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Advanced MPI
OpenMP/MPI Hybrid Programming
Load Balancing; Termination Detection

Parallel and Distributed Computing

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Monday, 27 March 2023

Outline

- Advanced MPI
- Hybrid programming
  - Combining OpenMP and MPI
- Load balancing
- Termination detection

Asynchronous Communication

- Blocking operations
  - `MPI_Send` only returns when the send buffer can be reused
    - Data has been received by destination
    - Or MPI has saved the data somewhere
  - `MPI_Recv` only returns when the receive buffer has been filled with valid data

- Non-blocking versions
  - `MPI_Isend` / `MPI_Irecv`
    - Buffers transferred in the background
    - Cannot use buffers until communication complete
  - allow overlap of computation and communication
  - use `MPI_Wait` / `MPI_Test` to check comm complete

Asynchronous Collectives

- Recent versions of MPI also provide asynchronous collective operations:

```
MPI_Isomething(<usual arguments>, MPI_Request *req)
```

- They return an `MPI_Request` reqect, similar to nonblocking point-to-point operations

- The user must call `MPI_Test` / `MPI_Wait` or their variants to complete the operation

- Multiple nonblocking collectives may be outstanding, but they must be called in the same order on all processes

Asynchronous Collectives

- Blocking and non-blocking don't match!
  - either all processes call the non-blocking version or all call the blocking one
  - Thus the following code is incorrect:

```
if(rank == root)
  MPI_Reduce( &x /* ... */ root, comm );
else
  MPI_Ireduce( &x /* ... */ root, comm, &req);
```

- Note that in point-to-point you can match an `MPI_Irecv` with an `MPI_Send`

Persistent Communication

```
for(i = 1; i < BIGNUM; i++){
    MPI_Irecv(buf1, cnt, tp, src, tag, com, &recv_req);

    do_work(buf1, buf2);

    MPI_Isend(buf2, cnt, tp, dst, tag, com, &send_req);

    // Wait for send to complete
    MPI_Wait(&send_req, status);
    // Wait for receive to finish (no deadlock!)
    MPI_Wait(&recv_req, status);
}
```

Persistent Communication

```
//Step 1) Initialize send/request objects
MPI_Recv_init(buf1, cnt, tp, src, tag, com, &recv_req);
MPI_Send_init(buf2, cnt, tp, dst, tag, com, &send_req);
for(i = 1; i < BIGNUM; i++){
    //Step 2) Use start in place of recv and send
    //MPI_Irecv (buf1, cnt, tp, src, tag, com, &recv_req);
    MPI_Start(&recv_req);

    do_work(buf1, buf2);

    //MPI_Isend (buf2, cnt, tp, dst, tag, com, &send_req);
    MPI_Start(&send_req);

    //Wait for send to complete
    MPI_Wait(&send_req, status);
    //Wait for receive to finish (no deadlock!)
    MPI_Wait(&recv_req, status);
}
MPI_Request_free(&recv_req);    //Step 3) Clean up the requests
MPI_Request_free(&send_req);
```

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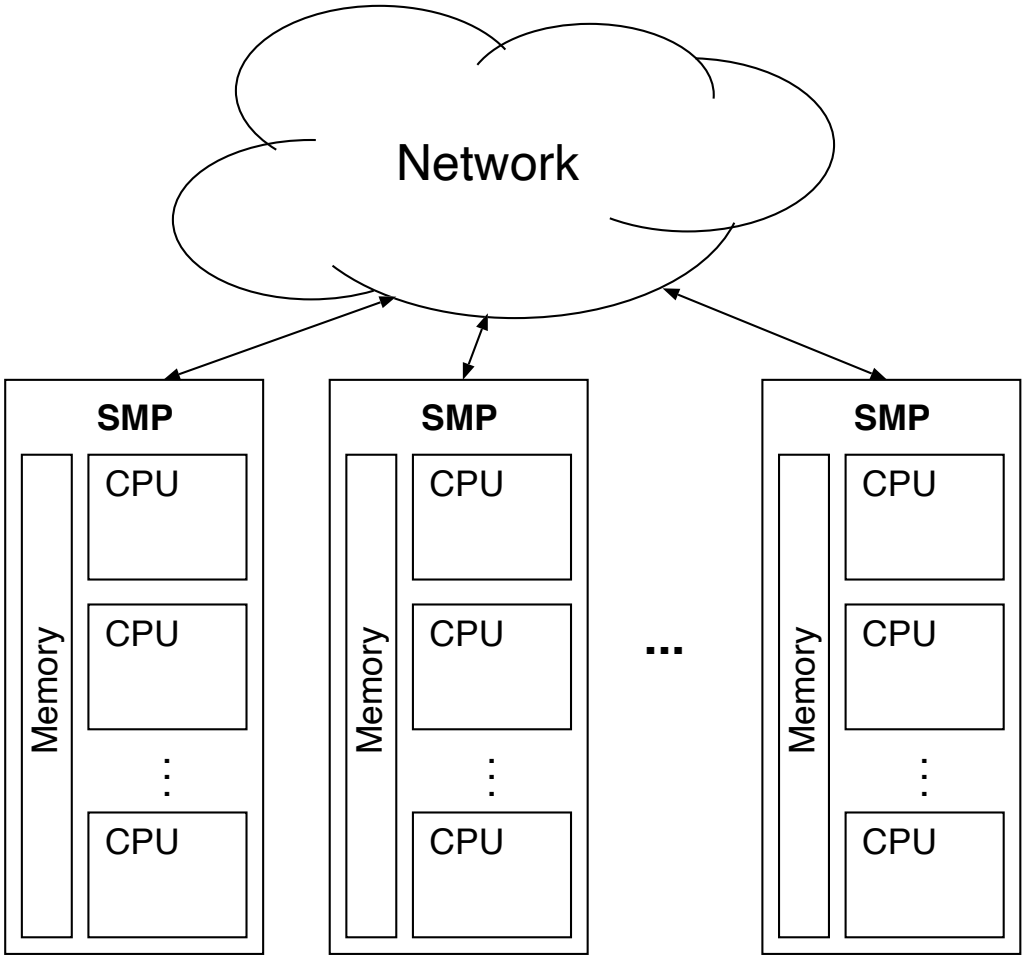
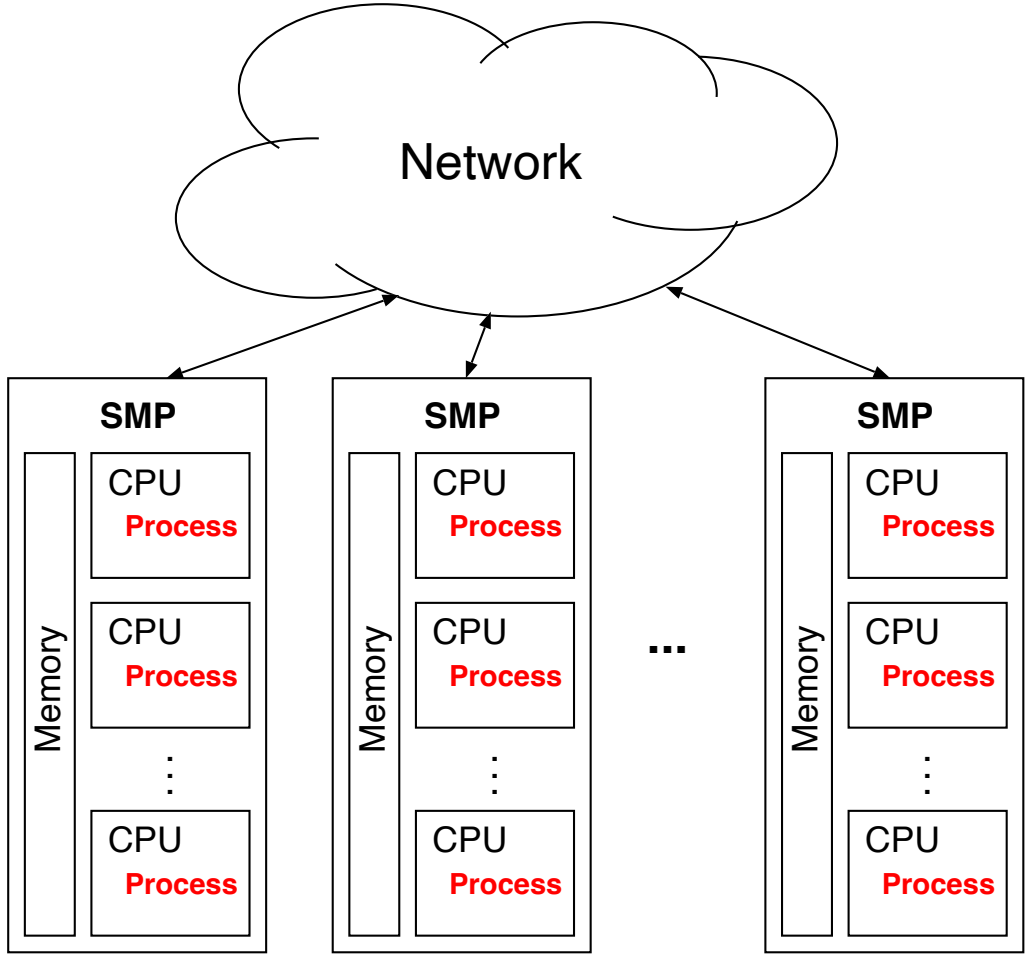
  - Dynamic load balancing is often difficult

