Parallel programming models

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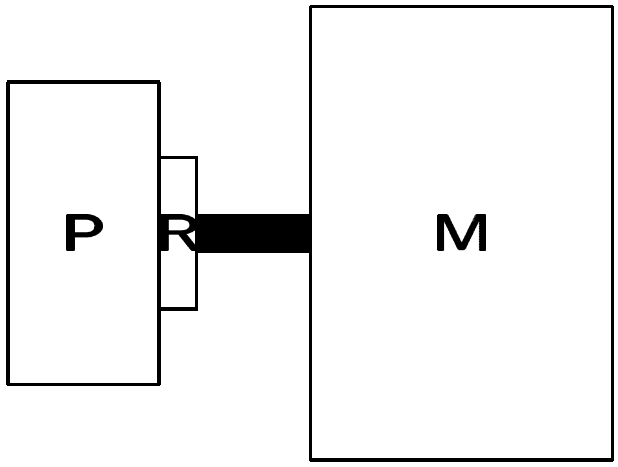
Overview

- Models of concurrency
- Overview of programming models: shared memory, distributed memory with remote memory access, message-passing
- Overview of the MPI programming interface
- Parallel programming considerations: communication and synchronization, domain decomposition
- Analyzing parallel algorithms: advection equation, Poisson equation
- Current research in parallel programming models

Sequential computing

The von Neumann model of computing conceptualizes the computer as consisting of a memory where instructions and data are stored, and a processing unit where the computation takes place. At each turn, we fetch an operator and its operands from memory, perform the computation, and write the results back to memory.

```
a = b + c
```



Computational limits

The speed of the computation is constrained by hardware limits:

- the rate at which instructions and operands can be loaded from memory, and results written back;

- and the speed of the processing units. The overall computation rate is limited by the slower of the two: memory.

Latency time to find a word.

Bandwidth number of words per unit time that can stream through the pipe.

Hardware trends

A processor clock period is currently $\sim$ 0.5-1 ns, Moore's constant is $4\times$/3 years.

RAM latency is $\sim$ 30 ns, Moore's constant is $1.3\times$/3 years.

Maximum memory bandwidth is theoretically the same as the clock speed, but far less for commodity memory.

Furthermore, since memory and processors are built basically of the same "stuff", there is no way to reverse this trend.

Concurrency

Within the raw physical limitations on processor and memory, there are algorithmic and architectural ways to speed up computation. Most involve doing more than one thing at once.

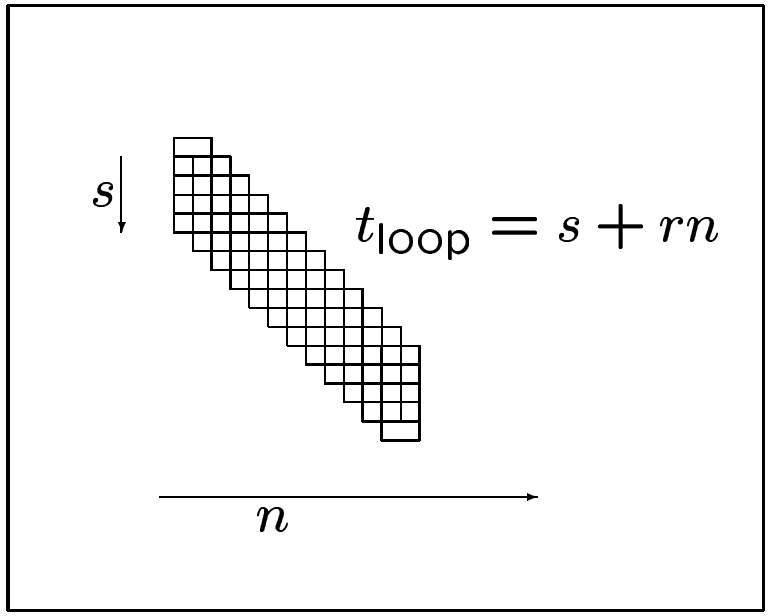
- Overlap separate computations and/or memory operations.
  - Pipelining.
  - Multiple functional units.
  - Overlap computation with memory operations.
  - Re-use already fetched information: **caching**.
  - Memory pipelining.
- Multiple computers sharing data.

The search for **concurrency** becomes a major element in the design of algorithms (and libraries, and compilers). Concurrency can be sought at different grain sizes.

Vector computing

Cray: if the same operation is *independently* performed on many different operands, schedule the operands to stream through the processing unit at a rate r = 1 per CP. Thus was born **vector processing**.

```
do i = 1,n
   a(i) = b(i) + c(i)
enddo
```



So long as the computations for each instance of the loop can be concurrently scheduled, the work within the loop can be made as complicated as one wishes.

The magic of vector computing is that for $s \gg rn$, $t_{\text{loop}} \approx s$ for any length n!

Of course in practice s depends on n if we consider the cost of fetching n operands from memory and loading the vector registers.

Vector machines tend to be expensive since they must use the fastest memory technology available to use the full potential of vector pipelining.

Real codes in general cannot be recast as a single loop of n concurrent sequences of arithmetic operations. There is lots of other stuff to be done (memory management, I/O, etc.) Since sustained memory bandwidth requirements over an entire code are somewhat lower, we can let multiple processors share the bandwidth, and seek concurrency at a coarser grain size.

```
!mic$ DO private(j)
do j = 1,n
   call ocean(j)
   call atmos(j)
enddo
```

Since the language standards do not specify parallel constructs, they are inserted through compiler directives. Historically, this began with Cray microtasking directives. More recently, community standards for directives (`!$OMP`, see `http://www.openmp.org`) have emerged. Stephane Ethier will be reviewing OpenMP next week.

Instruction-level parallelism

This is also based on the pipelining idea, but instead of performing the same operation on a vector of operands, we perform *different* operations simultaneously on different data streams.

```
a = b + c
d = e * f
```

The onus is on the compiler to detect ILP. Moreover, algorithms may not lend themselves to functional parallelism.

Amdahl's Law

Even a well-parallelized code will have some serial work, such as initialization, I/O operations, etc. The time to execute a parallel code on P processors is given by

$$t_P = t_s + \frac{t_{\|}}{P} \quad (1)$$

$$\frac{t_1}{t_P} = \frac{1}{s + \frac{1-s}{P}} \quad (2)$$

where $s \equiv \frac{t_s}{t_1}$ is the serial fraction.

Speedup of a 1% serial code is at most 100.

Load-balancing

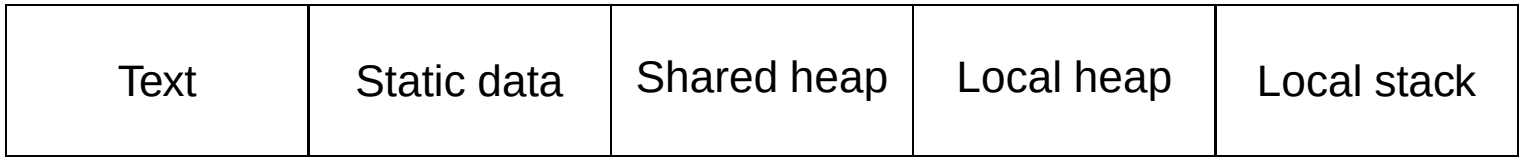
If the computational cost per instance of a parallel region unequal, the loop as a whole executes at the speed of the slowest instance (implicit synchronization at the end of a parallel region).

