Parallel Programming & Cluster Computing

Applications and Types of Parallelism

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Outline

- Monte Carlo: Client-Server
- N-Body: Task Parallelism
- Transport: Data Parallelism
Monte Carlo: Client-Server
Embarrassingly Parallel

An application is known as *embarrassingly parallel* if its parallel implementation:

1. can straightforwardly be broken up into roughly equal amounts of work per processor, AND
2. has minimal parallel overhead (for example, communication among processors).

We **love** embarrassingly parallel applications, because they get **near-perfect parallel speedup**, sometimes with modest programming effort.

Embarrassingly parallel applications are also known as **loosely coupled**.
Monte Carlo Methods

Monte Carlo is a European city where people gamble; that is, they play games of chance, which involve randomness. **Monte Carlo methods** are ways of simulating (or otherwise calculating) physical phenomena based on randomness. Monte Carlo simulations typically are embarrassingly parallel.
Monte Carlo Methods: Example

Suppose you have some physical phenomenon. For example, consider High Energy Physics, in which we bang tiny particles together at incredibly high speeds.

We want to know, say, the average properties of this phenomenon.

There are infinitely many ways that two particles can be banged together.

So, we can’t possibly simulate all of them.
Monte Carlo Methods: Example

Suppose you have some physical phenomenon. For example, consider High Energy Physics, in which we bang tiny particles together at incredibly high speeds.

There are infinitely many ways that two particles can be banged together. So, we can’t possibly simulate all of them.

Instead, we can **randomly choose a finite subset** of these infinitely many ways and simulate only the subset.
Monte Carlo Methods: Example

Suppose you have some physical phenomenon. For example, consider High Energy Physics, in which we bang tiny particles together at incredibly high speeds.

There are infinitely many ways that two particles can be banged together.

We randomly choose a finite subset of these infinitely many ways and simulate only the subset.

The average of this subset will be close to the actual average.
Monte Carlo Methods

In a Monte Carlo method, you randomly generate a large number of example cases (realizations) of a phenomenon, and then take the average of the properties of these realizations.

When the average of the realizations converges (that is, doesn’t change substantially if new realizations are generated), then the Monte Carlo simulation stops.
Monte Carlo simulations are embarrassingly parallel, because each realization is completely independent of all of the other realizations.

That is, if you’re going to run a million realizations, then:

1. you can straightforwardly break into roughly \((\text{Million} / N_p)\) chunks of realizations, one chunk for each of the \(N_p\) processors, AND

2. the only parallel overhead (for example, communication) comes from tracking the average properties, which doesn’t have to happen very often.
Serial Monte Carlo (C)

Suppose you have an existing serial Monte Carlo simulation:

```c
int main (int argc, char** argv)
{
    /* main */
    read_input(...);
    for (realization = 0;
        realization < number_of_realizations;
        realization++) {
        generate_random_realization(...);
        calculate_properties(...);
    } /* for realization */
    calculate_average(...);
} /* main */
```

How would you parallelize this?
Suppose you have an existing serial Monte Carlo simulation:

```fortran
PROGRAM monte_carlo
  CALL read_input(…)
  DO realization = 1, number_of_realizations
    CALL generate_random_realization(…)
    CALL calculate_properties(…)
  END DO
  CALL calculate_average(…)
END PROGRAM monte_carlo
```

How would you parallelize this?
Parallel Monte Carlo (C)

```c
int main (int argc, char** argv)
{ /* main */

    [MPI startup]
    if (my_rank == server_rank) {
        read_input(...);
    }

    mpi_error_code = MPI_Bcast(...);
    for (realization = 0;
        realization < number_of_realizations / number_of_processes;
        realization++) {
        generate_random_realization(...);
        calculate_realization_properties(...);
        calculate_local_running_average(...);
    } /* for realization */

    if (my_rank == server_rank) {
        [collect properties]
    }
    else {
        [send properties]
    }
    calculate_global_average_from_local_averages(...)
    output_overall_average(...)

    [MPI shutdown]
} /* main */
```
Parallel Monte Carlo (F90)

