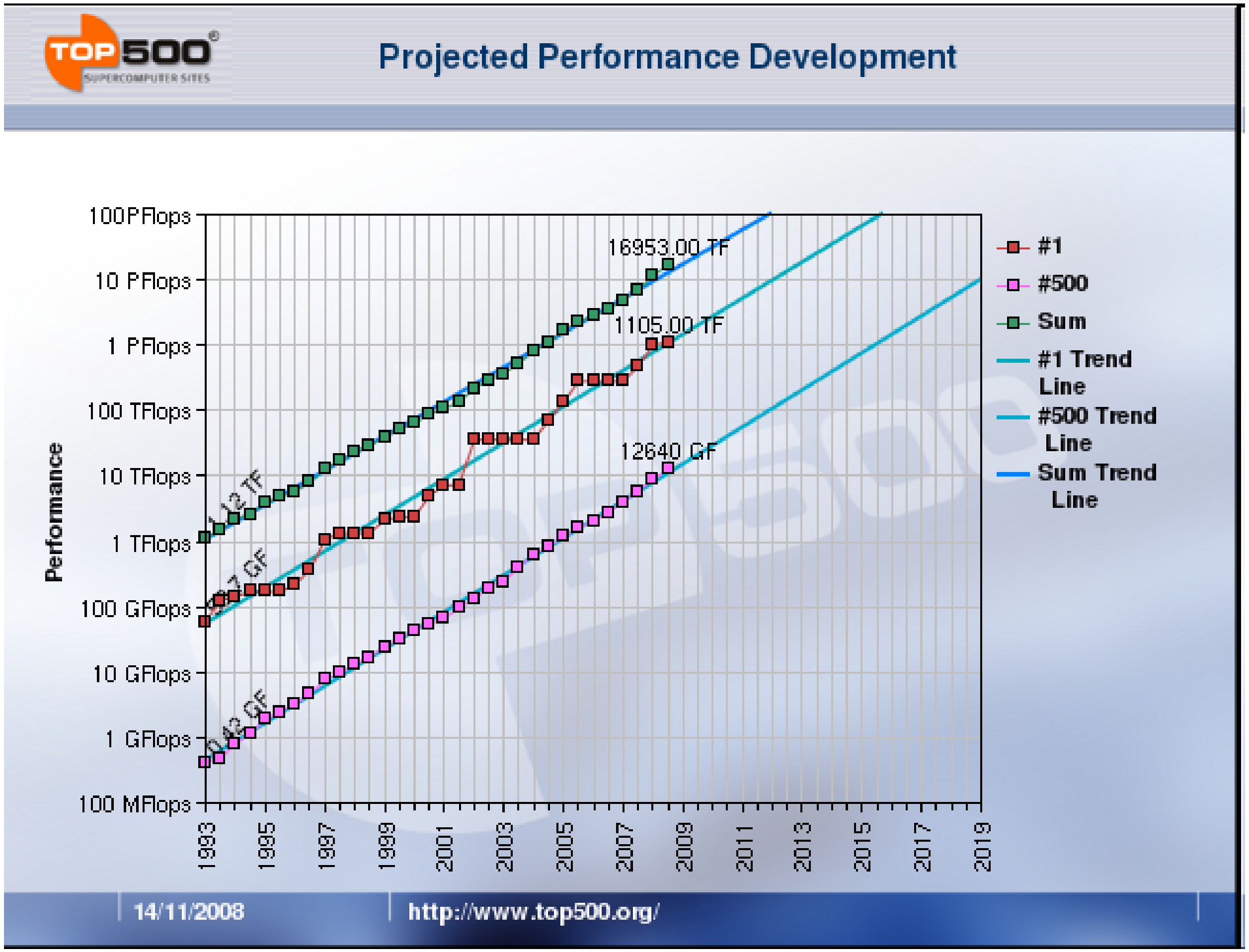
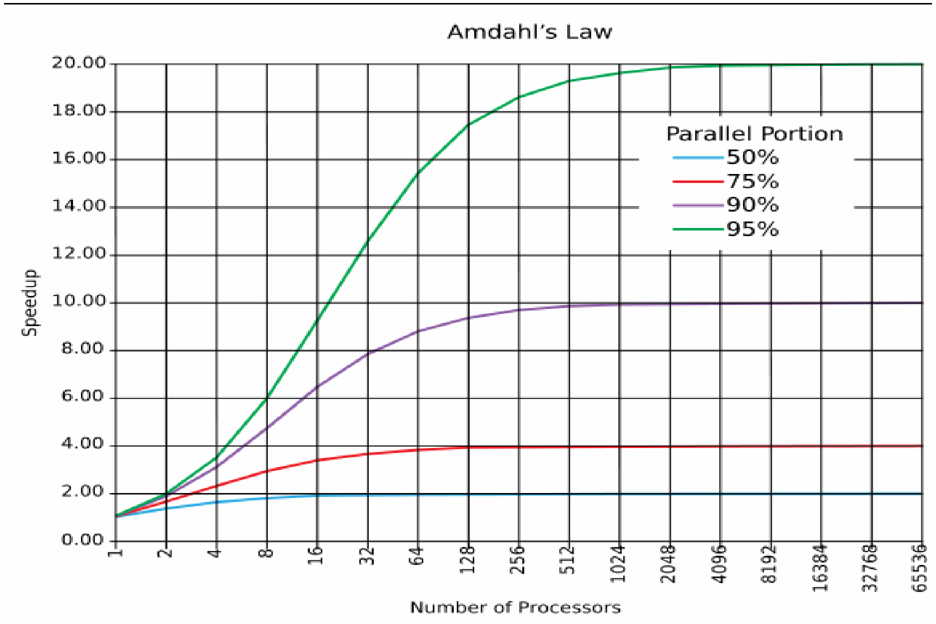
A crash course on MPI



Performance of laptop is only 12-14 years behind …
which is about the time it takes to complete PhD ….

