Announcements

• Assignment 6 (extra credit) on MPI has been posted
  • Due on Dec 6 11:59 pm

• Final exam is on Dec 16 10:30 am — 12:30 pm
  • In person, closed book/notes
Molecular Dynamics
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• Force calculations
  • Bonded interactions: bonds, angles, dihedrals
  • Non-bonded interactions: van der Waal’s and electrostatic forces
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- Number of atoms: thousands to millions
- Simulation step: \( \sim 1 \) femtosecond \( (10^{-15} \text{ s}) \)
- Used for drug design, materials design
Sequential Algorithm

- At every step, calculate forces on each atom
  - Calculate bonded and short-range forces every step
  - Calculate long-range non-bonded forces every few time steps (using PME or P3M etc.)

- Particle mesh Ewald (PME) summation:
  - Calculate long-range interactions in Fourier space

- Calculate velocities and new positions

- Repeat …
Traditional approaches to parallelization
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- Atom decomposition:
  - Partition the atoms across processes
Traditional approaches to parallelization

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  - Partition the atoms across processes

- Force decomposition:
  - Distribute the force matrix to processes
  - Matrix is sparse and non-uniform
Traditional approaches to parallelization

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- Spatial decomposition:
  - Assign a region of the 3D simulation space to each process
Hybrid parallelization

- Hybrid of spatial and force decomposition
- Decouple assignment of data and work to processes
- Distribute both atoms and the force calculations to different processes
Neutral territory (NT) methods

• Desmond’s mid-point method

SC23 Test-of-time award:
Particle mesh Ewald

• Replace direct force calculations by:
  • Calculate short-range forces in real space
  • Calculate long-range forces in Fourier space

• Create a 3D mesh/grid representing charge densities of atoms
  • Compute a 3D Fast Fourier Transform (FFT)

• FFT computes the discrete Fourier transform (DFT) or inverse DFT
  • Reduces the complexity from $O(N^2)$ to $O(N \log N)$
Parallelization of PME (3D FFT)
Parallelization of PME (3D FFT)

- Bring all the data to one process
Parallelization of PME (3D FFT)

- Bring all the data to one process
- 1D or slab decomposition
Parallelization of PME (3D FFT)

- 2D or pencil decomposition
Measles killed 200,000 in 2020 alone!

LARGE MEASLES OUTBREAKS
The epidemic in the Democratic Republic of the Congo is the largest single-nation outbreak for decades.

- Ukraine (2017–20) >115,000 cases >41 deaths
- Democratic Republic of the Congo (2019–20) 346,158 cases 841 deaths
- Madagascar (2018–20) 244,675 cases >1,000 deaths

Predictions say that 1.66 million people died of tuberculosis in 2020

https://www.nature.com/articles/d41586-020-01011-6

TERrible toll
By the end of July 2020, there had been 646,949 COVID-19 deaths worldwide. In the 32 countries and 4 major cities with relevant data, there were more excess deaths than COVID-19 deaths, suggesting that some COVID-19 deaths are misclassified or that other causes of death have also risen.

- Deaths attributed to COVID-19
- Excess deaths

32 countries and 4 major cities
- Worldwide

In August 2003, a heatwave in Europe caused 44,878 excess deaths

The global total of excess deaths is probably much higher than the number of COVID-19 deaths.

*Cumulative deaths from outbreak onset to latest available data, as of 18 August 2020.

https://www.nature.com/articles/d41586-020-02497-w
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Societal challenge

• Controlling the spread of infectious diseases is important

• Computational and mathematical modeling of epidemics important to assist governments in responding to outbreaks

• Made challenging due to:
  • increased and denser urbanization
  • increased local and global travel
  • increasingly immuno-comprised population
Approach: individual-based simulation

- Agent-based modeling to simulate epidemic diffusion
- Models agents (people) and interactions between them
- People interact when they visit the same location at the same time
- These “interactions” between pairs of people are represented as “visits” to locations
- Use a bi-partite graph of people and locations or a people-people interactivity graph
Serial algorithm

- At each timestep (typically a day):
  - Determine which people visit which locations
  - “Send” people to those locations
  - At each location “interactions” happen and transmission happens
  - Update people’s states at the end of the day and continue
- Interventions (vaccinations, school closures) can be added on certain days to change people’s susceptibility, movements etc.
Combination of network theory and discrete-event simulations