PROGRAM monte_carlo

  [MPI startup]
  IF (my_rank == server_rank) THEN
    CALL read_input(…)
  END IF
  CALL MPI_Bcast(…)
  DO realization = 1, number_of_realizations / number_of_processes
    CALL generate_random_realization(…)
    CALL calculate_realization_properties(…)
    CALL calculate_local_running_average(…)
  END DO
  IF (my_rank == server_rank) THEN
    [collect properties]
  ELSE
    [send properties]
  END IF
  CALL calculate_global_average_from_local_averages(…)
  CALL output_overall_average(…)
  [MPI shutdown]
END PROGRAM monte_carlo
$N$ Bodies
N-Body Problems

An $N$-body problem is a problem involving $N$ “bodies” – that is, particles (for example, stars, atoms) – each of which applies a force to all of the others.

For example, if you have $N$ stars, then each of the $N$ stars exerts a force (gravity) on all of the other $N-1$ stars.

Likewise, if you have $N$ atoms, then every atom exerts a force (nuclear) on all of the other $N-1$ atoms.
1-Body Problem

When $N$ is 1, you have a simple 1-Body Problem: a single particle, with no forces acting on it.

Given the particle’s position $P$ and velocity $V$ at some time $t_0$, you can trivially calculate the particle’s position at time $t_0 + \Delta t$:

$$P(t_0 + \Delta t) = P(t_0) + V\Delta t$$

$$V(t_0 + \Delta t) = V(t_0)$$
2-Body Problem

When \( N \) is 2, you have – surprise! – a 2-Body Problem: exactly 2 particles, each exerting a force that acts on the other.

The relationship between the 2 particles can be expressed as a differential equation that can be solved analytically, producing a closed-form solution.

So, given the particles’ initial positions and velocities, you can trivially calculate their positions and velocities at any later time.
When $N$ is 3, you have — surprise! — a 3-Body Problem: exactly 3 particles, each exerting a force that acts on the other 2.

The relationship between the 3 particles can be expressed as a differential equation that can be solved using an infinite series, producing a closed-form solution, due to Karl Fritiof Sundman in 1912.

However, in practice, the number of terms of the infinite series that you need to calculate to get a reasonable solution is so large that the infinite series is impractical, so you’re stuck with the generalized formulation.
N-Body Problems \((N > 3)\)

When \(N > 3\), you have a general \textit{N-Body Problem}: \(N\) particles, each exerting a force that acts on the other \(N-1\) particles.

The relationship between the \(N\) particles can be expressed as a differential equation that can be solved using an infinite series, producing a closed-form solution, due to Quidong Wang in 1991.

However, in practice, the number of terms of the infinite series that you need to calculate to get a reasonable solution is so large that the infinite series is impractical, so you’re stuck with the generalized formulation.
N-Body Problems ($N \geq 3$)

For $N \geq 3$, the relationship between the $N$ particles can be expressed as a differential equation that can be solved using an infinite series, producing a closed-form solution, but convergence takes so long that this approach is impractical. So, numerical simulation is pretty much the only way to study groups of 3 or more bodies.

Popular applications of N-body codes include:

- astronomy (that is, galaxy formation, cosmology);
- chemistry (that is, protein folding, molecular dynamics).

Note that, for $N$ bodies, there are on the order of $N^2$ forces, denoted $O(N^2)$. 
$N$ Bodies
Force #1
Force #2
Force #3
Force #4
Force #6
Force #N-1
N-Body Problems

Given $N$ bodies, each body exerts a force on all of the other $N - 1$ bodies.

Therefore, there are $N \cdot (N - 1)$ forces in total.

You can also think of this as $(N \cdot (N - 1)) / 2$ forces, in the sense that the force from particle A to particle B is the same (except in the opposite direction) as the force from particle B to particle A.
Aside: Big-O Notation

Let’s say that you have some task to perform on a certain number of things, and that the task takes a certain amount of time to complete.

Let’s say that the amount of time can be expressed as a polynomial on the number of things to perform the task on.

