Parallel *N* Body

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Outline

N-body problem

- Given initial positions and velocities of n bodies, compute their positions and velocities at given points in time
- n can be very large
- We want to compute in parallel

Equations of motion

Assume n particles, $0, 1, \ldots, n-1$
Particle q has position $\mathbf{s}_q(t)$, velocity $\mathbf{v}_q(t) = \mathbf{s}'_q(t)$ and acceleration $\mathbf{a}_q(t) = \mathbf{s}''_q(t)$
Bold denotes vectors; these are 3D (or 2D) vectors
Particle k exerts force on q

$$\mathbf{f}_{qk}(t) = -G\frac{m_q m_k}{\|\mathbf{s}_q(t) - \mathbf{s}_k(t)\|_2^3}[\mathbf{s}_q(t) - \mathbf{s}_k(t)],$$

where $G = 6.673 \times 10^{-11} m^3/(\text{kg} \cdot s^2)$ is the gravitational constant, and $\|\mathbf{s}_q(t) - \mathbf{s}_k(t)\|_2$ is the distance between particles q and k

Total force on q is

$$\mathbf{F}_q(t) = \sum_{\substack{k=0\\k\neq q}}^{n-1} \mathbf{f}_{qk}(t) = -Gm_q \sum_{\substack{k=0\\k\neq q}}^{n-1} \frac{m_k}{\|\mathbf{s}_q(t) - \mathbf{s}_k(t)\|_2^3}[\mathbf{s}_q(t) - \mathbf{s}_k(t)],$$

$q = 0, 1, \ldots n-1$
From Newton's second law of motion

$$\mathbf{F}_q(t) = m_q\mathbf{a}_q(t) = m_q\mathbf{s}_q''(t),$$

$$\begin{aligned}\mathbf{s}_q''(t) = \mathbf{F}_q(t)/m_q &= \frac{1}{m_q}\sum_{\substack{k=0\\k\neq q}}^{n-1} \mathbf{f}_{qk}(t)\\ &= -G\sum_{\substack{k=0\\k\neq q}}^{n-1} \frac{m_k}{\|\mathbf{s}_q(t) - \mathbf{s}_k(t)\|_2^3}[\mathbf{s}_q(t) - \mathbf{s}_k(t)]\end{aligned}$$

We have a system of second-order ordinary differential equations
We can write it as first order system

$$\begin{cases} \mathbf{s}_q'(t) & = \mathbf{v}_q(t) \\ \mathbf{v}_q'(t) & = \mathbf{F}_q(t)/m_q = -G \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \frac{m_k}{\|\mathbf{s}_q(t) - \mathbf{s}_k(t)\|_2^3} [\mathbf{s}_q(t) - \mathbf{s}_k(t)], \end{cases}$$

$q = 0, 1, \ldots, n-1$

Overall method

Given initial values for $\mathbf{s}_q(t)$ and $\mathbf{v}_q(t)$ for all q at initial time, e.g. $t_0 = 0$, we have an initial value problem
We advance in time from t_0 and compute at points t_i, $i > 0$
Assume $\mathbf{s}_{q,i}$ and $\mathbf{v}_{q,i}$ are computed up to t_i

On a time step from t_i to t_{i+1}
(1) compute total forces $\mathbf{F}_{q,i}$
(2) compute $\mathbf{v}_{q,i+1}$ and $\mathbf{s}_{q,i+1}$

We can do (2) using Runge-Kutta or a multistep method
Here we Euler's method, to keep the explanations simpler and focus on (1)

Euler's method

For simplicity, we use Euler's method
Assume $\mathbf{s}_{q,i}$ and $\mathbf{v}_{q,i}$ are given at t_i We compute at t_{i+1} by

$$\mathbf{v}_{q,i+1} = \mathbf{v}_{q,i} + h\mathbf{F}_{q,i}/m_q$$
$$\mathbf{s}_{q,i+1} = \mathbf{s}_{q,i} + h\mathbf{v}_{q,i},$$

where $h = t_{i+1} - t_i$ is stepsize; we use constant stepsize h

Computing forces

The total force for particle q is computed by

$$\mathbf{F}_{q,i} = \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \mathbf{f}_{qk,i} = -Gm_q \sum_{\substack{k=0 \\ k \neq q}}^{n-1} \frac{m_k}{\|\mathbf{s}_{q,i} - \mathbf{s}_{k,i}\|^3} [\mathbf{s}_{q,i} - \mathbf{s}_{q,i}]$$

Hence, on time step from t_i to t_{i+1} we need $\mathbf{v}_{q,i}$ and $\mathbf{s}_{q,i}$ for all q
How to compute these forces?

