Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

MCS 572 Lecture 29
Introduction to Supercomputing
Jan Verschelde, 17 March 2023

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

a fixed point formula

We want to solve $A\mathbf{x} = \mathbf{b}$ for $A \in \mathbb{R}^{n \times n}$, $\mathbf{b} \in \mathbb{R}^n$, for ***very large*** n.

Consider $A = L + D + U$, where

- $L = [\ell_{i,j}], \ell_{i,j} = a_{i,j}, i > j, \ell_{i,j} = 0, i \leq j$. L is lower triangular.
- $D = [d_{i,j}], d_{i,i} = a_{i,i} \neq 0, d_{i,j} = 0, i \neq j$. D is diagonal.
- $U = [u_{i,j}], u_{i,j} = a_{i,j}, i < j, u_{i,j} = 0, i \geq j$. U is upper triangular.

Then we rewrite $A\mathbf{x} = \mathbf{b}$ as

$$
\begin{aligned}
A\mathbf{x} = \mathbf{b} &\Leftrightarrow (L + D + U)\mathbf{x} = \mathbf{b} \\
&\Leftrightarrow D\mathbf{x} = \mathbf{b} - L\mathbf{x} - U\mathbf{x} \\
&\Leftrightarrow D\mathbf{x} = D\mathbf{x} + \mathbf{b} - L\mathbf{x} - U\mathbf{x} - D\mathbf{x} \\
&\Leftrightarrow D\mathbf{x} = D\mathbf{x} + \mathbf{b} - A\mathbf{x} \\
&\Leftrightarrow \mathbf{x} = \mathbf{x} + D^{-1}(\mathbf{b} - A\mathbf{x}).
\end{aligned}
$$

The fixed point formula $\mathbf{x} = \mathbf{x} + D^{-1}(\mathbf{b} - A\mathbf{x})$ is well defined if $a_{i,i} \neq 0$.

the Jacobi iterative method

The fixed point formula $\mathbf{x} = \mathbf{x} + D^{-1}(\mathbf{b} - A\mathbf{x})$ leads to

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \underbrace{D^{-1}\left(\mathbf{b} - A\mathbf{x}^{(k)}\right)}_{\Delta\mathbf{x}}, \quad k = 0, 1, \ldots$$

Writing the formula as an algorithm:

Input: A, $\mathbf{b}$, $\mathbf{x}^{(0)}$, ϵ, N.
Output: $\mathbf{x}^{(k)}$, k is the number of iterations done.

for k from 1 to N do
  $\Delta x := D^{-1}(\mathbf{b} - A\mathbf{x}^{(k)})$
  $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} + \Delta\mathbf{x}$
  exit when $(\|\Delta\mathbf{x}\| \leq \epsilon)$
end for.

cost and convergence

Counting the number of operations in

for k from 1 to N do
  $\Delta x := D^{-1}(\mathbf{b} - A\mathbf{x}^{(k)})$
  $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} + \Delta\mathbf{x}$
  exit when $(\|\Delta\mathbf{x}\| \leq \epsilon)$
end for.

we have a cost of $O(Nn^2)$, $O(n^2)$ for $A\mathbf{x}^{(k)}$, if A is dense.

Theorem (convergence of the Jacobi method)

The Jacobi method converges for strictly row-wise or column-wise diagonally dominant matrices, i.e.: if

$$|a_{i,i}| > \sum_{j \neq i} |a_{i,j}| \quad \text{or} \quad |a_{i,i}| > \sum_{j \neq i} |a_{j,i}|, \quad i = 1, 2, \ldots, n.$$

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

parallel version of Jacobi iterations

for k from 1 to N do
  $\Delta x := D^{-1}(\mathbf{b} - A\mathbf{x}^{(k)})$
  $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} + \Delta\mathbf{x}$
  exit when $(\|\Delta\mathbf{x}\| \leq \epsilon)$
end for.

