High-performance computing on distributed-memory architecture

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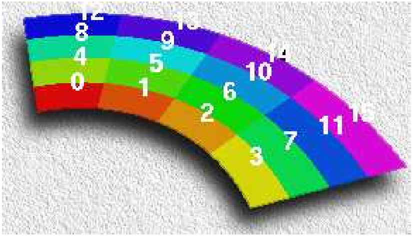
Outline

1. Overview of HPC
2. Introduction to MPI
3. Programming examples
4. High-level parallelization via DD



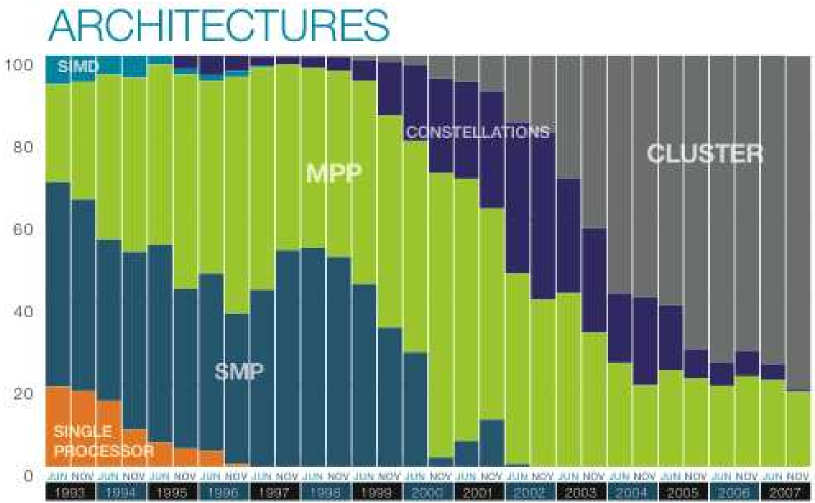
List of Topics

Motivation

- Nowadays, HPC refers to the use of parallel computers
- Memory performance is the No.1 limiting factor for scientific computing
  - size
  - speed
- Most parallel platforms have some level of distributed memory
  - distributed-memory MPP systems (tightly integrated)
  - commodity clusters
  - constellations
- Good utilization of distributed memory requires appropriate parallel algorithms and matching implementation

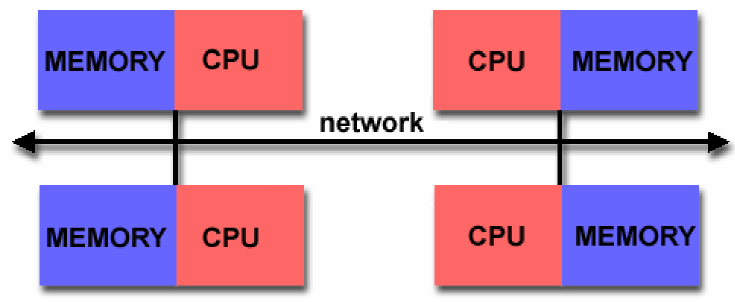
In this lecture, we will focus on distribued memory

Architecture development of Top500 list



http://www.top500.org

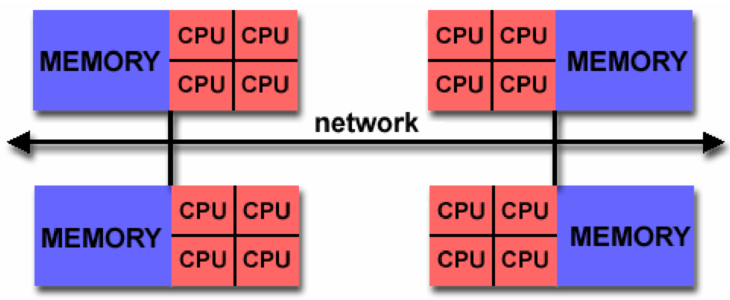
Distributed memory



A schematic view of distributed memory

Plot obtained from `https://computing.llnl.gov/tutorials/parallel_comp/`

Hybrid distributed-shared memory



A schematic view of hybrid distributed-shared memory

Plot obtained from `https://computing.llnl.gov/tutorials/parallel_comp/`

Main features of distributed memory

- Individual memory units share no physical storage
- Exchange of info is through explicit communication
- Messing passing is the de-facto programming style for distributed memory
- A programmer is often responsible for many details
  - identification of parallelism
  - design of parallel algorithm and data structure
  - breakup of tasks/data/subdomains
  - load balancing
  - insertion of communication commands