Parallel computing: a few things everyone should be familiar with…



- **Amdahl's law:**
  S_P – speed-up factor
  P - # of processors
  ξ - non parallelizable portion of a code

$$S_P = \frac{1}{\xi + (1-\xi)\frac{1}{P}} < \frac{T_1}{T_P}$$

- **Parallel efficiency**

$$\eta_P = \frac{P-1}{P \log_2 P}$$

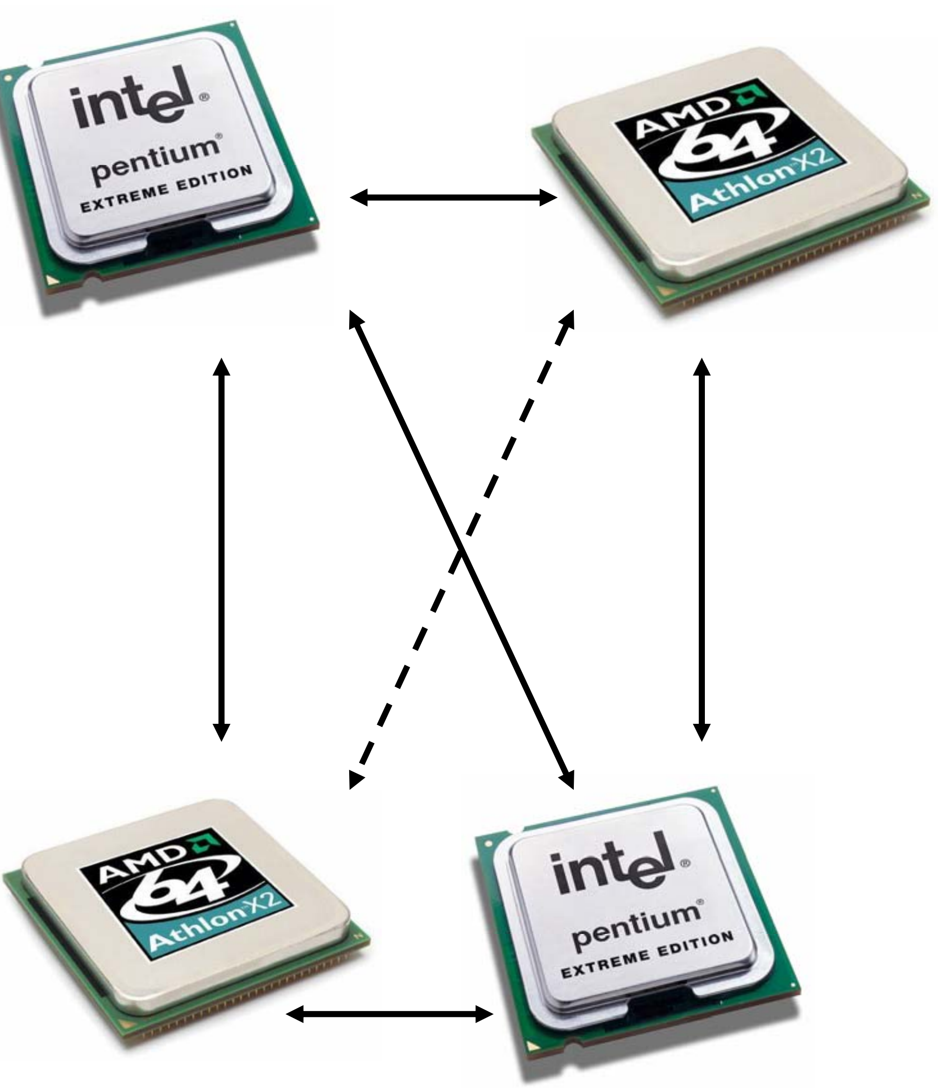
- **Communication cost**

$$C = L + \beta\, l$$

L – latency, *l* – message size,

β^{-1} - bandwidth

Message Passing Interface – MPI: what do we need it for?



The minimal MPI subset

1. MPI_Init()
2. MPI_Finalize()
3. MPI_Comm_size()
4. MPI_Comm_rank()
5. MPI_Send()
6. MPI_Recv()

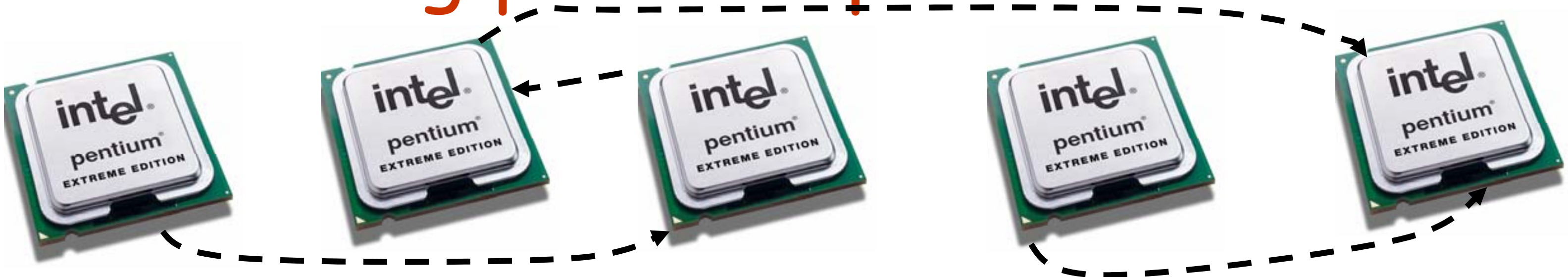
```
#include <stdio.h>
#include <mpi.h>

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

MPI_Init (&argc, &argv);
/* starts MPI */
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
/* get current process id */
MPI_Comm_size (MPI_COMM_WORLD, &size);
/* get number of processes */


printf( "Hello world from process %d of %d\n",
          rank, size );
MPI_Finalize();
return 0;
}
```