Work must be partitioned in a way that keeps the load on each parallel leg roughly equal.

If there is sufficient granularity (several instances of a parallel loop per processor), this can be automatically accomplished by implementing a global task queue.

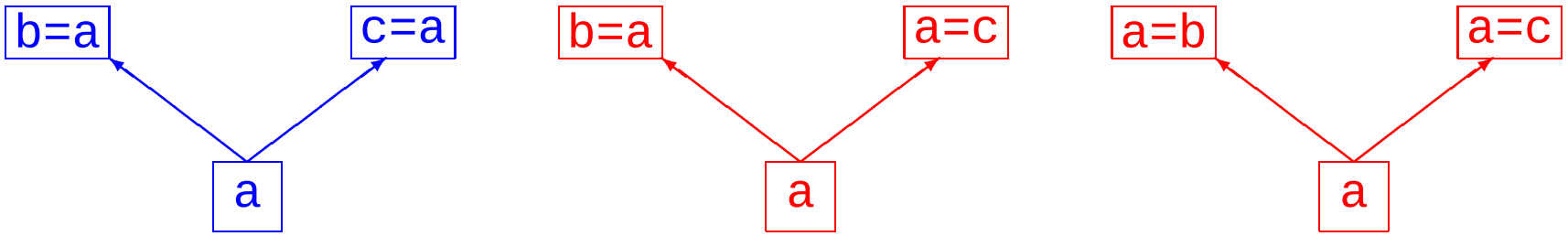
Memory model for shared memory parallelism

Every variable has a **scope**: global or local. Writing to global variables in a parallel region can result in a **race condition.**



- Static data is globally visible.
- Special forms of `malloc()` can place data in shared heap.

Race conditions



The second and third case result in a race condition and unpredictable results. The third case may be OK for certain reduction or search operations, defined within a **critical region.**

```
!mic$ CRITICAL
a = a + b
!mic$ END CRITICAL
```

Scalability of shared memory

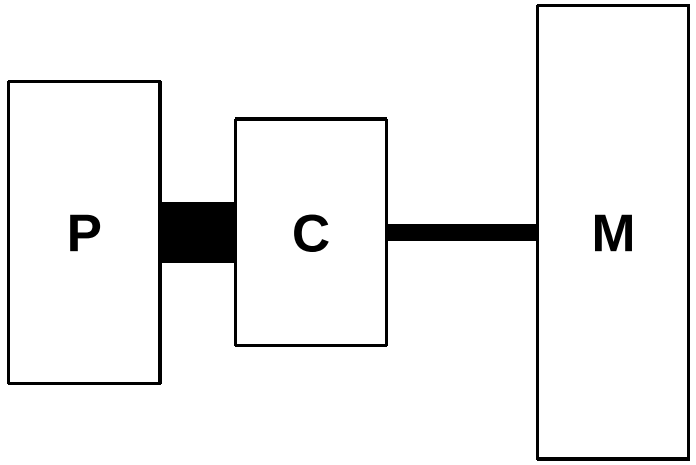
Shared memory parallelism with a **flat** or **uniform** memory model does not **scale** to large numbers of processors, because (again) of memory bandwidth. UMA memory access quickly runs out of aggregate bandwidth.

Scalability: the number of processors you can usefully add to a parallel system. It is also used to describe something like the degree of coarse-grained concurrency in a code or an algorithm, but this use is somewhat suspect, as this is almost always a function of problem size.

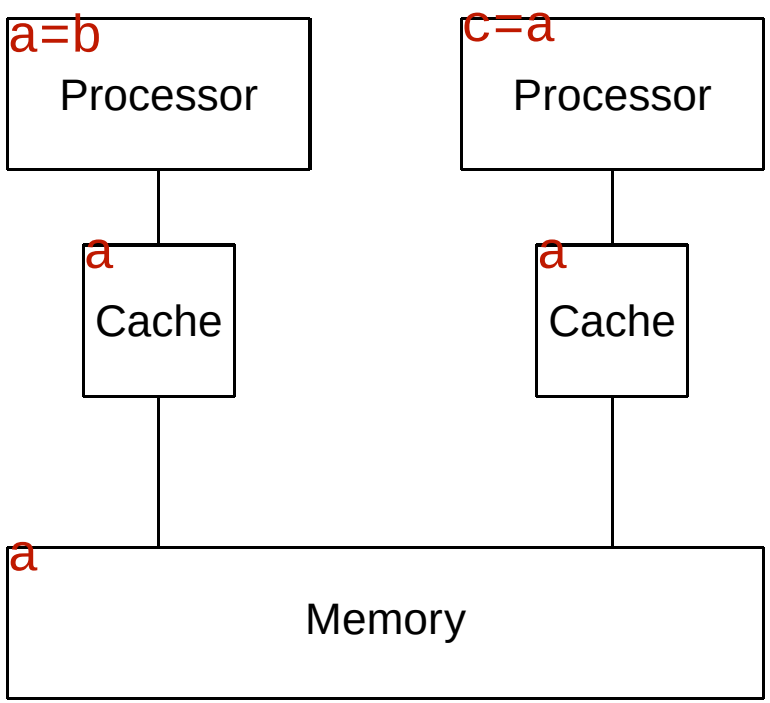
Caches

The memory bandwidth bottleneck may be alleviated by the use of caches.

Caches exploit **temporal locality** of memory access requests. Memory latency is also somewhat obscured by exploiting **spatial locality** as well: when a word is requested, adjacent words, constituting a **cache line**, are fetched as well.



In a multi-processor environment, extra overhead is incurred to maintain **cache coherency**.



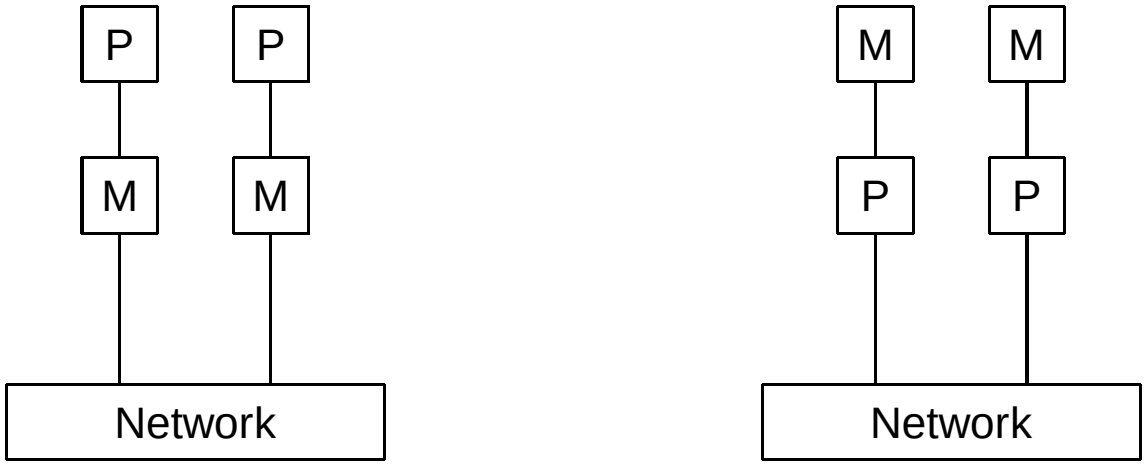
Limitations of pure shared memory

To summarize:

UMA architectures suffer from a crisis of aggregate memory bandwidth. The use of caches may alleviate the bandwidth problem, but require some form of communication between the disjoint members of the system: processors or caches.