Clusters of SMPs



Clusters of SMPs

- Using only MPI



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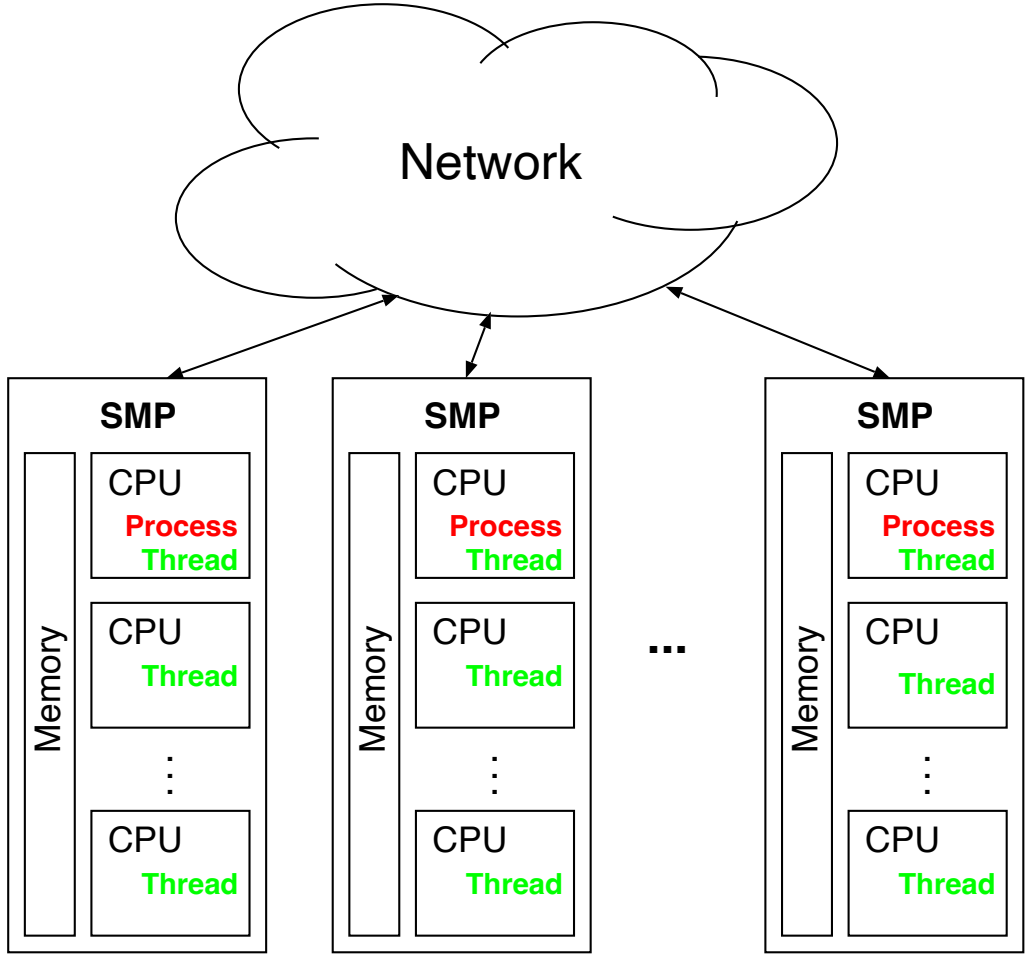

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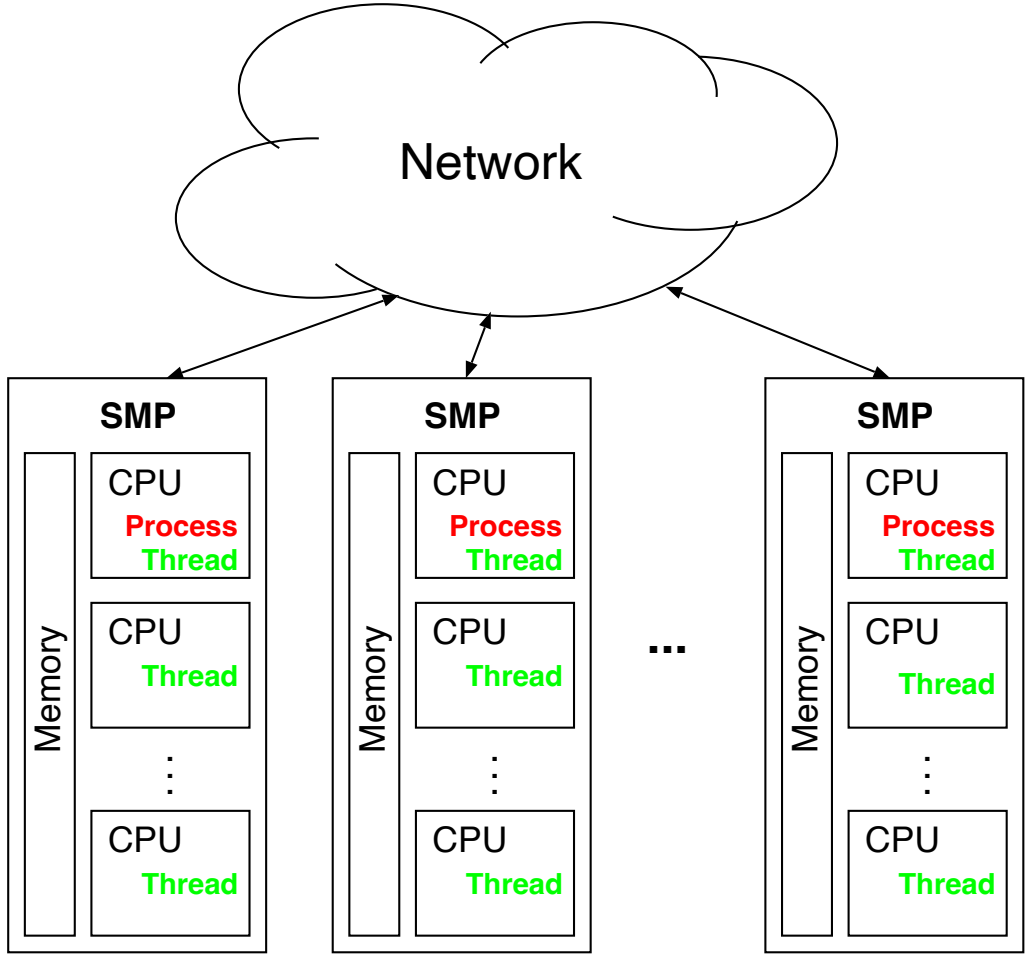

- Best of both worlds!

Hello World, in OpenMP+MPI

```
#include <stdio.h>
#include <mpi.h>
#include <omp.h>

int main(int argc, char *argv[])
{
  int numprocs, rank, namelen, iam, nt;
  char processor_name[MPI_MAX_PROCESSOR_NAME];

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Get_processor_name(processor_name, &namelen);

  #pragma omp parallel private(iam, nt)
  {
    nt = omp_get_num_threads();
    iam = omp_get_thread_num();
    printf("Hello from thread %d out of %d from process %d out of %d on %s\n”,
           iam, nt, rank, numprocs, processor_name);
  }
  MPI_Finalize();
}
```

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```
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Hello from thread 1 out of 2 from process 0 out of 1 on markov
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Hello from thread 1 out of 2 from process 0 out of 1 on markov
$ mpirun -n 3 ./HelloWorld
Hello from thread 0 out of 2 from process 0 out of 3 on markov
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A Common Execution Scenario

1. A single MPI process is launched on each SMP node in the cluster
2. Each process spawns N threads on each SMP node
3. At some global sync point, the master thread on each SMP communicate with one another
4. The threads belonging to each process continue until another sync point or completion

MPI Handling of Threads

- Replace `MPI_Init` by:

```
int MPI_Init_thread (
  int    argc,      /* command line arguments */
  char *argv[],
  int    desired,   /* desired level of thread support */
  int   *provided   /* level of thread support provided */
)
```

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  - `MPI_THREAD_MULTIPLE`: Multiple threads may call MPI, with no restrictions

Issues with `MPI_THREAD_MULTIPLE`

- An MPI implementation is not required to support levels higher than `MPI_THREAD_SINGLE`
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  - A fully thread-safe implementation will support `MPI_THREAD_MULTIPLE`

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- Blocking MPI calls will block only the calling thread and will not prevent other threads from running or executing MPI functions
- MPI calls by different threads must not share the same requests
- Collective operations using the same communicator must be correctly ordered among threads
  - Cannot call a broadcast on one thread and a reduce on another thread on the same communicator.

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- Some problems have two-level parallelism naturally
- Some problems could only use restricted number of MPI tasks
- Could have better scalability than both pure MPI and pure OpenMP

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- From sequential code
  - Decompose with MPI first, then add OpenMP
    - Simplest and least error-prone way is to use MPI outside parallel region, and allow only master thread to communicate between MPI tasks
- From OpenMP code, treat as serial code
  - Not as straightforward as adding OpenMP to an MPI application because global program state must be explicitly handled with MPI
  - Requires careful thought about how each process will communicate amongst one another
  - May require a complete reformulation of the parallelization, with a need to possibly redesign it from the ground up

Hybrid Parallelization Strategies

- From MPI code, add OpenMP
  - Is the easiest of the two options because the program state synchronization is already handled in an explicit way
  - Benefits depend on how many simple loops may be work-shared
  - The number of MPI processes per SMP node will depend on how many threads one wants to use per process

Example: Conjugate Gradient Method

- Conjugate Gradient Method: iterative method for efficiently solving linear systems of equations

$$Ax = b$$

- It can be demonstrated that the function

$$q(x) = \frac{1}{2}x^T Ax - x^T b + c$$

has a unique minimum, x, that is the solution to Ax=b.