To run the code above with p processors:

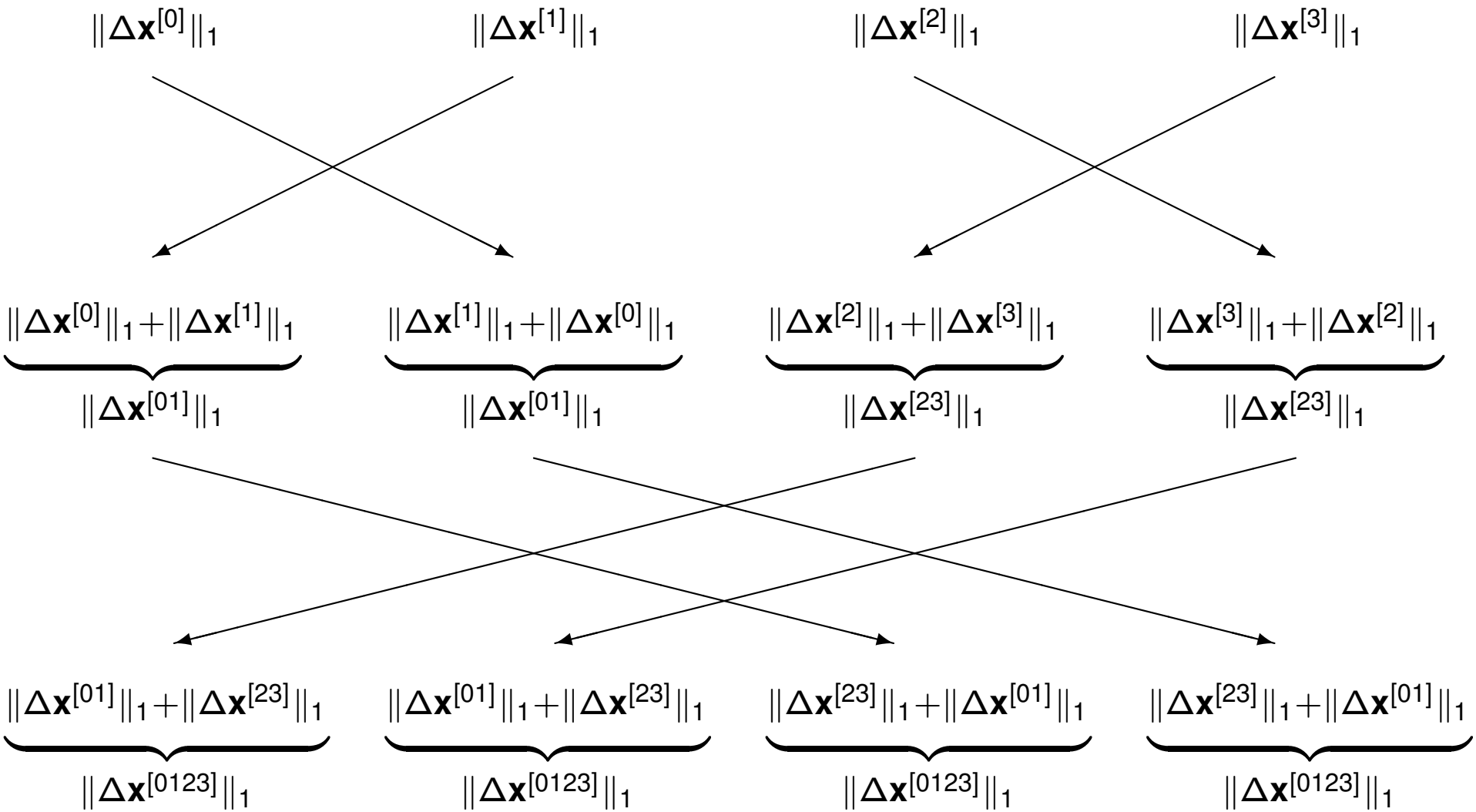
- The n rows of A are distributed evenly (e.g.: $p = 4$):