MPI Communications

- **Point-to-point communications**
  - Involves a sender and a receiver
  - Only the two processors participate in communication

- **Collective communications**
  - All processors within a communicator participate in communication (by calling same routine, may pass different arguments);
  - Barrier, reduction operations, gather, scatter…

Blocking point-to-point communication

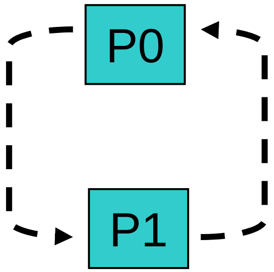



```
int MPI_Send(
    void *buf,     /* initial address of send buffer  */
    int count,     /* number of elements in send buffer (nonnegative integer) */
    MPI_Datatype datatype, /* datatype of each send buffer element */
    int dest,      /* rank of destination (integer)   */
    int tag,       /* message tag (integer)           */
    MPI_Comm comm  /* communicator                    */
);
```

```
int MPI_Recv(
    void *buf,     /* initial address of receive buffer  */
    int count,     /* number of elements in receive buffer (nonnegative integer) */
    MPI_Datatype datatype, /* datatype of each receive buffer element */
    int dest,      /* rank of source (integer)          */
    int tag,       /* message tag (integer)             */
    MPI_Comm comm,      /* communicator                 */
    MPI_Status   *status    /* status object            */
);
```

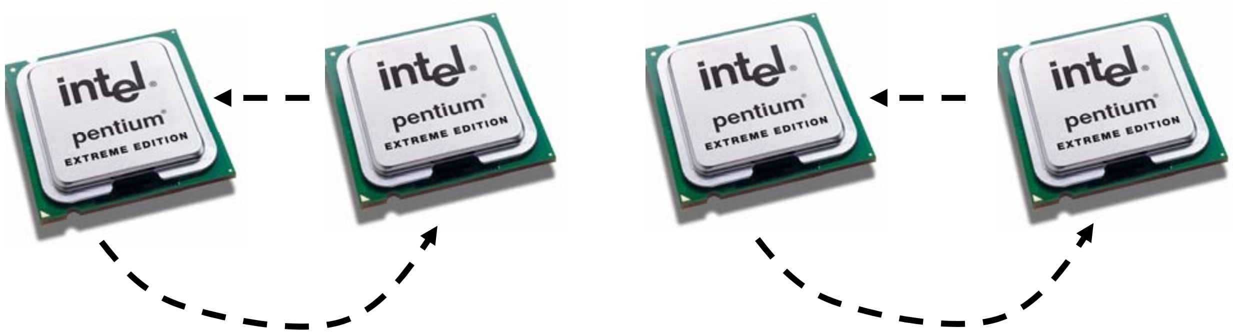
Deadlock

```
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
If(rank==0)
{
  MPI_Recv(buf1,count,MPI_DOUBLE,1,tag,comm);
  MPI_Send(buf2,count,MPI_DOUBLE,1,tag,comm);
}
else if (rank==1)
{
  MPI_Recv(buf1,count,MPI_DOUBLE,0,tag,comm);
  MPI_Send(buf2,count,MPI_DOUBLE,0,tag,comm);
}
```




```
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
If(rank==0)
{
  MPI_Recv(buf1,count,MPI_DOUBLE,1,tag,comm);
  MPI_Send(buf2,count,MPI_DOUBLE,1,tag,comm);
}
else if (rank==1)
{
  MPI_Send(buf2,count,MPI_DOUBLE,0,tag,comm);
  MPI_Recv(buf1,count,MPI_DOUBLE,0,tag,comm);
}
```

Blocking point-to-point communication




```
int MPI_Sendrecv(
    void *sendbuf,
    int sendcount,
    MPI_Datatype sendtype,
    int dest,
    int sendtag,

    void *recvbuf,
    int recvcount,
    MPI_Datatype recvtype,
    int source,
    int recvtag,

    MPI_Comm comm,
    MPI_Status *status
    );
```

Example

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

int main(int argc, char **argv)
{
  int my_rank, ncpus;
  int left_neighbor, right_neighbor;
  int data_received;
  int send_tag = 101, recv_tag=101;
  MPI_Status status;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
  MPI_Comm_size(MPI_COMM_WORLD, &ncpus);

  left_neighbor = (my_rank-1 + ncpus)%ncpus;
  right_neighbor = (my_rank+1)%ncpus;

  MPI_Sendrecv(&my_rank, 1, MPI_INT, left_neighbor, send_tag,
               &data_received, 1, MPI_INT, right_neighbor, recv_tag,
              MPI_COMM_WORLD, &status);

  printf("P%d received from right neighbor: P%d\n",
         my_rank, data_received);