Example: Conjugate Gradient Method

- Algorithm for Conjugate Gradient Method

1. Compute gradient: $g(t) = A\,x(t-1) - b$
2. If $g(t)^T g(t) < \epsilon$, stop
3. Compute direction vector: $d(t) = -g(t) + \frac{g(t)^T g(t)}{g(t-1)^T g(t-1)} d(t-1)$
4. Compute step size: $s(t) = -\frac{d(t)^T g(t)}{d(t)^T A d(t)}$
5. Compute new approximation of x: $x(t) = x(t-1) + s(t)d(t)$

Example: Conjugate Gradient Method

```
for(it = 0; it < n; it++) {
    denom1 = dot_product(g, g, n);
    matrix_vector_product(id, p, n, a, x, g);
    for(i = 0; i < n; i++) g[i] -= b[i];
    num1 = dot_product(g, g, n);

    /* When g is sufficiently close to 0, it is time to halt */
    if(num1 < EPSILON) break;

    for(i = 0; i < n; i++)
        d[i] = -g[i] + (num1/denom1) * d[i];
    num2 = dot_product(d, g, n);
    matrix_vector_product(id, p, n, a, d, tmpvec);
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    s = -num2 / denom2;
    for(i = 0; i < n; i++) x[i] += s * d[i];
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Example: Conjugate Gradient Method

- MPI implementation: program based on rowwise block decomposition of matrix A, and replication of vector b

- Results of profiling:

Function	1 CPU	8 CPUs
`matrix_vector_product`	99,5%	97,5%
`dot_product`	0,2%	1,1%
`cg`	0,3%	1,4%

Example: Conjugate Gradient Method

```
void matrix_vector_product (int id, int p, int n,
                            double **a, double *b, double *c)
{
  int i, j;
  double tmp;

  /* Accumulates sum */
  for(i = 0; i < BLOCK_SIZE(id,p,n); i++) {
    tmp = 0.0;
    for(j = 0; j < n; j++)
      tmp += a[i][j] * b[j];
    piece[i] = tmp;
  }
  replicate_vector(id, p, piece, n, c);
}
```

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    piece[i] = tmp;
  }
  replicate_vector(id, p, piece, n, c);
}
```

AllGather operation necessary to replicate the result vector

Example: Conjugate Gradient Method

- Adding OpenMP directives
  - Make outermost loop parallel
    - Outer loop may be executed in parallel if each thread has a private copy of `tmp` and `j`

```
#pragma omp parallel for private(j,tmp)
  for(i = 0; i < BLOCK_SIZE(id,p,n); i++)
```

  - Specify number of active threads per process

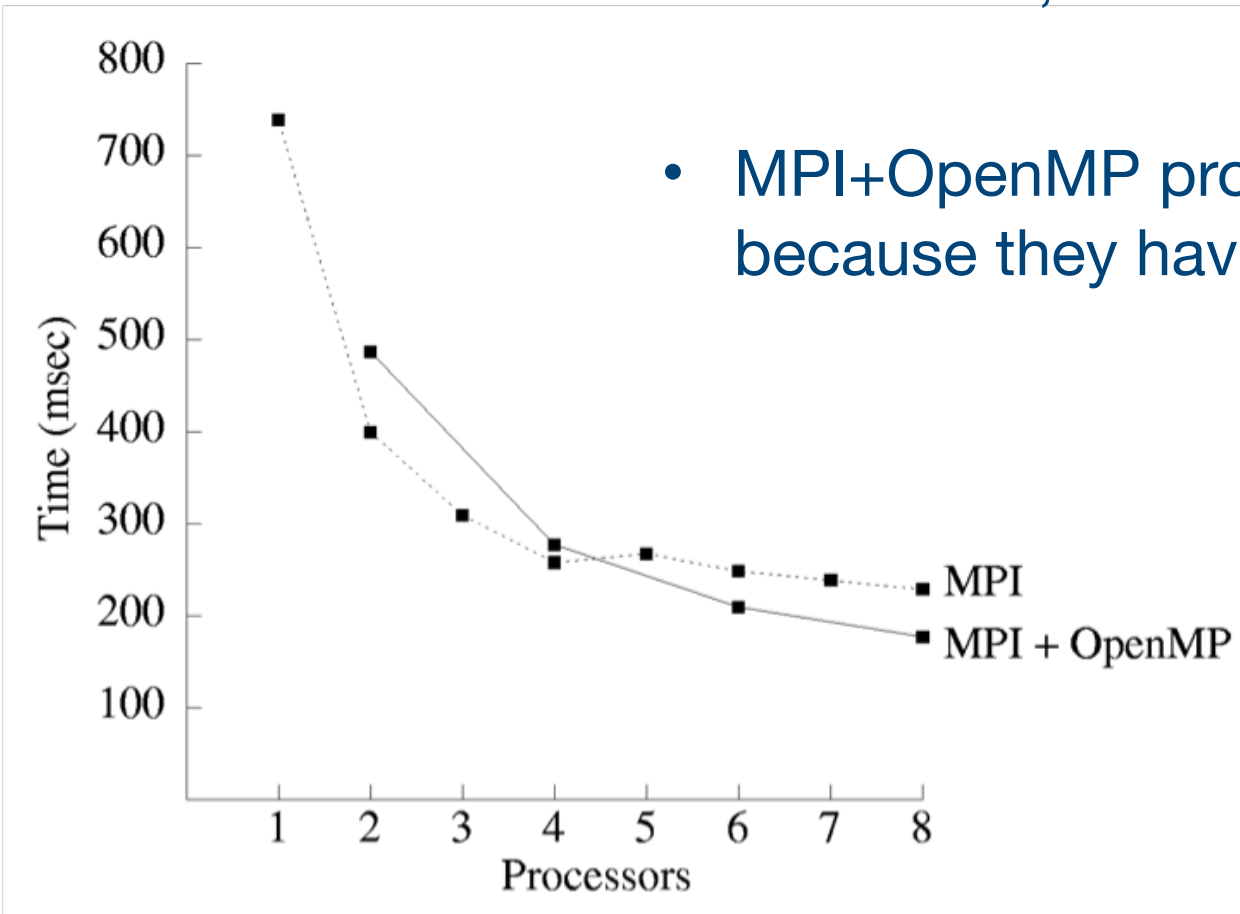
```
omp_set_num_threads(atoi(argv[3]));
```

Example: Conjugate Gradient Method

- Target system: a commodity cluster with four dual-processor nodes
- Pure MPI
  - Program executes on 1, 2, ..., 8 CPUs
  - On 1, 2, 3, 4 CPUs, each process on different node, maximizing memory bandwidth per CPU
- MPI + OpenMP
  - Program executes on 1, 2, 3, 4 processes, each process has two threads (program executes on 2, 4, 6, 8 threads)

Example: Conjugate Gradient Method

- MPI+OpenMP program slower on 2, 4 CPUs because threads are sharing memory bandwidth, while MPI processes are not



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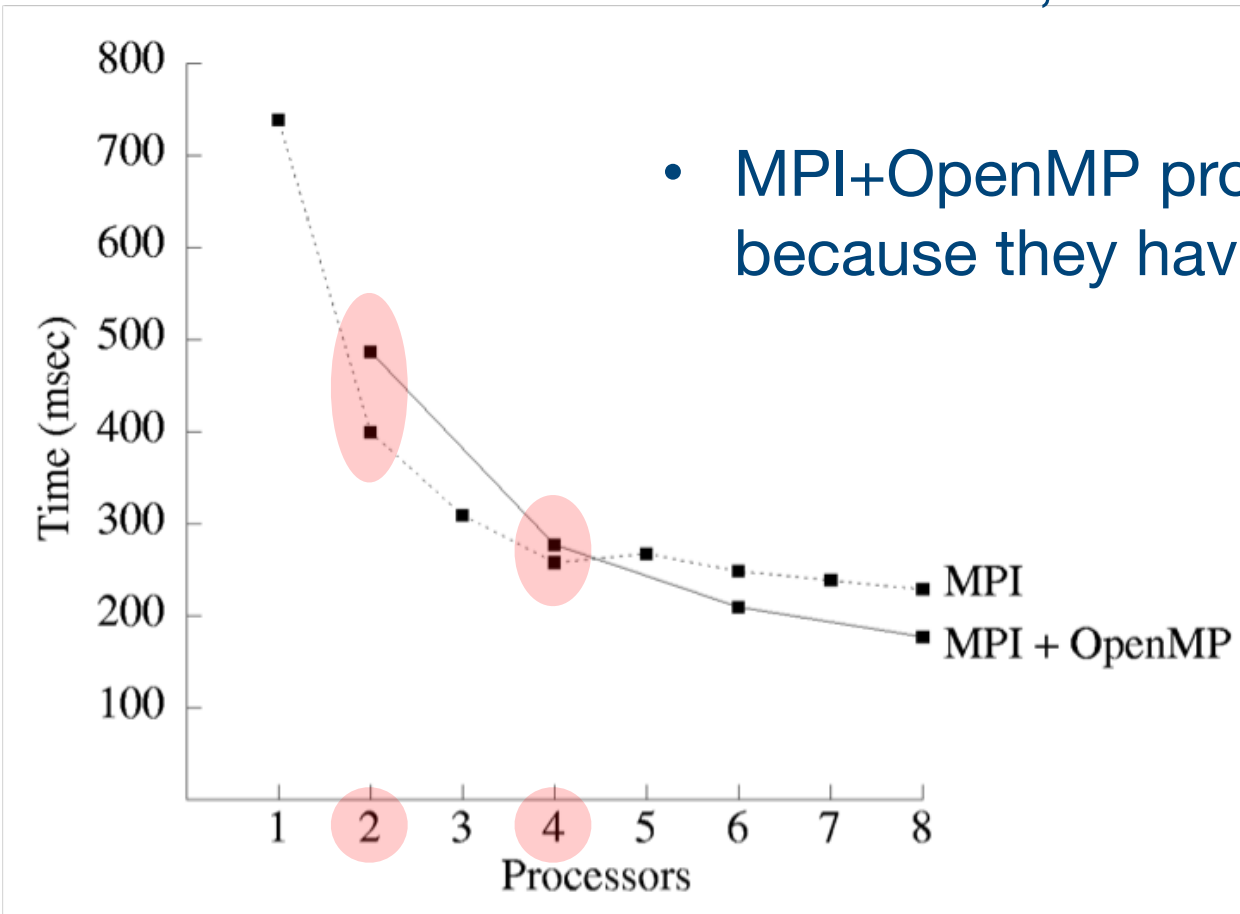