$$D \star \begin{bmatrix} \Delta\mathbf{x}^{[0]} \\ \hline \Delta\mathbf{x}^{[1]} \\ \hline \Delta\mathbf{x}^{[2]} \\ \hline \Delta\mathbf{x}^{[3]} \end{bmatrix} = \begin{bmatrix} \mathbf{b}^{[0]} \\ \hline \mathbf{b}^{[1]} \\ \hline \mathbf{b}^{[2]} \\ \hline \mathbf{b}^{[3]} \end{bmatrix} - \left[\begin{array}{cccc} A^{[0,0]} & A^{[0,1]} & A^{[0,2]} & A^{[0,3]} \\ \hline A^{[1,0]} & A^{[1,1]} & A^{[1,2]} & A^{[1,3]} \\ \hline A^{[2,0]} & A^{[2,1]} & A^{[2,2]} & A^{[2,3]} \\ \hline A^{[3,0]} & A^{[3,1]} & A^{[3,2]} & A^{[3,3]} \end{array}\right] \star \begin{bmatrix} \mathbf{x}^{[0],(k)} \\ \hline \mathbf{x}^{[1],(k)} \\ \hline \mathbf{x}^{[2],(k)} \\ \hline \mathbf{x}^{[3],(k)} \end{bmatrix}$$

- Synchronization is needed for $(\|\Delta\mathbf{x}\| \leq \epsilon)$.

butterfly synchronization

For $\|\cdot\|$, use $\|\Delta\mathbf{x}\|_1 = |\Delta x_1| + |\Delta x_2| + \cdots + |\Delta x_n|$.



communication and computation stages

The communication stages:

- At the start, every node must have $\mathbf{x}^{(0)}$, ϵ, N,
  - a number of rows of the matrix A; and
  - the corresponding part of the right hand side vector $\mathbf{b}$.
- After each update n/p elements of $\mathbf{x}^{(k+1)}$ must be scattered.
- The butterfly synchronization takes $\log_2(p)$ steps.

The scattering of $\mathbf{x}^{(k+1)}$ can coincide with the butterfly synchronization.

The computation effort: $O(n^2/p)$ in each stage.

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization

2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`

3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

the test system

For the dimension n, we consider the diagonally dominant system:

$$\begin{bmatrix} n+1 & 1 & \cdots & 1 \\ 1 & n+1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & n+1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} 2n \\ 2n \\ \vdots \\ 2n \end{bmatrix}.$$

The exact solution is $\mathbf{x}$: for $i = 1, 2, \ldots, n$, $x_i = 1$.

We start the Jacobi iteration method at $\mathbf{x}^{(0)} = \mathbf{0}$.

Parameters: $\epsilon = 10^{-4}$ and $N = 2n^2$.

running the program

```
$ time ./jacobi 1000
   0 : 1.998e+03
   1 : 1.994e+03
...
8405 : 1.000e-04
8406 : 9.982e-05
computed 8407 iterations
error : 4.986e-05

real    0m42.411s
user    0m42.377s
sys     0m0.028s
```

C code to run Jacobi iterations

```
void run_jacobi_method
  ( int n, double **A, double *b,
    double epsilon, int maxit,
    int *numit, double *x );
/*
 * Runs the Jacobi method for A*x = b.
 *
 * ON ENTRY :
 *    n         the dimension of the system;
 *    A         an n-by-n matrix A[i][i] /= 0;
 *    b         an n-dimensional vector;
 *    epsilon   accuracy requirement;
 *    maxit     maximal number of iterations;
 *    x         start vector for the iteration.
 *
 * ON RETURN :
 *    numit     number of iterations used;
 *    x         approximate solution to A*x = b. */
```