- Hybrid time-stepped and discrete-event simulation
Combination of network theory and discrete-event simulations

• Hybrid time-stepped and discrete-event simulation

Contact model at each location
Combination of network theory and discrete-event simulations

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Contact model at each location

Model for human transmission

Direct Contact
- Pathogens survive best inside the body
  - E.g., HIV, hepatitis, Ebola

Indirect Contact
- Pathogens survive in the environment
  - Pick up pathogen from surface or air
  - E.g., influenza, norovirus

Droplets
- Pathogens are in droplets, but do not survive long in air
  - E.g., Ebola, Rinderpest, parvovirus

Airborne
- Pathogens aerosolized and stay in the air
  - E.g., influenza, tuberculosis

WASH
- Through contaminated water or food
  - E.g., cholera, typhoid, hepatitis

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Disease model for each person

Contact model at each location

Model for human transmission

Combination of network theory and discrete-event simulations

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```python
while d < num_days:
    for each person:
        Send visit messages to locations

for each location:
    Process all visit messages
    Run discrete event simulation
    Send interaction messages

for each person:
    Process interactions
    Update disease state
```

Disease model for each person

Model for human transmission

Contact model at each location

Parallel simulation is challenging

- Size and scale of the social contact network (6 billion agents for a global simulation)
  - Unstructured networks and complicated dependencies lead to high communication cost
- Individuals and their behaviors are not identical
- Co-evolving epidemics, public policies and agent behaviors make it impossible to apply standard model reduction techniques
Parallel implementation: Loimos

- All the people and locations are distributed among all processes
- DES computation can be done locally in parallel
- Communication when sending visit and infection messages
- Uses Charm++, a message-driven model
Application software stack

- **Parallel programming model / runtime:**
  - MPI, OpenMP, Charm++, CUDA, …

- **Libraries**
  - Data and visualization libraries (mesh management, simulation output)
  - I/O libraries
  - Math/numerical libraries
  - Graph partitioning, load balancing …
Why use libraries?

- No need to reinvent the wheel
  - Libraries are highly optimized, have fewer bugs
- Avoids significant effort to write, optimize and maintain code
- Makes code more portable
Popular Libraries

• Data/visualization and I/O libraries
  - I/O: HDF5, pNetCDF, ADIOS

• Numerical libraries:
  - Fast Fourier transforms: FFTW
  - Dense linear algebra: BLAS, LAPACK, Intel MKL
  - Solvers for sparse systems: Hypre, PETSc, Trilinos

• Graph partitioning/load balancing:
  - METIS, Scotch, Zoltan, Chaco

https://events.prace-ri.eu/event/176/contributions/38/attachments/154/305/HPC_libraries.pdf
Domain-specific languages/frameworks

- Structured grids: SAMRAI, Chombo, AMReX
- Unstructured grids: MFEM, Quinoa
The $n$-body problem

- Simulate the motion of celestial objects interacting with one another due to gravitational forces
- Naive algorithm: $O(n^2)$
  - Every body calculates forces pair-wise with every other body (particle)

Data distribution in \( n \)-body problems

- Naive approach: Assign \( n/p \) particles to each process
- Other approaches?
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Space-filling curves

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Space-filling curves

Data distribution in $n$-body problems

- Let us consider a two-dimensional space with bodies/particles in it
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Data distribution in $n$-body problems

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Different parallelization methods

- Tree codes: Barnes-Hut simulations
- Fast multipole methods (FMM): Greengard and Rokhlin
- Particle mesh methods
- Particle-particle-particle-mesh (P³M) methods
Barnes-Hut simulation

- Represent the space containing the particles as an oct-tree
- Pairwise force calculations for nearby particles
- For tree nodes that are sufficiently far away, approximate the particles in the node by a single large particle at the center of mass
- $O(N \log N)$ algorithm

Fast multipole methods

- Use multipole expansion for distant particles
- Takes advantage of the fact that for nearby particles, multipole-expanded forces from distant particles are similar
- Reduces the time complexity further to $O(n)$
Particle-particle particle-mesh methods

- Explicit calculation of forces on nearby particles
- Fourier-based Ewald summation for calculating potentials on a grid
- Smoothed particle hydrodynamics
Abhinav Bhavele
5218 Brendan Iribe Center (IRB) / College Park, MD 20742
phone: 301.405.4507 / e-mail: bhatele@cs.umd.edu