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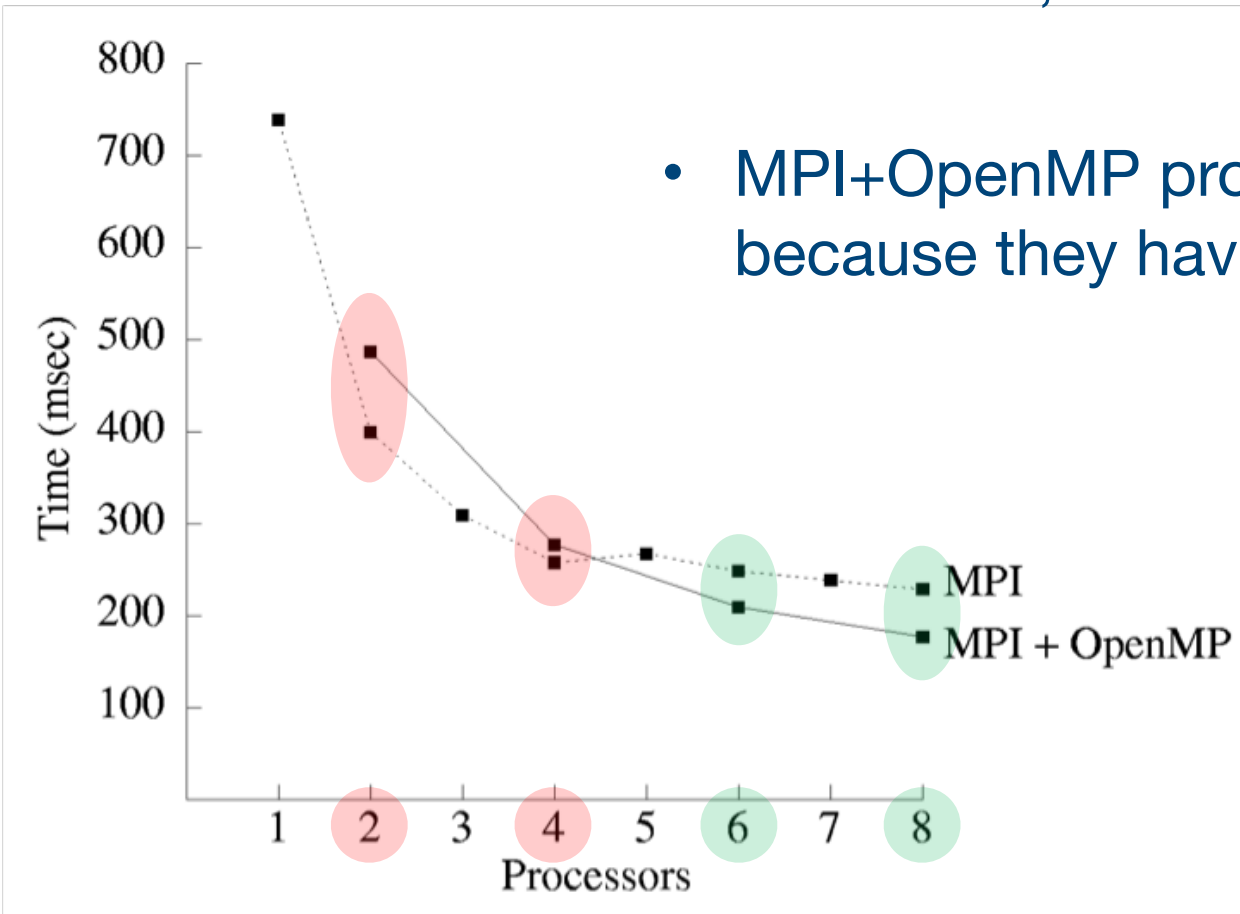

Foster's Design Methodology

- Development of scalable parallel algorithms by delaying machine-dependent decisions to later stages

Four steps:

- Partitioning
- Communication
- Agglomeration
- Mapping

Mapping

- Examples discussed in previous classes:
  - Circuit satisfiability
  - Sieve of Eratosthenes
  - All pairs shortest paths
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- So far, all primitive tasks require same amount of computation
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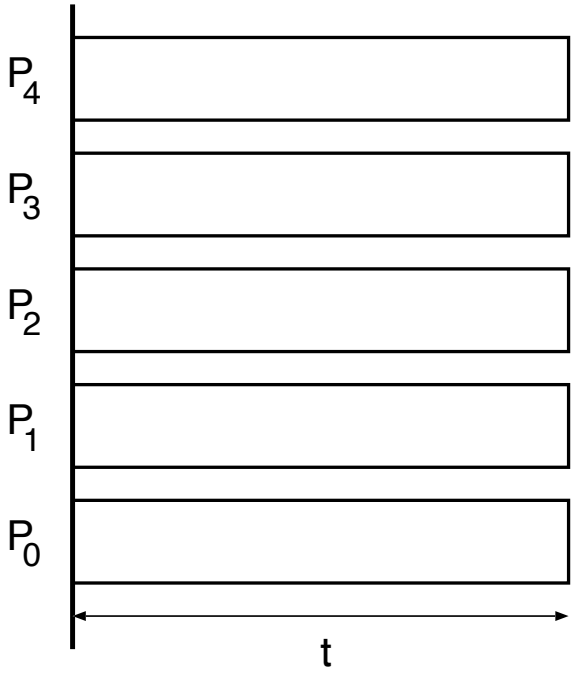
- What if we can not predict beforehand the amount of computation required per primitive task?

Load Balancing



Perfect load balancing

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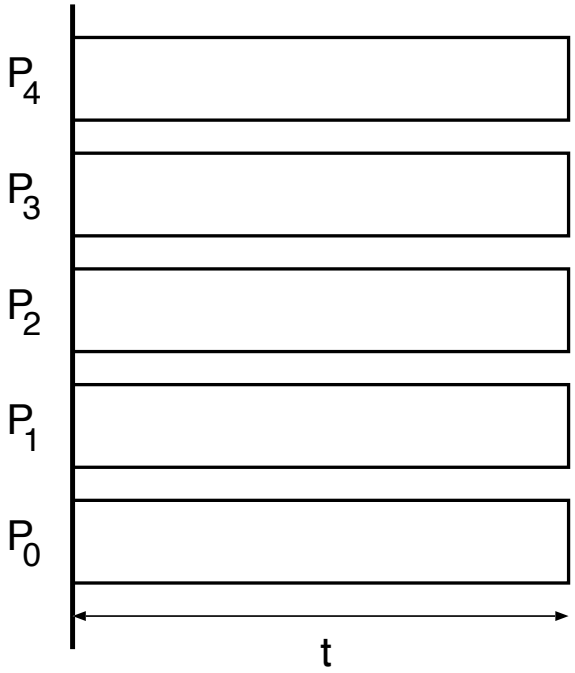

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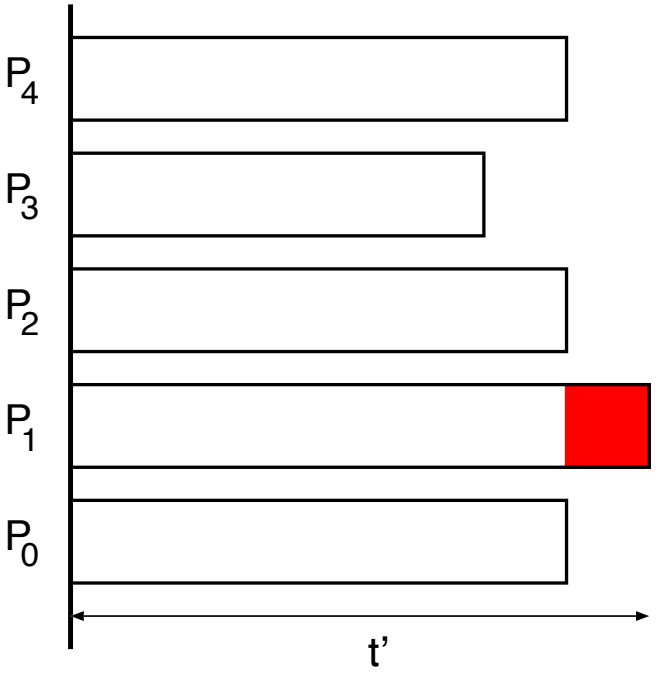