This suggests dispensing with the UMA model altogether: moving toward a model where memory segments are themselves distributed and communicate over a network. This involves a radical change to the programming model, since there is no longer a single **address space** in it. Instead communication between disjoint regions must be explicit: **remote memory access (RMA)** or **message passing.**

Distributed Memory



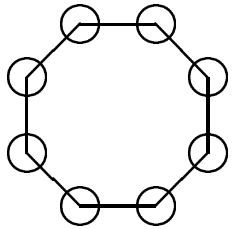
Tightly coupled systems memory closer to network than processor.

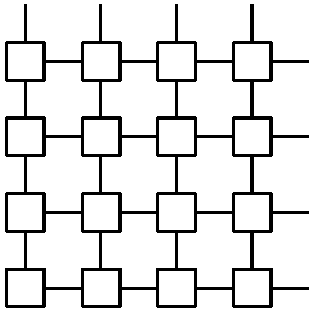
Loosely coupled systems processor closer to network than memory.

Loose coupling could include heterogeneous computing across a wide-area network.

Network Topologies

Ring, hypercube, torus.





A torus provides scalable connectivity: an n-dimensional torus of side p has p^n PEs with a maximum distance of $\frac{pn}{2}$.

Remote memory access with barriers

```
program test
integer :: me, right
me = my_pe()
call BARRIER()
call GET( right, me, 1, mod(my_pe()+1,num_pes()) )
call BARRIER()
print *, ’PE’, my_pe(), ’ says hi to its neighbour on the right,’, right
end
```

```
 PE 2  says hi to its neighbour on the right, 3
 PE 0  says hi to its neighbour on the right, 1
 PE 3  says hi to its neighbour on the right, 0
 PE 1  says hi to its neighbour on the right, 2
```

RMA synchronziation

`get()` synchronization:

```
b = ...
call BARRIER()
call GET( a, b, 1, remote_PE )
(useful work not dependent on a)
call BARRIER()
... = a
```

`put()` synchronization:

```
b = a
call PUT( a, b, 1, remote_PE )
(useful work not dependent on a)
call BARRIER()
a = ...
```

- `put()` and `get()` are *non-blocking*: return control to the sender after initiating communication.
- `barrier()` is a *blocking* operation.

Communication and synchronization

RMA is conceived with a tightly-coupled MPP in mind, where memory is close to the network. This permits the PE wishing to `get()` or `put()` data to a remote PE to proceed without interrupting the remote PE (if the hardware permits).

This requires a synchronization operation to make sure the transmitted data is available for the operation. Synchronization is effected with a `barrier()` call. On loosely-coupled systems barriers can be very expensive.

Distributed shared memory

More recently, with the advent of fast *hardware cache-coherency* techniques, the single-address-space programming model has been revived within the **ccNUMA** architectural model. Here memory is *physically* distributed, but *logically* shared. Since it still involves remote memory access (though perhaps hidden from the user), distributed memory is still a correct lens through which to view its performance.

```
b = ...
(useful work not dependent on a)
call BARRIER()
a = b
call BARRIER()
... = a
```

MPI: a communication model for loosely-coupled systems

For a loosely-coupled or heterogeneous system, direct operations to a remote memory cannot be permitted.

The communication model is a **rendezvous**.

```
call MPI_SEND( a, ..., to_pe,   ... )
call MPI_RECV( b, ..., from_pe, ... )
```

There is now another level of latency – **software latency** – in negotiating the communication.

Evolution of MPI

MPI was originally developed in an era when “the network is the computer” was the prevailing ideology.

Many algorithms and problems are not loosely coupled, however. And at the high-end, on tightly-coupled hardware, the software overhead. of MPI became apparent.

Later extensions (MPI-2) offered an implementation of RMA that could also run on loosely-coupled systems, but could be implemented efficiently on the right architecture, with overheads comparable to native libraries, such as SHMEM.

MPI-2 also provided a layer for expressing I/O from distributed data in succinct ways. Implementations suffer from the same problems as parallel I/O in general faces.

Parallel I/O

“I/O certainly has been lagging in the last decade.” – Seymour Cray, Public Lecture (1976).

“Also, I/O needs a lot of work.” – David Kuck, Keynote Address, 15th Annual Symposium on Computer Architecture (1988).

“I/O has been the orphan of computer architecture.” – Hennessy and Patterson, Computer Architecture - A Quantitative Approach. 2nd Ed. (1996).

The MPI_IO layer for parallel I/O provides useful constructs for dealing with distributed datatypes, but performance (and even uniform and portable implementation) is not guaranteed.

The MPI API: instantiation

Basic instantiation includes starting and stopping parallel execution, and to have each process uniquely identify itself and others.

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

int main(int argc, char **argv)
{
  int rank, size;

  MPI_Init(&argc, &argv);

  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &size);

  printf("I am PE %d of %d\n", rank, size);

  MPI_Finalize();
}
```

```
mpirun -np 2 a.out
```

Each MPI call has a context called a *communicator* with a certain size, and each process has a unique *rank* within it. To address a message to another PE, both are needed.

MPI: blocking send and receive

Blocked messages are the simplest mode of communication.

```
void *buf;
int count, dest, tag;
MPI_Datatype type;
MPI_Comm comm;
MPI_Status status;

MPI_Send( buf, count, type, pe, tag, comm);
MPI_Recv( buf, count, type, pe, tag, comm, status);
```

`count` words of type `type` are sent or received from `pe` within the context `comm`. `tag` is a user-supplied identifier for the message.

`type` can be a basic type (`MPI_INTEGER`, `MPI_FLOAT`, ...) or a more complex derived datatype for a complex message.

Problems with blocked communication: deadlock

- On PE 0:

```
MPI_Send( buf, count, type, 1, tag, comm);
MPI_Recv( buf, count, type, 1, tag, comm, &status);
```

- On PE 1:

```
MPI_Send( buf, count, type, 0, tag, comm);
MPI_Recv( buf, count, type, 0, tag, comm, &status);
```

The `send()` on PE 0 cannot complete until PE 1 calls `recv()`; and vice versa. Reversing the order of `send/recv` on one of the PEs will work.

Under the covers, MPI is using internal buffers to cache messages. A blocked comm pattern may work for some values of `count`, and then fail as `count` is increased.

MPI: non-blocking send and receive

A solution is to make at least one of `send/recv` non-blocking. A non-blocking call returns control to the caller after initiating communication. The status of the message buffer is undefined until a corresponding `wait()` call is posted to check the status of the message.

- On PE 0:

```
MPI_Request request;
MPI_Isend( buf, count, type, 1, tag, comm, &request);
... // other work that does not modify or free buf
MPI_Wait( &request, &status );
if( status == MPI_OK )
   buf = ...
```

- On PE 1:

```
MPI_Irecv( buf, count, type, 0, tag, comm, &request);
... // other work that does not require the contents of buf
MPI_Wait( &request, &status );
if( status == MPI_OK )
   ... = buf ...
```

`MPI_Wait()` is a blocking call. `MPI_Test()` can be used as an alternative to check if the pending communication is complete, without blocking.

MPI-2: RMA or one-sided communication

As mentioned earlier, the overhead of two-sided communication is easily seen on high-end communication fabrics. MPI-2 provided extensions to allow RMA, but the semantics permit it to be used on loosely coupled systems as well.

MPI-2 RMA uses a new object called a **window**, which exposes a region of memory to remote calls.

The **origin** is the process that performs the call, and the **target** the process in which the memory is accessed. Thus, in a `put` operation, source=origin and destination=target; in a `get` operation, source=target and destination=origin.

MPI-2 RMA API

- `MPI_Win_Create`
- `MPI_Put`: non-blocking put
- `MPI_Get`: non-blocking get
- `MPI_Accumulate`: non-blocking atomic accumulate.
- `MPI_Win_fence`: barrier.
- `MPI_Win_start`: request to write remote data.
- `MPI_Win_complete`: block until put is complete.
- `MPI_Win_post`: request to read remote data.
- `MPI_Win_wait`: block until get is complete.
- `MPI_Win_fence`: barrier.

MPI API summary

The basic calls within MPI have been described:

- instantiation: init, finalize, comm_rank, comm_size, ...
- communication: send, recv, isend, irecv, ...
- RMA: start/put/complete, post/get/wait ...

Other aspects of the API include:

- Creation of communicators and intracommunicators (MPI-2)
- Broadcast, gather, scatter
- Reduction operations (reduce, allreduce);
- etc.

The API is vast!

A programming model for MPPs

The model we will be looking at here consists of:

- *Distributed*, as opposed to shared, memory organization.
- *Local*, as opposed to global, address space.
- *Non-uniform*, as opposed to uniform, memory access.
- *Domain decomposition*, as opposed to functional decomposition.

Parallel programming model

A *task* is a sequential (or vector) program running on one processor using local memory.

A parallel computation consists of two more tasks executing concurrently.

Execution does not depend on particular assignment of tasks to processors. (More than one task may belong to a processor.)

Tasks requiring data from each other need to synchronize and exchange data as required. (We do not consider *embarrassingly parallel* problems here, where there is no need for synchronization and data exchange.)

Partitioning

Issues to consider in partitioning the problem into tasks:

- Data layout in memory.
- Cost of communication.
- Synchronization overhead.
- Load balance.

Communication model

A *message* consists of a block of data *contiguously laid out in memory*.

Communication consists of an non-blocking `send()` and a blocking `recv()` of a message. In loosely-coupled systems, PEs need to negotiate the communication, thus both a `send()` and a `recv()` are required. In tightly-coupled systems we can have a pure `send()` (`put()`) and a pure `recv()` (`get()`). The onus is on the user to ensure synchronization.

Communication costs: *latency* and *bandwidth*.

$$t_t = t_s + Lt_w \tag{3}$$

t_s can include *software latency* (cost of negotiating a two-sided transmission, gathering non-contiguous data from memory into a single message).

Note that we have considered t_t as being independent of inter-processor distance (generally well-verified).

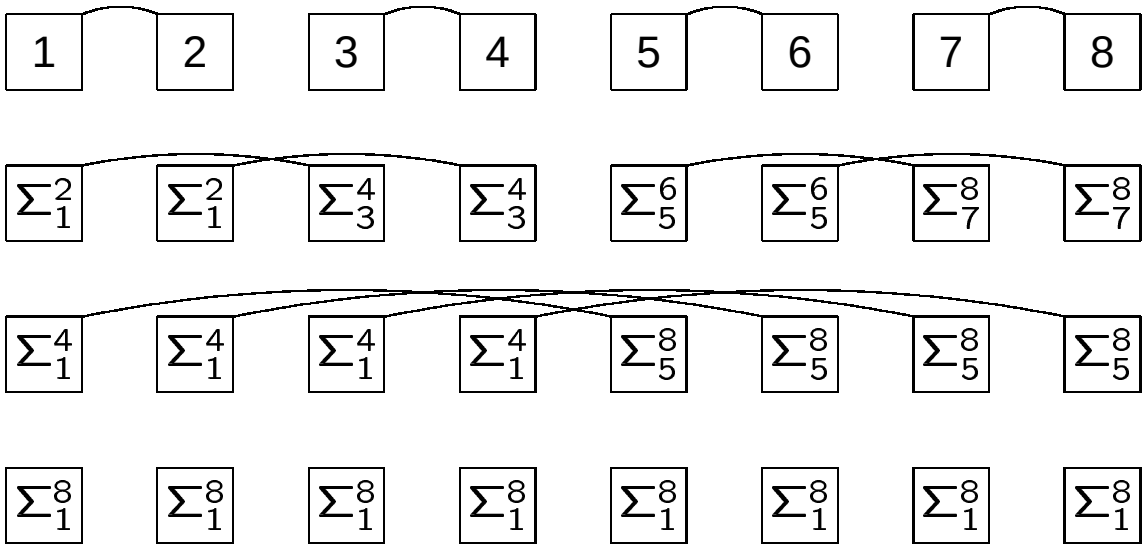
Global reduction

Sum the value of a on all PEs, every PE to have a copy of the result. Simplest algorithm: gather on PE 0, sum and broadcast.

```
program test
real :: a, sum
a = my_pe()
call BARRIER()
if( my_pe().EQ.0 )then
    sum = a
    do n = 1,num_pes()-1
       call GET( a, a, 1, n )
       sum = sum + a
    enddo
    do n = 1,num_pes()-1
       call PUT( sum, sum, 1, n )
    enddo
endif
call BARRIER()
print *, 'sum=', sum, ' on PE', my_pe()
end
```

This algorithm on p processors involves $2(p-1)$ communications and p summations, all sequential.

Here's another algorithm for doing the same thing: a binary tree. It executes in $\log_2 p$ steps, each step consisting of one communication and one summation.



There are two ways to perform each step:

```
if( mod(pe,2).EQ.0 )then !execute on even-numbered PEs
    call GET( a, sum, 1, pe+1 )
    sum = sum + a
    call PUT( sum, sum, 1, pe+1 )
endif

if( mod(pe,2).EQ.0 )then !execute on even-numbered PEs
    call GET( a, sum, 1, pe+1 )
    sum = sum + a
else                         !execute on odd-numbered PEs
    call GET( a, sum, 1, pe-1 )
    sum = sum + a
endif
```

The second is faster, even though a redundant computation is performed.