local variables

```
void run_jacobi_method
  ( int n, double **A, double *b,
    double epsilon, int maxit,
    int *numit, double *x )
{
    double *dx,*y;
    dx = (double*) calloc(n,sizeof(double));
    y = (double*) calloc(n,sizeof(double));
    int i,j,k;

    for(k=0; k<maxit; k++) { ... } /* main loop */

    *numit = k+1;
    free(dx); free(y);
}
```

the main loop in C

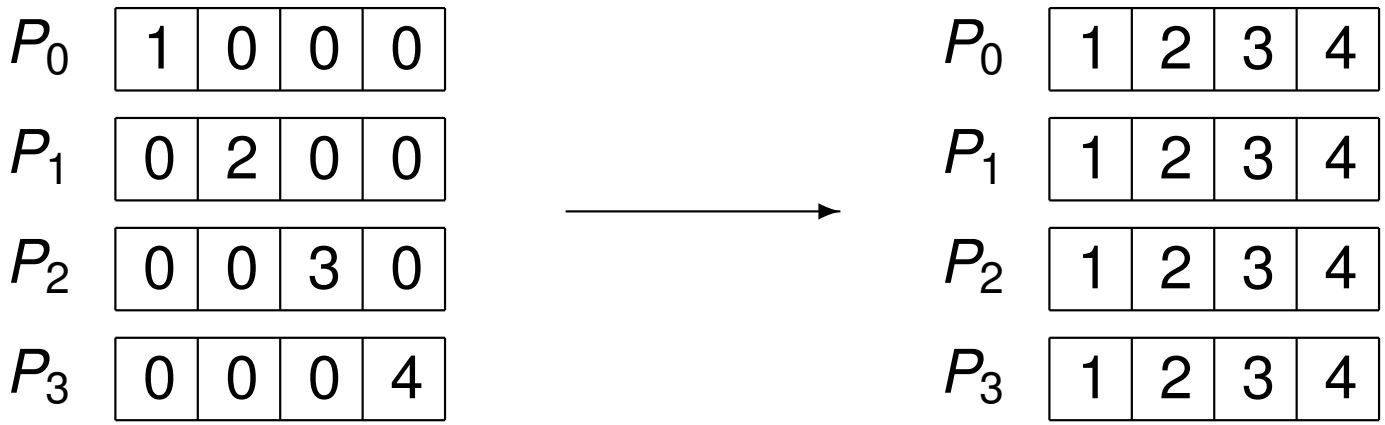
```
for(k=0; k<maxit; k++)
{
   double sum = 0.0;
   for(i=0; i<n; i++)
   {
      dx[i] = b[i];
      for(j=0; j<n; j++)
         dx[i] -= A[i][j]*x[j];
      dx[i] /= A[i][i];
      y[i] += dx[i];
      sum += ( (dx[i] >= 0.0) ? dx[i] : -dx[i]);
   }
   for(i=0; i<n; i++) x[i] = y[i];
   printf("%3d : %.3e\n",k,sum);
   if(sum <= epsilon) break;
}
```

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

gather-to-all

Gathering the four elements of a vector to four processors:



the `MPI_Allgather`

The syntax of the gather-to-all command is

```
MPI_Allgather(sendbuf,sendcount,sendtype,
              recvbuf,recvcount,recvtype,comm)
```

where the parameters are

sendbuf	starting address of send buffer
sendcount	number of elements in send buffer
sendtype	data type of send buffer elements
recvbuf	address of receive buffer
recvcount	number of elements received from any process
recvtype	data type of receive buffer elements
comm	communicator

running `use_allgather`

```
$ mpirun -np 4 ./use_allgather
data at node 0 : 1 0 0 0
data at node 1 : 0 2 0 0
data at node 2 : 0 0 3 0
data at node 3 : 0 0 0 4
data at node 3 : 1 2 3 4
data at node 0 : 1 2 3 4
data at node 1 : 1 2 3 4
data at node 2 : 1 2 3 4
$
```