For example, the amount of time it takes to read a book might be proportional to the number of words, plus the amount of time it takes to settle into your favorite easy chair.

\[ C_1 \cdot N + C_2 \]
Big-O: Dropping the Low Term

\[ C_1 \cdot N + C_2 \]

When \( N \) is very large, the time spent settling into your easy chair becomes such a small proportion of the total time that it’s virtually zero.

So from a practical perspective, for large \( N \), the polynomial reduces to:

\[ C_1 \cdot N \]

In fact, for any polynomial, if \( N \) is large, then all of the terms except the highest-order term are irrelevant.
Big-O: Dropping the Constant

\[ C_1 \cdot N \]

Computers get faster and faster all the time. And there are many different flavors of computers, having many different speeds.

So, computer scientists don’t care about the constant, only about the order of the highest-order term of the polynomial. They indicate this with Big-O notation:

\[ O(N) \]

This is often said as: “of order \( N \)”
N-Body Problems

Given $N$ bodies, each body exerts a force on all of the other $N - 1$ bodies. Therefore, there are $N \cdot (N - 1)$ forces total. In Big-O notation, that’s $O(N^2)$ forces.

So, calculating the forces takes $O(N^2)$ time to execute.

But, there are only $N$ particles, each taking up the same amount of memory, so we say that N-body codes are of:
- $O(N)$ spatial complexity (memory)
- $O(N^2)$ time complexity
Note that this picture shows only the forces between A and everyone else.
How to Calculate?

Whatever your physics is, you have some function, $F(B_i,B_j)$, that expresses the force between two bodies $B_i$ and $B_j$. For example, for stars and galaxies,

$$F(A,B) = G \cdot m_{B_i} \cdot m_{B_j} / \text{dist}(B_i, B_j)^2$$

where $G$ is the gravitational constant and $m$ is the mass of the body in question.

If you have all of the forces for every pair of particles, then you can calculate their sum, obtaining the force on every particle.

From that, you can calculate every particle’s new position and velocity.
How to Parallelize?

Okay, so let’s say you have a nice serial (single-CPU) code that does an N-body calculation. How are you going to parallelize it? You could:

- have a server feed particles to processes;
- have a server feed interactions (particle pairs) to processes;
- have each process decide on its own subset of the particles, and then share around the summed forces on those particles;
- have each process decide its own subset of the interactions, and then share around the summed forces from those interactions.
Do You Need a Server?

Let’s say that you have \( N \) bodies, and therefore you have \( \frac{1}{2} N (N - 1) \) interactions (every particle interacts with all of the others, but you don’t need to calculate both \( B_i \rightarrow B_j \) and \( B_j \rightarrow B_i \)).

Do you need a server?

Well, can each processor determine, on its own, either (a) which of the bodies to process, or (b) which of the interactions to process?

If the answer is yes, then you don’t need a server.
Parallelize How?

Suppose you have $N_p$ processors.

Should you parallelize:

- by assigning a subset of $N / N_p$ of the bodies to each processor, OR
- by assigning a subset of $N(N - 1) / N_p$ of the interactions to each processor?
Data vs. Task Parallelism

- **Data Parallelism** means parallelizing by giving a subset of the data to each process, and then each process performs the same tasks on the different subsets of data.

- **Task Parallelism** means parallelizing by giving a subset of the tasks to each process, and then each process performs a different subset of tasks on the same data.
Data Parallelism for N-Body?

If you parallelize an N-body code **by data**, then each processor gets $N / N_p$ pieces of data.

For example, if you have 8 bodies and 2 processors, then:

- Processor $P_0$ gets the first 4 bodies;
- Processor $P_1$ gets the second 4 bodies.

But, every piece of data (that is, every body) has to interact with every other piece of data, to calculate the forces.

So, every processor will have to send all of its data to all of the other processors, for every single interaction that it calculates.

That’s a lot of communication!
Task Parallelism for N-body?

If you parallelize an N-body code by task, then each processor gets all of the pieces of data that describe the particles (for example, positions, velocities, masses).

Then, each processor can calculate its subset of the interaction forces on its own, without talking to any of the other processors.

