Inter-node Communication Performance Tuning

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Introduction

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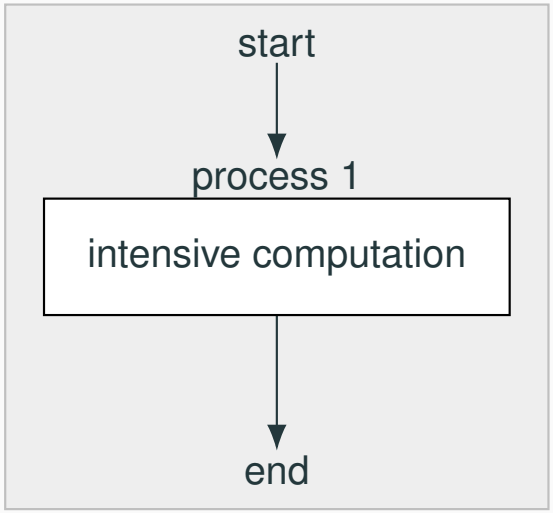

Figure 1: serial program design

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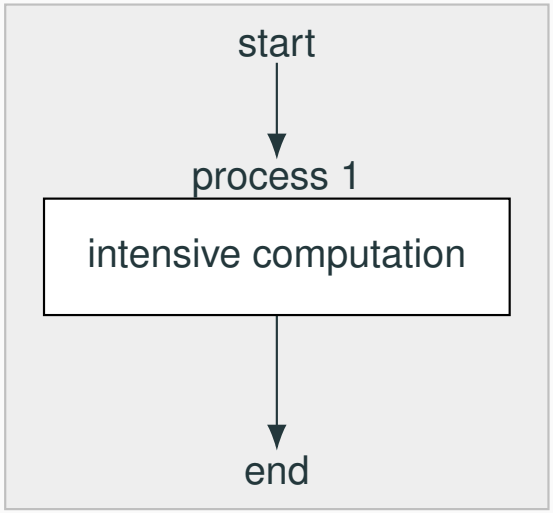

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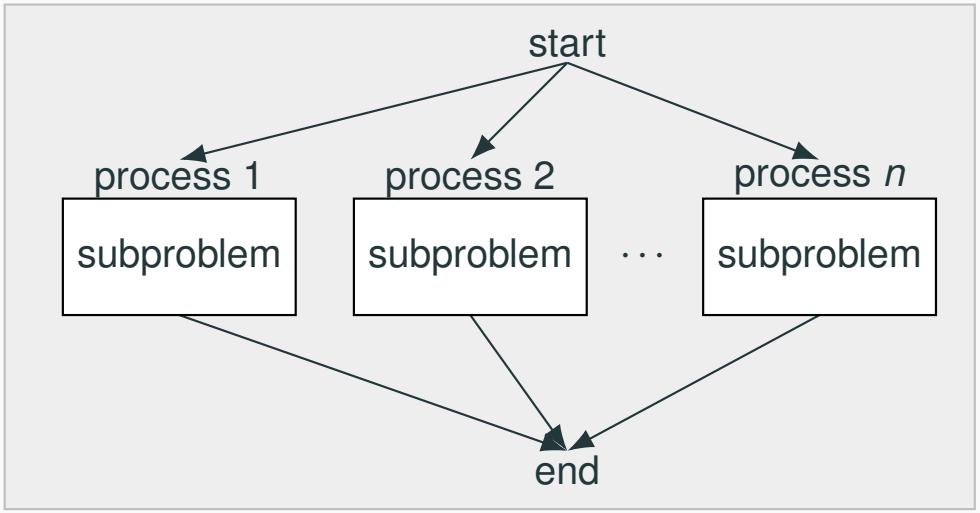

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Introduction

Message Passing Interface (MPI) is a standardized library that enables communication and coordination among multiple processes.

- Because of the extremely scalable context of MPI, thorough testing of a specific application is important to have confidence in optimization of message passing parallel programs.

Simulator - High Level Overview

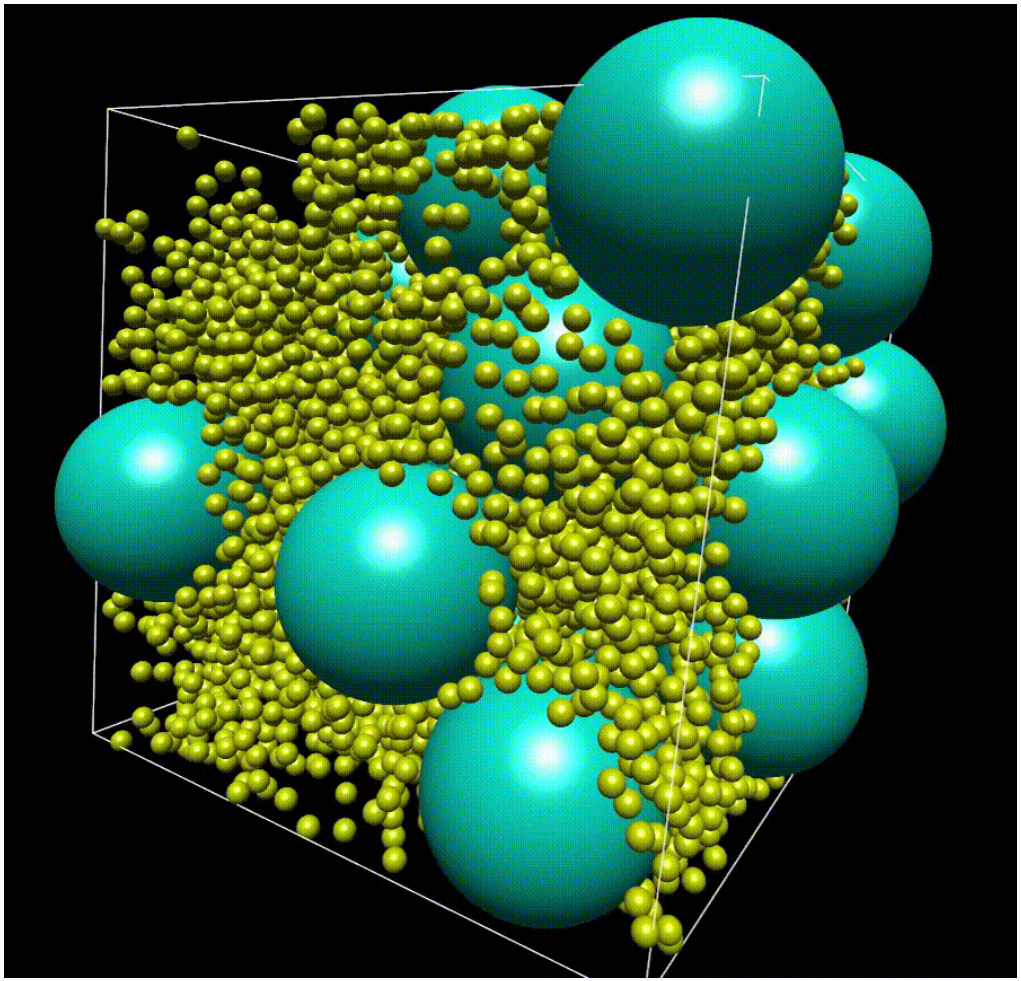

Figure 3: Quaternion Dissipative Particle Dynamics (QDPD) simulator output

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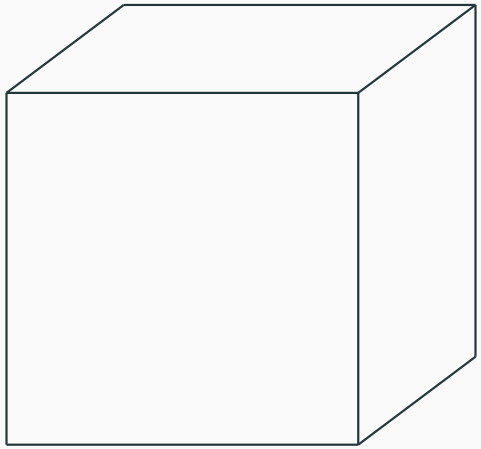

