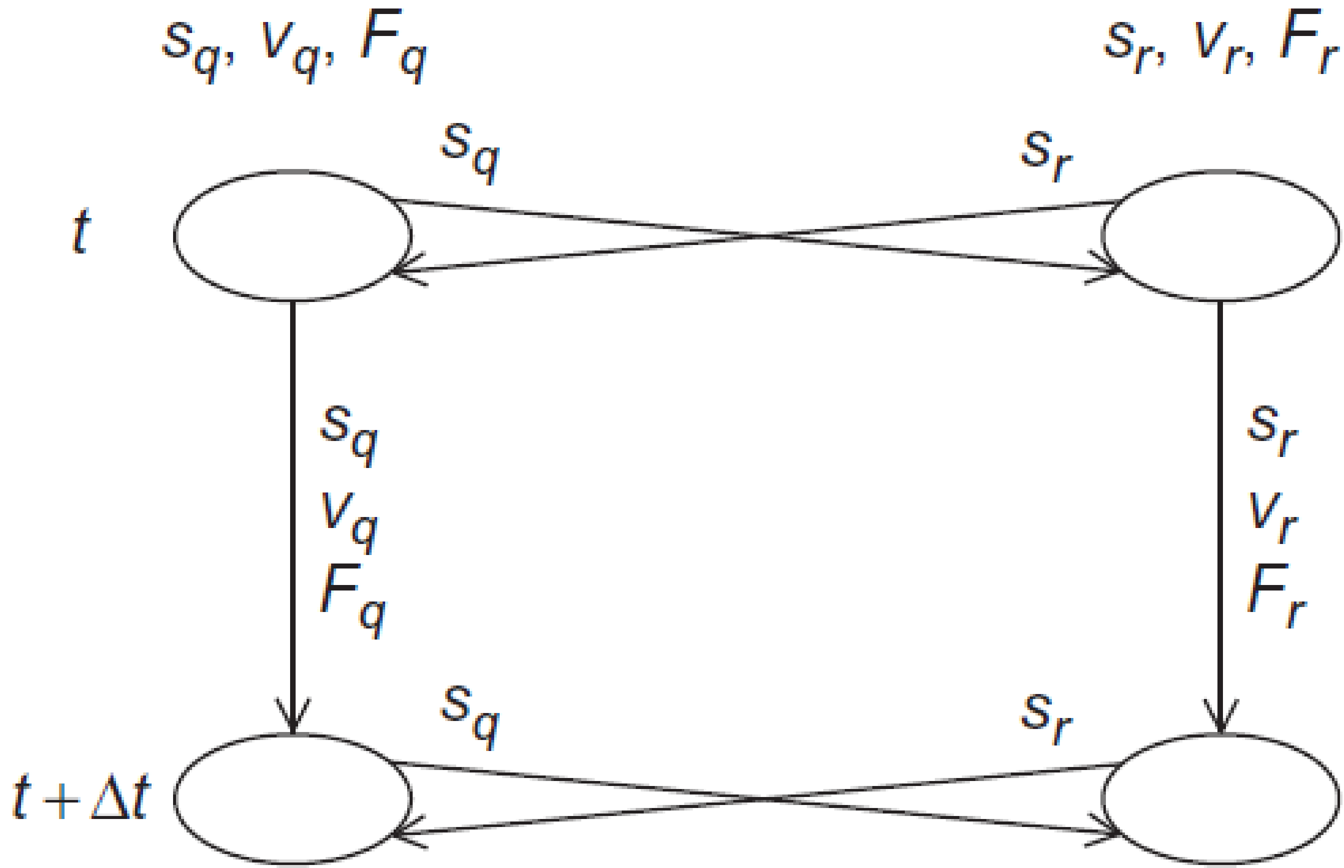
Parallelizing the N-Body Solvers

- Apply Foster's methodology.
- Initially, we want a lot of tasks.
- Start by making our tasks the computations of the positions, the velocities, and the total forces at each timestep.

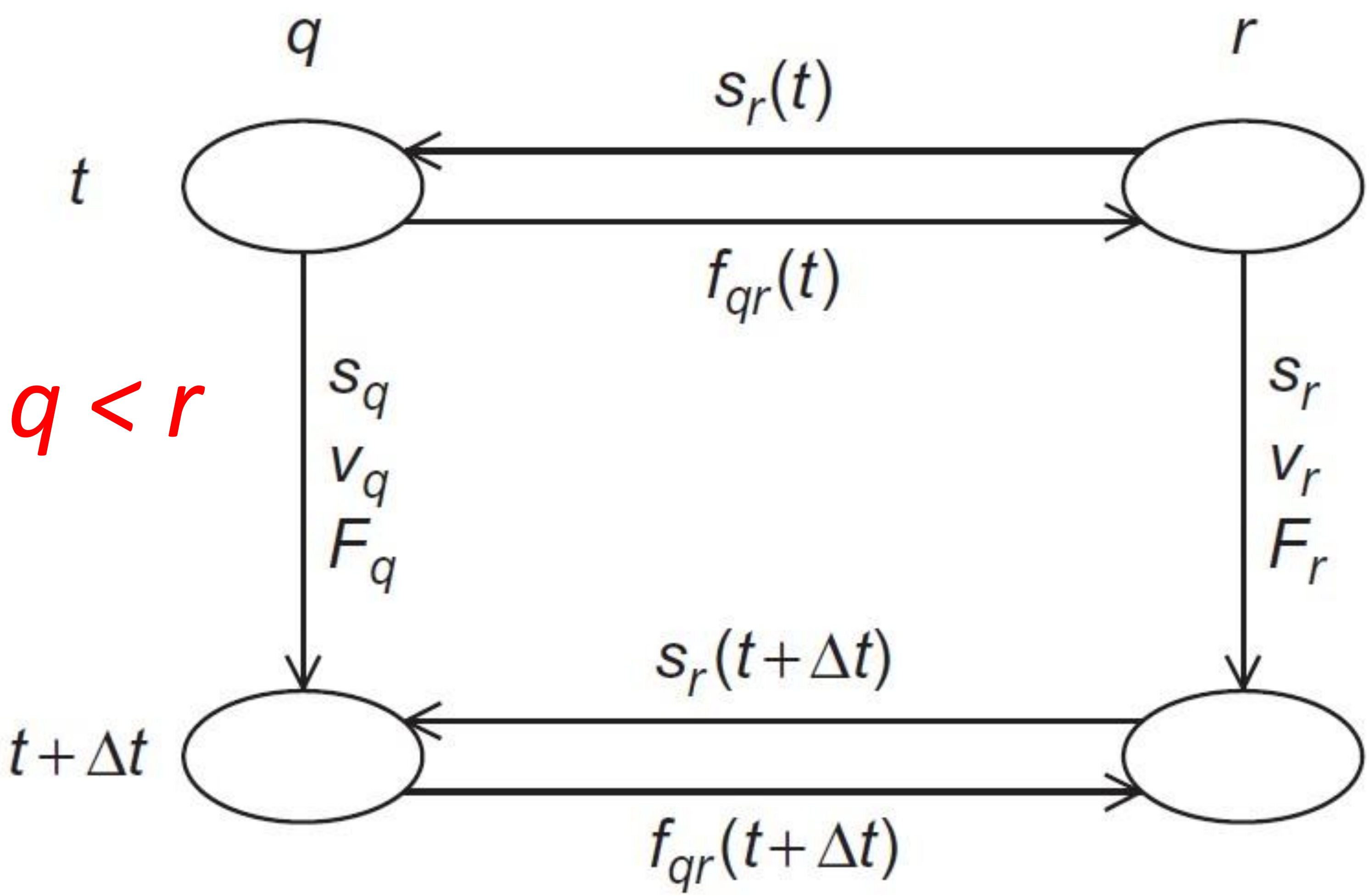
Communications Among Tasks in the Basic N-Body Solver



Communications Among Agglomerated Tasks in the Basic N-Body Solver



Communications Among Agglomerated Tasks in the **Reduced N-Body Solver**



Computing the total force on particle q in the reduced algorithm

```
for each particle k > q {
   x_diff = pos[q][X] − pos[k][X];
   y_diff = pos[q][Y] − pos[k][Y];
   dist = sqrt(x_diff*x_diff + y_diff*y_diff);
   dist_cubed = dist*dist*dist;
   force_qk[X] = G*masses[q]*masses[k]/dist_cubed * x_diff;
   force_qk[Y] = G*masses[q]*masses[k]/dist_cubed * y_diff;

   forces[q][X] += force_qk[X];
   forces[q][Y] += force_qk[Y];
   forces[k][X] −= force_qk[X];
   forces[k][Y] −= force_qk[Y];
}
```

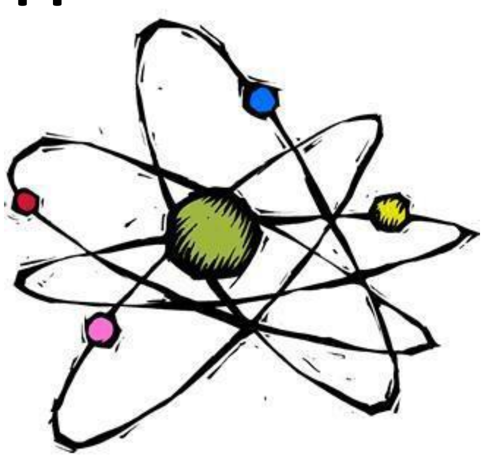
Serial pseudo-code

```
for each timestep {
   if (timestep output) Print positions and velocities of particles;
   for each particle q
      Compute total force on q;
   for each particle q
      Compute position and velocity of q;
}
```

iterating over particles

In principle, parallelizing the two inner for loops will map tasks/particles to cores.

