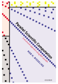
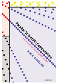
Message Passing Interface (MPI-1)

(PSC Appendix C, §C.1–C.2.4)



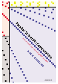
History of MPI

- 1994: Message Passing Interface (MPI) became available as a standard interface for parallel programming in C and Fortran 77.
- Designed by a committee called the MPI Forum consisting of computer vendors, users, computer scientists.
- Based on sending and receiving messages by a pair of processors. One processor sends; the other receives. Both are active in the communication.
- Underlying model: communicating sequential processes (CSP) proposed by Tony Hoare in 1978.
- MPI itself is not a model. BSP is a model.
- MPI is an interface for a communication library, like BSPlib.



Recent history of MPI

- 1997: MPI-2 standard defined. Added functionality:
  - one-sided communications (put, get, sum)
  - dynamic process management
  - parallel input/output
  - languages C++ and Fortran 90
- 2003: first full implementations of MPI-2 arrive, namely MPICH (Argonne National Labs) and LAM/MPI (Indiana University).
- 2004–: Open MPI. Open-source project, merges 3 MPI implementations: LAM/MPI, FT-MPI (University of Tennessee), LA-MPI (Los Alamos National Laboratory).
- 2012 MPI-3. Major update. More one-sided communications, nonblocking collective communications, sparse collective communications.

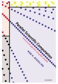


Why use MPI?

- It is available on almost every parallel computer, often in an optimised version provided by the vendor. Thus MPI is the most portable communication library.
- Many libraries are available written in MPI, such as the numerical linear algebra library ScaLAPACK.
- You can program in many different ways using MPI, since it is highly flexible.

Why not?

- It is huge: the full current MPI-3 standard has about 450 primitives. The user has to make many choices.
- It is not so easy to learn. Usually one starts with a small subset of MPI. Full knowledge of the standard is hard to attain.
- The one-sided communications of MPI-2 and MPI-3 are rather complicated. If you like one-sided communications you may want to consider BSPlib as an alternative.

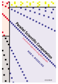


Ping pong benchmark

- The cost of communicating a message of length n is

  $$T(n) = t_{\mathrm{startup}} + n t_{\mathrm{word}}.$$

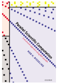
  Here, t_{startup} is a fixed startup cost and t_{word} is the additional cost per data word communicated.
- Communication of a message (in its blocking form) synchronises the sender and receiver. This is pairwise synchronisation, not global.
- Parameters t_{startup} and t_{word} are usually measured by sending a message from one processor to another and back: ping pong.
- The message length is varied in the ping pong benchmark.
- There is only one ping pong ball on the table.



Send and receive primitives

```
if (s==2)
  MPI_Send(x,5,MPI_DOUBLE,3,0,MPI_COMM_WORLD);
if (s==3)
  MPI_Recv(y,5,MPI_DOUBLE,2,0,MPI_COMM_WORLD,
           &status);
```

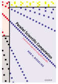
- Processor $P(2)$ sends 5 doubles to $P(3)$.
- $P(2)$ reads the data from its array `x`. After transmission, $P(3)$ writes these data into its array `y`.
- The integer ‘0’ is a tag for distinguishing between different messages from the same source processor to the same destination processor.
- `MPI_Send` and `MPI_Recv` are of fundamental importance in MPI.



Communicator: the whole processor world

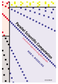
```
if (s==2)
  MPI_Send(x,5,MPI_DOUBLE,3,0,MPI_COMM_WORLD);
if (s==3)
  MPI_Recv(y,5,MPI_DOUBLE,2,0,MPI_COMM_WORLD,
           &status);
```

- A communicator is a subset of processors forming a communication environment with its own processor numbering.
- `MPI_COMM_WORLD` is the communicator consisting of all the processors.



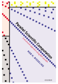
Send/Receive considered harmful

- 1968: Edsger Dijkstra, guru of structured programming, considered the Go To statement harmful in sequential programming.
- Go To was widely used in Fortran programming in those days. It caused spaghetti code: if you pull something here, something unexpected moves there.
- No one dares to use Go To statements any more.
- Send/Receive in parallel programming has the same dangers, and even more, since several diners eat from the same plate.
- Pull here, pull there, nothing moves: deadlock.
- Deadlock may occur if $P(0)$ wants to send a message to $P(1)$, and $P(1)$ to $P(0)$, and both processors want to send before they receive.