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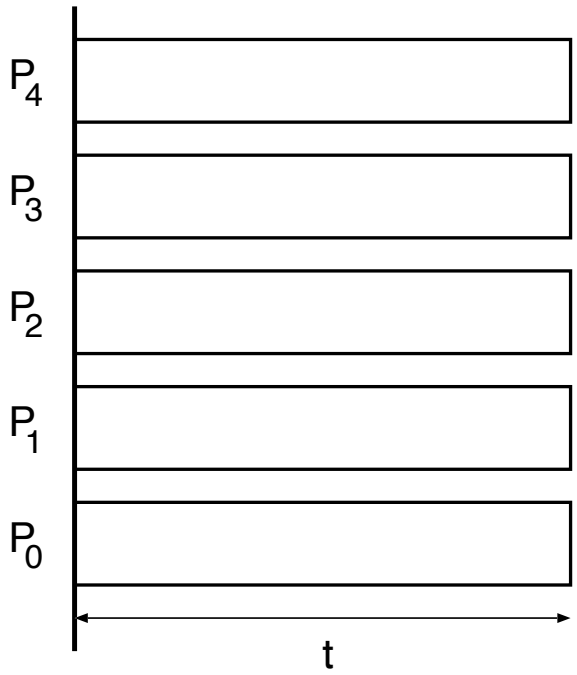

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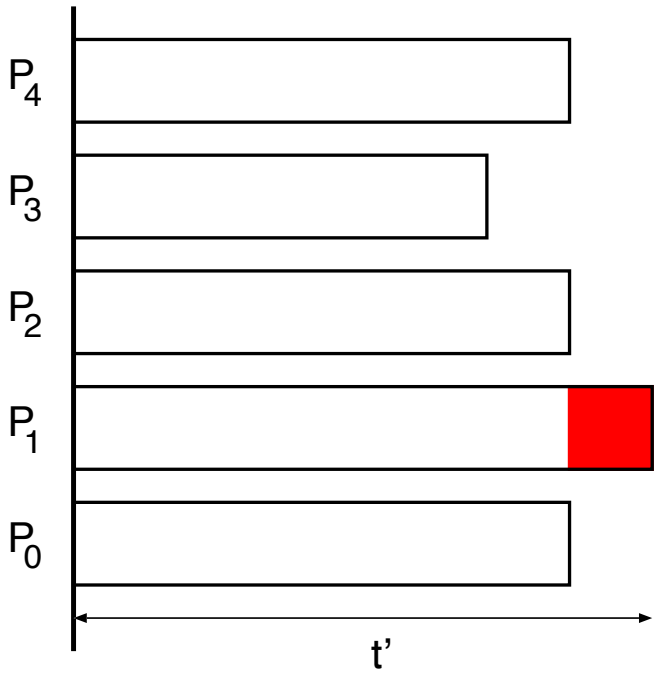

Imperfect load balancing

- Parallel execution time defined by last task to finish
- Parallel time minimized when load distributed evenly

Limitations of Static Load Balancing

- Computational effort of each task may not be known a-priori
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- Programs are subject to variable communication delays
- Performance of each processor may vary, and may not be known beforehand
- Dynamic load balancing overcomes these issues by making the division of the load dependent on the actual runtimes
  - → Penalty: additional overhead due to task management

Dynamic Load Balancing Management

- Centralized management
  - One process (master) is responsible for assigning tasks to slave processes
- Decentralized management
  - All processes are equal and divide work among them cooperatively

Centralized Dynamic Load Balancing

- Work Pool or Processor Farm model

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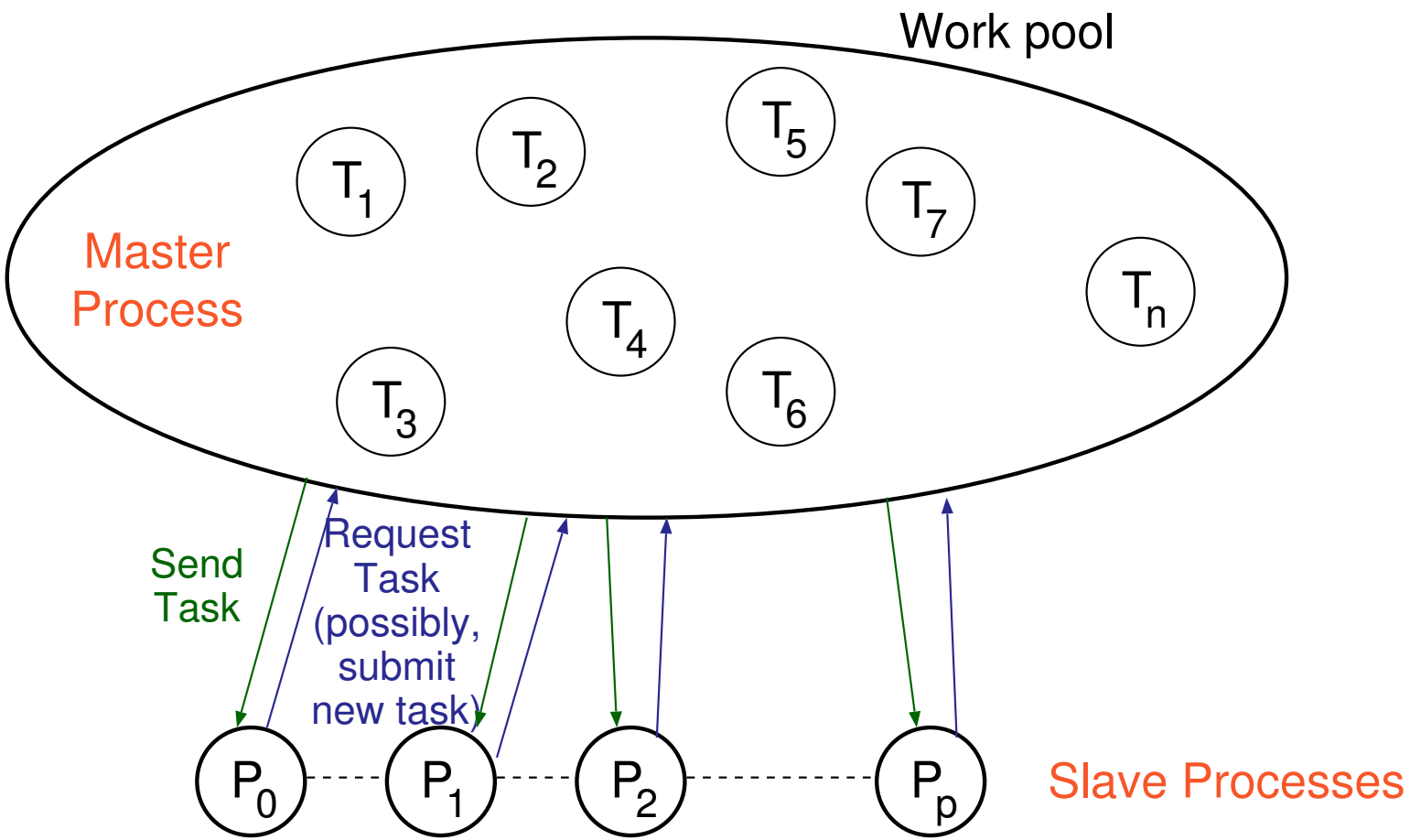

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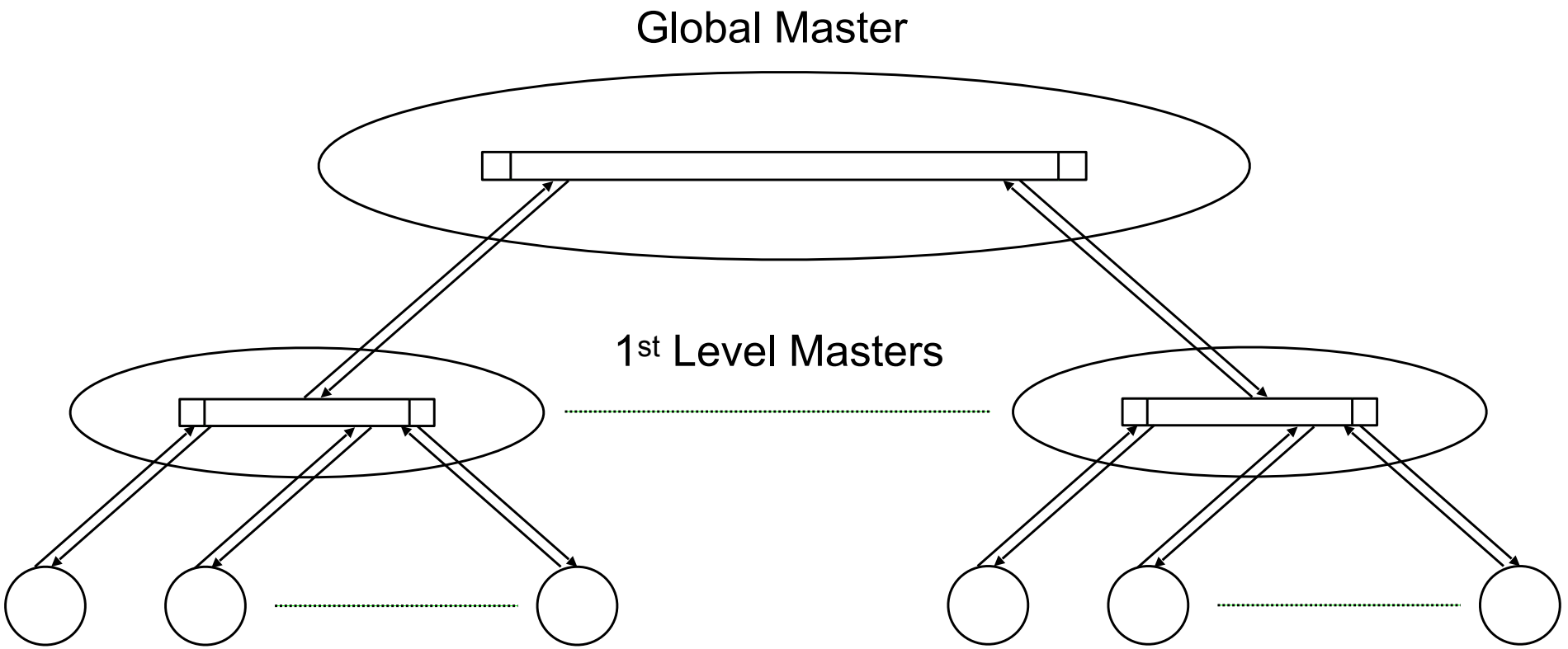
    - Not a significant problem if few slaves and/or computationally intensive tasks
    - For finer-grained tasks and many slaves, distribute task management

Decentralized Dynamic Load Balancing

- Initial approach can be simply to evolve the centralized system into a tree-like task management scheme
  - Main master distributes tasks to be managed by second-level masters
  - Each second-level master behaves as in the centralized method
- Naturally, this model can be extended to as many levels as desired

Decentralized Dynamic Load Balancing



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    - Better in high load systems
  - Sender-initiated method: process under heavy load sends tasks to processes willing to accept them

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    - Send to neighbors (dependent on network topology)

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    - Not so trivial...