```
do level = 0,lognpes-1    !level on tree
   pedist = 2**level      !distance to sum over
   b(:) = a(:)            !initialize b for each level of the tree
   call barrier()
   if( mod(pe,pedist*2).GE.pedist )then
       call GET( b, c, size(b), pe-pedist, pe-pedist )
       a(:) = b(:) + c(:)
   else
       call GET( b, c, size(b), pe+pedist, pe+pedist )
       a(:) = b(:) + c(:)
   endif
enddo
call barrier()
```

This algorithm performs the summation and distribution in $\log_2 p$ steps.

In general it is better to avoid designating certain PEs for certain tasks. Not only is a better work distribution likely to be available, it can be dangerous code:

```
if( pe.EQ.0 )call barrier()
```

While this is not necessarily incorrect (you could have

```
if( pe.NE.0 )call barrier()
```

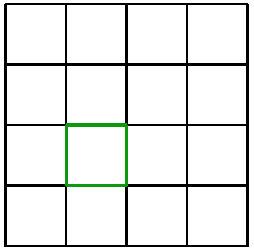
further down in the code), it is easy to go wrong.

Cost of constructing a “message”

```
real :: a(400,400), b(100,100), c(100,100,16)

b = a(101:200,101:200)
call BARRIER()
call GET( b, b, 10000, remote_PE )
call BARRIER()
a(101:200,101:200) = b

call GET( c(1,1,6), c(1,1,6), 10000, remote_PE )
```



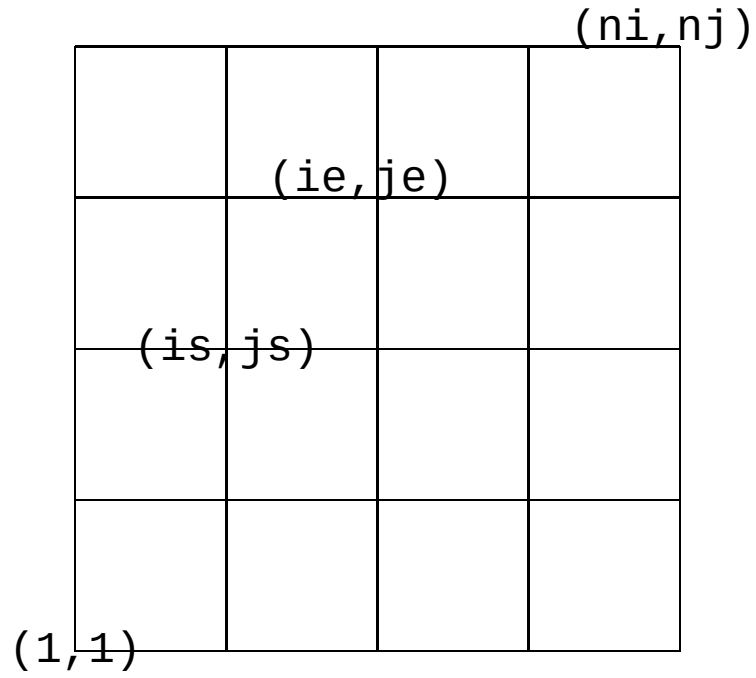
It is best to lay out data in suitable blocks.

Domain decomposition

```
do j = 1,nj
   do i = 1,ni
      a(i,j) = ...
   enddo
enddo
```

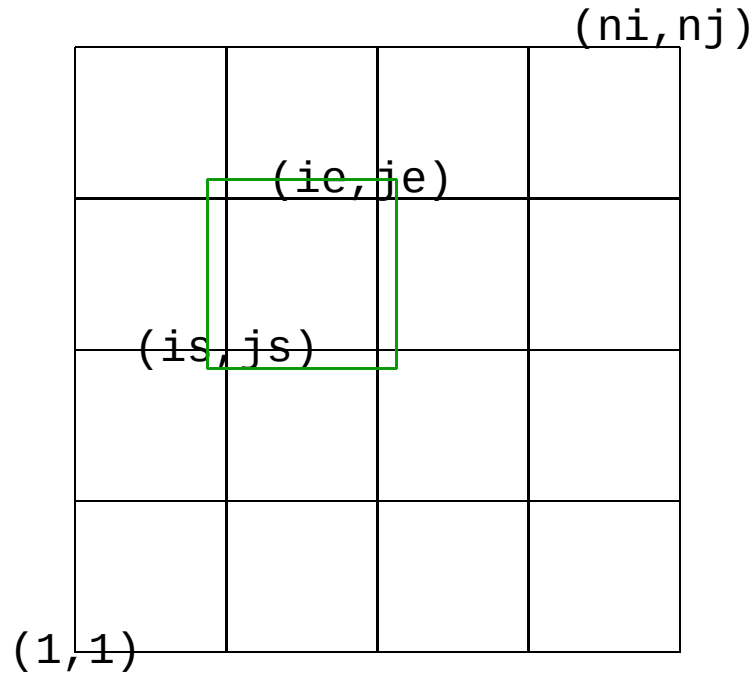
is replaced by

```
do j = js,je
   do i = is,ie
      a(i,j) = ...
   enddo
enddo
```



Computational and data domains

```
do j = js,je
   do i = is,ie
        a(i,j) = ...  + a(i-1,j+1) + ...
   enddo
enddo
```



The **computational domain** is the set of gridpoints that are computed on a domain. The **data domain** is the set of gridpoints needs to be available on-processor to carry out the computation, and includes a **halo** of a certain width.

Diffusion equation

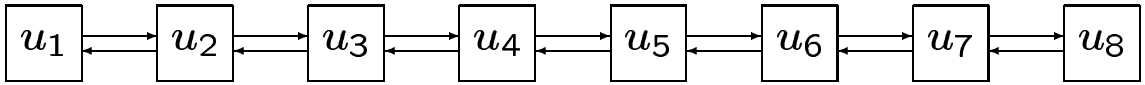
$$\frac{\partial u}{\partial t} + K\frac{\partial^2 u}{\partial x^2} = 0 \tag{4}$$

In discrete form:

$$u_i^{n+1} = u_i^n + c\frac{\Delta t}{2\Delta x}\left(u_{i+1}^n + u_{i-1}^n - 2u_i^n\right) \tag{5}$$

Assume $P < N$, and that P is an exact divisor of N.

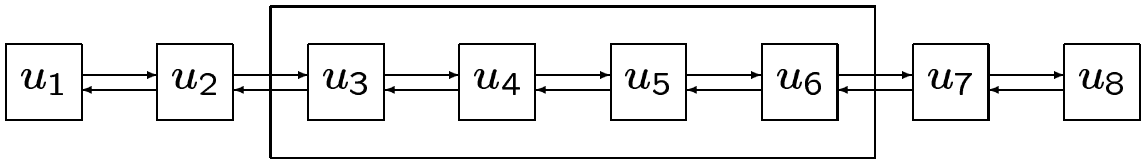
Round-robin allocation



Assign each u_i to a task. Assign each task by rotation to a different processor (*round-robin* allocation).

```
real :: u(1:N)
do i = 1,N
   if( my_pe().NE.pe(i) )cycle
!pass left,  send u(i) to task i-1, receive u(i+1) from task i+1
   call PUT( u(i), u(i), 1, pe(i-1) )
   call GET( u(i+1), u(i+1), 1, pe(i+1) )
!pass right, send u(i) to task i+1, receive u(i-1) from task i-1
   call PUT( u(i), u(i), 1, pe(i+1) )
   call GET( u(i-1), u(i-1), 1, pe(i-1) )
   call BARRIER()
   u(i) = u(i) + a*( u(i+1)+u(i-1)-2*u(i) )
enddo
```

Block allocation



We could also choose to assign N/P adjacent tasks to the same PE (*block* allocation).