Inner product program `mpiinprod`

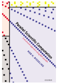
```
int main(int argc, char **argv){

    int p, s, n;

    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&p);
    MPI_Comm_rank(MPI_COMM_WORLD,&s);

    if (s==0){
        printf("Please enter n:\n");
        scanf("%d",&n);
        if(n<0)
            MPI_Abort(MPI_COMM_WORLD,-1);
    }
    MPI_Bcast(&n,1,MPI_INT,0,MPI_COMM_WORLD);
    ...
```



Collective communication: broadcast

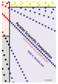
```
MPI_Bcast(&n, 1,    MPI_INT, 0, MPI_COMM_WORLD);

MPI_Bcast(buf,count,datatype,root,communicator);
```

- Broadcast `count` data items of a certain `datatype` from processor `root` to all others in the `communicator`, reading from location `buf` and also writing it there.
- All processors of the communicator participate.
- Extensive set of collective communications available in MPI. Using these reduces the size of program texts.



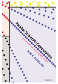
Inner product program mpiinprod (cont'd)

```
...
nl= nloc(p,s,n);
x= vecallocd(nl);
for (i=0; i<nl; i++){
    iglob= i*p+s;
    x[i]= iglob+1;
}
/* global sync for timing */
MPI_Barrier(MPI_COMM_WORLD);
time0=MPI_Wtime(); /* wall clock time */

alpha= mpiip(p,s,n,x,x);
MPI_Barrier(MPI_COMM_WORLD);
time1=MPI_Wtime();
...
MPI_Finalize();
exit(0);
```



Inner product function `mpiip`

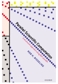
```
double mpiip(int p, int s, int n,
             double *x, double *y){

    double inprod, alpha;
    int i;

    inprod= 0.0;
    for (i=0; i<nloc(p,s,n); i++)
        inprod += x[i]*y[i];
    MPI_Allreduce(&inprod,&alpha,1,MPI_DOUBLE,
                  MPI_SUM,MPI_COMM_WORLD);

    return alpha;
}
```



Collective communication: reduce

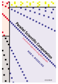
```
MPI_Allreduce(&inprod, &alpha,  1,  MPI_DOUBLE,
              MPI_SUM,   MPI_COMM_WORLD);

MPI_Allreduce(sendbuf, recvbuf, count, datatype,
              operation, communicator);
```

- The reduction operation by `MPI_Allreduce` sums the double-precision local inner products `inprod`, leaving the result `alpha` on all processors.
- One can also do this for an array instead of a scalar, by changing the parameter 1 to the array size `count`, or perform other operations, such as taking the maximum, by changing `MPI_SUM` to `MPI_MAX`.



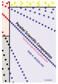
Benchmark: which primitive to measure?

- Benchmarking all communication primitives in MPI is a lot of work. This does not appeal to us.
- A typical MPI user would look first if there is a suitable collective-communication primitive that would do the job.
- This would lead to shorter program texts, and is good practice from the BSP point of view as well.
- Therefore, we choose a collective communication as the operation to be benchmarked.
- The BSP superstep, where every processor can communicate in principle with all others, is reflected best by the all-to-all primitives from MPI.
- Using an all-to-all primitive gives the MPI system the best opportunities for optimisation, similar to supersteps in BSPlib programs.



Measure time of `MPI_Alltoallv`

```
MPI_Barrier(MPI_COMM_WORLD);
time0= MPI_Wtime();

for (iter=0; iter<NITERS; iter++){
    MPI_Alltoallv(src,Nsend,Offset_send,MPI_DOUBLE,
                  dest,Nrecv,Offset_recv,MPI_DOUBLE,
                  MPI_COMM_WORLD);
    MPI_Barrier(MPI_COMM_WORLD);
}

time1= MPI_Wtime();
time= time1-time0;
```



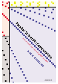
Syntax of MPI_Alltoallv

```
MPI_Alltoallv(src,  Nsend, Offset_send, datatype_send,
                    dest, Nrecv, Offset_recv, datatype_recv,
                    communicator);
```

- So-called vector variant allows a varying number of data to be sent (or even no data).
- The sender reads `Nsend[t]` data from array `src` starting at `Offset_send[t]` for each processor $P(t)$, $0 \leq t < p$, and sends these data.
- The receiver receives data from all processors, and stores them in array `dest`, with `Nrecv[t]` data arriving from processor $P(t)$ at offset `Offset_recv[t]`.
- All offsets are measured in units of the data type involved, e.g. `MPI_DOUBLE`. (Not in raw bytes, like in BSPlib.)