But, at the end of the force calculations, everyone has to share all of the forces that have been calculated, so that each particle ends up with the total force that acts on it (global reduction).
Here’s the C syntax for `MPI_Reduce`:

```c
mpi_error_code =
    MPI_Reduce(sendbuffer, recvbuffer,
               count, datatype, operation,
               root, communicator, mpi_error_code);
```

For example, to do a sum over all of the particle forces:

```c
mpi_error_code =
    MPI_Reduce(
               local_particle_force_sum,
               global_particle_force_sum,
               number_of_particles,
               MPI_DOUBLE, MPI_SUM,
               server_process, MPI_COMM_WORLD);
```
Here’s the Fortran 90 syntax for **MPI_Reduce**:

```fortran
CALL MPI_Reduce(sendbuffer, recvbuffer, &
                count, datatype, operation, &
                root, communicator, mpi_error_code)
```

For example, to do a sum over all of the particle forces:

```fortran
CALL MPI_Reduce( &
                local_particle_force_sum, &
                global_particle_force_sum, &
                number_of_particles, &
                MPI_DOUBLE_PRECISION, MPI_SUM, &
                server_process, MPI_COMM_WORLD, &
                mpi_error_code)
```
In the N-body case, we don’t want just one processor to know the result of the sum, we want every processor to know. So, we could do a reduce followed immediately by a broadcast. But, MPI gives us a routine that packages all of that for us: **MPI_Allreduce**.

**MPI_Allreduce** is just like **MPI_Reduce** except that every process gets the result (so we drop the **server_process** argument).
Here’s the C syntax for `MPI_Allreduce`:

```c
mpi_error_code = MPI_Allreduce(
    sendbuffer, recvbuffer, count, datatype, operation, communicator);
```

For example, to do a sum over all of the particle forces:

```c
mpi_error_code = MPI_Allreduce(
    local_particle_force_sum, global_particle_force_sum, number_of_particles, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
```
Here's the Fortran 90 syntax for \texttt{MPI\_Allreduce}:

\begin{verbatim}
CALL MPI\_Allreduce(
    & sendbuffer, recvbuffer, count, &
    & datatype, operation, &
    & communicator, mpi\_error\_code)
\end{verbatim}

For example, to do a sum over all of the particle forces:

\begin{verbatim}
CALL MPI\_Allreduce(
    & local\_particle\_force\_sum, &
    & global\_particle\_force\_sum, &
    & number\_of\_particles, &
    & MPI\_DOUBLE\_PRECISION, MPI\_SUM, &
    & MPI\_COMM\_WORLD, mpi\_error\_code)
\end{verbatim}
Collective Communications

A collective communication is a communication that is shared among many processes, not just a sender and a receiver.

MPI_Reduce and MPI_Allreduce are collective communications.

Others include: broadcast, gather/scatter, all-to-all.
Collectives Are Expensive

Collective communications are very expensive relative to point-to-point communications, because so much more communication has to happen.

But, they can be much cheaper than doing zillions of point-to-point communications, if that’s the alternative.
Transport:
Data Parallelism
What is a Simulation?

All physical science ultimately is expressed as calculus (for example, differential equations).

Except in the simplest (uninteresting) cases, equations based on calculus can’t be directly solved on a computer. Therefore, all physical science on computers has to be approximated.
I Want the Area Under This Curve!

How can I get the area under this curve?
A Riemann Sum

\[ A \approx \sum_{i=1}^{n} \Delta x \cdot y_i \]

Ceci n'est pas une pipe.

Parallel Programming: Apps & Par Types
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A Riemann Sum

Area under the curve \( \approx \sum_{i=1}^{n} y_i \Delta x \)

Ceci n’est pas un area under the curve: it’s **approximate**!
A Better Riemann Sum

Area under the curve \( \approx \sum_{i=1}^{n} y_i \Delta x \)

More, smaller rectangles produce a **better approximation**.
The Best Riemann Sum

Area under the curve \( = \sum_{i=1}^{\infty} y_i dx \equiv \int y dx \)

In the limit, infinitely many infinitesimally small rectangles produce the exact area.
The Best Riemann Sum

Area under the curve

\[ \sum \int \infty = \sum \int 1_i y \ dx \ dx \]

In the limit, infinitely many infinitesimally small rectangles produce the exact area.