```
real :: u(l-1:r+1)
!pass left,  send u(l) to task l-1, receive u(r+1) from task r+1
   call PUT( u(l), u(l), 1, pe(l-1) )
   call GET( u(r+1), u(r+1), 1, pe(r+1) )
!pass right, send u(r) to task r+1, receive u(l-1) from task l-1
   call PUT( u(r), u(r), 1, pe(r+1) )
   call GET( u(l-1), u(l-1), 1, pe(l-1) )
   call BARRIER()
   do i = l,r
      u(i) = u(i) + a*( u(i+1)+u(i-1)-2*u(i) )
   enddo
```

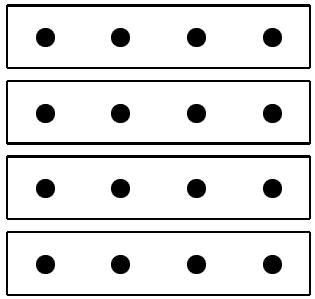
Communication is vastly reduced.

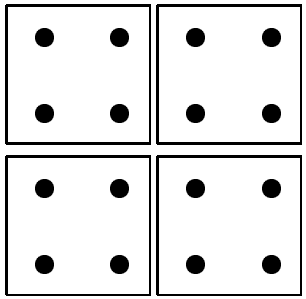
Overlapping communication and computation.

```
!pass left,  send u(l) to task l-1, receive u(r+1) from task r
   call PUT( u(l), u(l), 1, pe(l-1) )
   call GET( u(r+1), u(r+1), 1, pe(r+1) )
!pass right, send u(r) to task r+1, receive u(l-1) from task l
   call PUT( u(r), u(r), 1, pe(r+1) )
   call GET( u(l-1), u(l-1), 1, pe(l-1) )
   do i = l+1,r-1
      u(i) = u(i) + a*( u(i+1)+u(i-1)-2*u(i) )
   enddo
   call BARRIER()
   u(l) = u(l) + a*( u(l+1)+u(l-1)-2*u(l) )
   u(r) = u(r) + a*( u(r+1)+u(r-1)-2*u(r) )
```

The effective communication cost must be measured from the end of the do loop.

Domain decomposition in 2D





There are different ways to partition $N \times N$ points onto P processors.

1D or 2D decomposition?

Assume a problem size $N \times N \times K$, with a halo width of 1.

Cost per timestep with no decomposition:

$$t_0 = N^2 K t_c \tag{6}$$

Cost per timestep with 1D decomposition ($N \times \frac{N}{P} \times K$):

$$t_{1D} = \frac{N^2 K}{P} t_c + 2t_s + 4NKt_w \tag{7}$$

Cost per timestep with 2D decomposition ($\frac{N}{\sqrt{P}} \times \frac{N}{\sqrt{P}} \times K$):

$$t_{2D} = \frac{N^2 K}{P} t_c + 4t_s + \frac{8NK}{\sqrt{P}} t_w \tag{8}$$

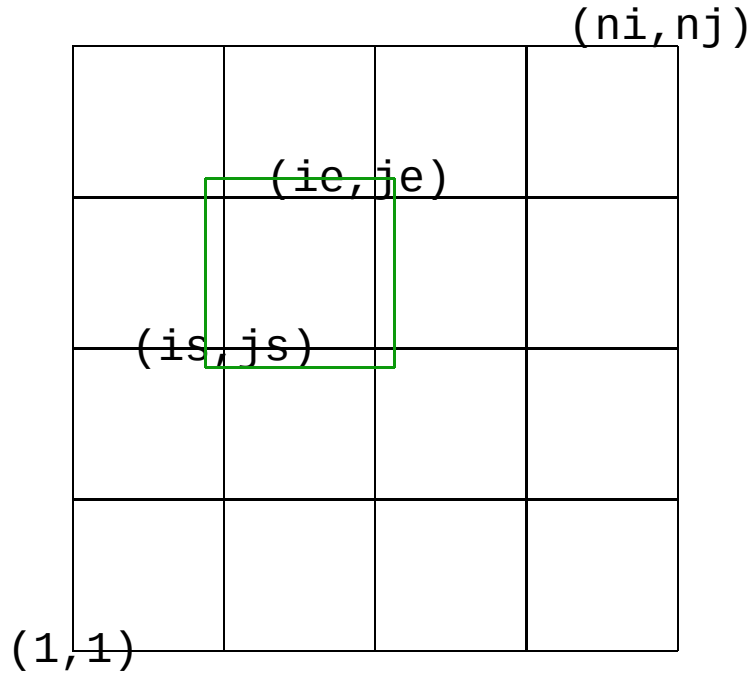
In the limit of asymptotic N, P (maintaining constant N^2/P), $t_{2D} \ll t_{1D}$.

The case for 2D decomposition is the argument that the communication to computation ratio is like a surface to volume ratio, which goes as $1/r$.

The flaw in this argument: outside the textbooks, only giant government sites (aka “spook sites”) are in the limit of asymptotic N and P!

For modest levels of parallelism, and realistic problem sizes, the additional cost incurred in software complexity may be hard to justify.

A second flaw, also serious, is that there is higher “software latency” associated with 2D halo exchanges, to gather non-contiguous data from memory into a single message.



Data layout in memory is a crucial issue (also for effective utilization of cache). The best method is to lay out data in memory to facilitate message-passing.

Elliptic equations

Consider a 2D Poisson equation:

$$\nabla^2 u(x, y) = f(x, y) \tag{9}$$

The solution at any point to a boundary value problem in general depends on all other points, therefore incurring a high communication cost on distributed systems.

Jacobi iteration

$$u_{ij}^{(n+1)} = \frac{1}{4}\left(u_{i-1,j}^{(n)} + u_{i+1,j}^{(n)} + u_{i,j-1}^{(n)} + u_{i,j+1}^{(n)} - \Delta x^2 f_{ij}\right) \qquad (10)$$

Iterate until $|u_{ij}^{(n+1)} - u_{ij}^{(n)}| < \epsilon$.

This method converges under known conditions, but convergence is slow.

Gauss-Seidel iteration

Update values on RHS as they become available:

$$u_{ij}^{(n+1)} = \frac{1}{4}\left(u_{i-1,j}^{(n+1)} + u_{i+1,j}^{(n+1)} + u_{i,j-1}^{(n)} + u_{i,j+1}^{(n)} - \Delta x^2 f_{ij}\right) \quad (11)$$

Iterate until $|u_{ij}^{(n+1)} - u_{ij}^{(n)}| < \epsilon$.

This method converges faster, but contains data dependencies that inhibit parallelization.