Termination Detection

- In general, termination at time *t* requires two conditions

  (1) Application-specific local termination conditions exist for all processes at time *t*

  (2) There are no messages in transit at time *t*

- Second condition is what makes this problem difficult
  - Wait long enough before assuming program has finished?

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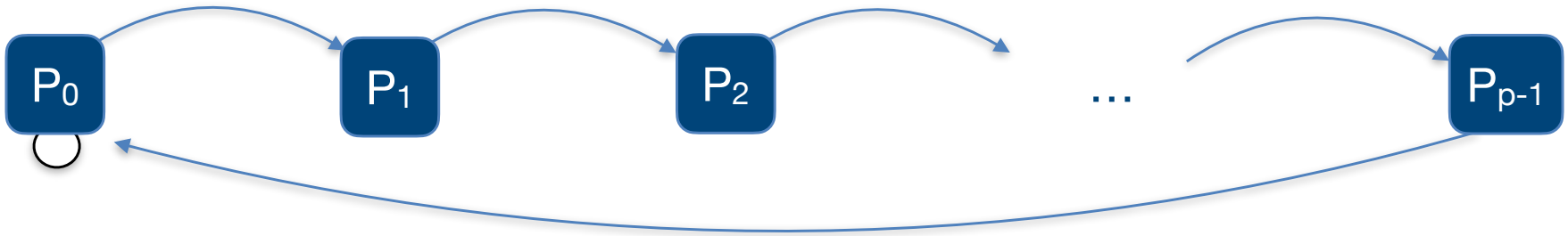

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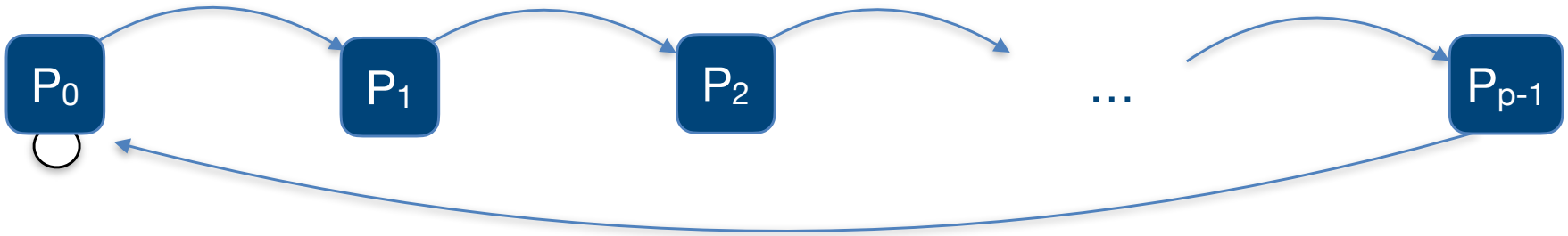

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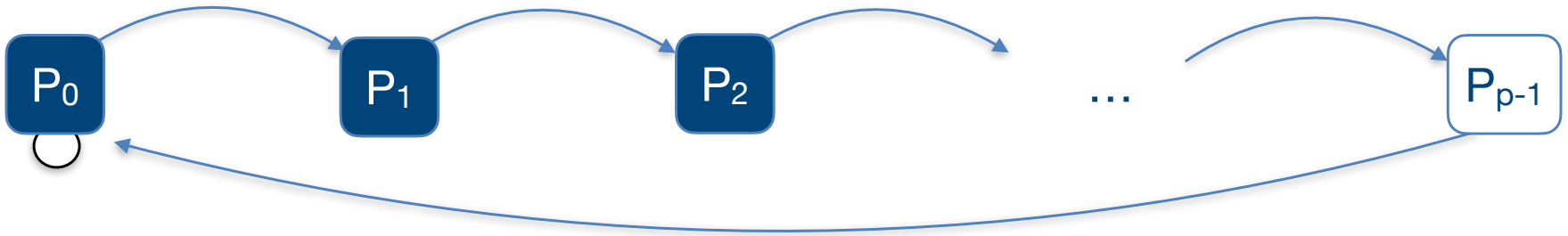

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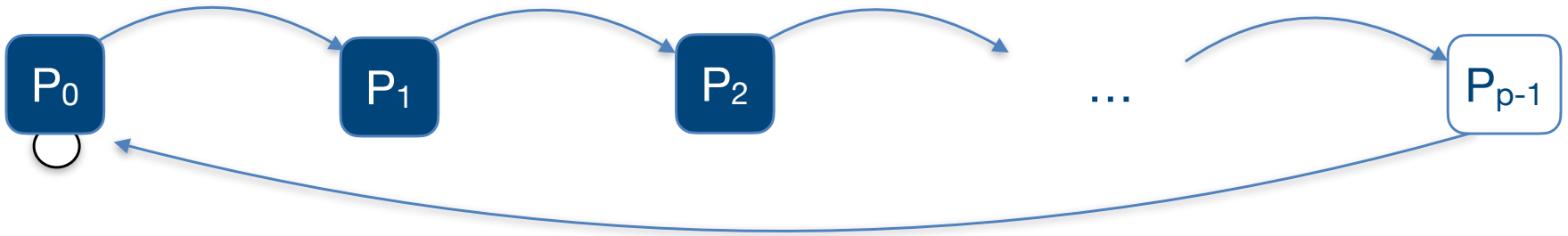

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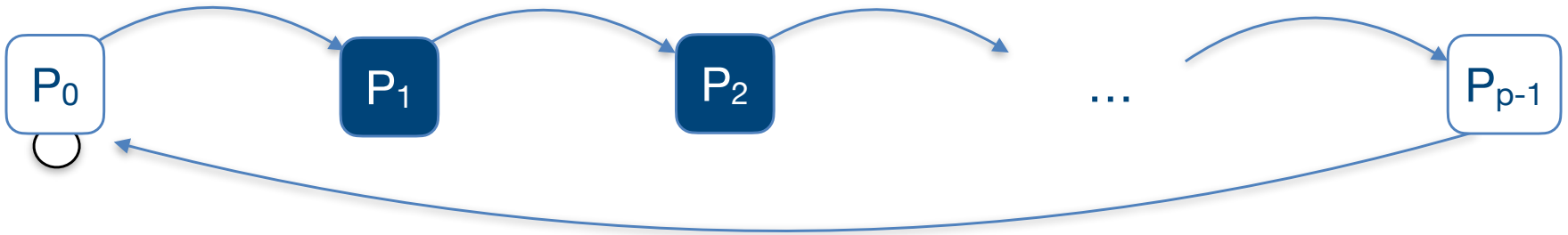

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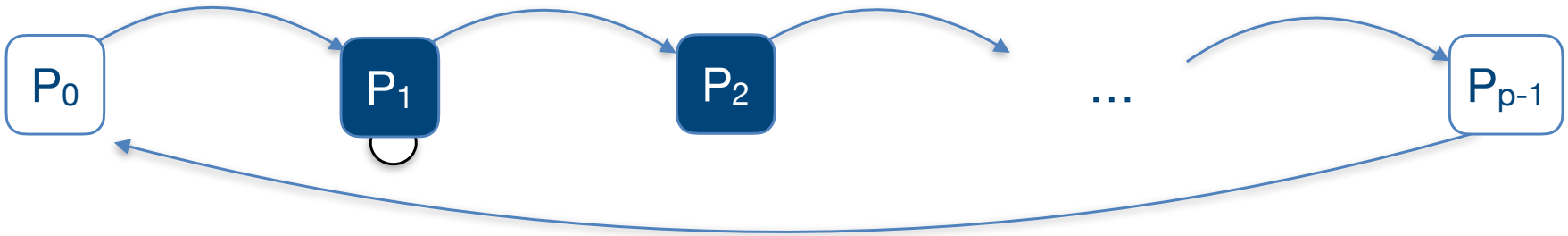

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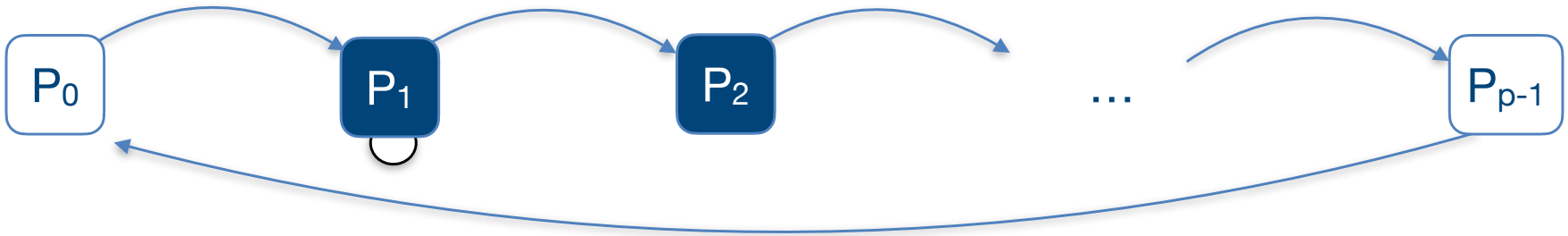