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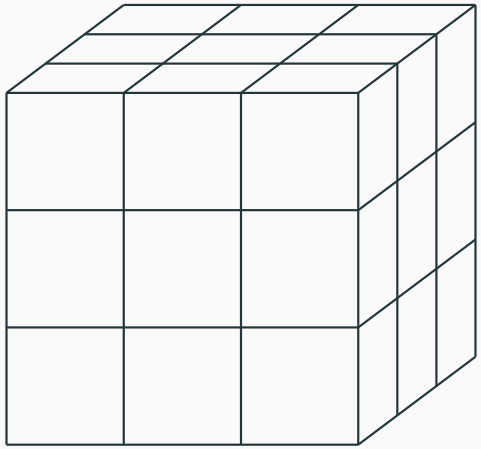

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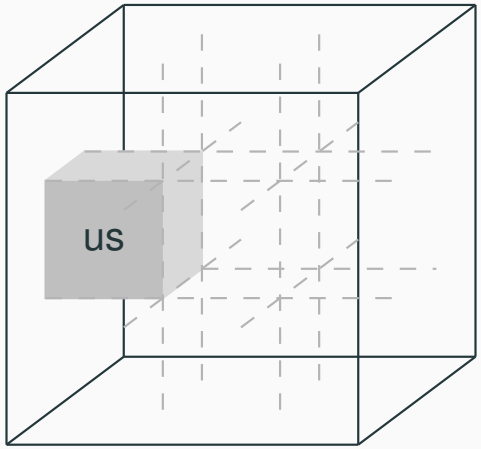

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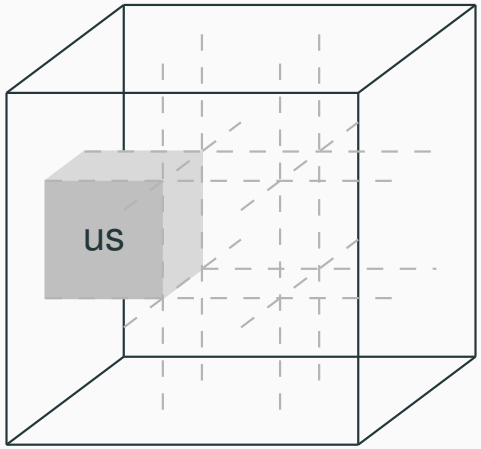

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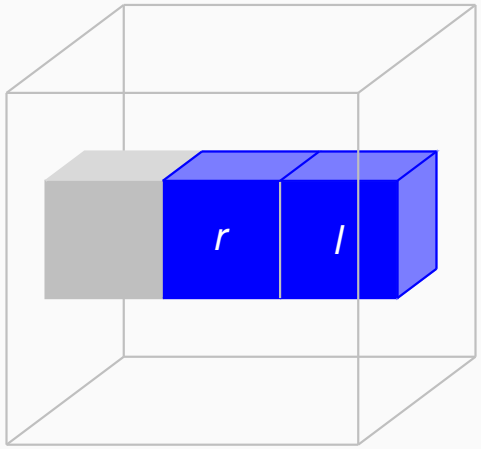

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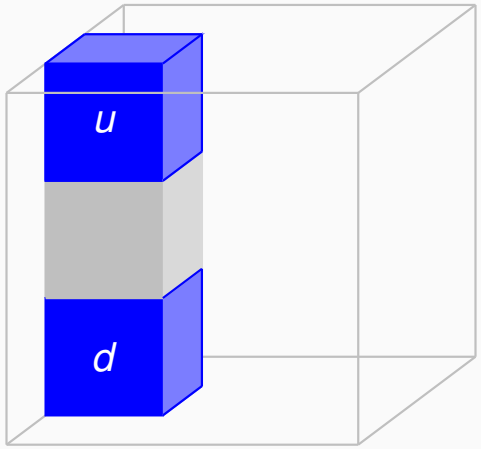

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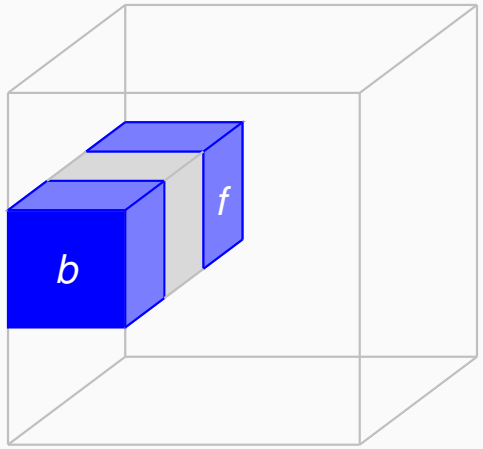

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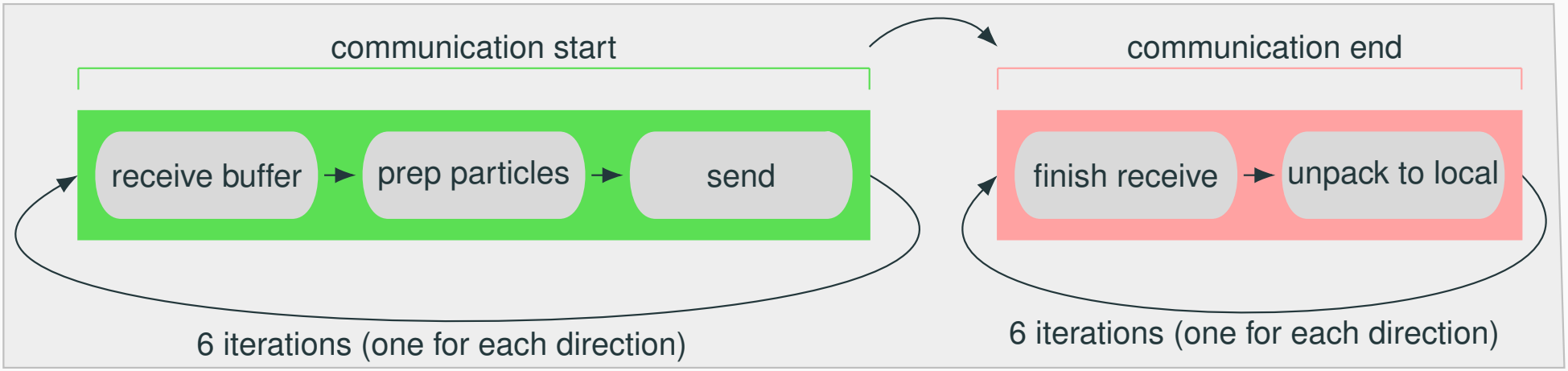

Figure 3: Each process' communication routine **per time step**

Objective

Possible Improvements

- 2 ways in question to prepare data to send between processes
- 2 MPI library implementations that we have access to: **Intel OneAPI** and **OpenMPI**
- Is it possible to perform computations while communicating, to improve efficiency?

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Questions:

- How can we optimize communication?
- Can we show overlap of computation and communication?

Two Methods of Preparing Data

Particle Structure

```c
typedef struct particle {
    int ints[50];
    double reals[100];
    struct particle* next;
} particle;
```