List of Topics

MPI (message passing interface)

MPI is a library standard for programming distributed memory

- MPI implementation(s) available on almost every major parallel platform (also on shared-memory machines)
- Portability, good performance & functionality
- Collaborative computing by a group of individual processes
- Each process has its own local memory
- Explicit message passing enables information exchange and collaboration between processes

More info: `http://www-unix.mcs.anl.gov/mpi/`

MPI basics

- The MPI specification is a combination of MPI-1 and MPI-2
- MPI-1 defines a collection of 120+ commands
- MPI-2 is an extension of MPI-1 to handle "difficult" issues
- MPI has language bindings for F77, C and C++
- There also exist, e.g., several MPI modules in Python (more user-friendly)
- Knowledge of entire MPI is not necessary

MPI language bindings

C binding

```
#include <mpi.h>

rc = MPI_Xxxxx(parameter, ... )
```

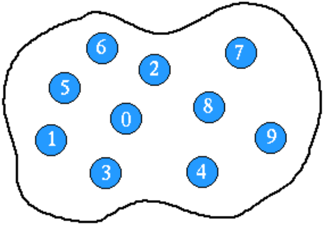
Fortran binding

```
include 'mpif.h'

CALL MPI_XXXXX(parameter,..., ierr)
```

MPI communicator

MPI_COMM_WORLD



- An MPI communicator: a "communication universe" for a group of processes
- `MPI_COMM_WORLD` – name of the default MPI communicator, i.e., the collection of all processes
- Each process in a communicator is identified by its rank
- Almost every MPI command needs to provide a communicator as input argument

MPI process rank

- Each process has a unique rank, i.e. an integer identifier, within a communicator
- The rank value is between 0 and `#procs-1`
- The rank value is used to distinguish one process from another
- Commands `MPI_Comm_size` & `MPI_Comm_rank` are very useful
- Example

```
int size, my_rank;
MPI_Comm_size (MPI_COMM_WORLD, &size);
MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

if (my_rank==0) {
   ...
}
```

MPI "Hello-world" example

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

int main (int nargs, char** args)
{
  int size, my_rank;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);
  printf("Hello world, I've rank %d out of %d procs.\n",
         my_rank,size);
  MPI_Finalize ();
  return 0;
}
```

MPI "Hello-world" example (cont'd)

- Compilation example: `mpicc hello.c`
- Parallel execution example: `mpirun -np 4 a.out`
- Order of output from the processes is not determined, may vary from execution to execution

```
Hello world, I've rank 2 out of 4 procs.
Hello world, I've rank 1 out of 4 procs.
Hello world, I've rank 3 out of 4 procs.
Hello world, I've rank 0 out of 4 procs.
```

The mental picture of parallel execution

The same MPI program is executed concurrently on each process

Process 0	Process 1	· · ·	Process P-1

Process 0:

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

int main (int nargs, char** args)
{
  int size, my_rank;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);
  printf("Hello world, I've rank %d out of %d procs.\n",
         my_rank,size);
  MPI_Finalize ();
  return 0;
}
```

Process 1:

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

int main (int nargs, char** args)
{
  int size, my_rank;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);
  printf("Hello world, I've rank %d out of %d procs.\n",
         my_rank,size);
  MPI_Finalize ();
  return 0;
}
```

Process P-1:

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

int main (int nargs, char** args)
{
  int size, my_rank;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);
  printf("Hello world, I've rank %d out of %d procs.\n",
         my_rank,size);
  MPI_Finalize ();
  return 0;
}
```

MPI point-to-point communication

- Participation of two different processes
- Several different types of send and receive commands
  - Blocking/non-blocking send
  - Blocking/non-blocking receive
  - Four modes of send operations
  - Combined send/receive

Standard MPI_send/MPI_recv

- To send a message

```
int MPI_Send(void *buf, int count, MPI_Datatype datatype,
             int dest, int tag, MPI_Comm comm);
```