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A differential equation is an equation in which differentials (for example, $dx$) appear as variables.

Most physics is best expressed as differential equations.

Very simple differential equations can be solved in “closed form,” meaning that a bit of algebraic manipulation gets the exact answer.

Interesting differential equations, like the ones governing interesting physics, can’t be solved in close form.

**Solution**: approximate!
### A Discrete Mesh of Data

![Diagram of a discrete mesh with data points](image-url)

Data live here!
A Discrete Mesh of Data

Thu, 25 May 2006, 8 am CDT (13Z)

Surface Temperature

Max Wind 32.57 kts
Finite Difference

A typical (though not the only) way of approximating the solution of a differential equation is through finite differencing: convert each $dx$ (infinitely thin) into a $\Delta x$ (has finite nonzero width).
Navier-Stokes Equation

\[ \frac{F_i}{V} = \frac{\partial}{\partial x_j} \left[ \eta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \delta_{ij} \nabla \cdot u \right] \]

Differential Equation

These are only here to frighten you ....

\[ \frac{F_i}{V} = \frac{\Delta}{\Delta x_j} \left[ \eta \left( \frac{\Delta u_i}{\Delta x_j} + \frac{\Delta u_j}{\Delta x_i} \right) + \lambda \delta_{ij} \nabla \cdot u \right] \]

Finite Difference Equation

The Navier-Stokes equations governs the movement of fluids (water, air, etc).
Cartesian Coordinates
A **structured mesh** is like the mesh on the previous slide. It’s nice and regular and rectangular, and can be stored in a standard Fortran or C or C++ array of the appropriate dimension and shape.

\[
\text{REAL,DIMENSION}(\text{nx,ny,nz}) :: u \\

\text{float u[nx][ny][nz];}
\]
Flow in Structured Meshes

When calculating flow in a structured mesh, you typically use a finite difference equation, like so:

\[ u_{\text{new}}_{i,j} = F(\Delta t, u_{\text{old}}_{i,j}, u_{\text{old}}_{i-1,j}, u_{\text{old}}_{i+1,j}, u_{\text{old}}_{i,j-1}, u_{\text{old}}_{i,j+1}) \]

for some function \( F \), where \( u_{\text{old}}_{i,j} \) is at time \( t \) and \( u_{\text{new}}_{i,j} \) is at time \( t + \Delta t \).

In other words, you calculate the new value of \( u_{i,j} \), based on its old value as well as the old values of its immediate neighbors.

Actually, it may use neighbors a few farther away.
Ghost Boundary Zones
Ghost Boundary Zones

We want to calculate values in the part of the mesh that we care about, but to do that, we need values on the boundaries. For example, to calculate $u_{new_{1,1}}$, you need $u_{old_{0,1}}$ and $u_{old_{1,0}}$. Ghost boundary zones are mesh zones that aren’t really part of the problem domain that we care about, but that hold boundary data for calculating the parts that we do care about.
A good basic algorithm for flow that uses ghost boundary zones is:

```c
for (timestep = 0; timestep < number_of_timesteps; timestep++) {
    fill_ghost_boundary(...);
    advance_to_new_from_old(...);
}
```

This approach generally works great on a serial code.
Using Ghost Boundary Zones (F90)

A good basic algorithm for flow that uses ghost boundary zones is:

```fortran
DO timestep = 1, number_of_timesteps
    CALL fill_ghost_boundary(…)
    CALL advance_to_new_from_old(…)
END DO
```

This approach generally works great on a serial code.
What if you want to parallelize a Cartesian flow code in MPI?

You’ll need to:

- decompose the mesh into *submeshes*;
- figure out how each submesh talks to its neighbors.
We want to split the data into chunks of equal size, and give each chunk to a processor to work on.