Figure 4: C Struct Representation of a Particle

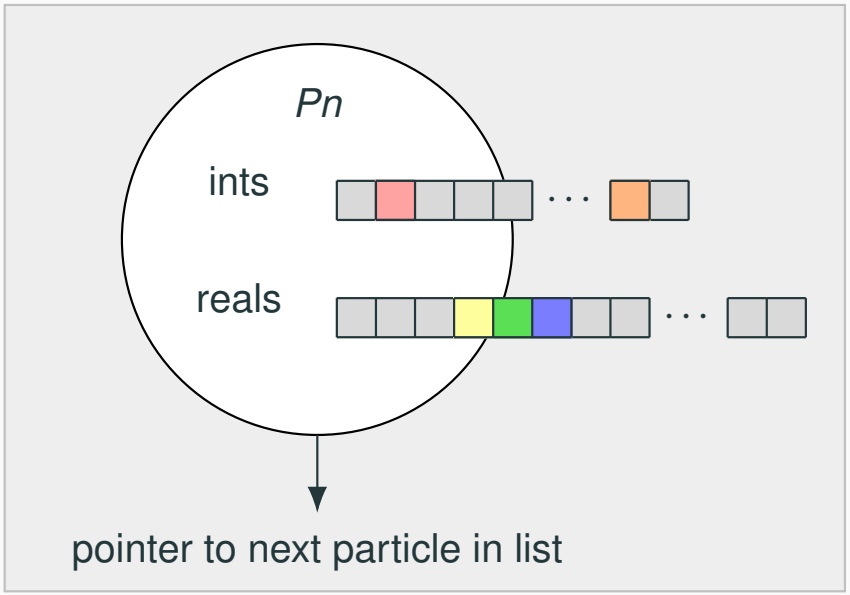
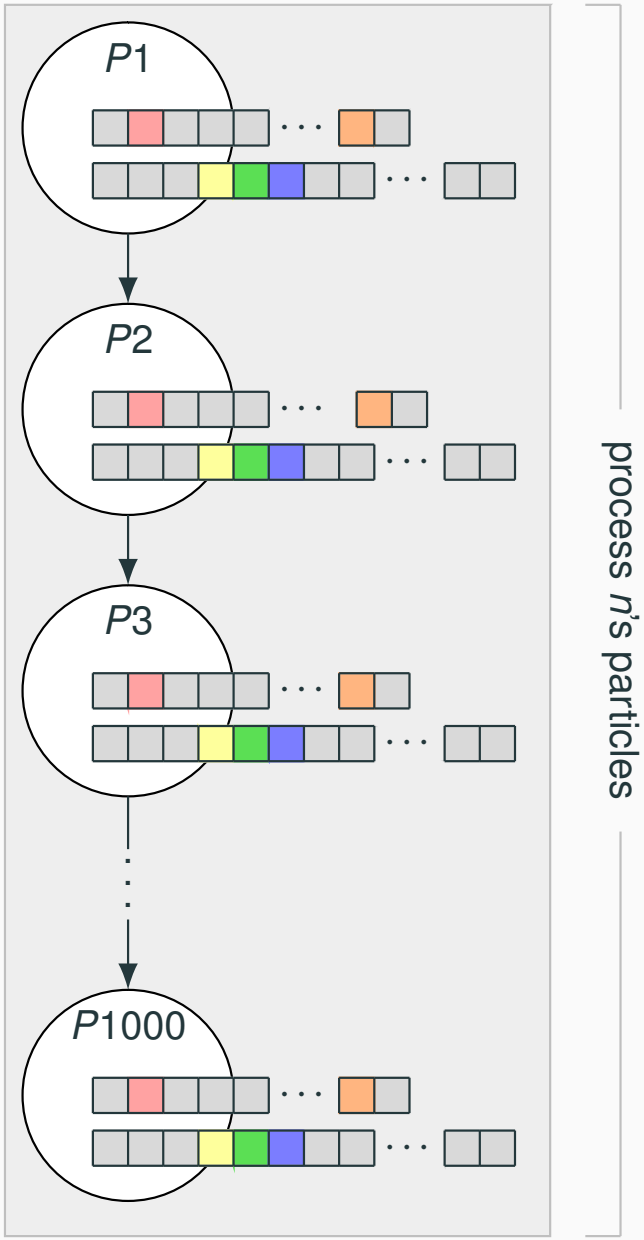


Figure 5: Graphical Representation of a Particle

ONLY data from the particle to send

Method 1 - packing a buffer



Particles to send: $[1, 3]$

SEND BUFFER

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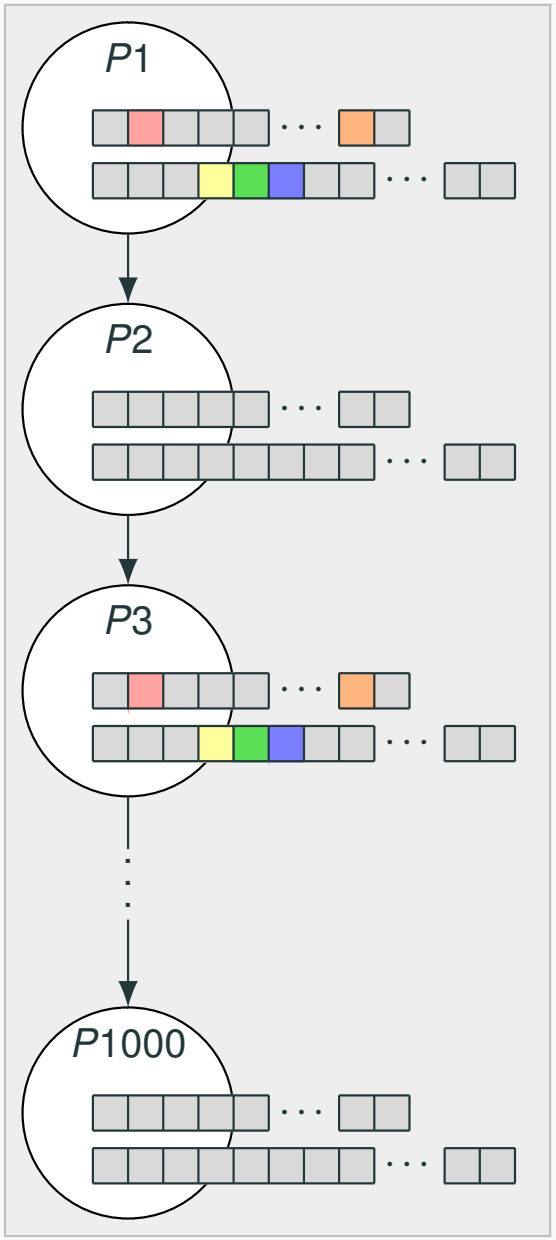

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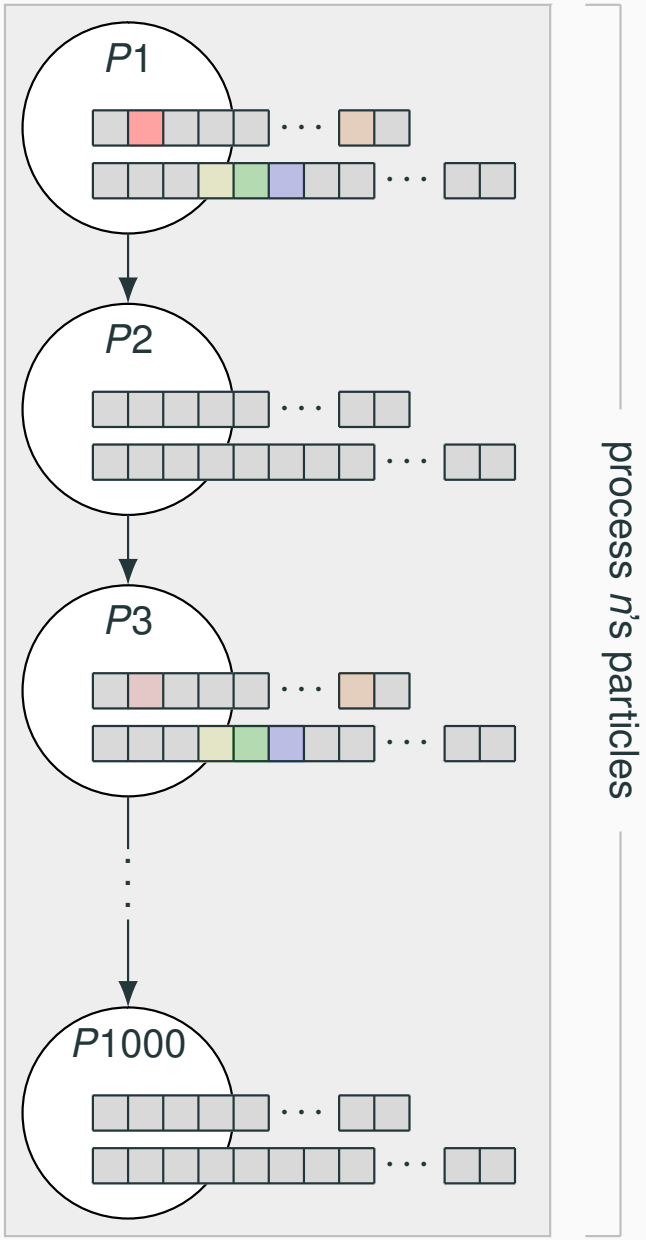