Serial algorithms

Basic algorithm

for $q = 0, 1, \ldots, n-1$
  $\mathbf{F}_{q,i} = 0$
  for $k = 0, 1, \ldots, n-1$
    if $k \neq q$
      compute $\mathbf{f}_{qk,i}$
      $\mathbf{F}_{q,i} = \mathbf{F}_{q,i} + \mathbf{f}_{qk,i}$

Reduced algorithm

for $q = 0, 1, \ldots, n-1$
  $\mathbf{F}_{q,i} = 0$
for $q = 0, 1, \ldots, n-1$
  for $k > q$
    compute $\mathbf{f}_{qk,i}$
    $\mathbf{F}_{q,i} = \mathbf{F}_{q,i} + \mathbf{f}_{qk,i}$
    $\mathbf{F}_{k,i} = \mathbf{F}_{k,i} - \mathbf{f}_{qk,i}$

From Newton's third law, $\mathbf{f}_{qk} = -\mathbf{f}_{kq}$

Example Consider four particles and the related forces

particles	0	1	2	3
0	–	$\mathbf{f}_{01}$	$\mathbf{f}_{02}$	$\mathbf{f}_{03}$
1	$-\mathbf{f}_{01}$	–	$\mathbf{f}_{12}$	$\mathbf{f}_{13}$
2	$-\mathbf{f}_{02}$	$-\mathbf{f}_{12}$	–	$\mathbf{f}_{23}$
3	$-\mathbf{f}_{03}$	$-\mathbf{f}_{13}$	$-\mathbf{f}_{23}$	–

Reduced algorithm computes

iteration 1, $q = 0$	iteration 2, $q = 1$	iteration 3, $q = 2$
$\mathbf{F}_0 = \mathbf{f}_{01} + \mathbf{f}_{02} + \mathbf{f}_{03}$		
$\mathbf{F}_1 = -\mathbf{f}_{01}$	$\mathbf{F}_1 = \mathbf{F}_1 + \mathbf{f}_{12} + \mathbf{f}_{13}$	
$\mathbf{F}_2 = -\mathbf{f}_{02}$	$\mathbf{F}_2 = \mathbf{F}_2 - \mathbf{f}_{12}$	$\mathbf{F}_2 = \mathbf{F}_2 + \mathbf{f}_{23}$
$\mathbf{F}_3 = -\mathbf{f}_{03}$	$\mathbf{F}_3 = \mathbf{F}_3 - \mathbf{f}_{13}$	$\mathbf{F}_3 = \mathbf{F}_3 - \mathbf{f}_{23}$

As the iteration number increases, the work decreases

Parallelization: block distribution

How to parallelize?
Assume block distribution, each process takes n/p particles
Basic algorithm: the work is the same per process
Reduced? Process 0 will do most of the work, then process 1, then process 2, and so on
Example: Consider $n = 6$ distributed on $p = 3$ processes:

PE	owns particles	stores
0	$0, 1$	$\mathbf{s}_0, \mathbf{s}_1$
1	$2, 3$	$\mathbf{s}_2, \mathbf{s}_3$
2	$4, 5$	$\mathbf{s}_4, \mathbf{s}_5$

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

	PE 0	PE 1	PE 2
owns	$\mathbf{s}_0, \mathbf{s}_1$	$\mathbf{s}_2, \mathbf{s}_3$	$\mathbf{s}_4, \mathbf{s}_5$
receives	$\mathbf{s}_2, \mathbf{s}_3$ from PE 1 $\mathbf{s}_4, \mathbf{s}_5$ from PE 2	$\mathbf{s}_4, \mathbf{s}_5$ from PE 2	
computes	$\mathbf{f}_{01}, \mathbf{f}_{02}, \mathbf{f}_{03}, \mathbf{f}_{04}, \mathbf{f}_{05}, \mathbf{f}_{12}, \mathbf{f}_{13}, \mathbf{f}_{14}, \mathbf{f}_{15}$	$\mathbf{f}_{23}, \mathbf{f}_{24}, \mathbf{f}_{25}, \mathbf{f}_{34}, \mathbf{f}_{35}$	$\mathbf{f}_{45}$
sends	$\mathbf{f}_{02}, \mathbf{f}_{03}, \mathbf{f}_{12}, \mathbf{f}_{13}$ to PE 1 $\mathbf{f}_{04}, \mathbf{f}_{05}, \mathbf{f}_{14}, \mathbf{f}_{15}$ to PE 2	$\mathbf{f}_{24}, \mathbf{f}_{25}, \mathbf{f}_{34}, \mathbf{f}_{35}$ to PE 2	

