Data Partitioning; Fan Out Data

1. Data Partitioning
   - functional and domain decomposition
2. Parallel Summation
   - applying divide and conquer
   - fanning out an array of data
   - fanning out with MPI
   - fanning in the results
3. An Application
   - computing hexadecimal expansions for π
4. Nonblocking Point-to-Point Communication
   - immediate send and receive
   - query the status of a communication

MCS 572 Lecture 9
Introduction to Supercomputing
Jan Verschelde, 16 September 2024

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functional and domain decomposition

To turn a sequential algorithm into a parallel one,
we distinguish between functional and domain decomposition:

Functional decomposition: distribute arithmetical operations among several processors.

Example: Monte Carlo simulations.

Domain decomposition: distribute data among several processors.

Example: Mandelbrot set computation.

Problem solving by parallel computers: the entire data set is often too large to fit into the memory of one computer.

Example: game tree for four in a row.

divide-and-conquer methods

Divide and conquer used to solve problems:

- break the problem in smaller parts,
- solve the smaller parts,
- assemble the partial solutions.

Often, divide and conquer is applied in a recursive setting where the smallest nontrivial problem is the base case.

Examples in sorting: mergesort and quicksort.

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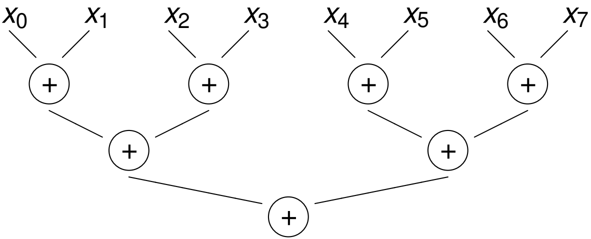
summing numbers with divide and conquer

$$
\begin{aligned}
\sum_{k=0}^{7} x_k &= (x_0 + x_1 + x_2 + x_3) + (x_4 + x_5 + x_6 + x_7) \\
&= ((x_0 + x_1) + (x_2 + x_3)) + ((x_4 + x_5) + (x_6 + x_7))
\end{aligned}
$$



With 4 processors, the summation of 8 numbers in done in 3 steps.

making partial sums

The size of the problem is n, where $S = \sum_{k=0}^{n-1} x_k$.

Assume we have 8 processors to make 8 partial sums:

$$\begin{aligned} S &= (S_0 + S_1 + S_2 + S_3) + (S_4 + S_5 + S_6 + S_7) \\ &= ((S_0 + S_1) + (S_2 + S_3)) + ((S_4 + S_5) + (S_6 + S_7)) \end{aligned}$$

where $m = \dfrac{n-1}{8}$ and $S_i = \sum_{k=0}^{m} x_{k+im}$

The communication pattern goes along divide and conquer:

- the numbers x_k are scattered in a *fan out* fashion,
- summing the partial sums happens in a *fan in* mode.

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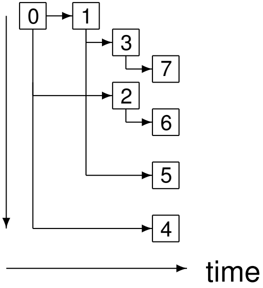
fanning out data



node	step 0	step 1	step 2	step 3
0	[0...7]	[0...3]	[0...1]	[0]
1		[4...7]	[4...5]	[4]
2			[2...3]	[2]
3			[6...7]	[6]
4				[1]
5				[5]
6				[3]
7				[7]

Algorithm: at step k, 2^k processors have data, and execute:

for j from 0 to $2^k - 1$ do

processor j sends $\frac{\text{data}}{2^{k+1}}$ to processor $j + 2^k$;

processor $j + 2^k$ receives $\frac{\text{data}}{2^{k+1}}$ from processor j.

refining the algorithm

In fanning out, we want to use the same array for all nodes, and use only one send/recv statement.

Observe the bit patterns in nodes and data locations:

	step				
node	0	1	2	3	data
000	[0...7]	[0...3]	[0...1]	[0]	000
001		[4...7]	[4...5]	[4]	100
010			[2...3]	[2]	010
011			[6...7]	[6]	110
100				[1]	001
101				[5]	101
110				[3]	011
111				[7]	111

At step 3, the node with label in binary expansion $b_2 b_1 b_0$ has data starting at index $b_0 b_1 b_2$.