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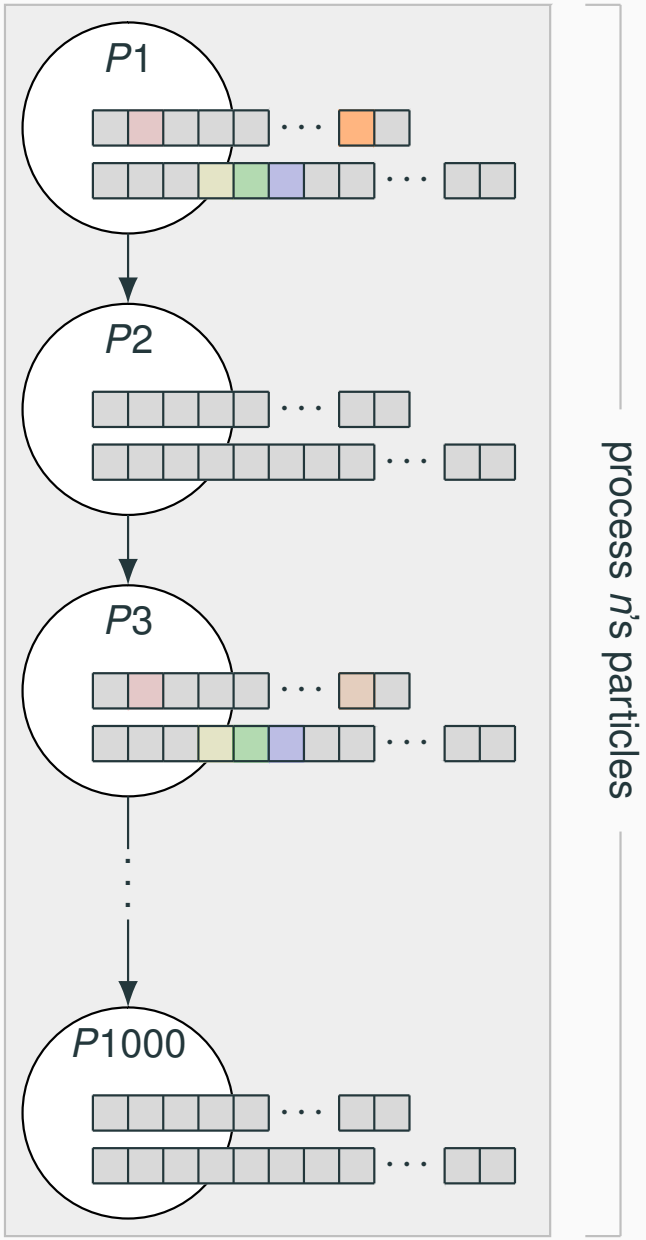

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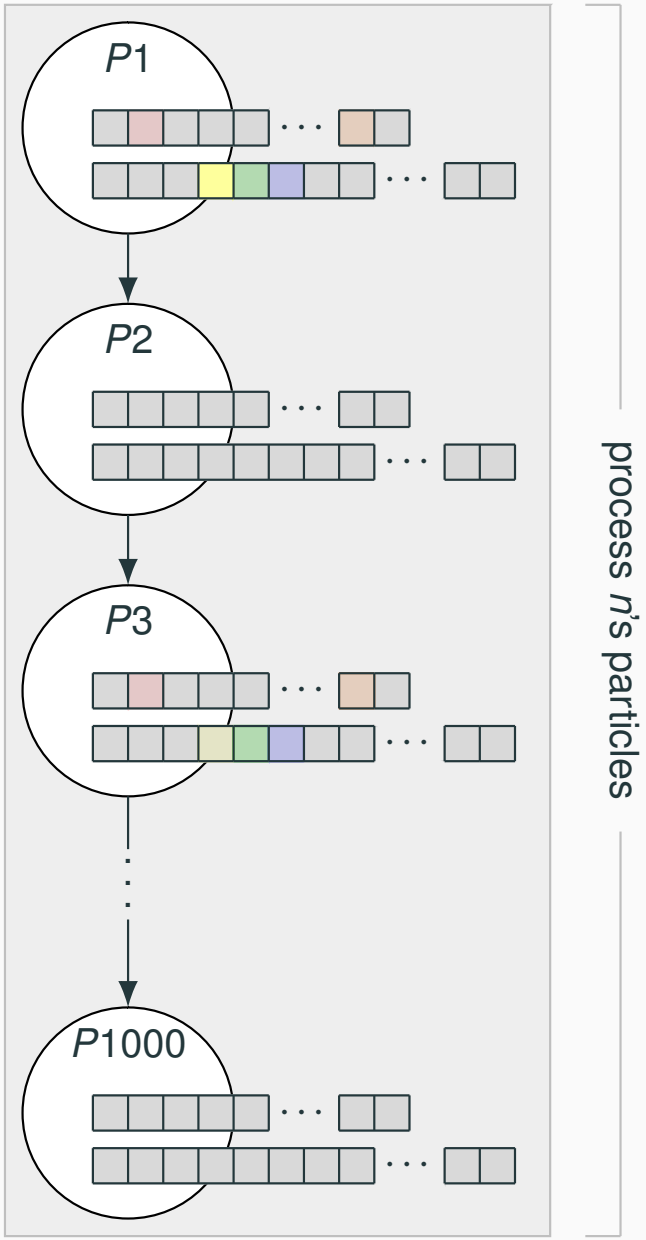

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dcK6={tK?z Q#]J9

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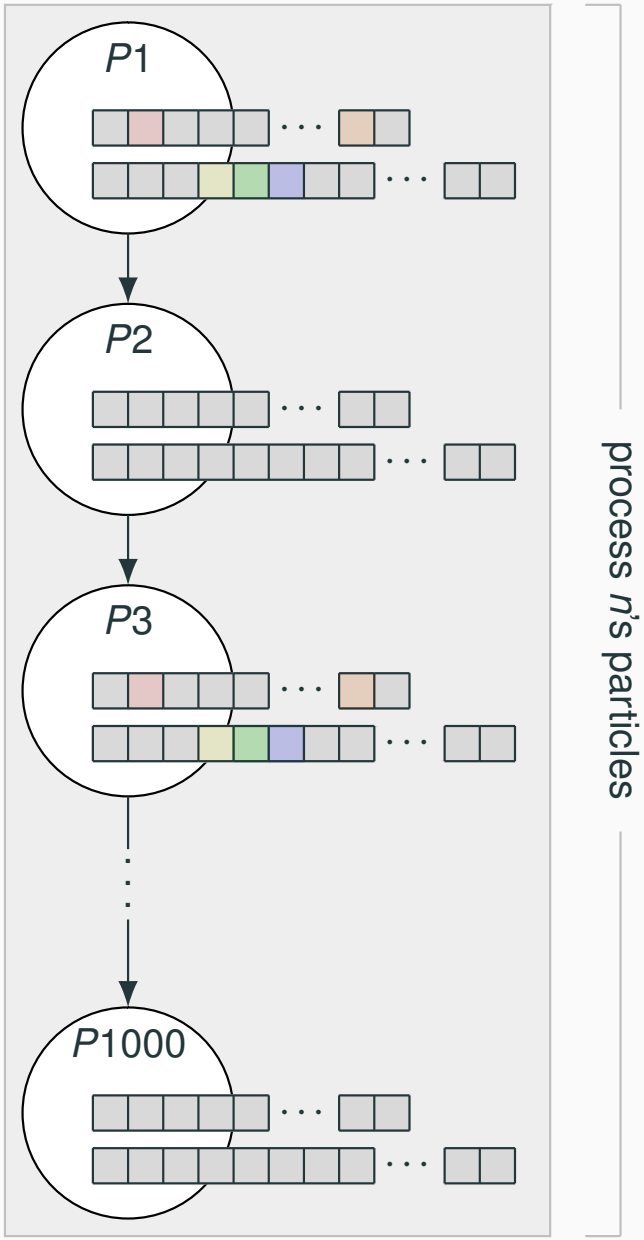

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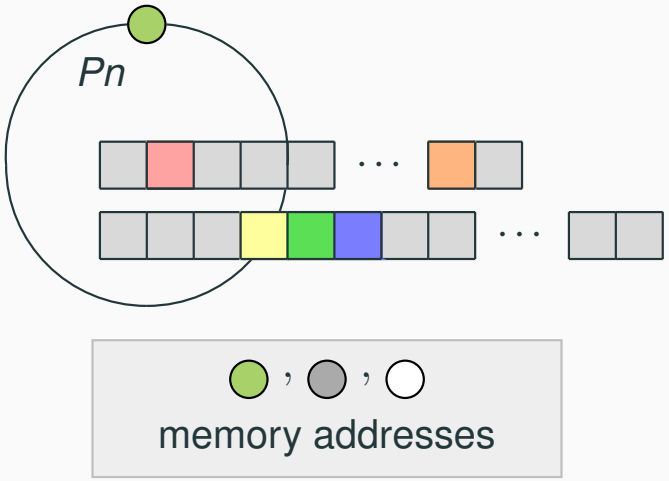
dcK6={tK?zQ#]J9w3R]F#knMK$9&V,(&mrJ{C0RMbR:W$C1K

- MPI_Pack() function encodes data as char* in the buffer
- This char* buffer is sent to an adjacent process
- MPI_Unpack() function can decode char* encoded data

Method 2 - Memory Address Offset Datatypes

- Recall a single particle's contents.