  // clean up
  MPI_Finalize();
  return 0;
}
```

Output:
P3 received from right neighbor: P0
P2 received from right neighbor: P3
P0 received from right neighbor: P1
P1 received from right neighbor: P2

Non-blocking point-to-point communication

```
int MPI_Isend(
    void *buf,       /* initial address of send buffer              */
    int     count,    /* number of elements in send buffer (nonnegative integer) */
    MPI_Datatype datatype, /* datatype of each send buffer element         */
    int     dest,      /* rank of destination (integer)               */
    int     tag,        /* message tag (integer)                        */
    MPI_Comm    comm,       /*  communicator                          */
    MPI_Request  *request   /*  communication request   */
);
```

```
int MPI_Irecv(
    void *buf,       /* initial address of receive buffer  */
    int     count,    /* number of elements in receive buffer (nonnegative integer) */
    MPI_Datatype datatype, /* datatype of each receive buffer element             */
    int     dest,       /* rank of source (integer)            */
    int     tag,         /* message tag (integer)               */
    MPI_Comm      comm,      /* communicator          */
    MPI_Request  *request /*  communication request */
);
```

What should we use?

MPI_Send + MPI_Recv

MPI_Send + MPI_Irecv

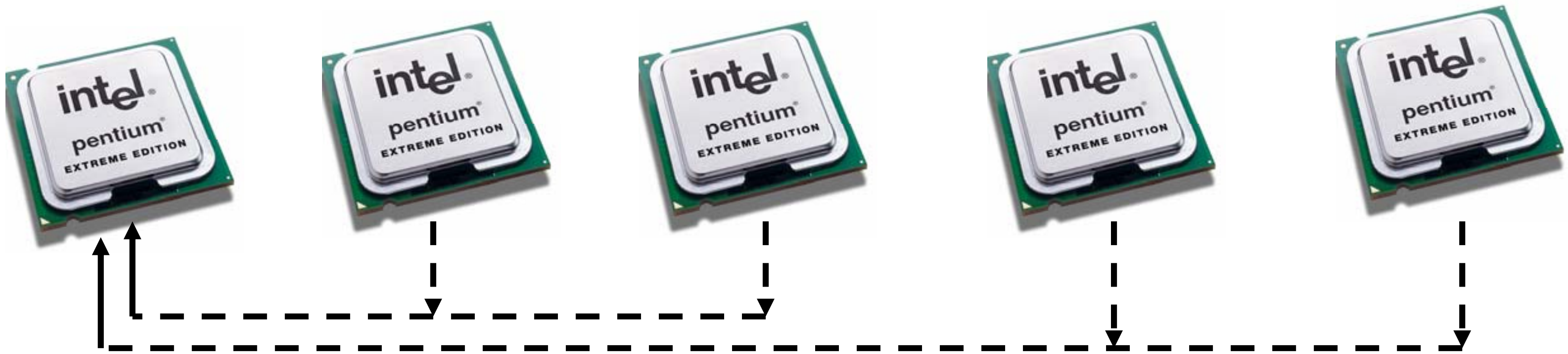
MPI_Isend + MPI_Recv

MPI_Isend + MPI_Irecv

MPI_Sendrecv

MPI_Alltoall

Collective communication

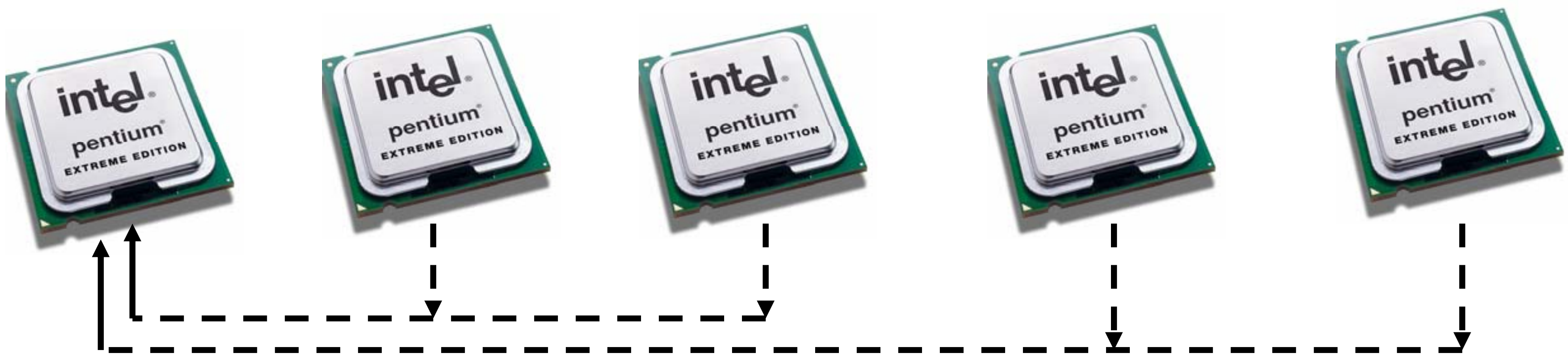