Initialise *h*-relation

```
for (i=0; i<h; i++)
    src[i]= (double)i;
if (p==1){
    Nsend[0]= Nrecv[0]= h;
} else {
    for (s1=0; s1<p; s1++)
        Nsend[s1]= h/(p-1);
    for (i=0; i < h%(p-1); i++)
        Nsend[(s+1+i)%p]++;   /* one extra */
    Nsend[s]= 0; /* no talking to yourself */

    for (s1=0; s1<p; s1++)
        Nrecv[s1]= h/(p-1);
    for (i=0; i < h%(p-1); i++)
        Nrecv[(s-1-i+p)%p]++;
    Nrecv[s]= 0;
}
```



Determine offsets

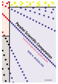
```
Offset_send[0]= 0;
Offset_recv[0]= 0;

for(s1=1; s1<p; s1++){
  Offset_send[s1]=Offset_send[s1-1]+Nsend[s1-1];
  Offset_recv[s1]=Offset_recv[s1-1]+Nrecv[s1-1];
}
```

Messages are stored in order of destination processor. Thus, offsets can be computed by a prefix operation.

LU decomposition function `mpilu`

```
void mpilu(int M, int N, int s, int t, int n,
           int *pi, double **a){

 MPI_Comm row_comm_s, col_comm_t;

 /* Create a new communicator for
    my processor row and column */
 MPI_Comm_split(MPI_COMM_WORLD,s,t,&row_comm_s);
 MPI_Comm_split(MPI_COMM_WORLD,t,s,&col_comm_t);
 ...
```

- 2D numbering directly available in MPI: create a communicator for every processor row and column by splitting the world communicator.

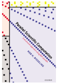


Splitting a communicator

```
MPI_Comm_split(MPI_COMM_WORLD,s,t,&row_comm_s);
```

- Processors that call `MPI_Comm_split` with the same value of s end up in the same communicator, which we call `row_comm_s`.
- Thus, we obtain M communicators, each corresponding to a processor row $P(s, *)$.
- Every processor obtains a processor number within its communicator. This number is by increasing value of the third parameter of the primitive, i.e., `t`.
- Broadcast of pivot value within processor column, i.e., within communicator `col_comm_t` now becomes:

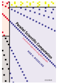
```
if (k%N==t)
  MPI_Bcast(&pivot,1,MPI_DOUBLE,smax,col_comm_t);
```



Swapping the permutation in $P(*,0)$

```
/* piece of code for k%M != r%M */
if (k%M==s){
    MPI_Send(&pi[k/M],1,MPI_INT,r%M,0,MPI_COMM_WORLD);
    MPI_Recv(&pi[k/M],1,MPI_INT,r%M,0,MPI_COMM_WORLD,
             &status);
}
if (r%M==s){
    MPI_Recv(&tmp,1,MPI_INT,k%M,0,MPI_COMM_WORLD,
             &status);
    MPI_Send(&pi[r/M],1,MPI_INT,k%M,0, MPI_COMM_WORLD);
    pi[r/M]= tmp;
}
```

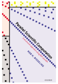
- Don't change the order of the sends and receives! (Punishment: deadlock on certain machines.)



Sender info must be initialised for FFT

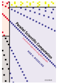
```
offset= 0;
j0= s%c0;        j2= s/c0;
for(j=0; j<npackets; j++){
    jglob= j2*c0*np + j*c0 + j0;
    destproc=  (jglob/(c1*np))*c1 + jglob%c1;
    Nsend[destproc]= 2*size;
    Offset_send[destproc]= offset;
    for(r=0; r<size; r++){
        tmp[offset + 2*r]=   x[2*(j+r*ratio)];
        tmp[offset + 2*r+1]= x[2*(j+r*ratio)+1];
    }
    offset += 2*size;
} ...
```

- `mpifft` is identical to `bspfft`, except for redistribution. Packets are the same.



Receiver info must also be initialised

```
...
/* Initialise receiver info */
offset= 0;
j0= s%c1;        j2= s/c1;
for(r=0; r<npackets; r++){
    j= r*size;
    jglob= j2*c1*np + j*c1 + j0;
    srcproc=  (jglob/(c0*np))*c0 + jglob%c0;
    Nrecv[srcproc]= 2*size;
    Offset_recv[srcproc]= offset;
    offset += 2*size;
}
MPI_Barrier(MPI_COMM_WORLD); /* for safety */
MPI_Alltoallv(tmp,Nsend,Offset_send,MPI_DOUBLE,
              x,  Nrecv,Offset_recv,MPI_DOUBLE,
              MPI_COMM_WORLD);
```



Summary

- The Message Passing Interface (MPI) is a highly portable communication library supported by most vendors of parallel computers.
- In MPI, you should try to use collective communications as much as possible. They reduce the size of program texts, and they also create supersteps, thus structuring the program in BSP style.
- MPI rule:

  collective communications may synchronise the processors, but you cannot rely on this.

  So feel free to add global synchronisations where needed.