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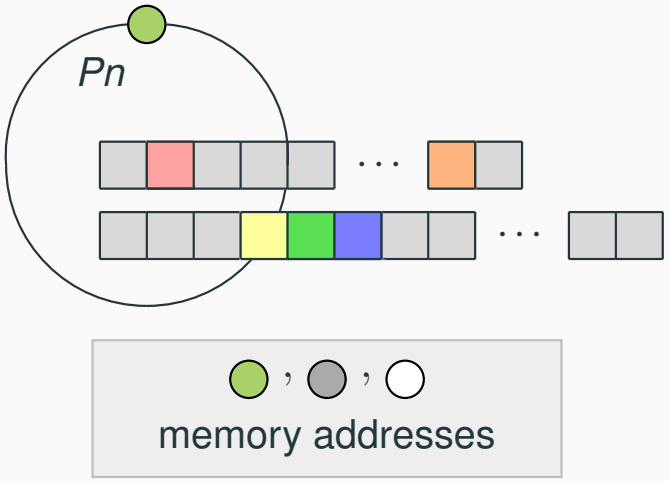

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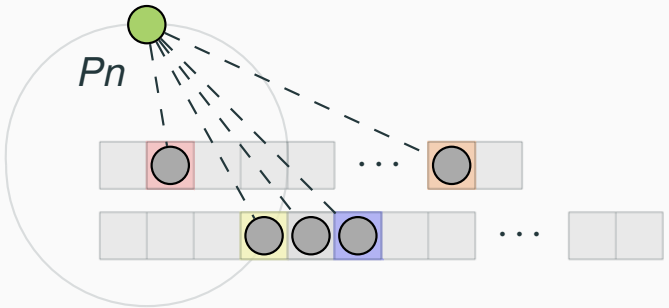

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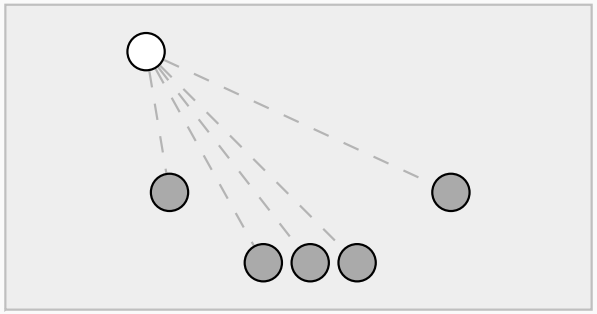

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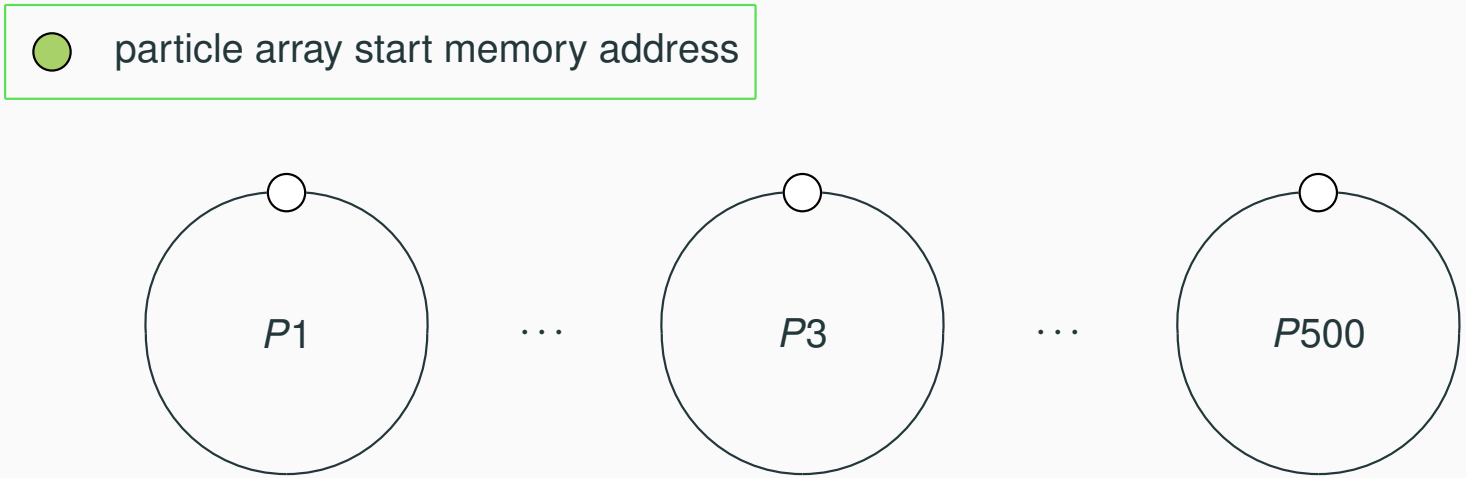

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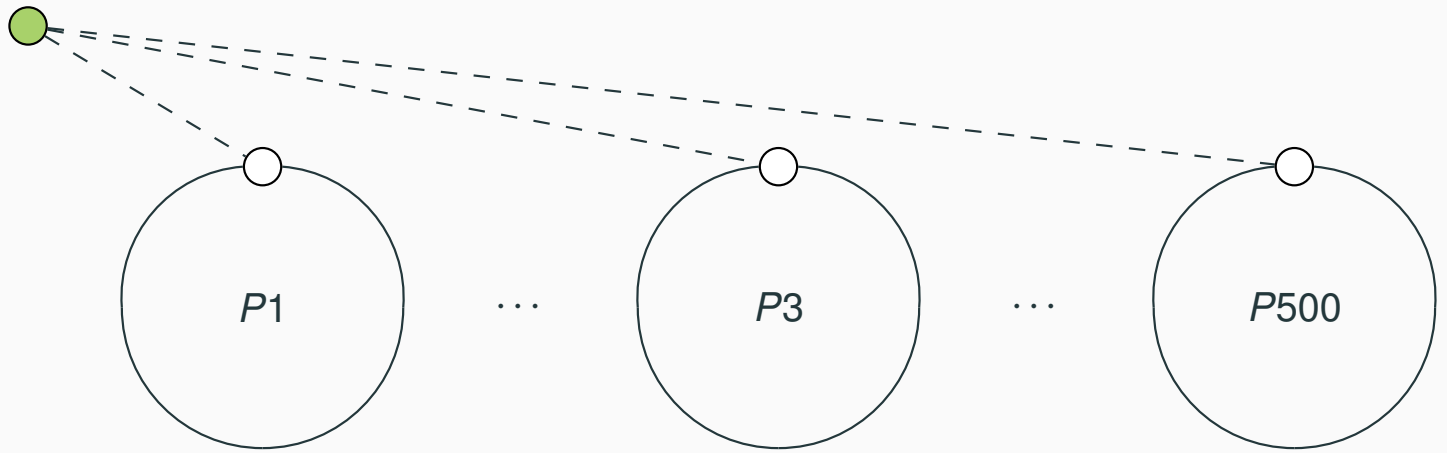