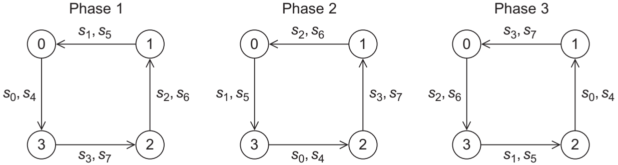
The work is not distributed evenly

Parallelization: ring pass communication

Process i

- sends to $(i - 1 + p) \mod p$
- receives from $(i + 1) \mod p$

Consider $n = 8$, $p = 4$ and cycling distribution[1]



PE	initial	receives		
		pass 1	pass 2	pass 3
0	$\mathbf{s}_0, \mathbf{s}_4$	$\mathbf{s}_1, \mathbf{s}_5$	$\mathbf{s}_2, \mathbf{s}_6$	$\mathbf{s}_3, \mathbf{s}_7$
1	$\mathbf{s}_1, \mathbf{s}_5$	$\mathbf{s}_2, \mathbf{s}_6$	$\mathbf{s}_3, \mathbf{s}_7$	$\mathbf{s}_0, \mathbf{s}_4$
2	$\mathbf{s}_2, \mathbf{s}_6$	$\mathbf{s}_3, \mathbf{s}_7$	$\mathbf{s}_0, \mathbf{s}_4$	$\mathbf{s}_1, \mathbf{s}_5$
3	$\mathbf{s}_3, \mathbf{s}_7$	$\mathbf{s}_0, \mathbf{s}_4$	$\mathbf{s}_1, \mathbf{s}_5$	$\mathbf{s}_2, \mathbf{s}_6$

[1] Figure is from P. Pacheco, An Introduction to Parallel Programming

Consider particles q and k

- If q is assigned to process P then P computes $\mathbf{f}_{qk}$ if
  - k is assigned to P or
  - positions of k are received on P

Example: Consider $n = 6$, $p = 3$, ring pass communication, and cycling distribution
After initial assignment

PE	initial	computes
0	$\mathbf{s}_0, \mathbf{s}_3$	$\mathbf{f}_{03}$
1	$\mathbf{s}_1, \mathbf{s}_4$	$\mathbf{f}_{14}$
2	$\mathbf{s}_2, \mathbf{s}_5$	$\mathbf{f}_{25}$

Then

PE	initial	pass 1	pass 2
0	$\mathbf{s}_0, \mathbf{s}_3$	$\mathbf{s}_1, \mathbf{s}_4$	$\mathbf{s}_2, \mathbf{s}_5$
computes	$\mathbf{f}_{03}$	$\mathbf{f}_{01}, \mathbf{f}_{04}, \mathbf{f}_{34}$	$\mathbf{f}_{02}, \mathbf{f}_{05}, \mathbf{f}_{35}$
1	$\mathbf{s}_1, \mathbf{s}_4$	$\mathbf{s}_2, \mathbf{s}_5$	$\mathbf{s}_0, \mathbf{s}_3$
computes	$\mathbf{f}_{14}$	$\mathbf{f}_{12}, \mathbf{f}_{15}, \mathbf{f}_{45}$	$\mathbf{f}_{13}$
2	$\mathbf{s}_2, \mathbf{s}_5$	$\mathbf{s}_0, \mathbf{s}_3$	$\mathbf{s}_1, \mathbf{s}_4$
computes	$\mathbf{f}_{25}$	$\mathbf{f}_{23}$	$\mathbf{f}_{24}$