the code use_allgather.c

```
int i,j,p;
MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD,&i);
MPI_Comm_size(MPI_COMM_WORLD,&p);
{
   int data[p];
   for(j=0; j<p; j++) data[j] = 0;
   data[i] = i + 1;
   printf("data at node %d :",i);
   for(j=0; j<p; j++) printf(" %d",data[j]);
   printf("\n");
   MPI_Allgather(&data[i],1,MPI_INT,
                 data,1,MPI_INT,MPI_COMM_WORLD);
   printf("data at node %d :",i);
   for(j=0; j<p; j++) printf(" %d",data[j]);
   printf("\n");
}
```

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

running `jacobi_mpi`

```
$ time mpirun -np 10 ./jacobi_mpi 1000
...
8405 : 1.000e-04
8406 : 9.982e-05
computed 8407 iterations
error : 4.986e-05

real    0m5.617s
user    0m45.711s
sys     0m0.883s
```

Recall the run with the sequential program:

```
real    0m42.411s
user    0m42.377s
sys     0m0.028s
```

Speedup: `42.411/5.617 = 7.550`.

the parallel `run_jacobi_method`

```
void run_jacobi_method
  ( int id, int p,
    int n, double **A, double *b,
    double epsilon, int maxit,
    int *numit, double *x )
{
    double *dx,*y;
    dx = (double*) calloc(n,sizeof(double));
    y = (double*) calloc(n,sizeof(double));
    int i,j,k;
    double sum[p];
    double total;
    int dnp = n/p;
    int istart = id*dnp;
    int istop = istart + dnp;
```

the main loop in `jacobi_mpi.c`

```
for(k=0; k<maxit; k++)
{
   sum[id] = 0.0;
   for(i=istart; i<istop; i++)
   {
      dx[i] = b[i];
      for(j=0; j<n; j++)
         dx[i] -= A[i][j]*x[j];
      dx[i] /= A[i][i];
      y[i] += dx[i];
      sum[id] += ( (dx[i] >= 0.0) ? dx[i] : -dx[i]);
   }
   for(i=istart; i<istop; i++) x[i] = y[i];
```

the all-to-all communication

```
      MPI_Allgather(&x[istart],dnp,MPI_DOUBLE,x,dnp,
                    MPI_DOUBLE,MPI_COMM_WORLD);
      MPI_Allgather(&sum[id],1,MPI_DOUBLE,sum,1,
                    MPI_DOUBLE,MPI_COMM_WORLD);
      total = 0.0;
      for(i=0; i<p; i++) total += sum[i];
      if(id == 0) printf("%3d : %.3e\n",k,total);
      if(total <= epsilon) break;
   }
   *numit = k+1;
   free(dx);
}
```

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

analysis

Computing $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} + D^{-1}(\mathbf{b} - A\mathbf{x}^{(k)})$ with p processors costs