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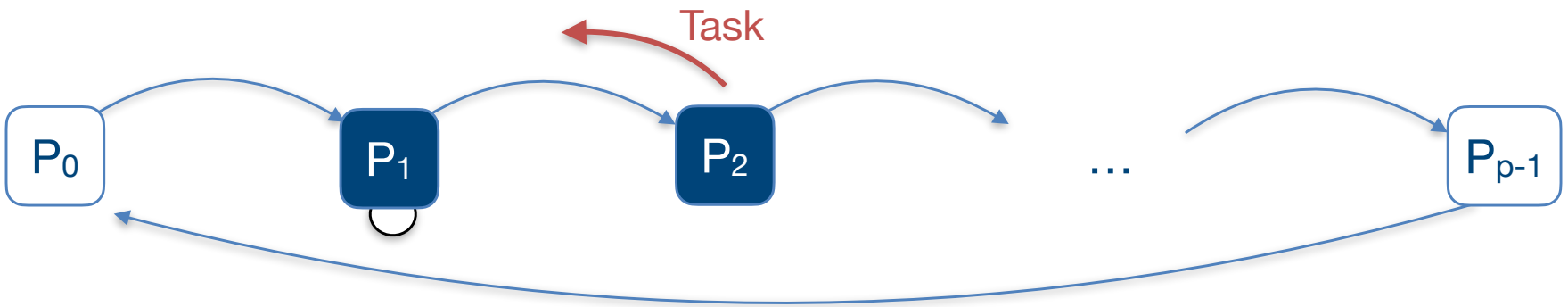

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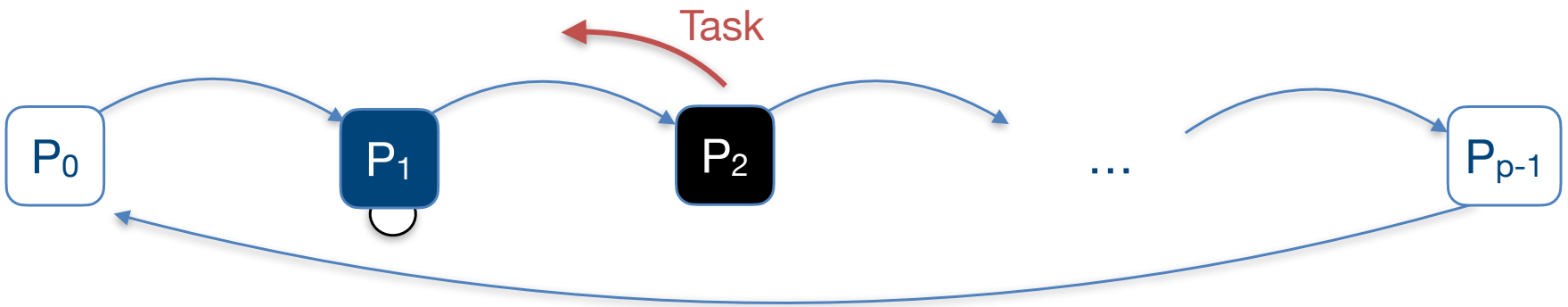

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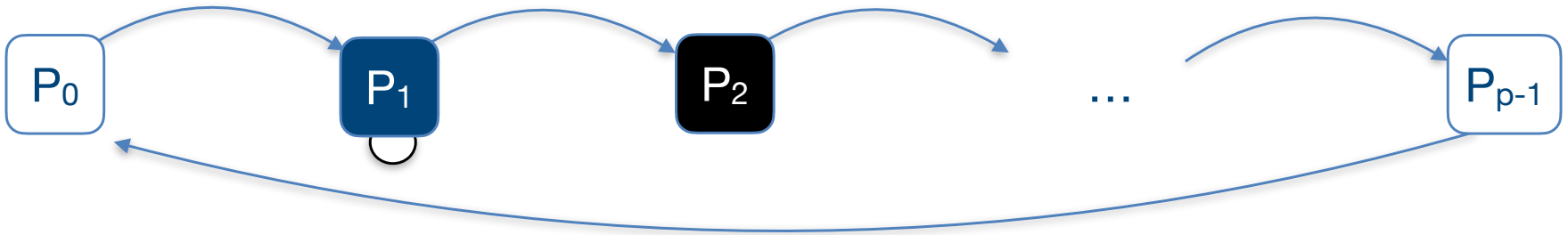

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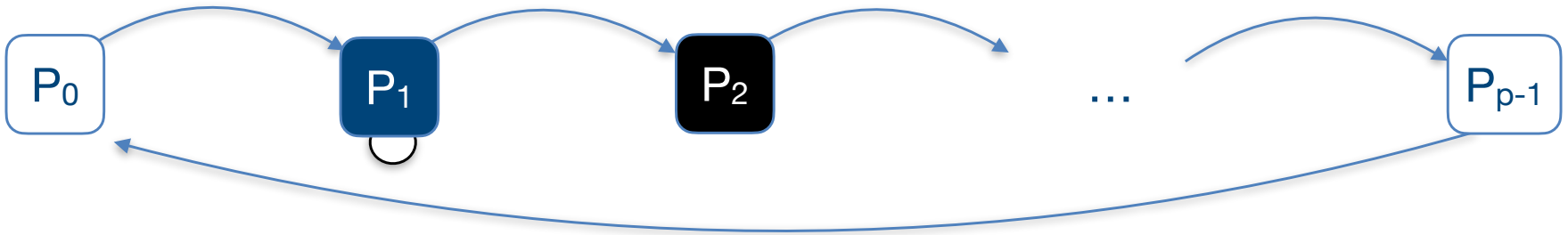

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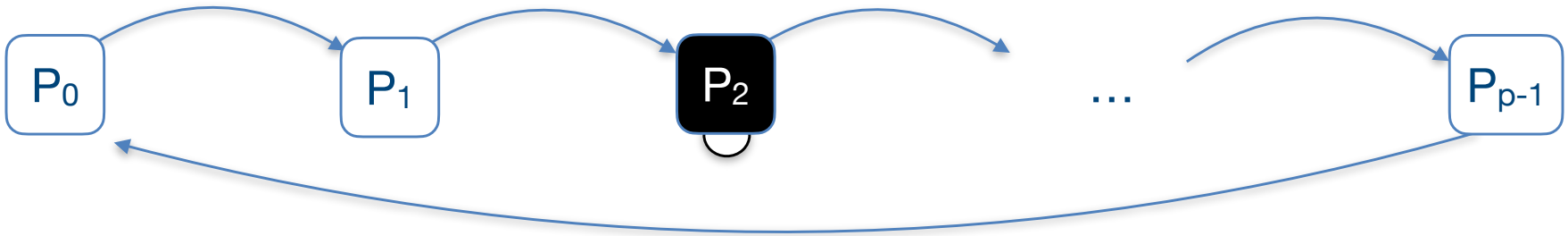

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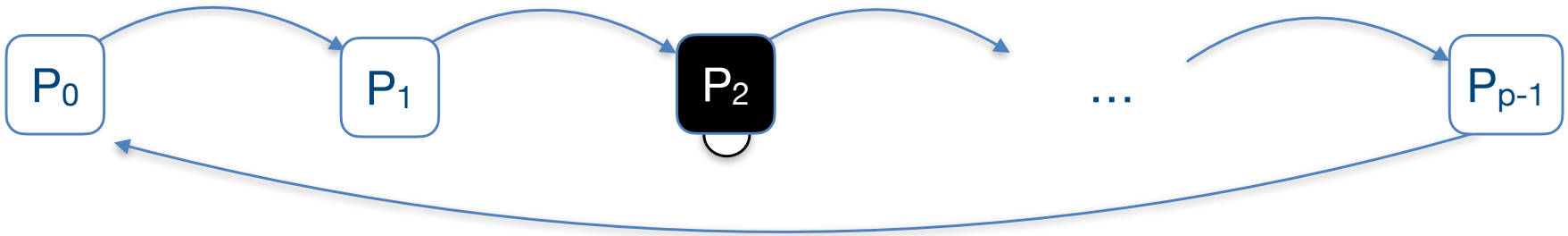

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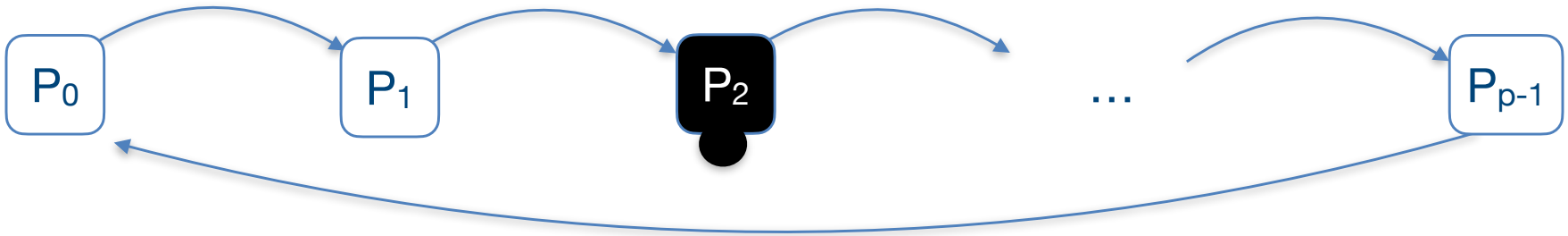