Parallelizing the Basic Solver using OpenMP



First attempt

```
for each timestep {
    if (timestep output) Print positions and velocities of particles;
#   pragma omp parallel for
    for each particle q
       Compute total force on q;
#   pragma omp parallel for
    for each particle q
       Compute position and velocity of q;
}
```

Let's check for race conditions caused by loop-carried dependences.

First loop

```
#   pragma omp parallel for
    for each particle q {
       forces[q][X] = forces[q][Y] = 0;
       for each particle k != q {
          x_diff = pos[q][X] − pos[k][X];
          y_diff = pos[q][Y] − pos[k][Y];
          dist = sqrt(x_diff*x_diff + y_diff*y_diff);
          dist_cubed = dist*dist*dist;
          forces[q][X] −= G*masses[q]*masses[k]/dist_cubed * x_diff;
          forces[q][Y] −= G*masses[q]*masses[k]/dist_cubed * y_diff;
       }
    }
```

No race conditions in parallelization of the first loop

- Only one thread will access forces[q] for any q.
- Accesses to *pos* and *masses* array are read.

Second loop

```
#   pragma omp parallel for
    for each particle q {
       pos[q][X] += delta_t*vel[q][X];
       pos[q][Y] += delta_t*vel[q][Y];
       vel[q][X] += delta_t/masses[q]*forces[q][X];
       vel[q][Y] += delta_t/masses[q]*forces[q][Y];
    }
```

No race conditions in parallelization of the second loop

- A single thread accesses pos[q], vel[q], masses[q], forces[q] for any particle q.
- Scalar variables are only read.

Repeated forking and joining of threads

The same team of threads will be used in both loops and for every iteration of the outer loop.

```
#   pragma omp parallel
    for each timestep {
       if (timestep output) Print positions and velocities of particles;
#      pragma omp for
       for each particle q
          Compute total force on q;
#      pragma omp for
       for each particle q
          Compute position and velocity of q;
    }
```

Problem: every thread will print all the positions and velocities.

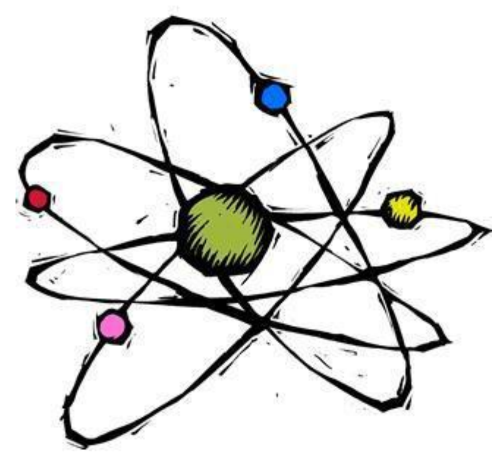
Adding the single directive

```
#   pragma omp parallel
    for each timestep {
        if (timestep output) {
#          pragma omp single
           Print positions and velocities of particles;
        }

#      pragma omp for
       for each particle q
          Compute total force on q;
#      pragma omp for
       for each particle q
          Compute position and velocity of q;
    }
```

Single: only one of the threads can execute the following block of code.

Parallelizing the Reduced Solver using OpenMP



Parallelizing the Reduced Solver Using OpenMP

```
#   pragma omp parallel
    for each timestep {
       if (timestep output) {
#         pragma omp single
          Print positions and velocities of particles;
       }
#      pragma omp for
       for each particle q
          forces[q] = 0.0;
#      pragma omp for
       for each particle q
          Compute total force on q;
#      pragma omp for
       for each particle q
          Compute position and velocity of q;
    }
```

Parallelization of the initialization of forces is fine, as there is no dependence among the iterations.

Problems

$$\mathbf{F}_3 = -\mathbf{f}_{03} - \mathbf{f}_{13} - \mathbf{f}_{23}$$

Updates to forces[3] create a **race condition**. **Why?**

Unlike basic version, in the reduced version, a thread ***may*** update elements in the forces array other than those corresponding to its assigned particles.

$$\begin{array}{l} \text{Thread 0} \\ \\ \text{Thread 1} \\ \\ \end{array} \begin{bmatrix} 0 & f_{01} & f_{02} & \boxed{f_{03}} \\ -f_{01} & 0 & f_{12} & \boxed{f_{13}} \\ -f_{02} & -f_{12} & 0 & \boxed{f_{23}} \\ -f_{03} & -f_{13} & -f_{23} & 0 \end{bmatrix}$$

Two threads attempt to access F_3

F_3 = forces[3]

First solution attempt

before all the ***updates*** to forces

```
#  pragma omp critical
   {
      forces[q][X] += force_qk[X];
      forces[q][Y] += force_qk[Y];
      forces[k][X] -= force_qk[X];
      forces[k][Y] -= force_qk[Y];
   }
```

Drawback: Access to the forces array will be effectively ***serialized!!!***

Second solution attempt

```
omp_set_lock(locks[q]);
forces[q][X] += force_qk[X];
forces[q][Y] += force_qk[Y];
omp_unset_lock(locks[q]);

omp_set_lock(locks[k]);
forces[k][X] -= force_qk[X];
forces[k][Y] -= force_qk[Y];
omp_unset_lock(locks[k]);
```

Use one lock for each particle.

The performance is not as good as serial code.

Third solution attempt

Solution: to carry out the computation of forces in two phases:

(Phase I) each thread performs calculations and stores results in its **own** array of forces;

(Phase II) the thread that has been assigned particle q will add the contributions that have been computed by different threads.

$$\mathbf{F}_3 = -\mathbf{f}_{03} \underbrace{- \mathbf{f}_{13}}_{\text{Thread 0}} \underbrace{- \mathbf{f}_{23}}_{\text{Thread 1}}$$

Revised algorithm – phase I

```
#  pragma omp for
   for each particle q {
      force_qk[X] = force_qk[Y] = 0;
      for each particle k > q {
         x_diff = pos[q][X] − pos[k][X];
         y_diff = pos[q][Y] − pos[k][Y];
         dist = sqrt(x_diff*x_diff + y_diff*y_diff);
         dist_cubed = dist*dist*dist;
         force_qk[X] = G*masses[q]*masses[k]/dist_cubed * x_diff;
         force_qk[Y] = G*masses[q]*masses[k]/dist_cubed * y_diff;

         loc_forces[my_rank][q][X] += force_qk[X];
         loc_forces[my_rank][q][Y] += force_qk[Y];
         loc_forces[my_rank][k][X] −= force_qk[X];
         loc_forces[my_rank][k][Y] −= force_qk[Y];
      }
   }
```

(1) each thread performs calculations and stores results in its **own** array of forces;

Revised algorithm – phase II

```
#   pragma omp for
    for (q = 0; q < n; q++) {
       forces[q][X] = forces[q][Y] = 0;
       for (thread = 0; thread < thread_count; thread++) {
          forces[q][X] += loc_forces[thread][q][X];
          forces[q][Y] += loc_forces[thread][q][Y];
       }
    }
```

(2) the thread that has been assigned particle q will **add the contributions** that have been computed by **different** threads.

Another example

- 6 particles, 3 threads, block partition

$$
\begin{array}{c}
\text{Thread 0} \left\{ \begin{array}{c} \\ \\ \end{array} \right. \\
\text{Thread 1} \left\{ \begin{array}{c} \\ \\ \end{array} \right. \\
\text{Thread 2} \left\{ \begin{array}{c} \\ \\ \end{array} \right.
\end{array}
\begin{bmatrix}
0 & f_{01} & f_{02} & f_{03} & f_{04} & f_{05} \\
-f_{01} & 0 & f_{12} & f_{13} & f_{14} & f_{15} \\
-f_{02} & -f_{12} & 0 & f_{23} & f_{24} & f_{25} \\
-f_{03} & -f_{13} & -f_{23} & 0 & f_{34} & f_{35} \\
-f_{04} & -f_{14} & -f_{24} & -f_{34} & 0 & f_{45} \\
-f_{05} & -f_{15} & -f_{25} & -f_{35} & -f_{45} & 0
\end{bmatrix}
\begin{array}{l}
\text{Particle 0} \\
\text{Particle 1} \\
\text{Particle 2} \\
\text{Particle 3} \\
\text{Particle 4} \\
\text{Particle 5}
\end{array}
$$

First Phase Computations for Reduced Algorithm with Block Partition

		Thread		
Thread	Particle	0	1	2
0	0	$\mathbf{f}_{01} + \mathbf{f}_{02} + \mathbf{f}_{03} + \mathbf{f}_{04} + \mathbf{f}_{05}$	0	0
	1	$-\mathbf{f}_{01} + \mathbf{f}_{12} + \mathbf{f}_{13} + \mathbf{f}_{14} + \mathbf{f}_{15}$	0	0
1	2	$-\mathbf{f}_{02} - \mathbf{f}_{12}$	$\mathbf{f}_{23} + \mathbf{f}_{24} + \mathbf{f}_{25}$	0
	3	$-\mathbf{f}_{03} - \mathbf{f}_{13}$	$-\mathbf{f}_{23} + \mathbf{f}_{34} + \mathbf{f}_{35}$	0
2	4	$-\mathbf{f}_{04} - \mathbf{f}_{14}$	$-\mathbf{f}_{24} - \mathbf{f}_{34}$	$\mathbf{f}_{45}$
	5	$-\mathbf{f}_{05} - \mathbf{f}_{15}$	$-\mathbf{f}_{25} - \mathbf{f}_{35}$	$-\mathbf{f}_{45}$