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running with 8 processes

```
$ mpirun -np 8 ./fan_out_integers
stage 0, d = 1 :
0 sends 40 integers to 1 at 40, start 40
1 received 40 integers from 0 at 40, start 40
stage 1, d = 2 :
0 sends 20 integers to 2 at 20, start 20
2 received 20 integers from 0 at 20, start 20
1 sends 20 integers to 3 at 60, start 60
3 received 20 integers from 1 at 60, start 60
stage 2, d = 4 :
0 sends 10 integers to 4 at 10, start 10
7 received 10 integers from 3 at 70, start 70
3 sends 10 integers to 7 at 70, start 70
4 received 10 integers from 0 at 10, start 10
1 sends 10 integers to 5 at 50, start 50
2 sends 10 integers to 6 at 30, start 30
6 received 10 integers from 2 at 30, start 30
5 received 10 integers from 1 at 50, start 50
```

run continued

```
data at all nodes :
1 has 10 integers starting at 40 with 40, 41, 42
2 has 10 integers starting at 20 with 20, 21, 22
7 has 10 integers starting at 70 with 70, 71, 72
5 has 10 integers starting at 50 with 50, 51, 52
0 has 10 integers starting at 0 with 0, 1, 2
6 has 10 integers starting at 30 with 30, 31, 32
3 has 10 integers starting at 60 with 60, 61, 62
4 has 10 integers starting at 10 with 10, 11, 12
```

MPI_Barrier to synchronize printing

To synchronize across all members of a group we apply

```
MPI_Barrier(comm)
```

where `comm` is the communicator (`MPI_COMM_WORLD`).

`MPI_Barrier` blocks the caller until all group members have called the statement.

The call returns at any process only after all group members have entered the call.

computing the offset

```
int parity_offset ( int n, int s );
/* returns the offset of node with label n
 * for data of size s based on parity of n */

int parity_offset ( int n, int s )
{
   int offset = 0;
   s = s/2;
   while(n > 0)
   {
      int d = n % 2;
      if(d > 0) offset += s;
      n = n/2;
      s = s/2;
   }
   return offset;
}
```

start of the main program

```
/* include headers omitted */
#define size 80     /* size of the problem */
#define tag 100     /* tag of send/recv */
#define v 1         /* verbose flag */

int main ( int argc, char *argv[] )
{
   int myid,p,s,i,j,d,b;
   int A[size];

   MPI_Status status;
   MPI_Init(&argc,&argv);
   MPI_Comm_size(MPI_COMM_WORLD,&p);
   MPI_Comm_rank(MPI_COMM_WORLD,&myid);

   if(myid == 0) /* manager initializes */
      for(i=0; i<size; i++) A[i] = i;
```

the main loop

```
s = size;
for(i=0,d=1; i<3; i++,d*=2) /* A is fanned out */
{
   s = s/2;
   if(v>0) MPI_Barrier(MPI_COMM_WORLD);
   if(myid == 0)
      if(v > 0) printf("stage %d, d = %d :\n",i,d);
   if(v>0) MPI_Barrier(MPI_COMM_WORLD);
   for(j=0; j<d; j++)
   {
      b = parity_offset(myid,size);
```

the inner loop

```
for(j=0; j<d; j++){
   b = parity_offset(myid,size);
   if(myid == j){
      if(v>0)
         printf("%d sends %d integers to %d at %d, \
                 start %d\n",j,s,j+d,b+s,A[b+s]);
      MPI_Send(&A[b+s],s,MPI_INT,j+d,tag,MPI_COMM_WORLD);
   }
   else if(myid == j+d){
      MPI_Recv(&A[b],s,MPI_INT,j,tag,
               MPI_COMM_WORLD,&status);
      if(v>0)
         printf("%d received %d integers from %d at %d, \
                 start %d\n",j+d,s,j,b,A[b]);
   }
}
```

the end of the program

```
    }
    if(v > 0) MPI_Barrier(MPI_COMM_WORLD);
    if(v > 0) if(myid == 0) printf("data at all nodes :\n");
    if(v > 0) MPI_Barrier(MPI_COMM_WORLD);
    printf("%d has %d integers starting at %d with %d, %d, \
            %d\n", myid,size/p,b,A[b],A[b+1],A[b+2]);
    MPI_Finalize();
    return 0;
}
```

using mpi4py and numpy

```
import numpy as np
from mpi4py import MPI
COMM = MPI.COMM_WORLD
SIZE = 80                    # size of the problem

def main(verbose=True):
    """
    Fans out 80 integers to 8 processors.
    """
    myid = COMM.Get_rank()
    p = COMM.Get_size()
    # manager initializes, workers allocate space
    if myid == 0:
        data = np.arange(SIZE, dtype='i')
    else:
        data = np.empty(SIZE, dtype='i')
```

code without verbose statements

```
d = 1                       # depth
s = SIZE                    # size of a slice
b = 0                       # begin index
for i in range(3):          # in 3 steps for 8 nodes
    s = s//2
    for j in range(d):
        b = parity_offset(myid, SIZE);
        if myid == j:
            slice = data[b+s: b+2*s]
            COMM.Send([slice, MPI.INT], dest=j+d)
        elif myid == j+d:
            slice = data[b: b+s]
            COMM.Recv([slice, MPI.INT], source=j)
    d = 2*d
```

fanning out with MPI.jl

The Python code translates directly into Julia,
see the program fan_out_integers.jl.