```
int MPI_Reduce (
     void               *sendbuf,
     void               *recvbuf,
     int                 count,
     MPI_Datatype datatype,
     MPI_Op              op,
     int                 root,
     MPI_Comm       comm
);
```

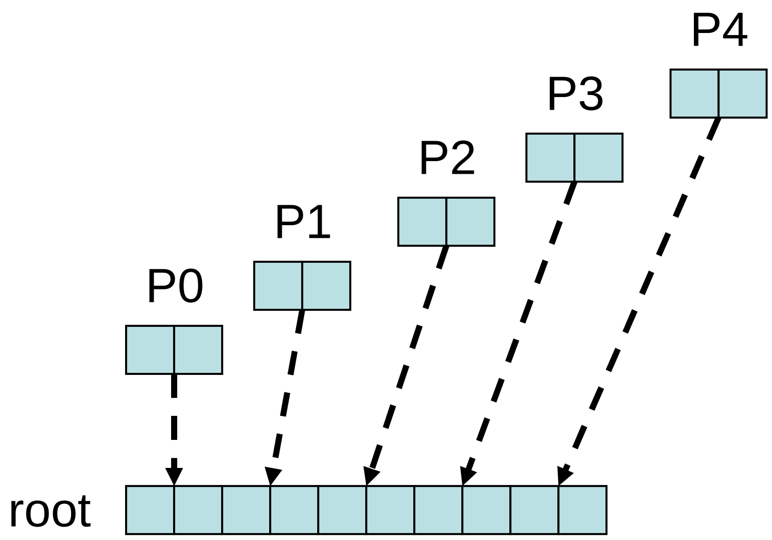
MPI function	Math Meaning
MPI_MAX maximum,	max
MPI_MIN minimum,	min
MPI_MAXLOC	maximum and location of maximum
MPI_MINLOC	minimum and location of minimum
MPI_SUM	sum
MPI_PROD	product
MPI_LAND	logical and
MPI_LOR	logical or
MPI_LXOR	logical exclusive or
MPI_BAND	bitwise and
MPI_BOR	bitwise or
MPI_BXOR	bitwise exclusive or

Implemented in integration, dot products, finding maxima or minima ….

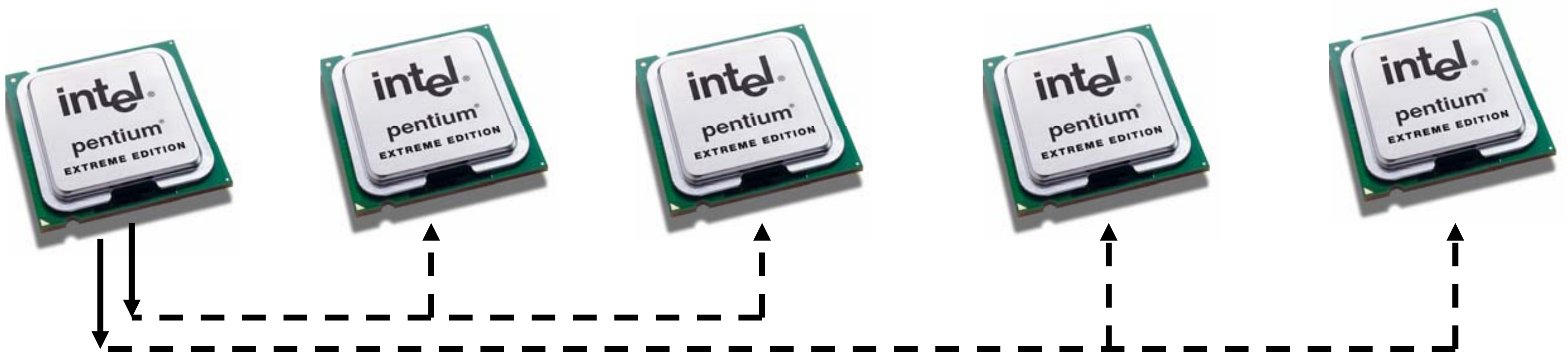
Collective communication



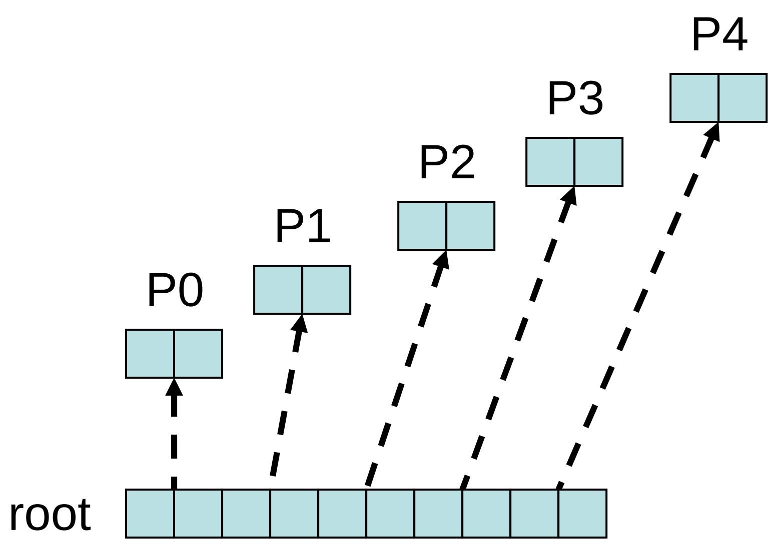
```
int MPI_Gather (
   void              *sendbuf,
   int                sendcnt,
   MPI_Datatype sendtype,
   void              *recvbuf,
   int                recvcount,
   MPI_Datatype recvtype,
   int                root,
   MPI_Comm      comm
);
```



Collective communication