Imbalanced workload among three threads

Another example - continued

- 6 particles, 3 threads, cyclic partition

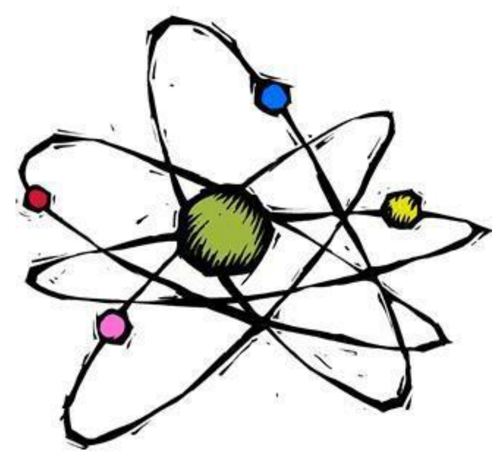
$$
\begin{array}{l}
\textbf{Thread 0} \\
\textbf{Thread 1} \\
\textbf{Thread 2} \\
\textbf{Thread 0} \\
\textbf{Thread 1} \\
\textbf{Thread 2}
\end{array}
\begin{bmatrix}
0 & f_{01} & f_{02} & f_{03} & f_{04} & f_{05} \\
-f_{01} & 0 & f_{12} & f_{13} & f_{14} & f_{15} \\
-f_{02} & -f_{12} & 0 & f_{23} & f_{24} & f_{25} \\
-f_{03} & -f_{13} & -f_{23} & 0 & f_{34} & f_{35} \\
-f_{04} & -f_{14} & -f_{24} & -f_{34} & 0 & f_{45} \\
-f_{05} & -f_{15} & -f_{25} & -f_{35} & -f_{45} & 0
\end{bmatrix}
\begin{array}{l}
\text{Particle 0} \\
\text{Particle 1} \\
\text{Particle 2} \\
\text{Particle 3} \\
\text{Particle 4} \\
\text{Particle 5}
\end{array}
$$

First Phase Computations for Reduced Algorithm with Cyclic Partition

		Thread		
Thread	Particle	0	1	2
0	0	$\mathbf{f}_{01}+\mathbf{f}_{02}+\mathbf{f}_{03}+\mathbf{f}_{04}+\mathbf{f}_{05}$	0	0
1	1	$-\mathbf{f}_{01}$	$\mathbf{f}_{12}+\mathbf{f}_{13}+\mathbf{f}_{14}+\mathbf{f}_{15}$	0
2	2	$-\mathbf{f}_{02}$	$-\mathbf{f}_{12}$	$\mathbf{f}_{23}+\mathbf{f}_{24}+\mathbf{f}_{25}$
0	3	$-\mathbf{f}_{03}+\mathbf{f}_{34}+\mathbf{f}_{35}$	$-\mathbf{f}_{13}$	$-\mathbf{f}_{23}$
1	4	$-\mathbf{f}_{04}-\mathbf{f}_{34}$	$-\mathbf{f}_{14}+\mathbf{f}_{45}$	$-\mathbf{f}_{24}$
2	5	$-\mathbf{f}_{05}-\mathbf{f}_{35}$	$-\mathbf{f}_{15}-\mathbf{f}_{45}$	$-\mathbf{f}_{25}$

More balanced workload among three threads with cyclic partition

Parallelizing the Solvers using Pthreads



Parallelizing the Solvers Using Pthreads

- By default, local variables in Pthreads are private.
- All shared variables are global in the Pthreads.
- The principle data structures in the Pthreads version are identical to those in the OpenMP version
- Startup for Pthreads is basically the same as the startup for OpenMP

Parallelizing the Solvers Using Pthreads

- The main difference between Pthreads and OpenMP is in the details of parallelizing the inner loops.

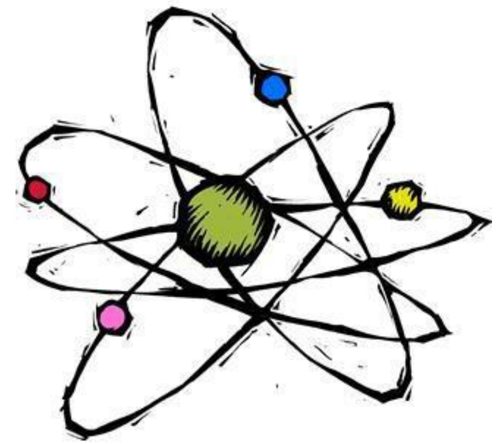
- We must explicitly determine which values of the loop variables correspond to each thread's calculations.

Parallelizing the Solvers Using Pthreads

- Another difference between the Pthreads and the OpenMP versions has to do with barriers.
  - At the end of a parallel for OpenMP has an implied barrier.
  - We need to add explicit barriers after the inner loops when a race condition can arise.

- The Pthreads standard includes a barrier. However, some systems don't implement it.

Parallelizing the Solvers using MPI



Parallelizing the Basic Solver Using MPI

- Choices with respect to the data structures:
  - Each process stores the entire global array of particle masses.
  - Each process only uses a single n-element array for the positions.
  - Each process uses a pointer loc_pos that refers to the start of its block of pos.
  - On process 0 local_pos = pos;

    on process 1 local_pos = pos + loc_n;

    etc.

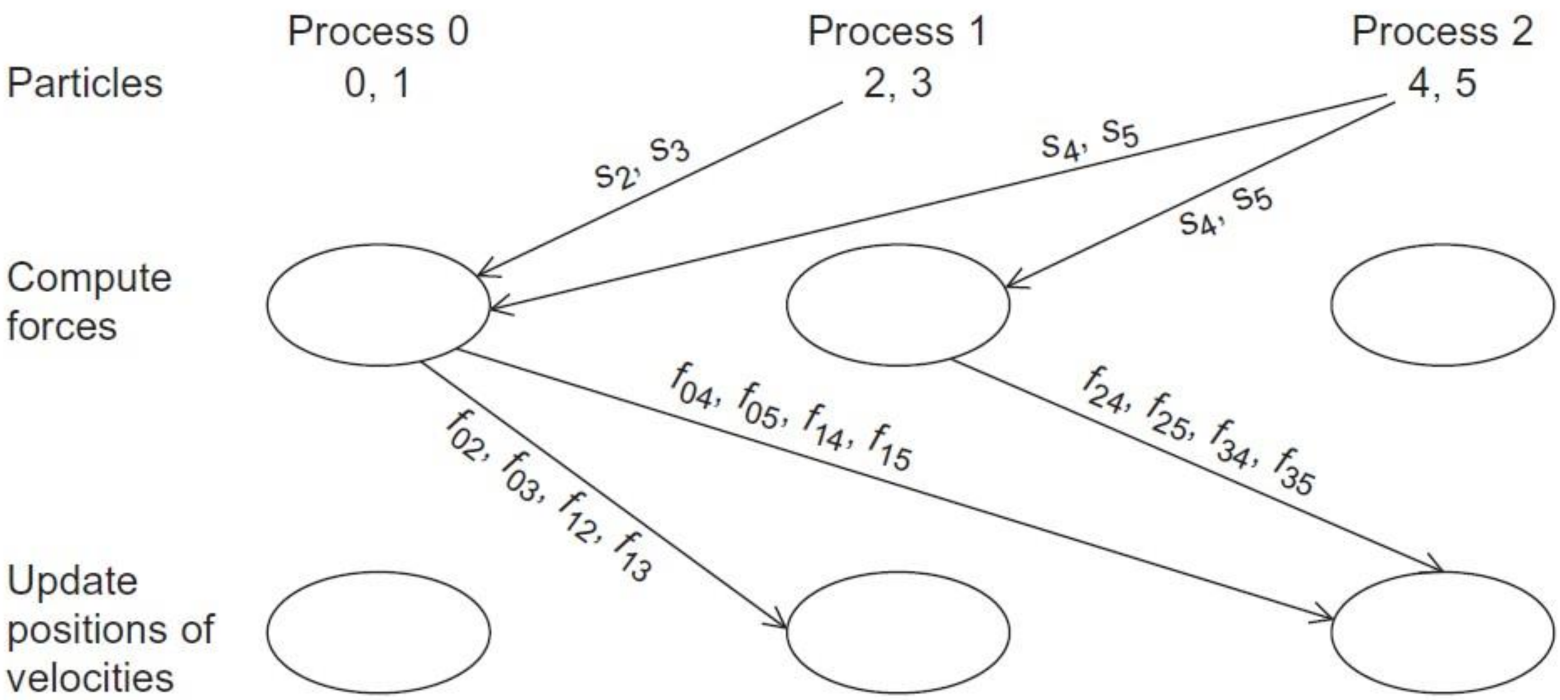
Pseudo-code for the MPI version of the basic n-body solver

```
Get input data;
for each timestep {
   if (timestep output)
      Print positions and velocities of particles;
   for each local particle loc_q
      Compute total force on loc_q;
   for each local particle loc_q
      Compute position and velocity of loc_q;
   Allgather local positions into global pos array;
}
Print positions and velocities of particles;
```