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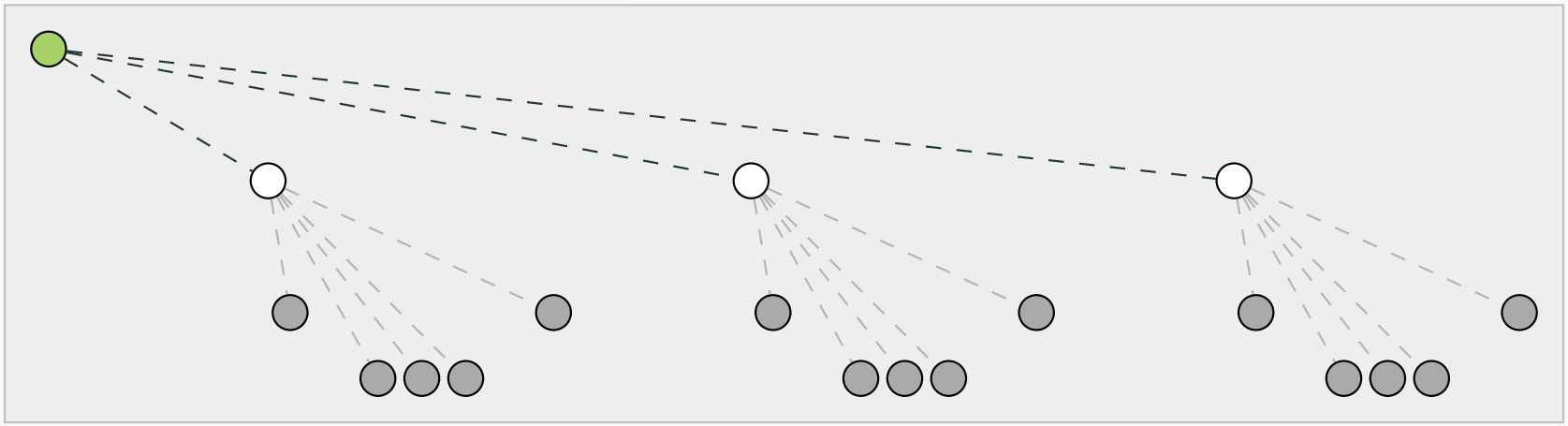

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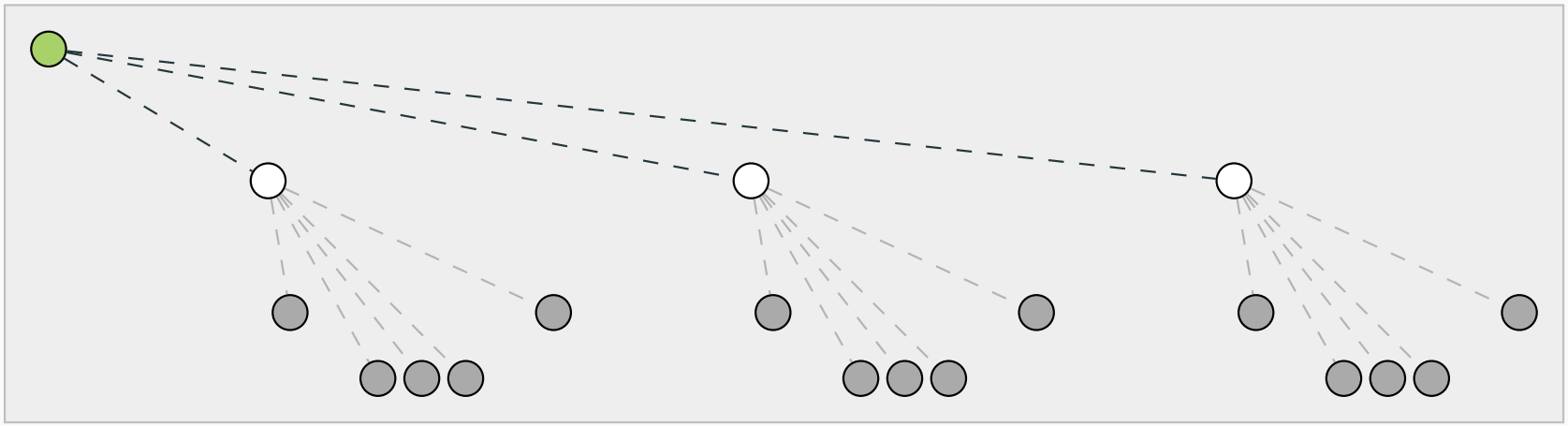

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- Send one instance of the 2nd derived datatype
  - As long as we send to a particle* buffer, the received data will be readable.

Methodology

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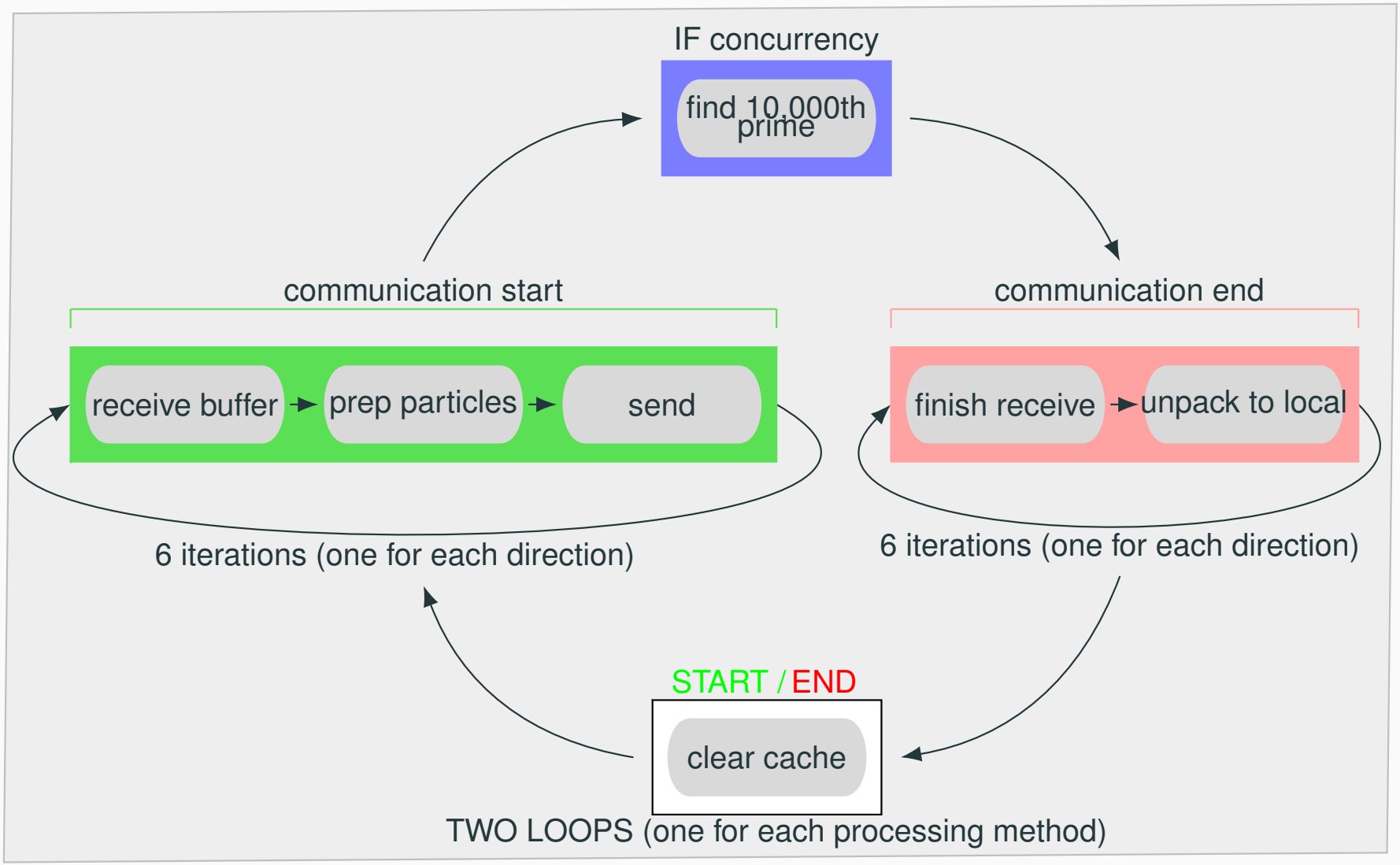
1. An input csv file specifies input data for a test run.
    - The number of particles to send to each adjacent process (2 - 8192).
    - Whether communication and computation should be performed concurrently.
2. Process 0 reads the input file and broadcasts this input data to the other processes with an MPI function call.
3. Each process is assigned a unique subvolume of the global volume and its adjacent processes are taken note of.
4. Each process is then given the same linked list of 5000 unique particles.