```
int MPI_Scatter (
   void              *sendbuf,
   int                sendcnt,
   MPI_Datatype sendtype,
   void              *recvbuf,
   int                recvcount,
   MPI_Datatype recvtype,
   int                root,
   MPI_Comm      comm
);
```



Collective communication

To operate on messages of unequal length:

- MPI_Scatter**v**
- MPI_Gather**v**

To obtain results on all processors:

- MPI_Allreduce
- MPI_Allgather (**v**)

To Send data from all to all processes

- MPI_Alltoall(**v**)

To broadcast message

- MPI_Bcast

To synchronize between processors

- MPI_Barrier

Good programming

- **Reliability** – The code does not have errors and can be trusted to compute what it is supposed to compute.

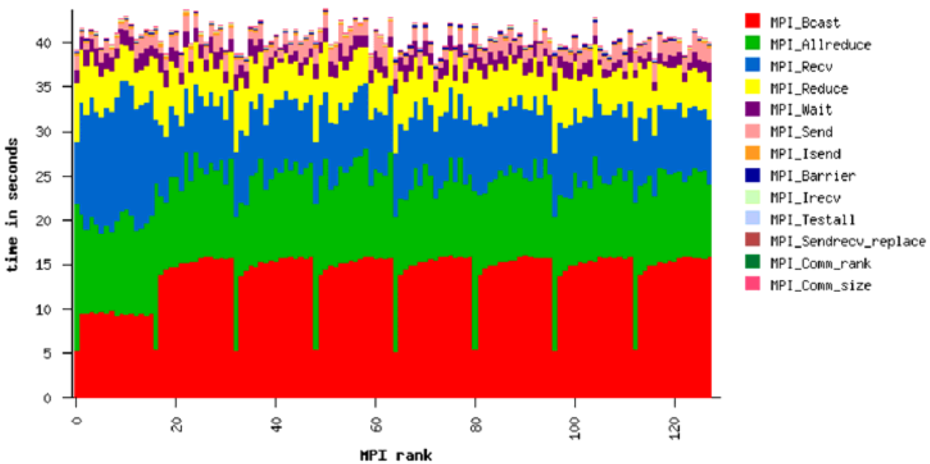