Pseudo-code for output

```
Gather velocities onto process 0;
if (my_rank == 0) {
   Print timestep;
   for each particle
      Print pos[particle] and vel[particle]
}
```

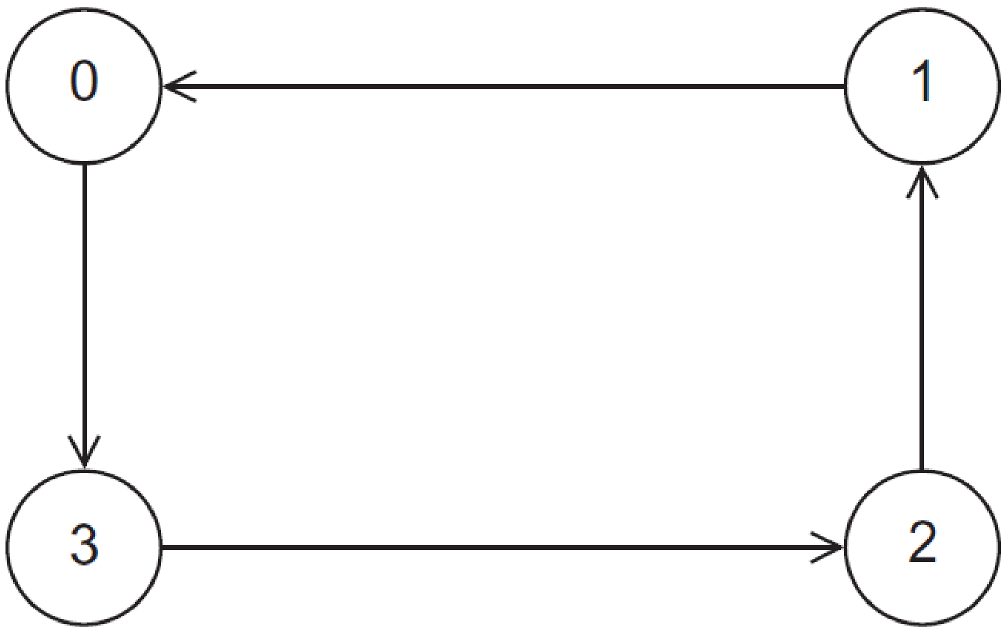
Communication In A Possible MPI Implementation of the N-Body Solver
(for a reduced solver)



Complicated!

Unless the implementation were very carefully done, it would probably be very slow.

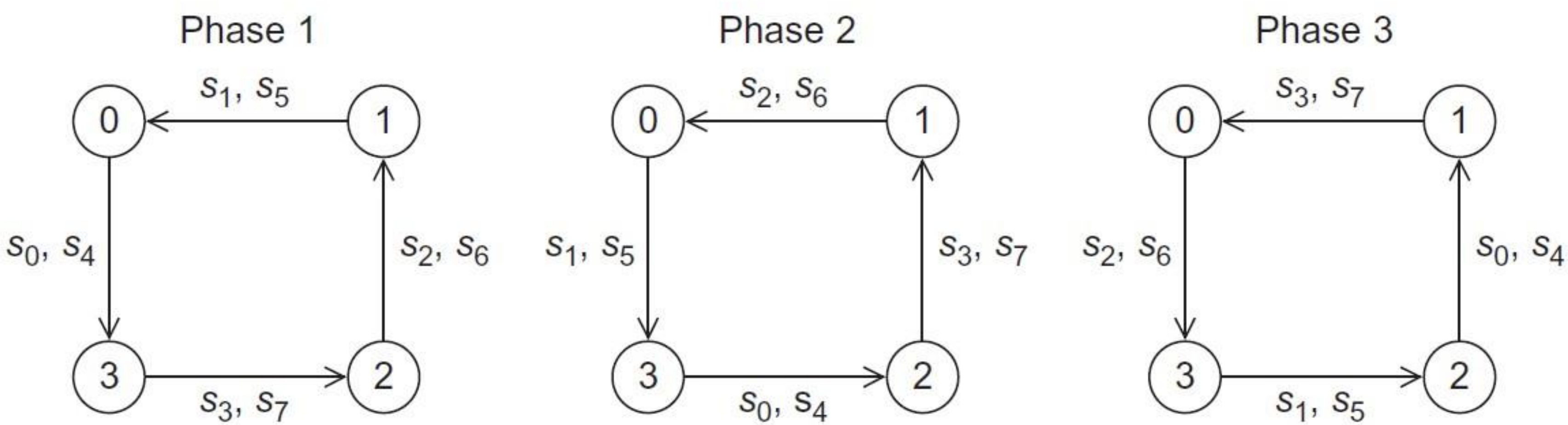
A Ring of Processes



By repeatedly sending and receiving data using the ring, each process has access to positions of all the particles.

Ring Pass of Positions

4 processes, 8 particles, cyclic partition



Phase 1: each process will send positions of its assigned particles to its "lower-ranked" neighbor and receive positions of particles assigned to its "higher-ranked" neighbor

Phase 2: each process will forward the positions it received in the first phase.

Computation of Forces in Ring Pass

In each phase, a process can

(1)compute inter-particle forces resulting from interaction between its assigned particles and the particles whose positions it has received;

(2)once an inter-particle force has been computed, the process can add the force into a local array of forces, and subtract the force from the received array of forces.

Computation of Forces in Ring Pass

2 processes, 4 particles, cyclic partition

Time	Variable	Process 0	Process 1
Start	loc_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	loc_forces	$0, 0$	$0, 0$
	tmp_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	tmp_forces	$0, 0$	$0, 0$
After Comp of Forces	loc_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	loc_forces	$\mathbf{f}_{02}, 0$	$\mathbf{f}_{13}, 0$
	tmp_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	tmp_forces	$0, -\mathbf{f}_{02}$	$0, -\mathbf{f}_{13}$
After First Comm	loc_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	loc_forces	$\mathbf{f}_{02}, 0$	$\mathbf{f}_{13}, 0$
	tmp_pos	$\mathbf{s}_1, \mathbf{s}_3$	$\mathbf{s}_0, \mathbf{s}_2$
	tmp_forces	$0, -\mathbf{f}_{13}$	$0, -\mathbf{f}_{02}$
After Comp of Forces	loc_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	loc_forces	$\mathbf{f}_{01} + \mathbf{f}_{02} + \mathbf{f}_{03}, \mathbf{f}_{23}$	$\mathbf{f}_{12} + \mathbf{f}_{13}, 0$
	tmp_pos	$\mathbf{s}_1, \mathbf{s}_3$	$\mathbf{s}_0, \mathbf{s}_2$
	tmp_forces	$-\mathbf{f}_{01}, -\mathbf{f}_{03} - \mathbf{f}_{13} - \mathbf{f}_{23}$	$0, -\mathbf{f}_{02} - \mathbf{f}_{12}$
After Second Comm	loc_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	loc_forces	$\mathbf{f}_{01} + \mathbf{f}_{02} + \mathbf{f}_{03}, \mathbf{f}_{23}$	$\mathbf{f}_{12} + \mathbf{f}_{13}, 0$
	tmp_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	tmp_forces	$0, -\mathbf{f}_{02} - \mathbf{f}_{12}$	$-\mathbf{f}_{01}, -\mathbf{f}_{03} - \mathbf{f}_{13} - \mathbf{f}_{23}$
After Comp of Forces	loc_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	loc_forces	$\mathbf{f}_{01} + \mathbf{f}_{02} + \mathbf{f}_{03}, -\mathbf{f}_{02} - \mathbf{f}_{12} + \mathbf{f}_{23}$	$-\mathbf{f}_{01} + \mathbf{f}_{12} + \mathbf{f}_{13}, -\mathbf{f}_{03} - \mathbf{f}_{13} - \mathbf{f}_{23}$
	tmp_pos	$\mathbf{s}_0, \mathbf{s}_2$	$\mathbf{s}_1, \mathbf{s}_3$
	tmp_forces	$0, -\mathbf{f}_{02} - \mathbf{f}_{12}$	$-\mathbf{f}_{01}, -\mathbf{f}_{03} - \mathbf{f}13 - \mathbf{f}_{23}$

Final phase: carry out a vector sum

Pseudo-code for the MPI implementation of the reduced n-body solver

```
source = (my_rank + 1) % comm_sz;
dest = (my_rank - 1 + comm_sz) % comm_sz;
Copy loc_pos into tmp_pos;
loc_forces = tmp_forces = 0;

Compute forces due to interactions among local particles;
for (phase = 1; phase < comm_sz; phase++) {
   Send current tmp_pos and tmp_forces to dest;
   Receive new tmp_pos and tmp_forces from source;
   /* Owner of the positions and forces we're receiving */
   owner = (my_rank + phase) % comm_sz;
   Compute forces due to interactions among my particles
      and owner's particles;
}
Send current tmp_pos and tmp_forces to dest;
Receive new tmp_pos and tmp_forces from source;
```

Performance of the MPI n-body solvers

Processes	Basic	Reduced
1	17.30	8.68
2	8.65	4.45
4	4.35	2.30
8	2.20	1.26
16	1.13	0.78

(in seconds)

Reduced solver is better than basic solver

Run-Times for OpenMP and MPI N-Body Solvers

(in seconds)

Processes/ Threads	OpenMP		MPI	
	Basic	Reduced	Basic	Reduced
1	15.13	8.77	17.30	8.68
2	7.62	4.42	8.65	4.45
4	3.85	2.26	4.35	2.30

Basic OpenMP solver is faster than basic MPI solver.