$$t_{\text{comp}} = \frac{n(2n+3)}{p}.$$

We count $2n+3$ operations because of

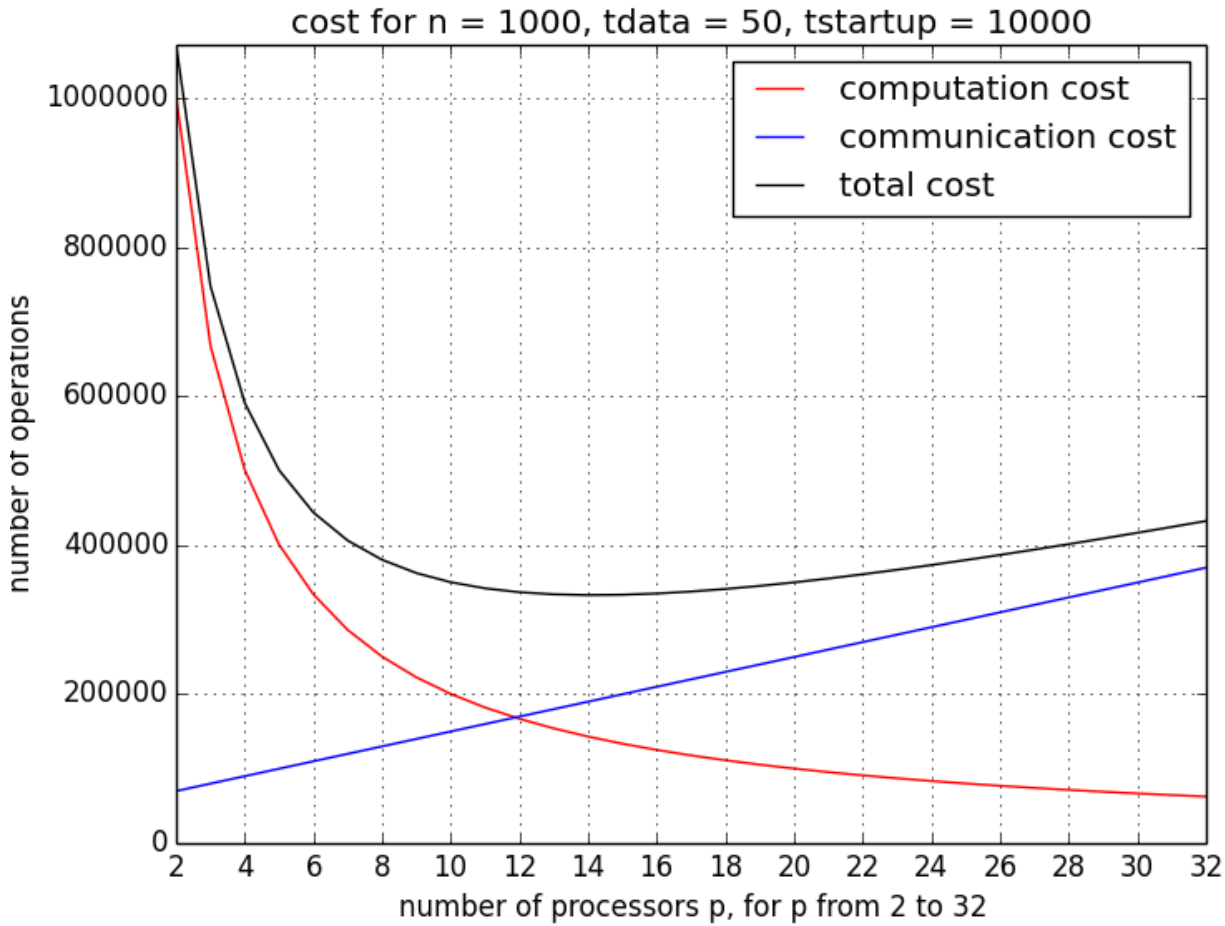
- one $-$ and one $\star$ when running over the columns of A; and
- one $/$, one $+$ for the update and one $+$ for the $\|\cdot\|_1$.

The communication cost is

$$t_{\text{comm}} = p\left(t_{\text{startup}} + \frac{n}{p}t_{\text{data}}\right).$$