- **Robustness**, which is closely related to reliability – The code has a wide range of applicability as well as the ability to detect bad data, “singular” or other problems that it can not be expected to handle, and other abnormal situations, and deal with them in a way that is satisfactory to user.

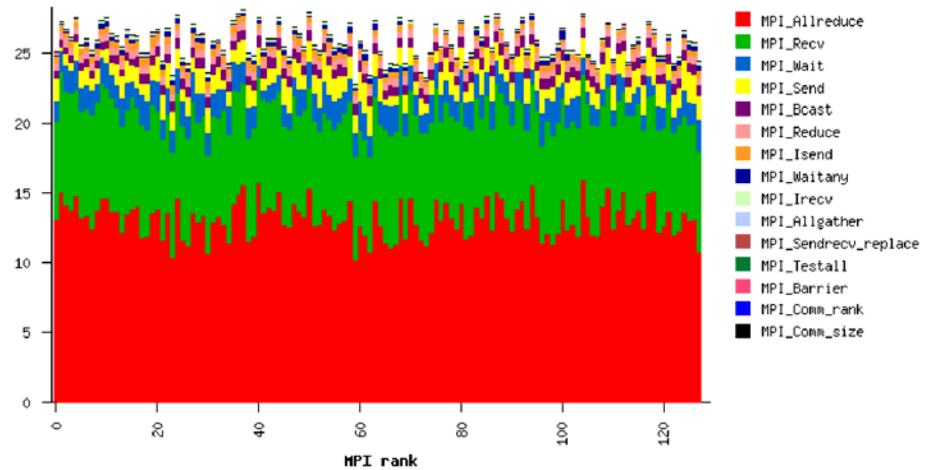
- **Portability** – The code can be transferred from one computer to another with a minimum effort and without loosing reliability. Usually this means that the code has been written in a general high-level language like FORTRAN (C++) and uses no “tricks” that are dependent on the characteristic of a particular computer. Any machine characteristics that must be used are clearly delineated.

- **Maintainability** – Any code will necessary need to be changed from time to time, either to make corrections or to add enhancements, and this should be possible with minimum effort.