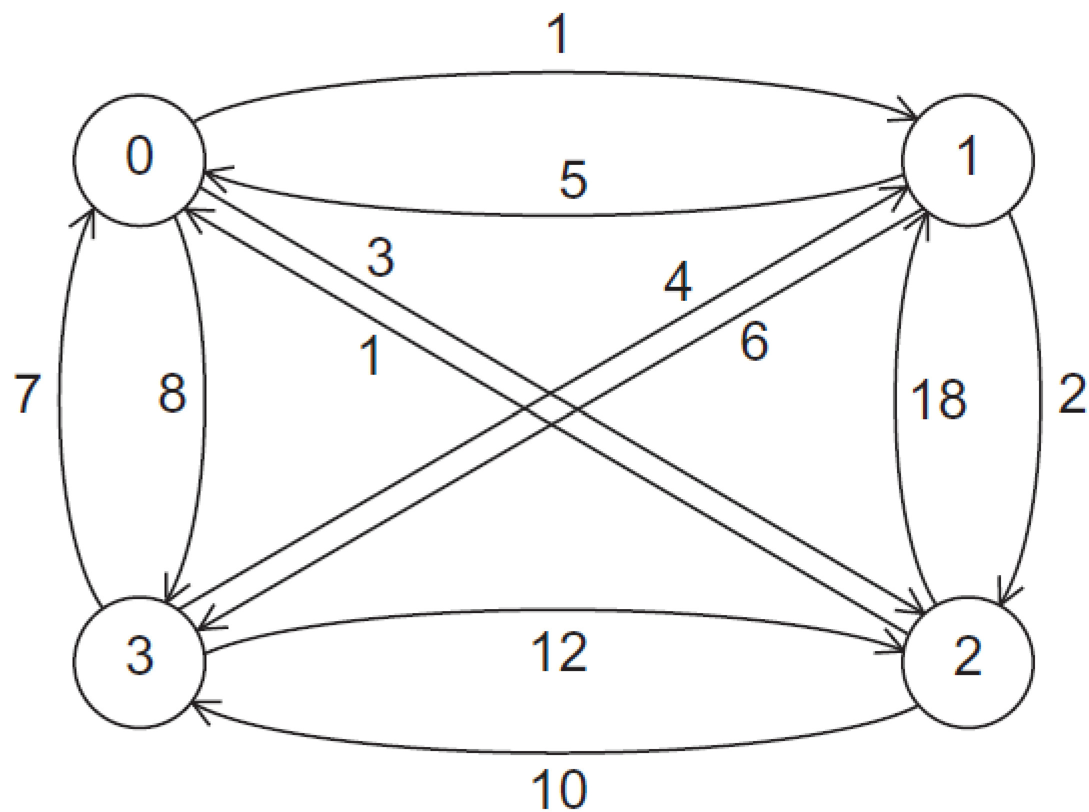
Reduced solver: OpenMP $\approx$ MPI

Tree search

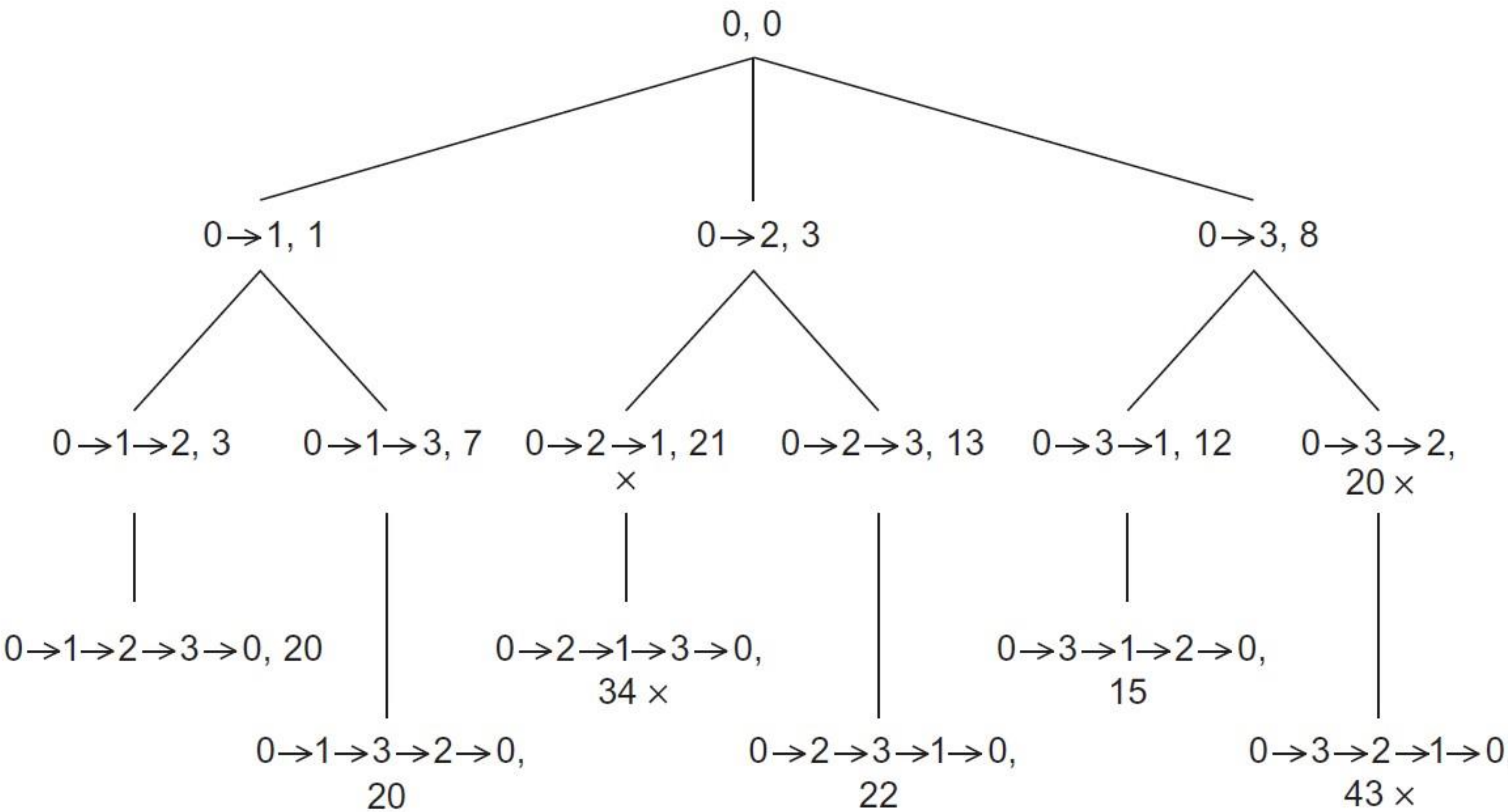
Tree search problem (TSP)

- An NP-complete problem.
- No known solution to TSP that is better in all cases than exhaustive search.
- Ex., the travelling salesperson problem, finding a minimum cost tour.

A Four-City TSP



Search Tree for Four-City TSP



Pseudo-code for a recursive solution to TSP using depth-first search

```
void Depth_first_search(tour_t tour) {
   city_t city;

   if (City_count(tour) == n) {
      if (Best_tour(tour))
         Update_best_tour(tour);
   } else {
      for each neighboring city
         if (Feasible(tour, city)) {
            Add_city(tour, city);
            Depth_first_search(tour);
            Remove_last_city(tour);
         }
   }
}  /* Depth_first_search */
```

To see if there are n cities in the partial tour

To see if the complete tour has a lower cost than the current "best tour"

Replace the current best tour with the tour

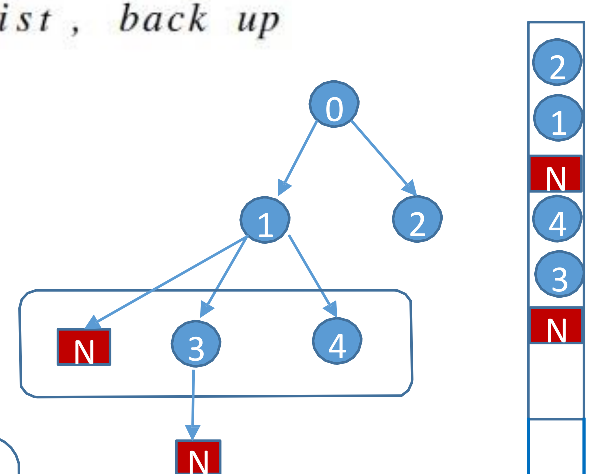
To see if city has been visited, and if not, whether the city can possibly lead to a least-cost tour.

Remove city from the tour, as it shouldn't be included in the tour in subsequent recursive calls.