```
!receive halo from south and west
   call recv(...)
   call recv(...)
!do computation
   do j = js,je
      do i = is,ie
         u(i,j) = u(i-1,j)+u(i,j-1)+u(i+1,j)+u(i,j+1)-a*f(i,j)
      enddo
   enddo
!pass halo to north and west
   call send(...)
   call send(...)
```

4	5	6	7
3	4	5	6
2	3	4	5
1	2	3	4

Red-Black Gauss-Seidel method

```
do parity = red,black
   if( parity.NE.my_parity(pe) )cycle
!receive halo from south and west
   call recv(...)
   call recv(...)
!do red domains on odd passes, black domains on even passes
   do j = js,je
      do i = is,ie
         u(i,j) = u(i-1,j)+u(i,j-1)+u(i+1,j)+u(i,j+1)-a*f(i,j)
      enddo
   enddo
!pass halo to north and west
   call send(...)
   call send(...)
enddo
```

2	1	2	1
1	2	1	2
2	1	2	1
1	2	1	2

More sophisticated methods of hastening the convergence are generally hard to parallelize. The conjugate gradient method accelerates this by computing at each step the optimal vector in phase space along which to converge. Unfortunately, computing the direction involves a global reduction.

In summary, if there are alternatives to solving an elliptic equation over distributed data, they should be given very serious consideration.

Conclusions

Considerations in implementing parallel algorithms:

- Uniformity of workload. Designated PEs for some operations can be useful in certain circumstances, but in general a better division of work can probably be found.

- Design data layout in memory to facilitate message passing and cache behaviour. Sometimes redundantly computing data on all PEs is preferable to communication.

- Be wary of asymptotic scalability theory. The cost of achieving maximal parallelism often includes a considerable complexity burden, with dubious returns at modest levels of parallelism.

Current research: uniform memory models

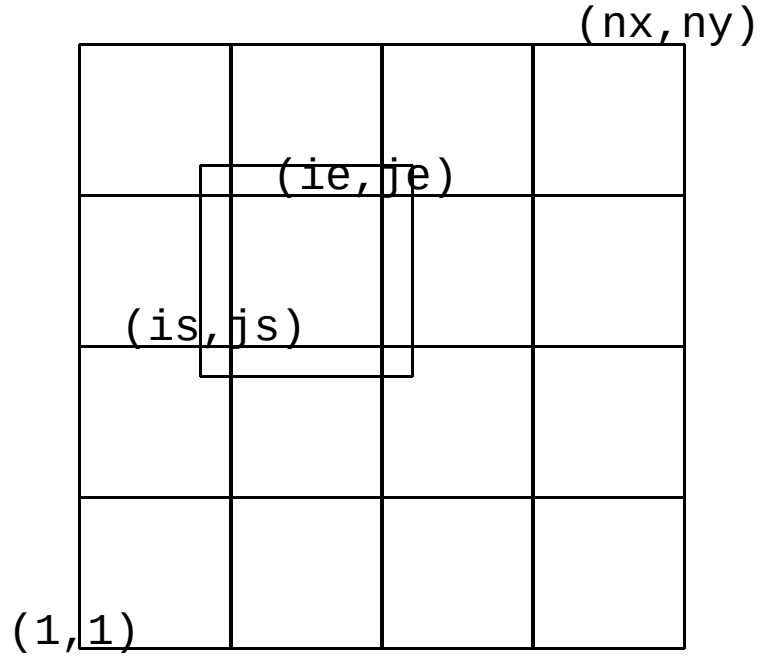
Shared memory signal parallel and critical regions, private and shared variables. Canonical architecture: UMA, limited scalability.

Distributed memory domain decomposition, local caches of remote data (“halos”), copy data to/from remote memory (“message passing”). Canonical architecture: NUMA, scalable at cost of code complexity.

Distributed shared memory or ccNUMA message-passing, shared memory or remote memory access (RMA) semantics. Processor-to-memory distance varies across address space, must be taken into account in coding for performance. Canonical architecture: cluster of SMPs. Scalable at large cost in code complexity.

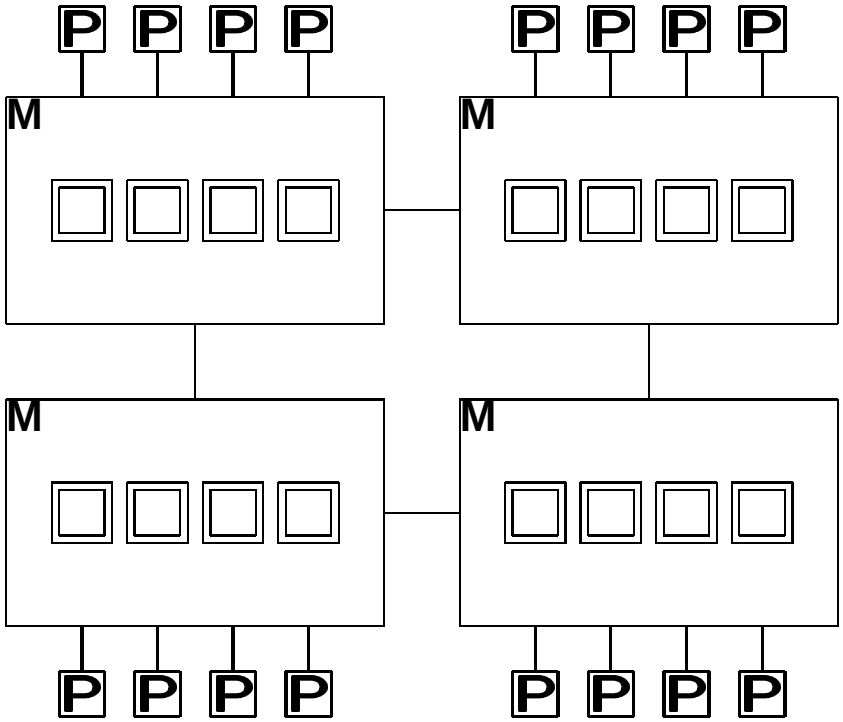
Uniform memory models seek hide these differences from the user.

A 2D example



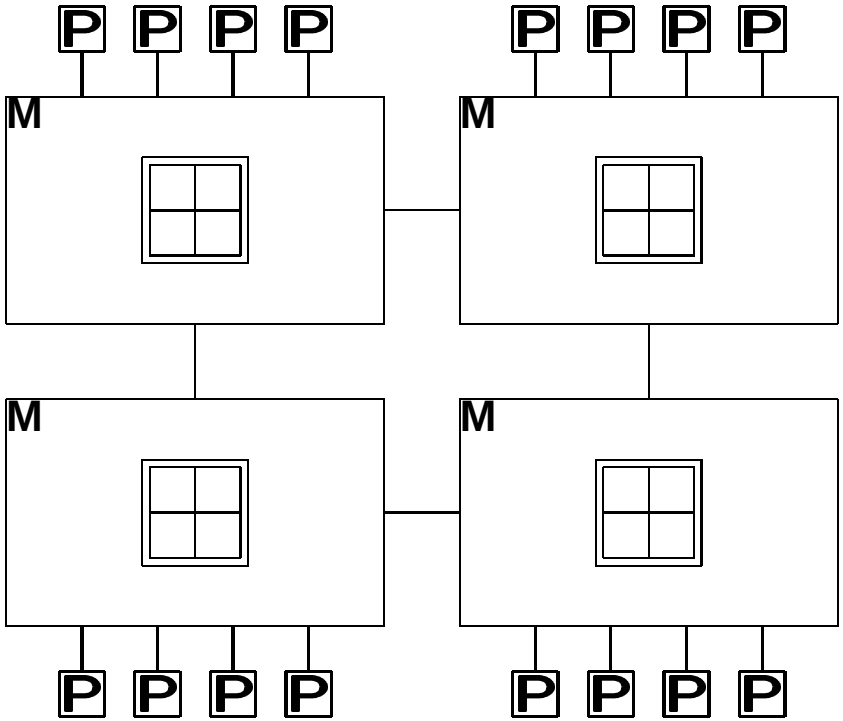