Gene Golub, James M. Ortega, **Scientific computing**: an introduction with **parallel computing,** 1993**.**

Code optimization through code profiling

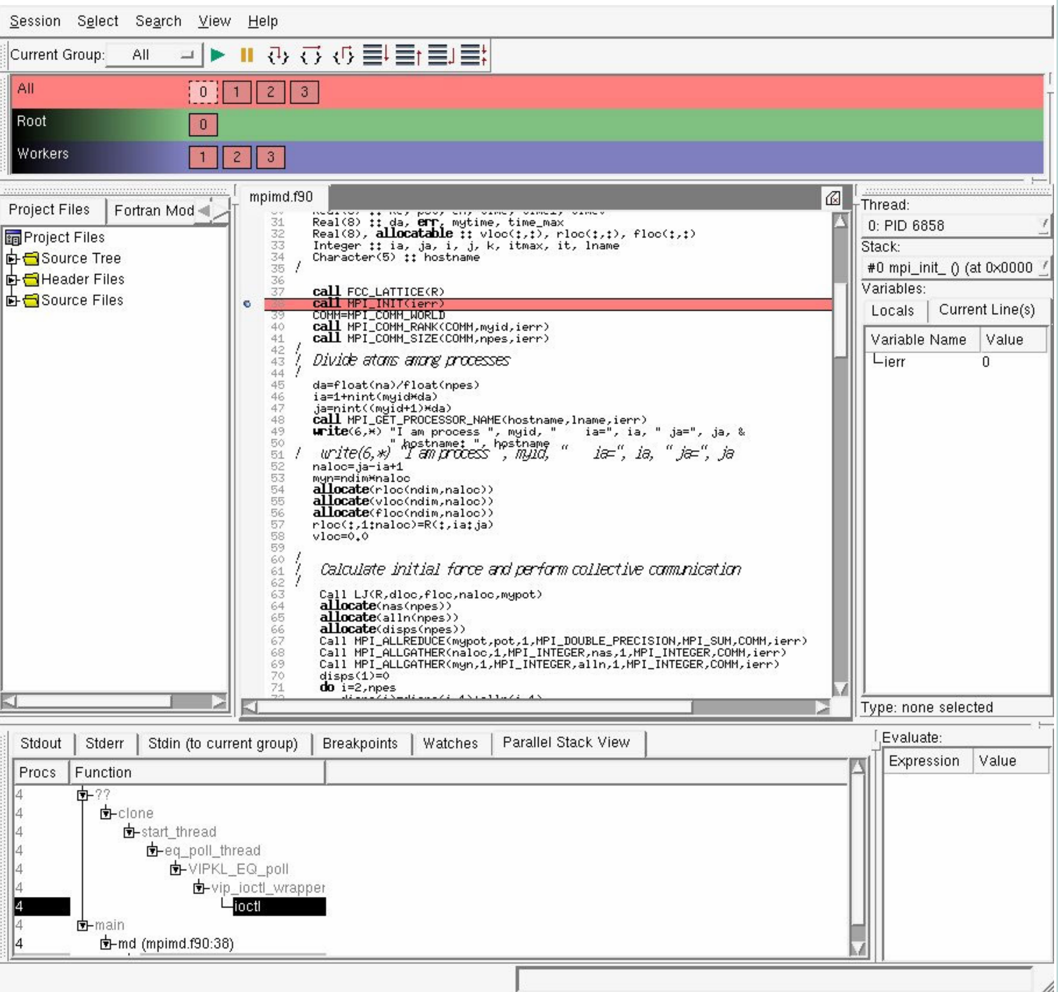




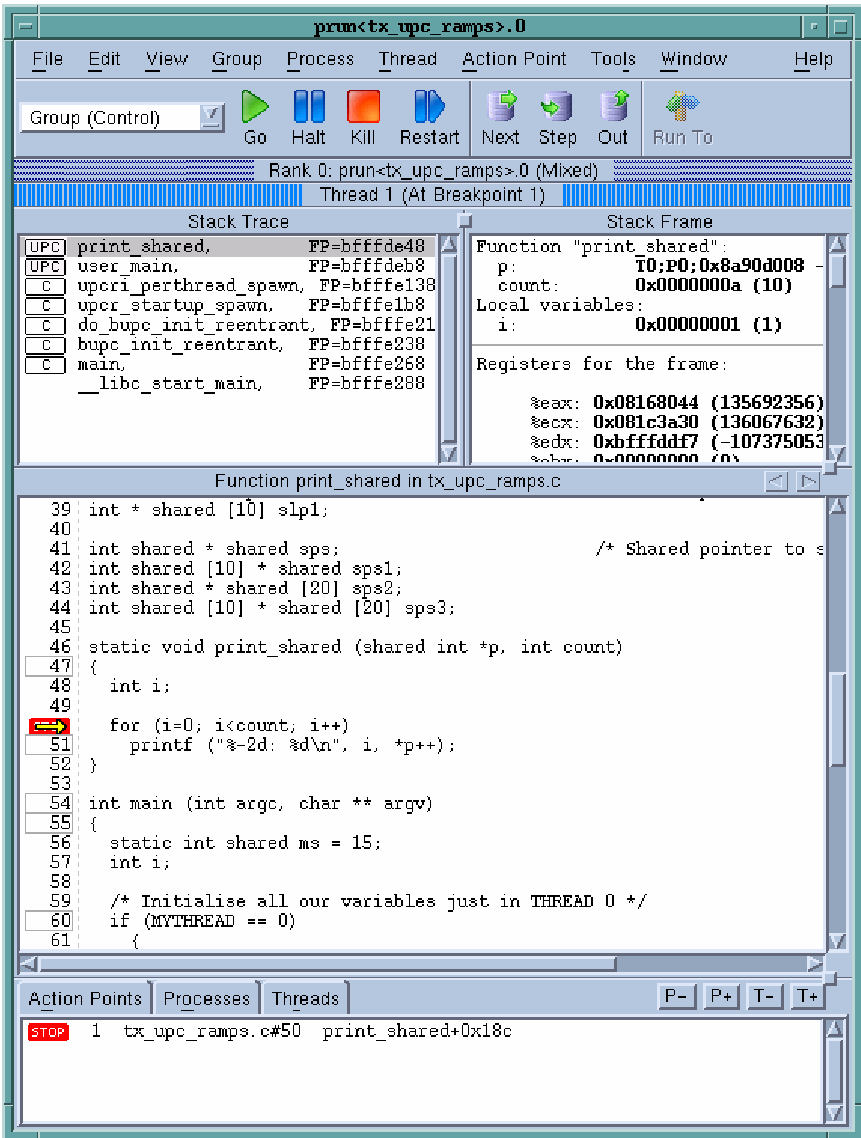
Difference: 40 sec → 25 sec

Debugging parallel code

DDT

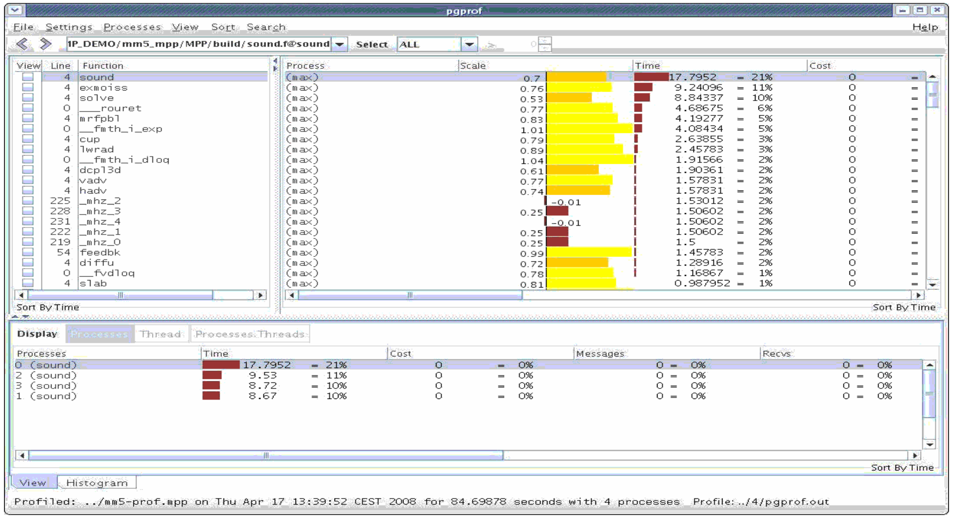


Totalview

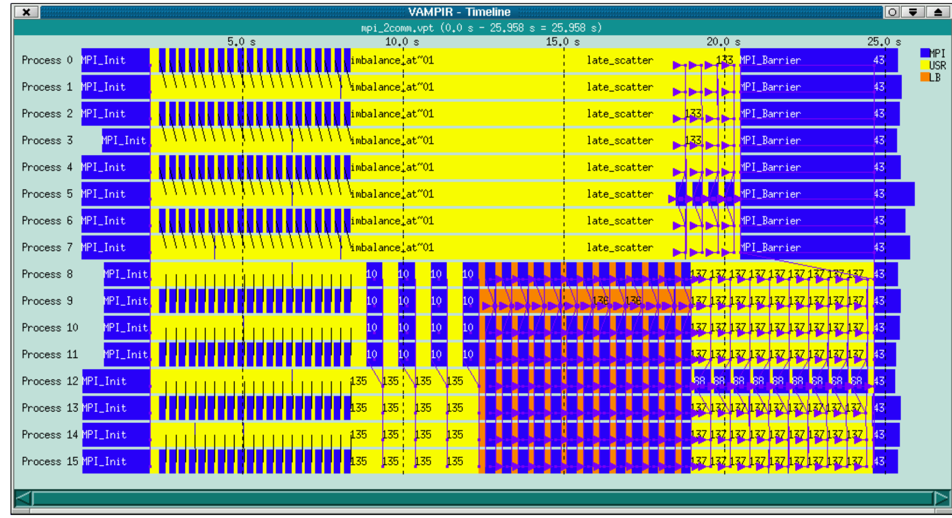


Performance analysis tools

pgprof



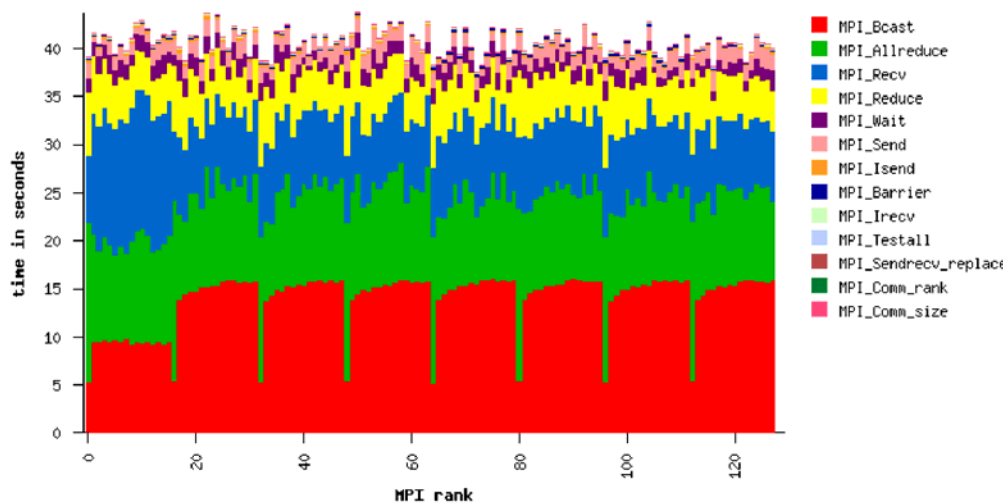
vampire



crayPAT

100.0%	100.0%	512	Total
59.8%	**59.8%**	**306**	**stepfx_**
17.6%	**77.3%**	**90**	**getrusage**
8.0%	85.4%	41	stepfy_
6.2%	91.6%	32	integr_
2.0%	93.6%	10	gradco_
1.0%	94.5%	5	__write
0.8%	95.3%	4	filerx_

IMP



How to learn MPI programming?

Just do it!