Methodology

5. Each process chooses different particles to send to the 6 directions based off of a RNG seeded with the PID.
6. Obtain elapsed times for each primary functionality in the flowchart above.



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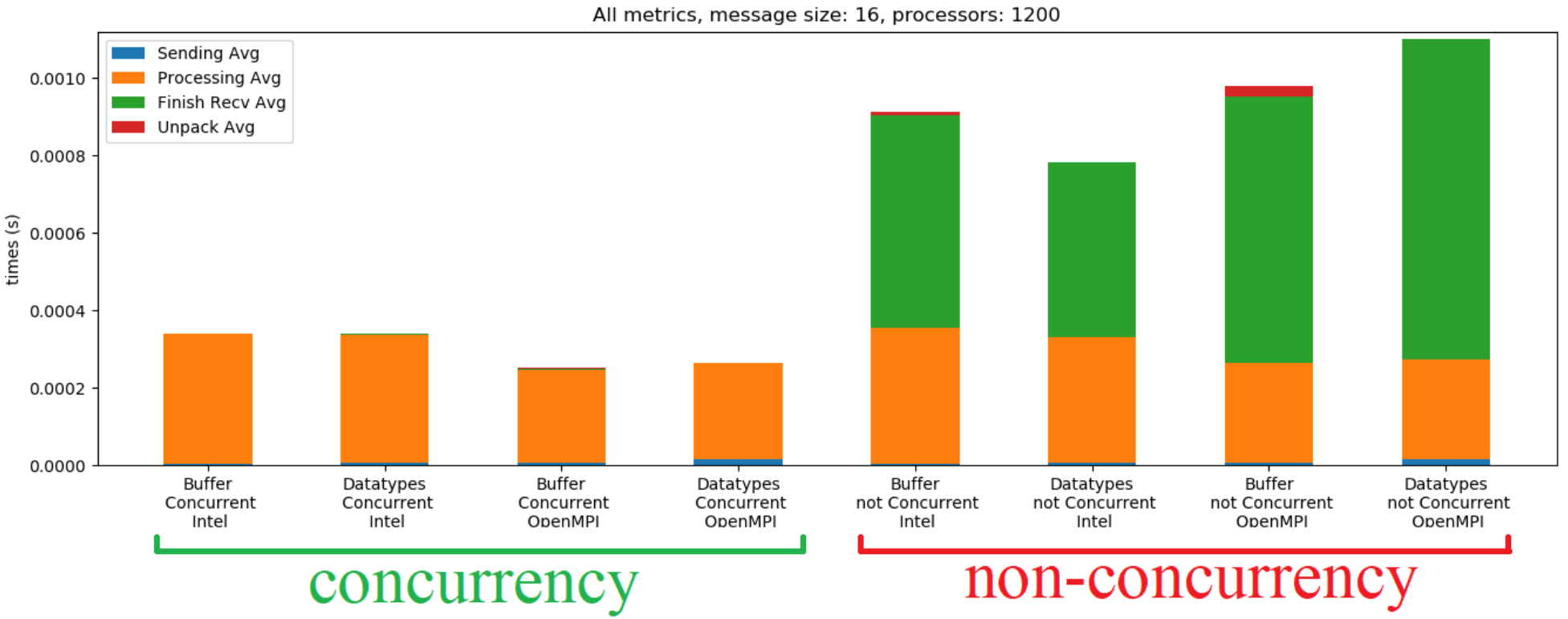

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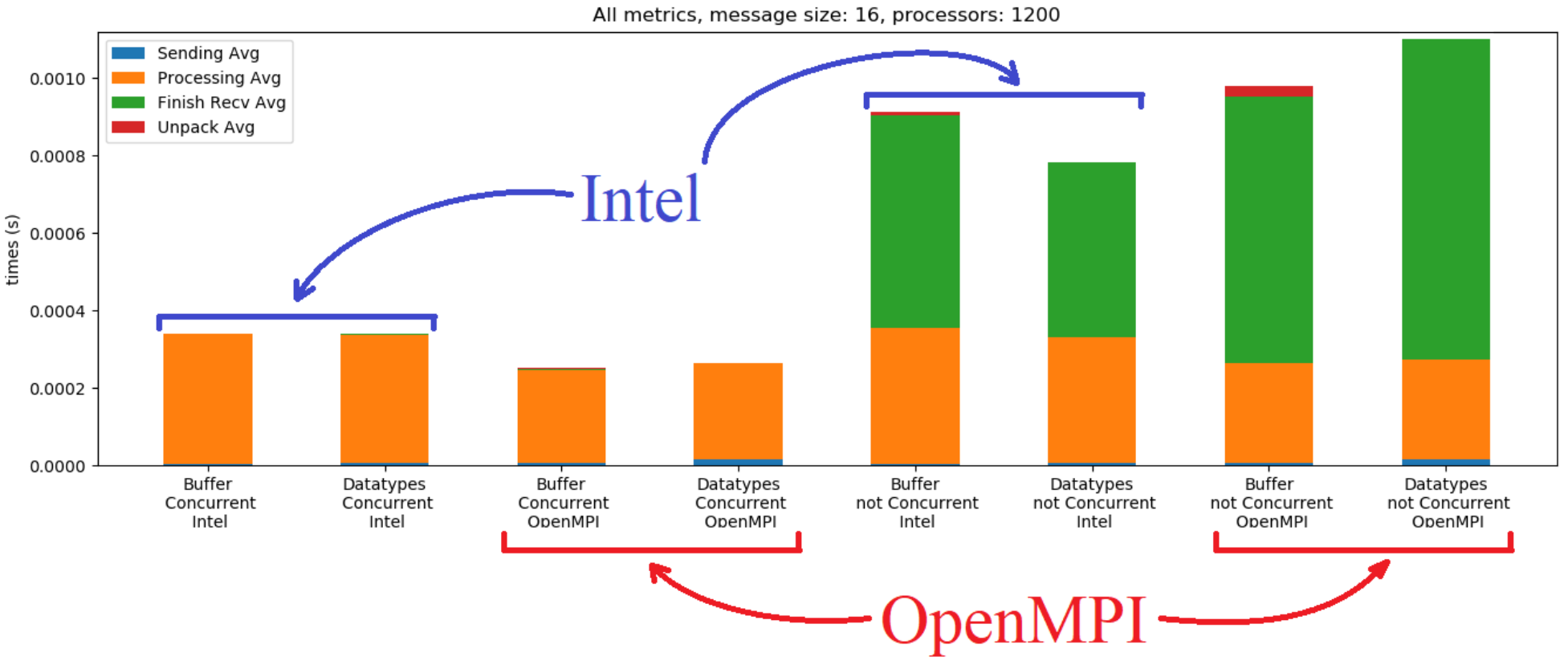