Consider a platform consisting of 16 PEs consisting of 4 mNodes of 4 PEs each. We also assume that the the entire 16-PE platform is a DSM or cc-NUMA aNode. We can then illustrate 3 ways to implement a `DistributedArray`. One PET is scheduled on each PE.

Distributed memory



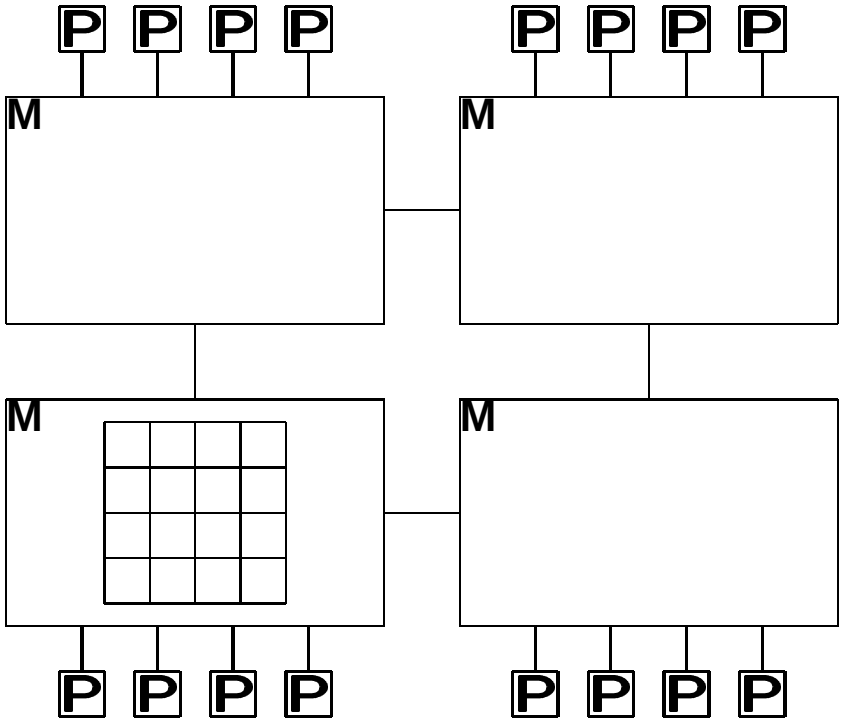
- each domain allocated as a separate array with halo, even within the same mNode.
- Performance issues: the message-passing call stack underlying MPI or another library may actually serialize when applied within an mNode.

Hybrid memory model



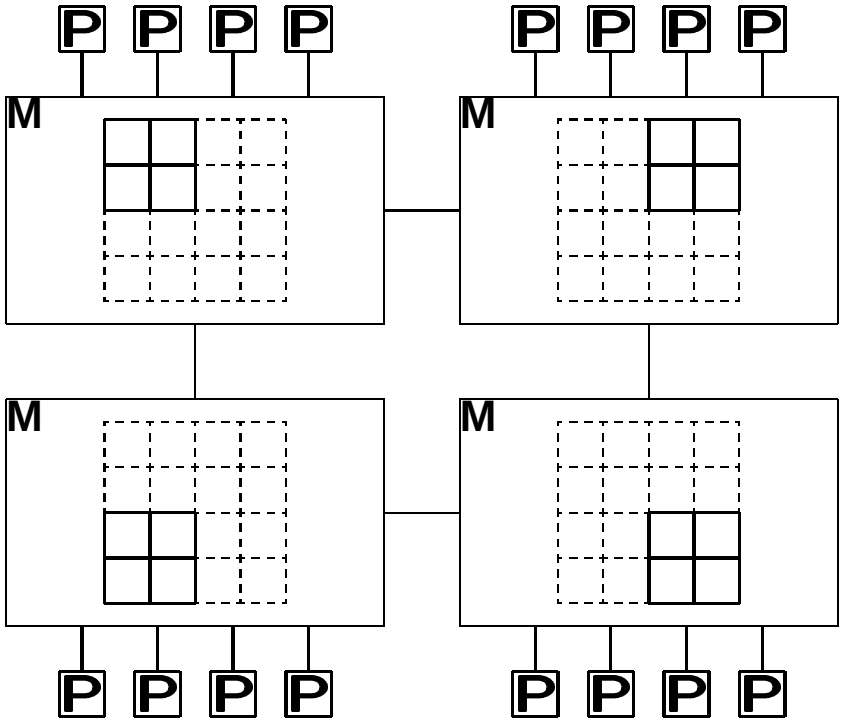
- shared across an mNode, distributed among mNodes.
- fewer and larger messages than distributed memory, may be less latency-bound.

Pure shared memory



Array is local to one mNode: other mNodes requires remote loads and stores. OK on platforms that are well-balanced in bandwidth and latency for local and remote accesses. ccNUMA ensures cache coherence across the aNode.

Intelligent memory allocation on DSM



Better memory locality: allocate each block of 4 domains on a separate page, and assign pages to different mNodes, based on processor-memory affinity.

New programming models

- UMM and the ESMF virtual machine.
- Co-Array Fortran and Unified Parallel C.
- The ARMCI library: intelligent RMA primitives.

Review

- Concurrency and its limitations: Amdahl's law, load imbalance.
- Memory models: shared, distributed, distributed shared.
- Communication primitives: RMA, blocking vs. non-blocking.
- Synchronization: global vs. point-to-point.
- Pitfalls: deadlocks and hangs, race conditions, implicit serialization.
- Algorithms: reducing remote data dependencies.
- Current research: high-level programming models that hide the underlying memory model and configure themselves to the architecture.

References

- `http://www-unix.mcs.anl.gov/mpi/`, a good starting point for standards, manuals, examples, etc.
- Designing and Building Parallel Programs: by Ian Foster.
- Using MPI, 2nd Edition, by William Gropp, Ewing Lusk, and Anthony Skjellum.
- MPI: The Complete Reference, by Marc Snir, Steve Otto, Steven Huss-Lederman, David Walker, and Jack Dongarra, The MIT Press.
- MPI: The Complete Reference - 2nd Edition: Volume 2 - The MPI-2 Extensions , by William Gropp, Steven Huss-Lederman, Andrew Lumsdaine, Ewing Lusk, Bill Nitzberg, William Saphir, and Marc Snir, The MIT Press.
- Many online tutorials: Cornell Theory Center, Minnesota Supercomputing Institute, Argonne, ...

More references: There's more to life than MPI

- ARMCI: `http://www.emsl.pnl.gov/docs/parsoft/armci/`
- Co-Array Fortran: `http://www.co-array.org/`
- `http://www.pmodels.org`
- In search of clusters, Pfister. Idiosyncratic and interesting book.