- To receive a message

```
int MPI_Recv(void *buf, int count, MPI_Datatype datatype,
             int source, int tag, MPI_Comm comm,
             MPI_Status *status);
```

An MPI message is an array of data elements "inside an envelope"

- *Data*: start address of the message buffer, counter of elements in the buffer, data type
- *Envelope*: source/destination process, message tag, communicator

Example of MPI_send/MPI_recv

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

int main (int nargs, char** args)
{
  int size, my_rank, flag;
  MPI_Status status;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

  if (my_rank>0)
    MPI_Recv (&flag, 1, MPI_INT,
              my_rank-1, 100, MPI_COMM_WORLD, &status);

  printf("Hello world, I've rank %d out of %d procs.\n",my_rank,siz

  if (my_rank<size-1)
    MPI_Send (&my_rank, 1, MPI_INT,
              my_rank+1, 100, MPI_COMM_WORLD);

  MPI_Finalize ();
  return 0;
```

Example of MPI_send/MPI_recv (cont´d)

Process 0 Process 1 · · · Process P-1

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

int main (int nargs, char** args)
{
  int size, my_rank, flag;
  MPI_Status status;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

  if (my_rank>0)
    MPI_Recv (&flag, 1, MPI_INT,
              my_rank-1, 100, MPI_COMM_WORLD, &status);

  printf("Hello world, I've rank %d out of %d procs.\n",my_rank,size);

  if (my_rank<size-1)
    MPI_Send (&my_rank, 1, MPI_INT,
              my_rank+1, 100, MPI_COMM_WORLD);

  MPI_Finalize ();
  return 0;
}
```

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

int main (int nargs, char** args)
{
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  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

  if (my_rank>0)
    MPI_Recv (&flag, 1, MPI_INT,
              my_rank-1, 100, MPI_COMM_WORLD, &status);

  printf("Hello world, I've rank %d out of %d procs.\n",my_rank,size);

  if (my_rank<size-1)
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  MPI_Finalize ();
  return 0;
}
```
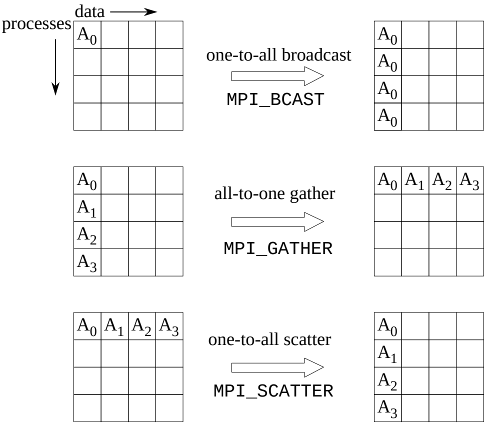

```
#include <stdio.h>
#include <mpi.h>

int main (int nargs, char** args)
{
  int size, my_rank, flag;
  MPI_Status status;
  MPI_Init (&nargs, &args);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

  if (my_rank>0)
    MPI_Recv (&flag, 1, MPI_INT,
              my_rank-1, 100, MPI_COMM_WORLD, &status);

  printf("Hello world, I've rank %d out of %d procs.\n",my_rank,size);

  if (my_rank<size-1)
    MPI_Send (&my_rank, 1, MPI_INT,
              my_rank+1, 100, MPI_COMM_WORLD);

  MPI_Finalize ();
  return 0;
}
```

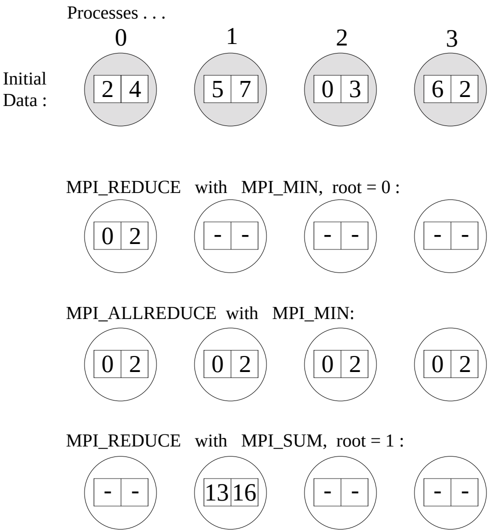
- Enforcement of ordered output by passing around a "semaphore", using MPI_send and MPI_recv
- Successful message passover requires a matching pair of MPI_send and MPI_recv

MPI collective communication

A collective operation involves *all* the processes in a communicator: (1) synchronization (2) data movement (3) collective computation



Collective communication (cont´d)



MPI example of collective communication

Inner-product between two vectors: $c = \sum_{i=1}^{n} a(i)b(i)$