Pseudo-code for an implementation of a depth-first solution to TSP without recursion

```
for (city = n-1; city >= 1; city--)
   Push(stack, city);
while (!Empty(stack)) {
   city = Pop(stack);
   if (city == NO_CITY) // End of child list, back up
      Remove_last_city(curr_tour);
   else {
      Add_city(curr_tour, city);
      if (City_count(curr_tour) == n) {
         if (Best_tour(curr_tour))
            Update_best_tour(curr_tour);
         Remove_last_city(curr_tour);
      } else {
         Push(stack, NO_CITY);
         for (nbr = n-1; nbr >= 1; nbr--)
            if (Feasible(curr_tour, nbr))
               Push(stack, nbr);
      }
   } /* if Feasible */
} /* while !Empty */
```

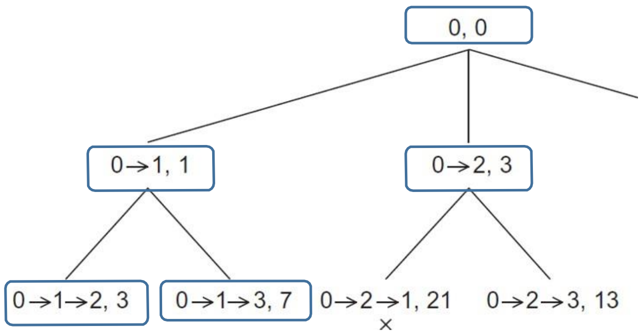
NO_CITY is a marker so that we can tell when we've visited all children of a tree node

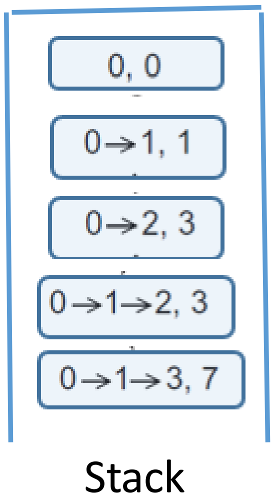


Before pushing all children of a node, we push NO_CITY marker

Pseudo-code for a second solution to TSP that doesn't use recursion

```
Push_copy(stack, tour);   // Tour that visits only the hometown
while (!Empty(stack)) {
   curr_tour = Pop(stack);
   if (City_count(curr_tour) == n) {
      if (Best_tour(curr_tour))
         Update_best_tour(curr_tour);
   } else {
      for (nbr = n-1; nbr >= 1; nbr--)
         if (Feasible(curr_tour, nbr)) {
            Add_city(curr_tour, nbr);
            Push_copy(stack, curr_tour);
            Remove_last_city(curr_tour);
         }
   }
   Free_tour(curr_tour);
}
```





Using pre-processor macros

```
/* Find the ith city on the partial tour */
int Tour_city(tour_t tour, int i) {
   return tour->cities[i];
}  /* Tour_city */
```

```
/* Find the ith city on the partial tour */
#define Tour_city(tour, i) (tour->cities[i])
```

Run-Times of the Three Serial Implementations of Tree Search

(in seconds)

Recursive	First Iterative	Second Iterative
30.5	29.2	32.9

- First iterative solution is faster, as it eliminates some overhead due to repeated function calls.
- Second iterative solution is slower because of repeated copying of tour data structure.
- The second iterative one is easy to parallelize.

Making sure we have the "best tour" (1)

- When a process finishes a tour, it needs to check if it has a better solution than recorded so far.

- The global Best_tour function only reads the global best cost, so we don't need to tie it up by locking it. There's no contention with other readers.

- If the process does not have a better solution, then it does not attempt an update.

Making sure we have the “best tour” (2)

- If another thread is updating while we read, we may see the old value or the new value.

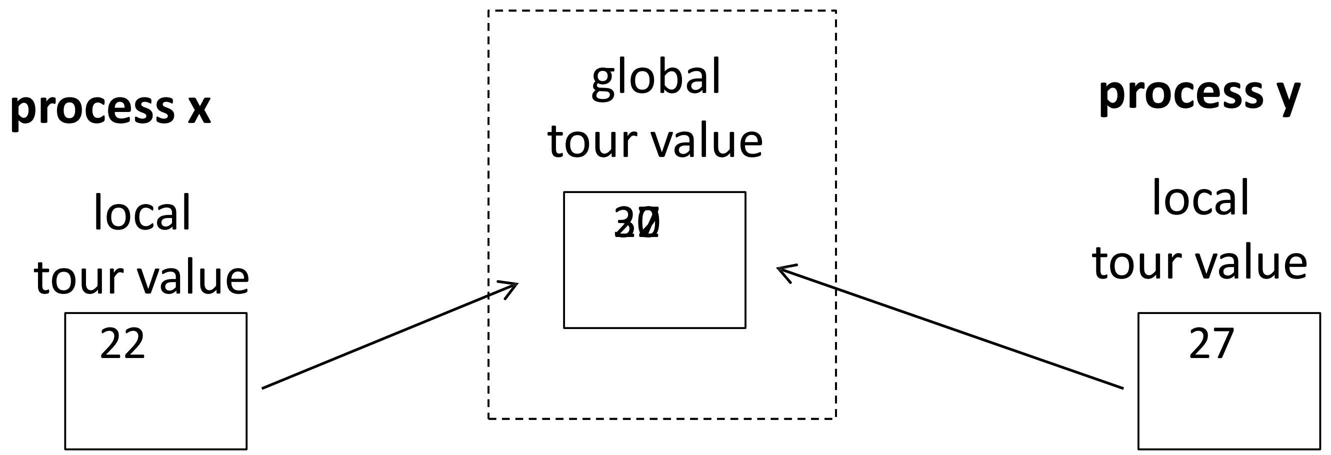
- The new value is preferable, but to ensure this would be more costly than it is worth.

Making sure we have the "best tour" (3)

- In the case where a thread tests and decides it has a better global solution, we need to ensure two things:
  - 1) That the process locks the value with a mutex, preventing a race condition.
  - 2) In the possible event that the first check was against an old value while another process was updating, we do not put a worse value than the new one that was being written.

- We handle this by locking, then testing again.

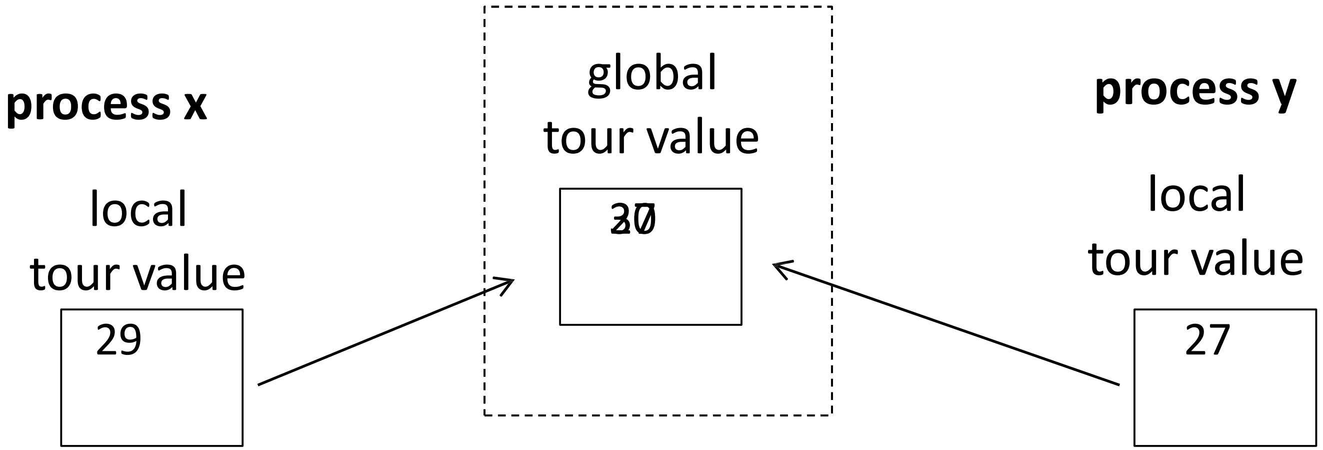
First scenario



3. test
6. lock
7. test again
8. update
9. unlock

1. test
2. lock
4. update
5. unlock

Second scenario



process x:

3. test
6. lock
7. **test again**
8. unlock

process y:

1. test
2. lock
4. update
5. unlock

Parallelizing the Tree Search Programs Using Pthreads

Static Parallelization of Tree Search using Pthreads

- **Idea:** a single thread use BFS to generate at least thread_count partial tours to distribute among threads, then each thread takes its partial tours and runs iterative tree search on them.

- Four **differences** compared with iterative serial one:
  - The use of my_stack instead of stack;
  - Initialization of the stack;
  - Implementation of Best_tour func;
  - Implementation of Update_best_tour func.

Pseudo-code for a Pthreads implementation of a statically parallelized solution to TSP

```
Partition_tree(my_rank, my_stack);

while (!Empty(my_stack)) {
   curr_tour = Pop(my_stack);
   if (City_count(curr_tour) == n) {
      if (Best_tour(curr_tour)) Update_best_tour(curr_tour);
   } else {
      for (city = n-1; city >= 1; city--)
         if (Feasible(curr_tour, city)) {
            Add_city(curr_tour, city);
            Push_copy(my_stack, curr_tour);
            Remove_last_city(curr_tour)
         }
   }
   Free_tour(curr_tour);
}
```

Dynamic Parallelization of Tree Search using Pthreads

Basic Idea:

(1) when a thread runs out of work, it waits to see if another thread can provide more work.

(2) if a thread still has work and finds that there is at least one thread without work, it can split its stack and provide work for one of the threads.

Note: using pthread_cond_wait, pthread_cond_signal, pthread_cond_broadcast for implementation.