Then, each processor can work independently of all of the others, except when it’s exchanging boundary data with its neighbors.
MPI supports exactly this kind of calculation, with a set of functions _MPI_Cart_*:

- _MPI_Cart_create_
- _MPI_Cart_coords_
- _MPI_Cart_shift_

These routines create and describe a new communicator, one that replaces _MPI_COMM_WORLD_ in your code.
MPI_Sendrecv

MPI_Sendrecv is just like an MPI_Send followed by an MPI_Recv, except that it’s much better than that.

With MPI_Send and MPI_Recv, these are your choices:

- Everyone calls MPI_Recv, and then everyone calls MPI_Send.
- Everyone calls MPI_Send, and then everyone calls MPI_Recv.
- Some call MPI_Send while others call MPI_Recv, and then they swap roles.
Why not `Recv` then `Send`?

Suppose that everyone calls `MPI_Recv`, and then everyone calls `MPI_Send`.

```c
MPI_Recv(incoming_data, ...);
MPI_Send(outgoing_data, ...);
```

Well, these routines are *blocking*, meaning that the communication has to complete before the process can continue on farther into the program.

That means that, when everyone calls `MPI_Recv`, they’re waiting for someone else to call `MPI_Send`.

We call this *deadlock*.

Officially, the MPI standard guarantees that **THIS APPROACH WILL ALWAYS FAIL**.
Why not **Send** then **Recv**?

Suppose that everyone calls `MPI_Send`, and then everyone calls `MPI_Recv`:

```
MPI_Send(outgoing_data, ...);
MPI_Recv(incoming_data, ...);
```

Well, this will only work if there’s enough **buffer space** available to hold everyone’s messages until after everyone is done sending.

Sometimes, there isn’t enough buffer space.

Officially, the MPI standard allows MPI implementers to support this, but **it isn’t part of the official MPI standard**; that is, a particular MPI implementation doesn’t have to allow it, so **THIS WILL SOMETIMES FAIL**.
Alternate Send andRecv?

Suppose that some processors call `MPI_Send` while others call `MPI_Recv`, and then they swap roles:

```c
if (((my_rank % 2) == 0) {
    MPI_Send(outgoing_data, ...);
    MPI_Recv(incoming_data, ...);
} else {
    MPI_Recv(incoming_data, ...);
    MPI_Send(outgoing_data, ...);
}
```

This will work, and is sometimes used, but it can be painful to manage – especially if you have an odd number of processors.
MPI_Sendrecv allows each processor to simultaneously send to one processor and receive from another. For example, P₁ could send to P₀ while simultaneously receiving from P₂. (Note that the send and receive don’t have to literally be simultaneous, but we can treat them as so in writing the code.)

This is exactly what we need in Cartesian flow: we want the boundary data to come in from the east while we send boundary data out to the west, and then vice versa. These are called shifts.
MPI_Sendrecv

mpi_error_code =
    MPI_Sendrecv(
        westward_send_buffer,
        westward_send_size, MPI_REAL,
        west_neighbor_process, westward_tag,
        westward_recv_buffer,
        westward_recv_size, MPI_REAL,
        east_neighbor_process, westward_tag,
        cartesian_communicator, mpi_status);

This call sends to west_neighbor_process the data in westward_send_buffer, and at the same time receives from east_neighbor_process a bunch of data that end up in westward_recv_buffer.
Why MPI_Sendrecv?

The advantage of MPI_Sendrecv is that it allows us the luxury of no longer having to worry about who should send when and who should receive when.

This is exactly what we need in Cartesian flow: we want the boundary information to come in from the east while we send boundary information out to the west – without us having to worry about deciding who should do what to who when.
MPI_Sendrecv

Concept in Principle

Concept in practice
**MPI_Sendrecv**

**Concept in practice**

**Actual Implementation**

`westward_send_buffer`  

`westward_recv_buffer`
What About Edges and Corners?

If your numerical method involves faces, edges and/or corners, don’t despair.

It turns out that, if you do the following, you’ll handle those correctly:

- When you send, send the entire ghost boundary’s worth, including the ghost boundary of the part you’re sending.
- Do in this order:
  - all east-west;
  - all north-south;
  - all up-down.
- At the end, everything will be in the correct place.
Thanks for your attention!

Questions?
References