```
MPI_Comm_size (MPI_COMM_WORLD, &num_procs);
MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

my_start = n/num_procs*my_rank;
my_stop = n/num_procs*(my_rank+1);

my_c = 0.;
for (i=my_start; i<my_stop; i++)
  my_c = my_c + (a[i] * b[i]);

MPI_Allreduce (&my_c, &c, 1, MPI_DOUBLE,
               MPI_SUM, MPI_COMM_WORLD);
```

List of Topics

Parallel programming overview

- Decide a "breakup" of the global problem
  - functional decomposition – a set of concurrent tasks
  - data parallelism – sub-arrays, sub-loops, sub-domains
- Choose a parallel algorithm (e.g. based on modifying a serial algorithm)
- Design local data structure, if needed
- Standard serial programming plus insertion of MPI calls

Calculation of π

Want to numerically approximate the value of π

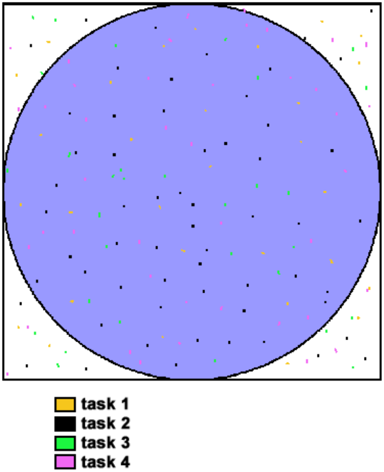
- Area of a circle: $A = \pi R^2$
- Area of the largest circle that fits into the unit square: $\frac{\pi}{4}$, because $R = \frac{1}{2}$
- Estimate of the area of the circle $\Rightarrow$ estimate of π
- How?
  - Throw a number of random points into the unit square
  - Count the percentage of points that lie in the circle by

$$\left((x-\frac{1}{2})^2 + (y-\frac{1}{2})^2\right) \leq \frac{1}{4}$$

  - The percentage is an estimate of the area of the circle
- $\pi \approx 4\,A$

Parallel calculation of π

```
num = npoints/P;
my_circle_pts = 0;

for (j=1; j<=num; j++) {
  generate random 0<=x,y<=1
  if (x,y) inside circle
    my_circle_pts += 1
}

MPI_Allreduce(&my_circle_pts,
              &total_count,
              1,MPI_INT,MPI_SUM,
              MPI_COMM_WORLD);

pi = 4.0*total_count/npoints;
```



The issue of load balancing

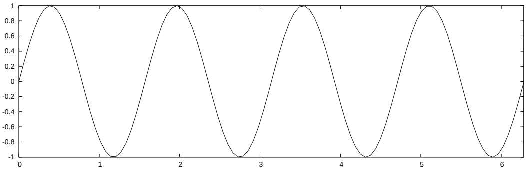
What if `npoints` is not divisible by `P`?

- Simple solution of load balancing