Example

$p = 3$, $n = 9$

PE	initial	pass 1	pass 2
0	$\mathbf{s}_0, \mathbf{s}_3, \mathbf{s}_6$	$\mathbf{s}_1, \mathbf{s}_4, \mathbf{s}_7$	$\mathbf{s}_2, \mathbf{s}_5, \mathbf{s}_8$
computes	$\mathbf{f}_{03}, \mathbf{f}_{06}, \mathbf{f}_{36}$	$\mathbf{f}_{01}, \mathbf{f}_{04}, \mathbf{f}_{07}, \mathbf{f}_{34}, \mathbf{f}_{37}, \mathbf{f}_{67}$	$\mathbf{f}_{02}, \mathbf{f}_{05}, \mathbf{f}_{08}, \mathbf{f}_{35}, \mathbf{f}_{38}, \mathbf{f}_{68}$
1	$\mathbf{s}_1, \mathbf{s}_4, \mathbf{s}_7$	$\mathbf{s}_2, \mathbf{s}_5, \mathbf{s}_8$	$\mathbf{s}_0, \mathbf{s}_3, \mathbf{s}_6$
computes	$\mathbf{f}_{14}, \mathbf{f}_{17}, \mathbf{f}_{47}$	$\mathbf{f}_{12}, \mathbf{f}_{15}, \mathbf{f}_{18}, \mathbf{f}_{45}, \mathbf{f}_{48}, \mathbf{f}_{78}$	$\mathbf{f}_{13}, \mathbf{f}_{16}, \mathbf{f}_{46}$
2	$\mathbf{s}_2, \mathbf{s}_5, \mathbf{s}_8$	$\mathbf{s}_0, \mathbf{s}_3, \mathbf{s}_6$	$\mathbf{s}_1, \mathbf{s}_4, \mathbf{s}_7$
computes	$\mathbf{f}_{25}, \mathbf{f}_{28}, \mathbf{f}_{58}$	$\mathbf{f}_{23}, \mathbf{f}_{26}, \mathbf{f}_{56}$	$\mathbf{f}_{24}, \mathbf{f}_{27}, \mathbf{f}_{57}$

particle	PE								
0	0	$\mathbf{f}_{01}$	$\mathbf{f}_{02}$	$\mathbf{f}_{03}$	$\mathbf{f}_{04}$	$\mathbf{f}_{05}$	$\mathbf{f}_{06}$	$\mathbf{f}_{07}$	$\mathbf{f}_{08}$
1	1		$\mathbf{f}_{12}$	$\mathbf{f}_{13}$	$\mathbf{f}_{14}$	$\mathbf{f}_{15}$	$\mathbf{f}_{16}$	$\mathbf{f}_{17}$	$\mathbf{f}_{18}$
2	2			$\mathbf{f}_{23}$	$\mathbf{f}_{24}$	$\mathbf{f}_{25}$	$\mathbf{f}_{26}$	$\mathbf{f}_{27}$	$\mathbf{f}_{28}$
3	0				$\mathbf{f}_{34}$	$\mathbf{f}_{35}$	$\mathbf{f}_{36}$	$\mathbf{f}_{37}$	$\mathbf{f}_{38}$
4	1					$\mathbf{f}_{45}$	$\mathbf{f}_{46}$	$\mathbf{f}_{47}$	$\mathbf{f}_{48}$
5	2						$\mathbf{f}_{56}$	$\mathbf{f}_{57}$	$\mathbf{f}_{58}$
6	0							$\mathbf{f}_{67}$	$\mathbf{f}_{68}$
7	1								$\mathbf{f}_{78}$
8	2								

red: initial; blue: pass 1; green: pass 2

particle	PE	computes							
0	0	f_{01}	f_{02}	f_{03}	f_{04}	f_{05}	f_{06}	f_{07}	f_{08}
3	0				f_{34}	f_{35}	f_{36}	f_{37}	f_{38}
6	0							f_{67}	f_{68}
1	1		f_{12}	f_{13}	f_{14}	f_{15}	f_{16}	f_{17}	f_{18}
4	1					f_{45}	f_{46}	f_{47}	f_{48}
7	1								f_{78}
2	2			f_{23}	f_{24}	f_{25}	f_{26}	f_{27}	f_{28}
5	2						f_{56}	f_{57}	f_{58}
8	2								

red: initial; blue: pass 1; green: pass 2