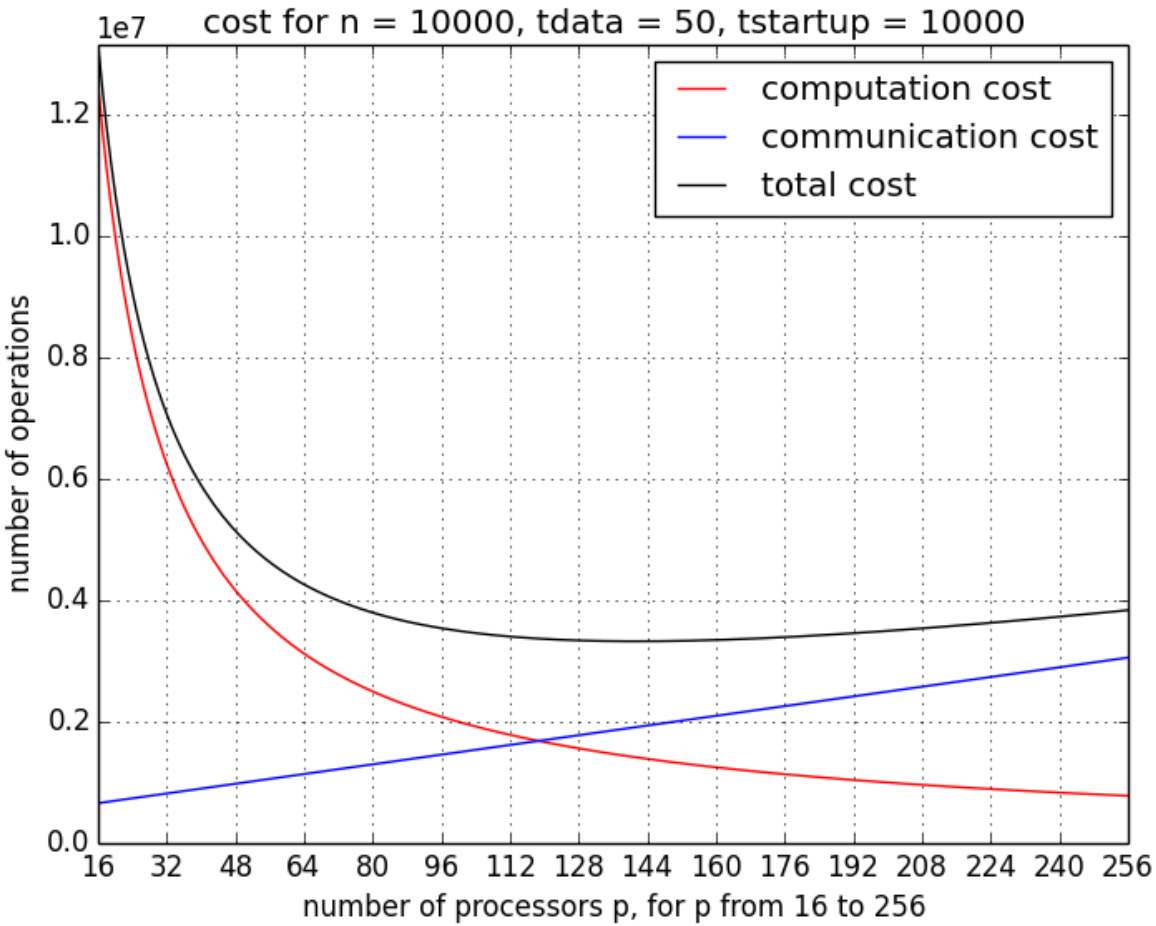
In the examples, the time unit is the cost of one arithmetical operation. Then the costs t_{startup} and t_{data} are multiples of this unit.

finding the p with the minimum total cost



The computation, communication, and total cost for p from 2 to 32, for 1 iteration, $n = 1,000$, $t_{\text{startup}} = 10,000$, and $t_{\text{data}} = 50$.

investigating the scalability



The computation, communication, and total cost for p from 16 to 256, for 1 iteration, $n = 10,000$, $t_{\text{startup}} = 10,000$, and $t_{\text{data}} = 50$.

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

a parallel matrix-vector product

Copied from the MPI for Python documentation:

```
from mpi4py import MPI
import numpy

def matvec(comm, A, x):
    m = A.shape[0] # local rows
    p = comm.Get_size()
    xg = numpy.zeros(m*p, dtype='d')
    comm.Allgather([x, MPI.DOUBLE],
                   [xg, MPI.DOUBLE])
    y = numpy.dot(A, xg)
    return y
```

Lisandro Dalcin: *MPI for Python*. Release 3.0.3, Oct 01, 2020.