Dynamic Parallelization of Tree Search Using Pthreads

- Code executed by a thread before it splits:
  - It checks that it has at least two tours in its stack.
  - It checks that there are threads waiting.
  - It checks whether the new_stack variable is NULL.

- Termination issues.
  - Only when all the threads have run out of work.
  - **Terminated function** is used instead of Empty(stack)

Pseudo-Code for Pthreads Terminated Function (1)

```
if (my_stack_size >= 2 && threads_in_cond_wait > 0 &&
      new_stack == NULL) {
   lock term_mutex;
   if (threads_in_cond_wait > 0 && new_stack == NULL) {
      Split my_stack creating new_stack;
      pthread_cond_signal(&term_cond_var);
   }
   unlock term_mutex;
   return 0;  /* Terminated = False; don't quit */
} else if (!Empty(my_stack)) { /* Stack not empty, keep working */
   return 0;  /* Terminated = false; don't quit */
} else { /* My stack is empty */
   lock term_mutex;
   if (threads_in_cond_wait == thread_count-1) { /* Last thread   */
                                                  /* running       */
      threads_in_cond_wait++;
      pthread_cond_broadcast(&term_cond_var);
      unlock term_mutex;
      return 1;  /* Terminated = true; quit */
```

Pseudo-Code for Pthreads Terminated Function (2)

```
   } else { /* Other threads still working, wait for work */
      threads_in_cond_wait++;
      while (pthread_cond_wait(&term_cond_var, &term_mutex) != 0);
      /* We've been awakened */
      if (threads_in_cond_wait < thread_count) { /* We got work */
         my_stack = new_stack;
         new_stack = NULL;
         threads_in_cond_wait--;
         unlock term_mutex;
         return 0;  /* Terminated = false */
      } else {  /* All threads done */
         unlock term_mutex;
         return 1;  /* Terminated = true; quit */
      }
   }  /* else wait for work */
}  /* else my_stack is empty */
```

Grouping the termination variables

```
typedef struct {
    my_stack_t new_stack;
    int threads_in_cond_wait;
    pthread_cond_t term_cond_var;
    pthread_mutex_t term_mutex;
} term_struct;
typedef term_struct* term_t;

term_t term; // global variable
```

Run-times of Pthreads tree search programs

15-city problems

Threads	First Problem			Second Problem		
	Serial	Static	Dynamic	Serial	Static	Dynamic
1	32.9	32.7	34.7 (0)	26.0	25.8	27.5 (0)
2		27.9	28.9 (7)		25.8	19.2 (6)
4		25.7	25.9 (47)		25.8	9.3 (49)
8		23.8	22.4 (180)		24.0	5.7 (256)

(in seconds)

numbers of times stacks were split

Parallelizing the Tree Search Programs Using OpenMP

Parallelizing the Tree Search Programs Using OpenMP

- Same basic issues implementing the static and dynamic parallel tree search programs as Pthreads.
- A few small changes can be noted.

Pthreads

```
if (my_rank == whatever)
```

```
#  pragma omp single
```

OpenMP

OpenMP emulated condition wait

```
/* Global vars */
int awakened_thread = -1;
work_remains = 1;  /* true */
. . .
omp_unset_lock(&term_lock);
while (awakened_thread != my_rank && work_remains);
omp_set_lock(&term_lock);
```

Busy-waiting !

Performance of OpenMP and Pthreads implementations of tree search

	First Problem						Second Problem					
	Static		Dynamic				Static		Dynamic			
Th	OMP	Pth	OMP		Pth		OMP	Pth	OMP		Pth	
1	32.5	32.7	33.7	(0)	34.7	(0)	25.6	25.8	26.6	(0)	27.5	(0)
2	27.7	27.9	28.0	(6)	28.9	(7)	25.6	25.8	18.8	(9)	19.2	(6)
4	25.4	25.7	33.1	(75)	25.9	(47)	25.6	25.8	9.8	(52)	9.3	(49)
8	28.0	23.8	19.2	(134)	22.4	(180)	23.8	24.0	6.3	(163)	5.7	(256)

(in seconds)

For most parts, OpenMP implementation is comparable to Pthreads implementation.

Implementation of Tree Search Using MPI and Static Partitioning

Implementation using MPI and static partitioning

- Read the adjacency matrix on process 0, and broadcast it to all the processes;
- Partitioning the tree
- Checking and updating the best tour
- After the search has terminated, making sure that process 0 has a copy of the best tour for output

Partitioning the tree

- **MPI_Scatter**: cannot be used, as # of initial partial tours may not be evenly divisible by comm_sz.
- **MPI_Scatterv**: a variant of MPI_Scatter, which can send different # of objects to different processes.

```
int MPI_Scatterv(
      void*         sendbuf        /* in  */,
      int*          sendcounts     /* in  */,
      int*          displacements  /* in  */,
      MPI_Datatype  sendtype       /* in  */,
      void*         recvbuf        /* out */,
      int           recvcount      /* in  */,
      MPI_Datatype  recvtype       /* in  */,
      int           root           /* in  */,
      MPI_Comm      comm           /* in  */)
```

Data sent to process q will begin in location (sendtype = MPI_INT)

sendbuf + displacement[q]

Gathering a different number of objects from each process in the communicator

- **MPI_Gatherv**: a variant of MPI_Gather, which can gather different # of objects from different processes.

```
int MPI_Gatherv(
      void*          sendbuf          /* in   */,
      int            sendcount        /* in   */,
      MPI_Datatype   sendtype         /* in   */,
      void*          recvbuf          /* out  */,
      int*           recvcounts       /* in   */,
      int*           displacements    /* in   */,
      MPI_Datatype   recvtype         /* in   */,
      int            root             /* in   */,
      MPI_Comm       comm             /* in   */)
```

Maintaining the best tour

- When a process finds a new best tour, it should send it to other processes.
- **MPI_Bcast** cannot be used, as it is **blocking**.
- New tour should be sent in a way that the sender won't block indefinitely.

Maintaining the best tour

- **MPI_Iprobe:** checking to see if a message is available
  - It doesn't actually try to receive a message

```
int MPI_Iprobe(
        int           source        /* in  */,
        int           tag           /* in  */,
        MPI_Comm      comm          /* in  */,
        int*          msg_avail_p   /* out */,
        MPI_Status*   status_p      /* out */);
```

If such a msg is available,*msg_avail_p is assigned TRUE

Status_p->MPI_SOURCE will be assigned the rank of message source

MPI code to check for new best tour costs

```
MPI_Iprobe(MPI_ANY_SOURCE, NEW_COST_TAG,   comm,
      &msg_avail, &status);
while(msg_avail)
{
      MPI_Recv(&received_cost, 1, MPI_INT, status.MPI_SOURCE,
            NEW_COST_TAG, comm, MPI_STATUS_IGNORE );
      if (received_cost < best_tour_cost)
            best_tour_cost = received_cost;
      MPI_Iprobe(MPI_ANY_SOURCE, NEW_COST_TAG, comm,
            &msg_avail, &status);
}
```

Modes and Buffered Sends - 1

- MPI provides four modes for sends.
  - **Standard**: MPI_Send
  - **Synchronous:** MPI_Ssend
  - **Ready:** MPI_Rsend
  - **Buffered:** MPI_Bsend

Modes and Buffered Sends - 2

- **Standard: MPI_Send**
  - MPI implementation decides whether to copy the message content into its own storage, or to block until a matching receive is posted.

- **Synchronous: MPI_Ssend**
  - The send will block until a matching receive is posted

Modes and Buffered Sends - 3

- **Ready: MPI_Rsend**
  - The send is erroneous unless a matching Receive is posted *before* the Send is started.

- **Buffered: MPI_Bsend**
  - MPI implementation must copy the message into local temporary storage if a matching Receive hasn't been posted.
  - The temporary storage must be provided by the user program, not MPI implementation.

Printing the best tour

- Have each process store its local best tour
- After completing searches, call MPI_Allreduce
- The process with the global best tour can then send it to process 0 for output

```
struct {
   int cost;
   int rank;
} loc_data, global_data;
```

```
loc_data.cost = Tour_cost(loc_best_tour);
loc_data.rank = my_rank;
```