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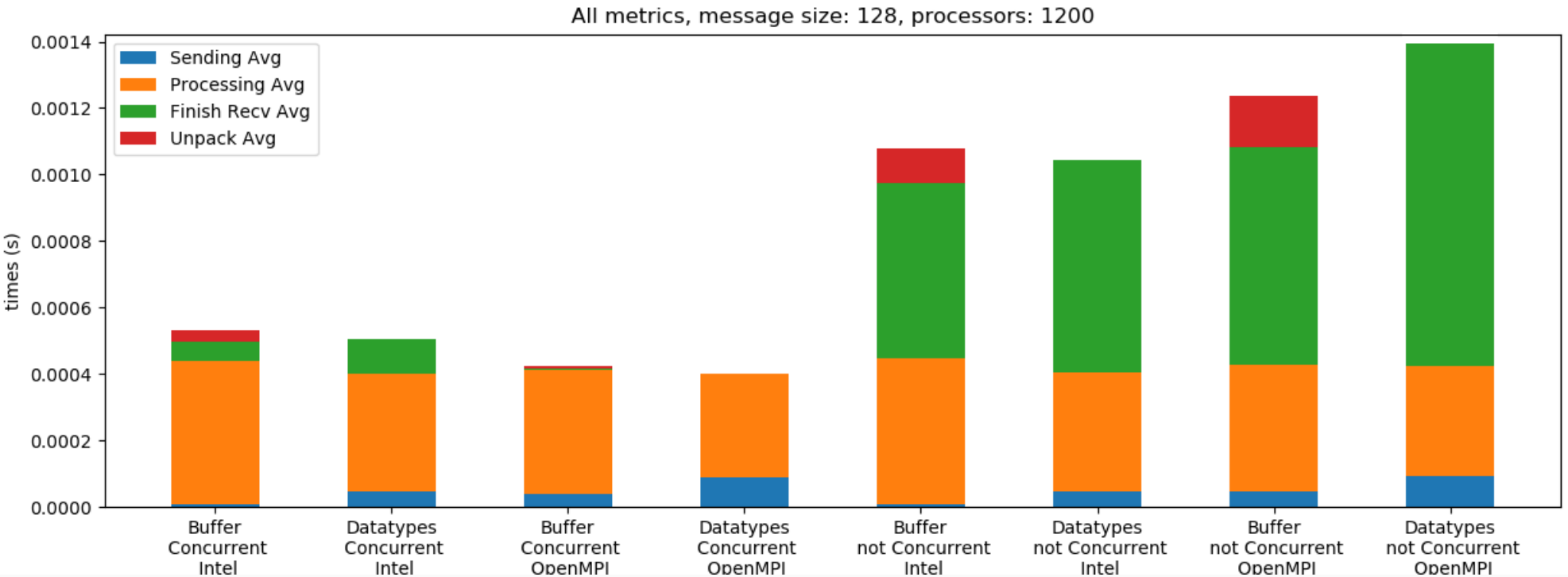

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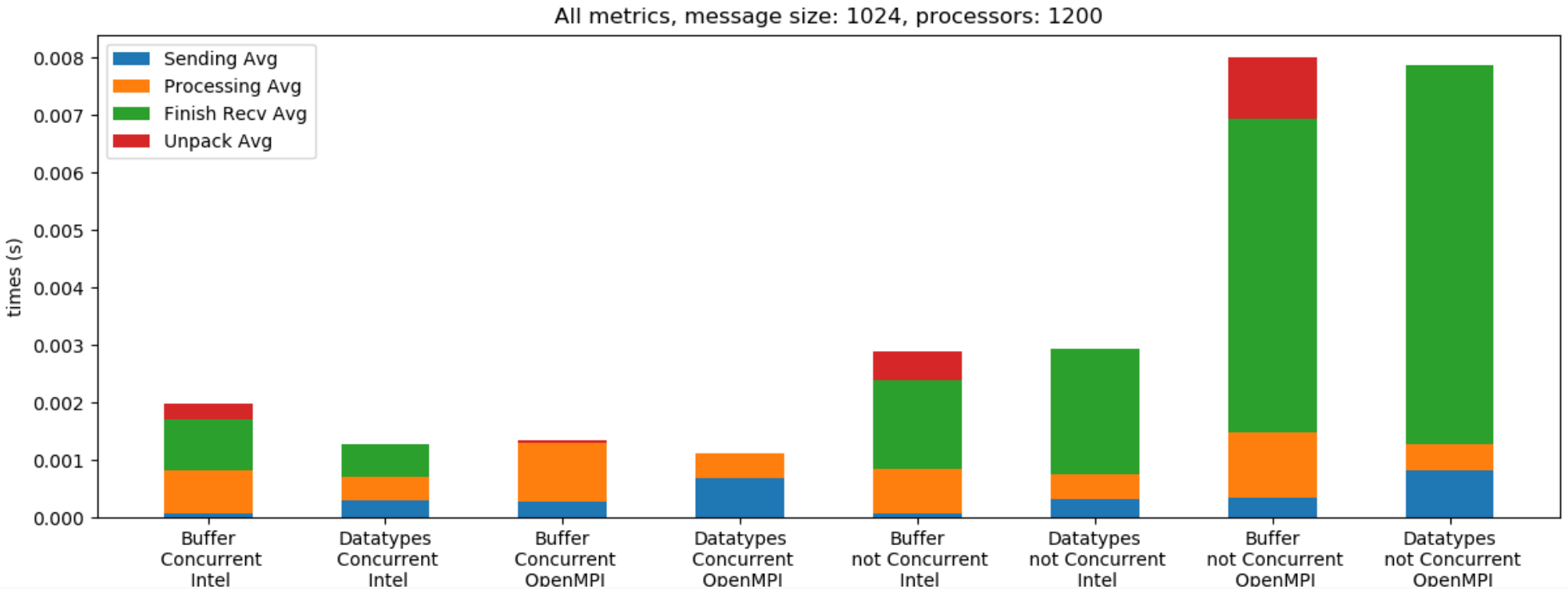

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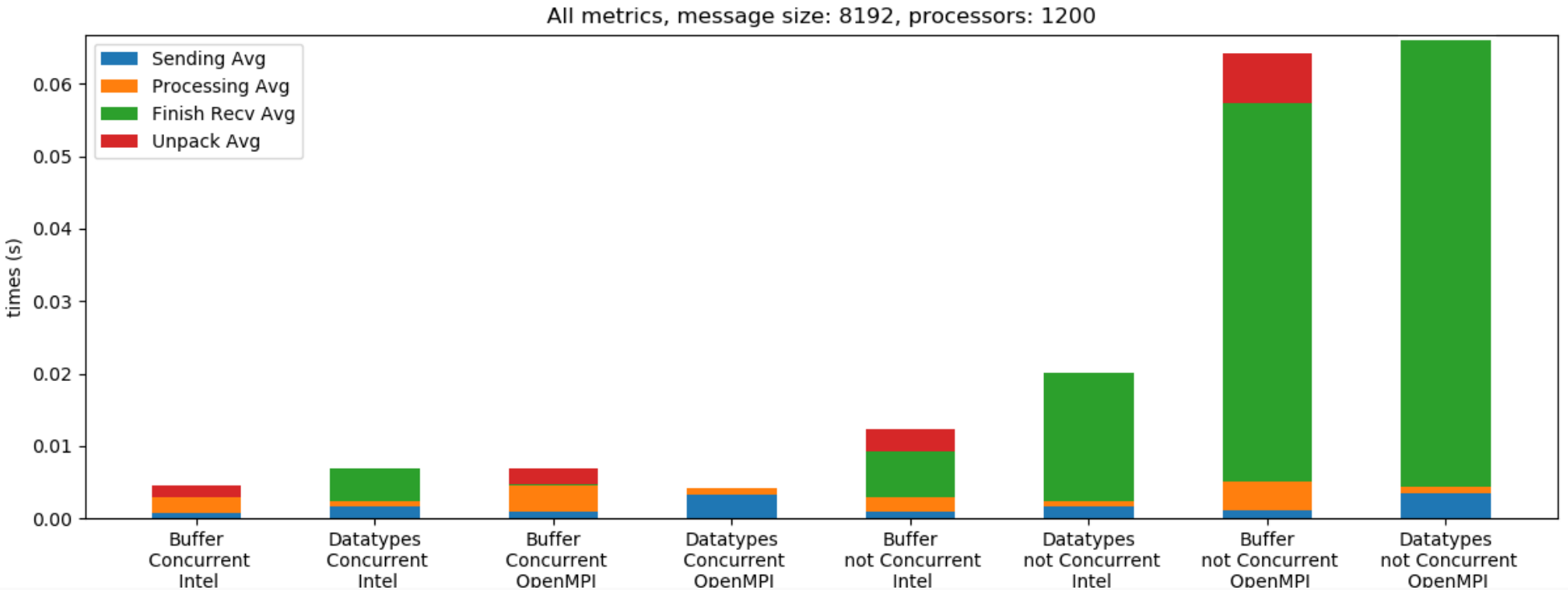

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Conclusions

- Communication **can** overlap with computation.
- The communication benchmark performance is not as simple as expected.
  - compiler
  - compiler options
  - MPI implementation
  - OS
  - other OS processes
  - network hardware
  - memory heirarchy

Future Work

- Overlap communication and computation whenever possible in the simulator
- Control some of the other variables mentioned in future tests.

Questions?