Parallel Iterative Methods for Linear Systems

1. Jacobi iterations
   - derivation of the formulas
   - parallel version with butterfly synchronization
2. a Parallel Implementation with MPI
   - the sequential program
   - gather-to-all with `MPI_Allgather`
   - the parallel program
   - analysis of the computation and communication cost
   - collective communications with `mpi4py`
3. A Multithreaded Julia Program
   - strip partitioning and reduce barriers

strip partitioning

If the dimension of the matrix is a multiple of the number of threads, for some matrix `A` and vectors `x`, `y`:

```
nt = nthreads()
size = 10
dim = nt*size

@threads for i=1:nt
    tdx = threadid()
    idxstart = 1 + (tdx-1)*size
    idxend = tdx*size
    @inbounds y[idxstart:idxend]
          = A[idxstart:idxend, :]*x
end
```

reduce barriers

```
using Base.Threads
using SyncBarriers

nt = nthreads()
nb = [k for k=1:nt]
barrier = reduce_barrier(+, Int, nt)
s = 0
@threads for i=1:nt
    tdx = threadid()
    global s = reduce!(barrier[tdx], nb[tdx])
end
println("The sum of ", nb, " is ", s, ".")
```

The output of `julia -t 4 mtreduce.jl` is

```
The sum of [1, 2, 3, 4] is 10.
```

a multithreaded method of Jacobi

In a multithreaded Jacobi method, with p threads:

1. The i-th thread
   1. computes the i-th strip of the update $\Delta \mathbf{x}_i$,
   2. updates the i-th strip of $\mathbf{x}_i$ with $\Delta \mathbf{x}_i$,
   3. computes the norm of the i-th update $\|\Delta \mathbf{x}_i\|$.
2. Given $(\|\Delta \mathbf{x}_1\|, \|\Delta \mathbf{x}_2\|, \ldots, \|\Delta \mathbf{x}_p\|)$, a reduce barrier computes

$$\|\Delta \mathbf{x}\|_1 = \|\Delta \mathbf{x}_1\| + \|\Delta \mathbf{x}_2\| + \cdots + \|\Delta \mathbf{x}_p\|$$

   and that $\|\Delta \mathbf{x}\|_1$ is used by every thread as the stop criterion.

See the Julia program `mtjacobi.jl`, posted at the course web site.

three runs on pascal

```
time julia -t 2 mtjacobi.jl 8000
number of iterations : 40
the error : 1.9681077347290746e-5

real    0m15.390s
user    11m35.441s
sys     4m51.916s
$ time julia -t 4 mtjacobi.jl 8000
number of iterations : 20
the error : 2.3621495916454325e-5

real    0m5.400s
user    2m13.138s
sys     1m18.059s
$ time julia -t 8 mtjacobi.jl 8000
number of iterations : 39
the error : 1.7918058060438385e-5

real    0m5.400s
user    2m10.425s
sys     1m13.413s
```

Summary + Exercises

We covered §6.3.1 in the book of Wilkinson and Allen.
Because of its slow convergence, the Jacobi method is seldomly used.

Exercises:

1. Use mpi4py or MPI.jl for the parallel Jacobi method.
   Compare with the C version to demonstrate the correctness.
2. Use OpenMP to write a parallel version of the Jacobi method.
   Do you observe a better speedup than with MPI?
3. The power method to compute the largest eigenvalue of a matrix A uses the formulas $\mathbf{y} := A\mathbf{x}^{(k)}$; $\mathbf{x}^{(k+1)} := \mathbf{y}/\|\mathbf{y}\|$.
   Describe a parallel implementation of the power method.
4. Consider the formula for the total cost of the Jacobi method for an n-dimensional linear system with p processors.
   Derive an analytic expression for the optimal value of p.
   What does this expression tell about the scalability?