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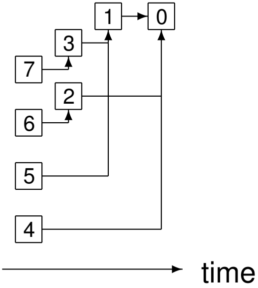
fanning in results



Algorithm: at step k, 2^k processors send results and execute:

for j from 0 to $2^k - 1$ do
processor $j + 2^k$ sends the result to processor j;
processor j receives the result from processor $j + 2^k$.

We run the algorithm for decreasing values of k: $k = 2, 1, 0$.

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the BBP algorithm for π

Computing π to trillions of digits
is a benchmark problem for supercomputers.

One of the remarkable discoveries made by the PSLQ Algorithm
(PSLQ = Partial Sum of Least Squares, or integer relation detection)
is a simple formula that allows to calculating any binary digit
of π without calculating the digits preceding it:

$$\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right).$$

BBP stands for Bailey, Borwein and Plouffe.

Instead of adding numbers, we concatenate strings.

some readings on calculations for π

- David H. Bailey, Peter B. Borwein and Simon Plouffe: **On the Rapid Computation of Various Polylogarithmic Constants.** *Mathematics of Computation* 66(218): 903–913, 1997.
- David H. Bailey: **the BBP Algorithm for Pi**. September 17, 2006. `http://crd-legacy.lbl.gov/~dhbailey/dhbpapers/`.
- Daisuke Takahashi: **Parallel implementation of multiple-precision arithmetic and 2, 576, 980, 370, 000 decimal digits of pi calculation.** *Parallel Computing* 36(8): 439-448, 2010.

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nonblocking point-to-point communication

The MPI_SEND and MPI_RECV are ***blocking***:

- The sender must wait till the message is received.
- The receiver must wait till the message is sent.

For synchronized computations, this is desirable.

To overlap the communication with the computation,
we may prefer the use of ***nonblocking*** communication operations:

- MPI_ISEND for the Immediate send; and
- MPI_IRECV for the Immediate receive.

The status of the immediate send/receive

- can be queried with MPI_TEST; or
- we can wait for its completion with MPI_WAIT.

MPI_ISEND specification

```
MPI_ISEND(buf, count, datatype, dest,
          tag, comm, request)
```

parameter	description
`buf`	address of the send buffer
`count`	number of elements in send buffer
`datatype`	datatype of each send buffer element
`dest`	rank of the destination
`tag`	message tag
`comm`	communicator
`request`	communication request (output)

The sender should not modify any part of the send buffer after a nonblocking send operation is called, until the send completes.

MPI_IRECV specification

```
MPI_IRECV (buf, count, datatype, source,
           tag, comm, request)
```

parameter	description
`buf`	address of the receive buffer
`count`	number of elements in receive buffer
`datatype`	datatype of each receive buffer element
`source`	rank of source or `MPI_ANY_SOURCE`
`tag`	message tag or `MPI_ANY_TAG`
`comm`	communicator
`request`	communication request (output)

The receiver should not access any part of the receive buffer after a nonblocking receive operation is called, until the receive completes.

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waiting for a nonblocking communication

After the call to MPI_ISEND or MPI_IRECV, the request can be used to query the status of the communication or wait for its completion.

To wait for the completion of a nonblocking communication:

MPI_WAIT (request, status)

parameter	description
request	communication request
status	status object

To test the status of the communication:

MPI_TEST (request, flag, status)

parameter	description
request	communication request
flag	true if operation completed
status	status object

Summary + Exercises

The material in this lecture is based on chapter 4 of the text book by Wilkinson and Allen.

Exercises:

1. Adjust the fanning out of the array of integers so it works for any number p of processors where $p = 2^k$ for some k.
   You may take the size of the array as an integer multiple of p.
2. Run the program of the previous exercise on the supercomputer, for $p = 8, 16, 32, 64$, and 128.
   For each run, report the wall clock time.
3. Complete the summation and the fanning in of the partial sums, extending the program. You may leave $p = 8$.