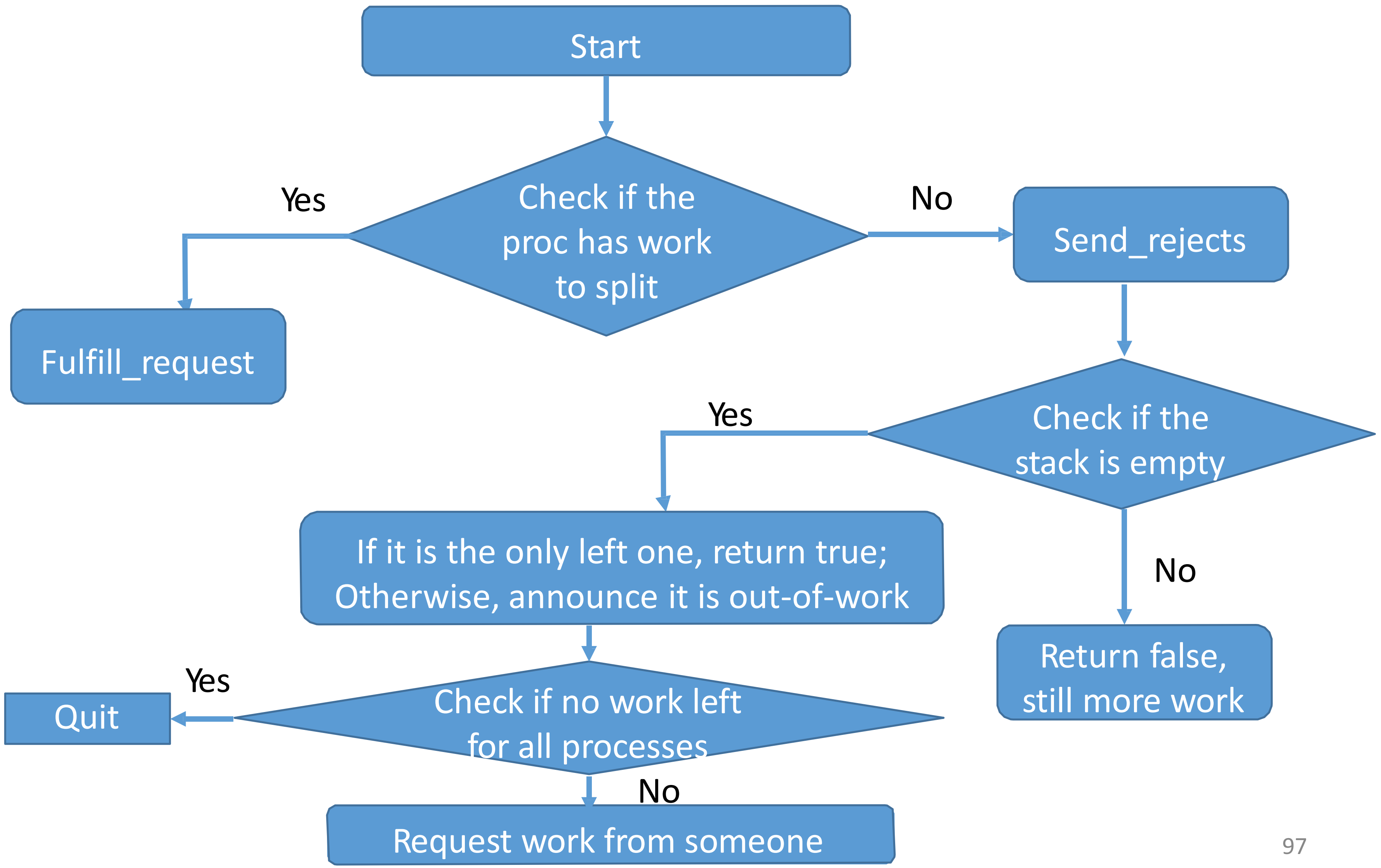
```
MPI_Allreduce(&loc_data, &global_data, 1, MPI_2INT, MPI_MINLOC, comm);
if (global_data.rank == 0) return; /* 0 already has the best tour */
if (my_rank == 0)
   Receive best tour from process global_data.rank;
else if (my_rank == global_data.rank)
   Send best tour to process 0;
```

Implementation of Tree Search Using MPI and Dynamic Partitioning

Using MPI and Dynamic Partitioning

- **Key difference** with OpenMP/pthreads:
  - There is no central repository of information on which processes are waiting for work.
  - Rather than simply going into a busy-wait or termination, a process that has run out of work should send a request for work to another process.

Terminated function for a Dynamically Partitioned TSP solver that Uses MPI



Terminated Function for a Dynamically Partitioned TSP solver with MPI (1)

```
if (My_avail_tour_count(my_stack) >= 2) {
   Fulfill_request(my_stack);
   return false;  /* Still more work */
} else { /* At most 1 available tour */
   Send_rejects();  /* Tell everyone who's requested */
                    /* work that I have none        */
   if (!Empty_stack(my_stack)) {
      return false;  /* Still more work */
   } else {  /* Empty stack */
      if (comm_sz == 1) return true;
      Out_of_work();
      work_request_sent = false;
      while (1) {
         Clear_msgs();  /* Messages unrelated to work, termination */
         if (No_work_left()) {
            return true;  /* No work left.  Quit */
```

the proc has work to split

the proc has no more work to split

the proc has work to do, cannot terminate

Only one proc is left, and it has no work, quit

When stack is empty, announce it is out-of-work

If all procs have no work left, quit

Terminated Function for a Dynamically Partitioned TSP solver with MPI (2)

Send work request to other proc

```
      } else if (!work_request_sent) {
         Send_work_request();  /* Request work from someone */
         work_request_sent = true;
      } else {
         Check_for_work(&work_request_sent, &work_avail);
         if (work_avail) {
            Receive_work(my_stack);
            return false;
         }
      }
   }  /* while */
  }  /* Empty stack */
} /* At most 1 available tour */
```

Check for work, if there is work available, receive work from the remote proc.

Splitting the stack and data packing

- **MPI_Pack:** Packing data into a buffer of contiguous memory
- **Split_stack** packs the contents of new stack into contiguous memory and send the block of contiguous memory to the receiver

```
int MPI_Pack(
      void*          data_to_be_packed    /* in     */,
      int            to_be_packed_count   /* in     */,
      MPI_Datatype   datatype             /* in     */,
      void*          contig_buf           /* out    */,
      int            contig_buf_size      /* in     */,
      int*           position_p           /* in/out */,
      MPI_Comm       comm                 /* in     */)
```

```
int MPI_Unpack(
      void*          contig_buf           /* in     */,
      int            contig_buf_size      /* in     */,
      int*           position_p           /* in/out */,
      void*          unpacked_data        /* out    */,
      int            unpack_count         /* in     */,
      MPI_Datatype   datatype             /* in     */,
      MPI_Comm       comm                 /* in     */)
```

Distributed Termination Detection

- *Out_of_work()* and *No_work_left()* implements the termination detection algorithm.
- The termination detection algorithm used in shared-memory programs will have problems in MPI.
- Suppose each proc stores a variable *oow* to indicate the number of processes that are out of work
  - Initially, oow = 0
  - Each time a process runs out of work (or receive work), it sends a message to other processes, so that others will update their copies of oow.

Table 6.10 Termination Events that Result in an Error

Time	Process 0	Process 1	Process 2
0	Out of Work Notify 1, 2 oow = 1	Out of Work Notify 0, 2 oow = 1	Working oow = 0
1	Send request to 1 oow = 1	Send Request to 2 oow = 1	Recv notify fr 1 oow = 1
2	oow = 1	Recv notify fr 0 oow = 2	Recv request fr 1 oow = 1
3	oow = 1	oow = 2	Send work to 1 oow = 0
4	oow = 1	Recv work fr 2 oow = 1	Recv notify fr 0 oow = 1
5	oow = 1	Notify 0 oow = 1	Working oow = 1
6	oow = 1	Recv request fr 0 oow = 1	Out of work Notify 0, 1 oow = 2
7	Recv notify fr 2 oow = 2	Send work to 0 oow = 0	Send request to 1 oow = 2
8	Recv 1st notify fr 1 oow = 3	Recv notify fr 2 oow = 1	oow = 2
9	Quit	Recv request fr 2 oow = 1	oow = 2

The **error** here is that the work sent from process 1 to process 0 is lost

The reason is that proc 0 receives notification that proc 2 is out of work before it receives notification that proc 1 has received work.

A simple distributed termination detection algorithm

- **Idea**: keeping track of a quantity that is conserved and can be measured precisely (e.g., energy)

- **Algorithm:**
  - Initially, each process has 1 unit of energy
  - When a process runs out of work, it sends its energy to process 0.
  - When a process fulfills a request for work, it divides its energy in half, keeping half for itself, and sending half to another
  - The program should terminate when process 0 receives a total energy of comm_sz units

Performance of MPI and Pthreads implementations of tree search

(in seconds)

Th/Pr	First Problem						Second Problem					
	Static		Dynamic				Static		Dynamic			
	Pth	MPI	Pth		MPI		Pth	MPI	Pth		MPI	
1	35.8	40.9	41.9	(0)	56.5	(0)	27.4	31.5	32.3	(0)	43.8	(0)
2	29.9	34.9	34.3	(9)	55.6	(5)	27.4	31.5	22.0	(8)	37.4	(9)
4	27.2	31.7	30.2	(55)	52.6	(85)	27.4	31.5	10.7	(44)	21.8	(76)
8		35.7			45.5	(165)		35.7			16.5	(161)
16		20.1			10.5	(441)		17.8			0.1	(173)

- Pthreads outperforms MPI implementation for small shared-memory systems.
- For large problems, MPI program is much more scalable and can provide better performance.

Concluding Remarks (1)

- In developing the reduced MPI solution to the n-body problem, the "ring pass" algorithm proved to be much easier to implement and is probably more scalable.

- In a distributed memory environment in which processes send each other work, determining when to terminate is a nontrivial problem.

Concluding Remarks (2)

- When deciding which API to use, we should consider whether to use shared- or distributed-memory.

- We should look at the memory requirements of the application and the amount of communication among the processes/threads.

Concluding Remarks (3)

- If the memory requirements are great or the distributed memory version can work mainly with cache, then a distributed memory program is likely to be much faster.

- On the other hand if there is considerable communication, a shared memory program will probably be faster.

Concluding Remarks (3)

- In choosing between OpenMP and Pthreads, if there's an existing serial program and it can be parallelized by the insertion of OpenMP directives, then OpenMP is probably the clear choice.

- However, if complex thread synchronization is needed then Pthreads will be easier to use.