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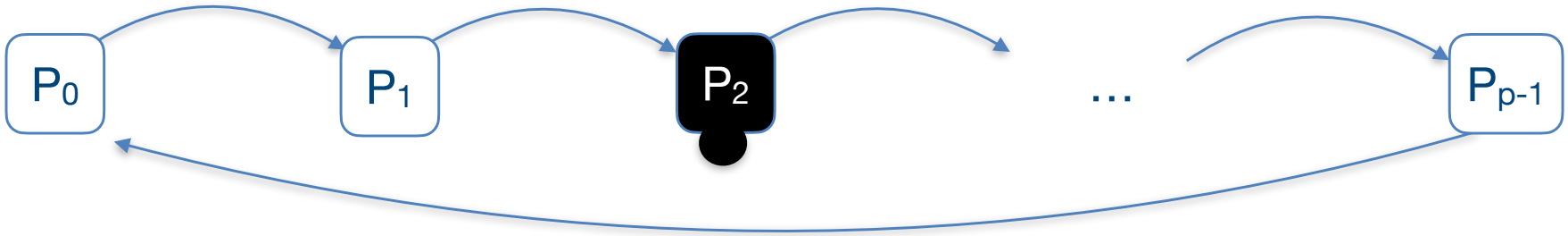

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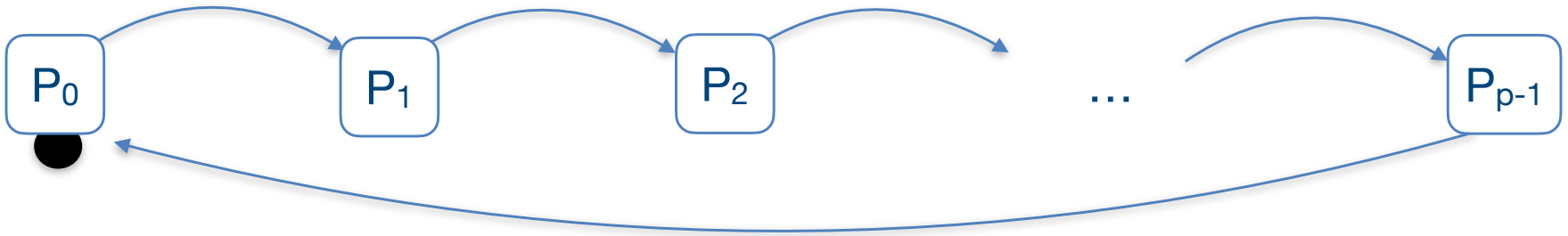

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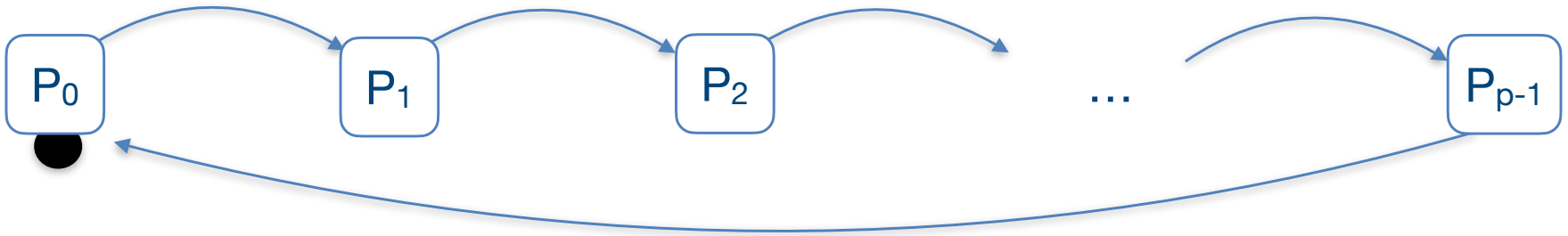

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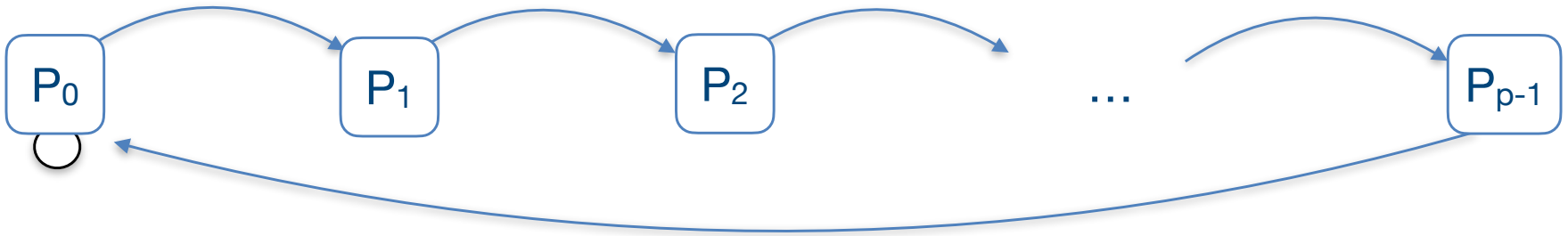

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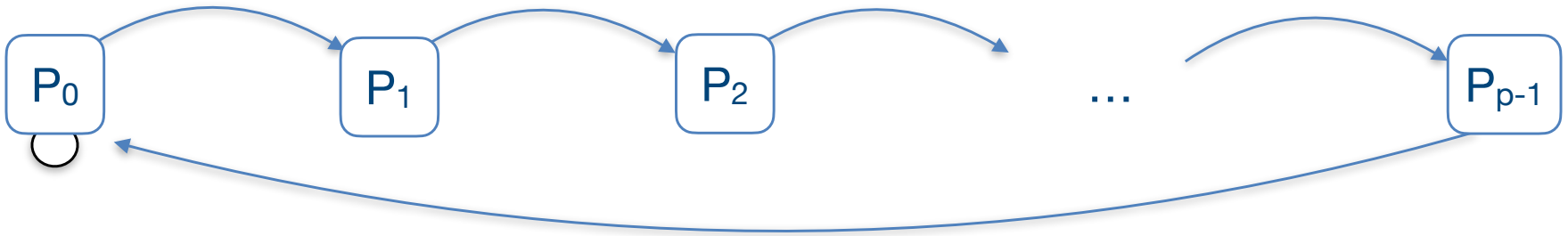

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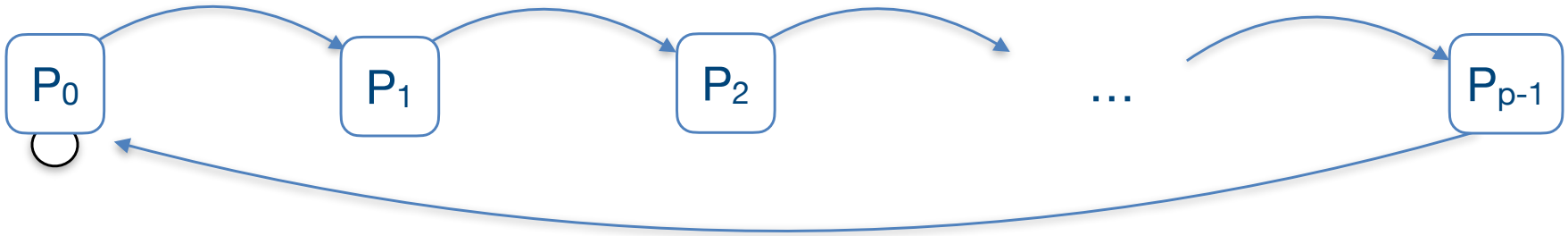

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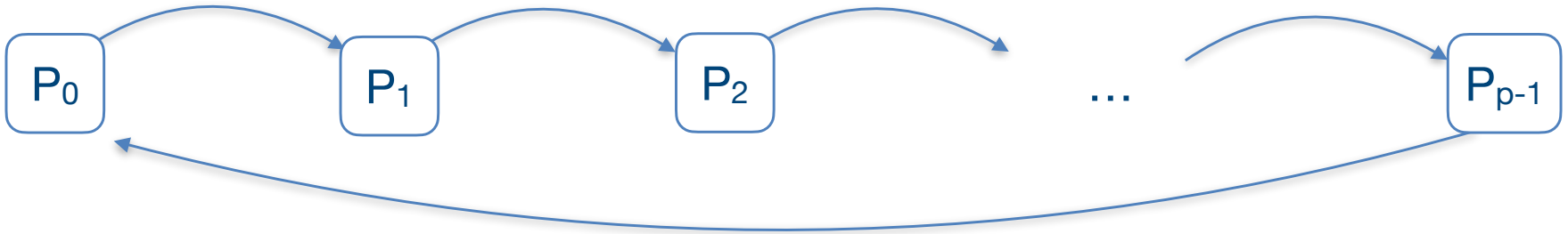

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Review

- Advanced MPI
- Hybrid programming
  - Combining OpenMP and MPI
- Load balancing
- Termination detection

Next Class …

- Methods for Solving Linear Systems
  - Direct Methods: solution is sought directly, at once
    - Gaussian Elimination
    - LU Factorization
  - Iterative Methods: solution is sought iteratively, by improvement
    - Relaxation Methods
    - Krylov Methods
    - Preconditioning
- Linear Second-order Partial Differential Equations (PDEs)
  - Finite difference methods
  - Example: steady-state heat distribution
  - Ghost points