



MPI Communication Optimization

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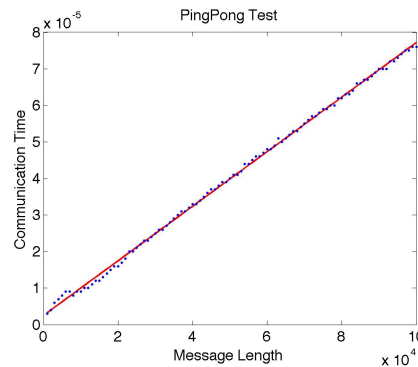


Parallel Code Optimization:

- **Algorithm**
 - Need to have efficient algorithms
(Also optimize the serial performance)
- **Communication**
 - Need to minimize communication time
- **Load balance**
 - Need to have equal work load



Communication overhead



$T_{\text{Comm}}(n) = t_s + n t_w$, $t_s = 2.5 \mu\text{s}$, $\beta = 10.7 \text{ GB/s}$, ($t_w = 1/\beta$)
 $\Rightarrow T_{\text{Comm}}(1) = 2500 \text{ ns} + 0.7 \text{ ns}$, latency \gg transfer time
 Compare: 37 GFlop/s \Rightarrow 92500 operations/latency

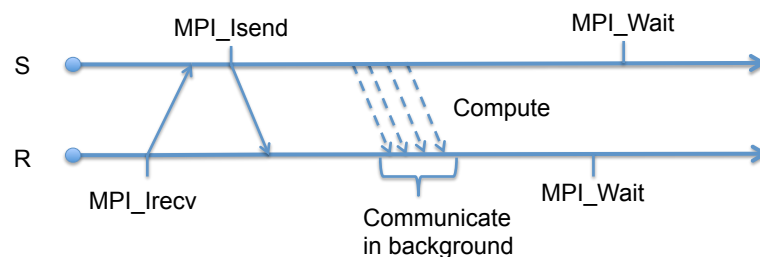
\Rightarrow **Need to minimize and/or hide the latency**
 (and keep the total communication volume down) !



Communication optimization:

1. Non-blocking/buffered communication

Overlap computations and communication



\Rightarrow Avoid synchronization and hide latency
 (and data transfer time).



2. Derived datatypes

Send non-contiguous data in one call

- `MPI_Type_vector(...)` -- Regular distribution
- `MPI_Type_indexed(...)` -- Irregular distribution
- `MPI_Type_struct(...)` -- Different datatypes

=> Reduce number of communication calls (latency)



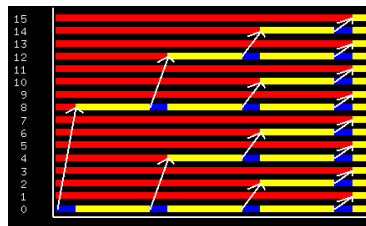
```
MPI_Type_vector(4,3,5,MPI_DOUBLE,&strided);
MPI_Type_commit(&strided);
MPI_Send(A,1,strided,to,tag,comm);
```



3. Collective communication calls

Uses efficient algorithms to communicate with many processors in one call:

- `MPI_Bcast(...)`
- `MPI_Scatter(...)`
- `MPI_Gather(...)`
- `MPI_Allgather(...)`
- `MPI_Alltoall(...)`
- `MPI_Reduce(...)`



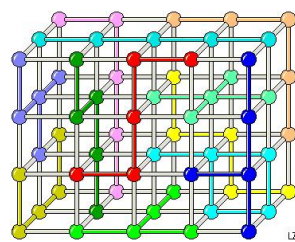
=> Parallelize the communication (reduce latency)



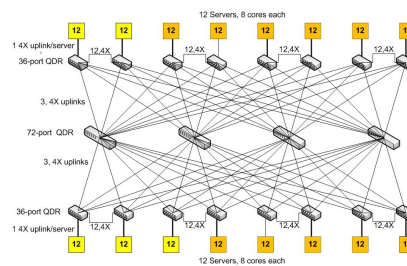
4. Virtual topologies

Communicator with structure. Makes a mapping to physical topology optimizing (localizing) the communication. Helps in algorithm construction reflecting the communication pattern.

- `MPI_Cart_create(...)`
- `MPI_Graph_create(...)`



Virtual topology



Physical topology



5. Persistent communication

Initiate communication once and activate repeatedly
 ⇒ Reduces initialization overhead (latency), useful when we have many calls and complicated patterns.

```

MPI_Send_init(...);
MPI_Recv_init(...);
etc (many calls)

for (i=0; i<n; i++)
{
    MPI_Startall(...);
    Compute
    MPI_Waitall(...)
    Use data
}
  
```



6. Message probing

Reduce synchronization OH by not ordering messages, use first-come first-serve.
Avoid sending length in a separate call.

```
while (i < nproc)
{
    MPI_Probe(MPI_ANY_SOURCE, ... , &stat);
    MPI_Get_count(&stat, type, &len);
    MPI_Recv(data, len, type, stat.MPI_SOURCE, ... );
    i++;
}
```



Example: Numerical PDE Solver

Consider the Hyperbolic PDE:

$$u_t + u_x + u_y = F(t, x, y) \quad 0 \leq x \leq 1, 0 \leq y \leq 1$$

$$\begin{cases} u(t, 0, y) = h_1(t, y) & 0 \leq y \leq 1 \\ u(t, x, 0) = h_2(t, x) & 0 \leq x \leq 1 \end{cases} \quad \text{Boundary Conditions}$$

$$u(0, x, y) = g(x, y) \quad \text{Initial Conditions}$$

Solve with explicit finite difference method,
for example Leap-Frog



Core of the computations:

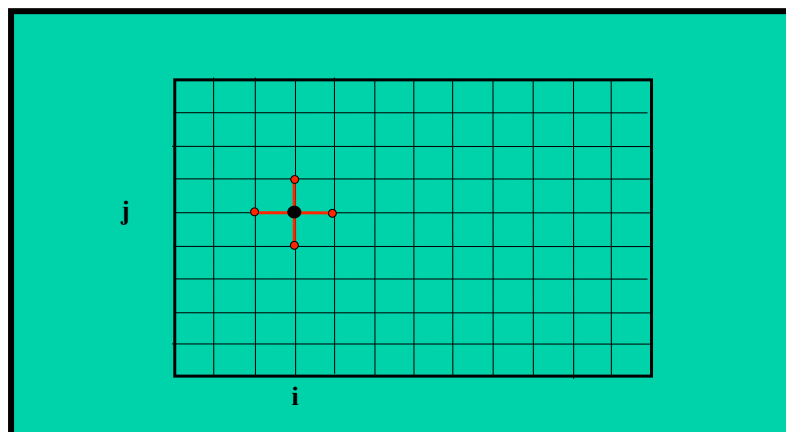
```

do k=2,Nt
  t=k*dt; Uold=U; U=Unew;
  do j=1,Ny-1
    do i=1,Nx-1
      x=i/Nx; y=j/Ny
      Unew(i,j)=Uold(i,j)+2*dt*(F(t,x,y)-
        (U(i+1,j)-u(i-1,j))/(2*dx)-
        (U(i,j+1)-U(i,j-1))/(2*dy))
    end do
  end do
end do

```

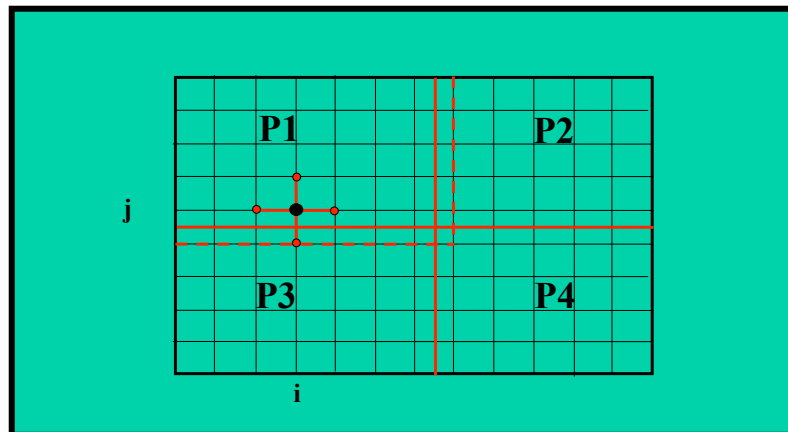


Computational stencil:






Parallelization, partition grid:



Message Passing Version:

```
do k=2,Nt
  t=k*dt; Uold=U; U=Unew;
  update partition boundary - communicate
  do j=j1,j2
    do i=i1,i2
      x=i/Nx; y=j/Ny
      Unew(i,j)=Uold(i,j)+2*dt*(F(t,x,y)-
        (U(i+1,j)-U(i-1,j))/(2*dx)-
        (U(i,j+1)-U(i,j-1))/(2*dy))
    end do
  end do
end do
```




Compute 'left, right, up, down' node

```
! Send and receive left-right
if ('not at left boundary')
  call mpi_send(left, ... )
end if

if ('not at right boundary')
  call mpi_recv(right, ... )
  call mpi_send(right, ... )
end if

if ('not at left boundary')
  call mpi_recv(left, ... )
end if

! Send and receive up-down
...
```



Note:

- **Structured domain decomposition**
Use cartesian processor topology
(simplifies communication)
- **The communication is repeated**
Use persistent communication objects
(mpi_send_init, mpi_startall, mpi_waitall)
- **Inner domain independent of neighbors**
Overlap communication with computations
(asynchronous communication)



```

! Create virtual topology
mpi_cart_create( ... )
mpi_cart_shift(dim1,left,right, ... )
...

! Initiate communication
mpi_send_init(left, ... )
mpi_recv_init(left, ... )
mpi_send_init(right, ... )
...

! Timestepping
do k=2,Nt
  mpi_startall( ... )
  update inner points
  mpi_waitall( ... )
  update partition boundary
end do

```



PDE Solver (lab MPI):

Program files:

- [wave.c](#) -- Main program
- [initcomm.c](#) -- Persistent communication
- [diffop.c](#) -- Computational core

(+ some additional files)

Task: Study implementation details and measure the parallel performance for different problem sizes. Compare performance running within one server and using several servers (out of node communication).



Real example: Combustion simulation

HPC User: Michael Liberman, Physics dept UU

Problem:

Navier-Stokes 2D, chemical reaction terms
Modeling of deflagration-to-detonation transition
(i.e. knocking which must be avoided in engines)
=> Efficient burning and good fuel economy

Needs:

Requires a very accurate numerical resolution
of the flame front => Efficiently parallelized code
for a large number of processors



Results:

Original code parallelized with MPI, standard
MPI_Send/MPI_Recv, and 1D partitioning

- Changed standard calls to non-blocking persistent communication objects
- Extended to 2D partitioning, virtual topology
- Extended to multi-block partitioning, (allows for AMR and two-level parallelization)
- Efficient load balancing for multi-block grids

=> Very high parallel efficiency
(Super linear on SunFire 15K)