```
num = npoints/P;
if (my_rank < (npoints%P))
  num += 1;
```

- Load balancing is very important for performance
- Homogeneous processes should have as even disbribution of work load as possible
- (Dynamic) load balancing is nontrivial for real-world parallel computation

Example: 1D standard wave equation



Consider the 1D wave equation:

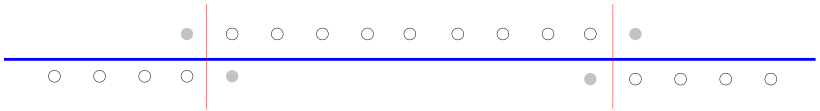
$$
\begin{aligned}
\frac{\partial^2 u}{\partial t^2} &= \gamma^2 \frac{\partial^2 u}{\partial x^2}, \quad x \in (0,1), \; t > 0, \\
u(0,t) &= U_L, \\
u(1,t) &= U_R, \\
u(x,0) &= f(x), \\
\frac{\partial}{\partial t} u(x,0) &= 0\,.
\end{aligned}
$$

Explicit FDM for 1D wave equation

Define time step Δt, spatial cell Δx, and $C = \gamma \Delta t / \Delta x$,

$$
\begin{aligned}
u_i^0 &= f(x_i), \quad i = 0, \ldots, n+1, \\
u_i^{-1} &= u_i^0 + \frac{1}{2} C^2 (u_{i+1}^0 - 2u_i^0 + u_{i-1}^0), \quad i = 1, \ldots, n \\
u_i^{k+1} &= 2u_i^k - u_i^{k-1} + C^2 (u_{i+1}^k - 2u_i^k + u_{i-1}^k), \\
&\qquad\qquad\qquad i = 1, \ldots, n, \ k \geq 0, \\
u_0^{k+1} &= U_L, \quad k \geq 0, \\
u_{n+1}^{k+1} &= U_R, \quad k \geq 0.
\end{aligned}
$$

Each processor computes on a subinterval



- The global domain is partitioned into subdomains
- Each subdomain has a set of inner points, plus 2 ghost points shared with neighboring subdomains
- First, u_i^{k+1} is updated on the inner points
- Then values on the leftmost and rightmost inner points are sent to the left and right neighbors
- Values from neighbors are received for the left and right ghost points

Multi-dimensional standard wave equation

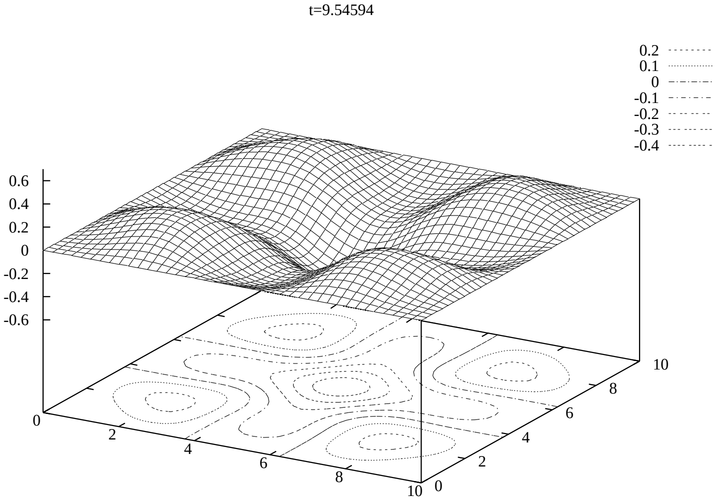
$$\frac{\partial^2 u}{\partial t^2} = \nabla \cdot \left(c^2(\mathbf{x})\nabla u\right) + f(\mathbf{x}, t)$$

- 2nd-order centered differences in time and space
- $\Rightarrow$ explicit scheme (point-wise update):

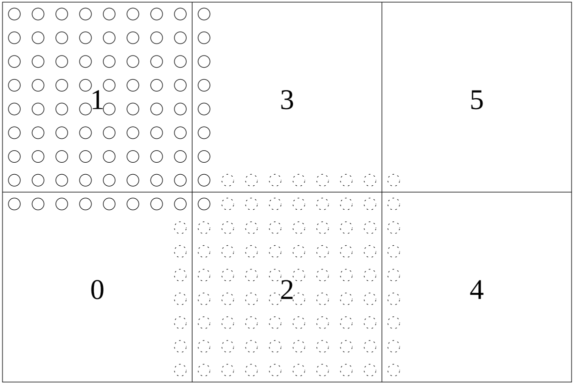
$$u_{i,j}^{k+1} = S(u_{i,j\pm1}^{k}, u_{i\pm1,j}^{k}, u_{i,j}^{k}, u_{i,j}^{k-1}, \mathbf{x}_{i,j}, t_k)$$

- Can compute all new $u_{i,j}^{k+1}$ values independently
- Parallelism arises from subdomain decomposition

Let us look at the parallel algorithm in 2D

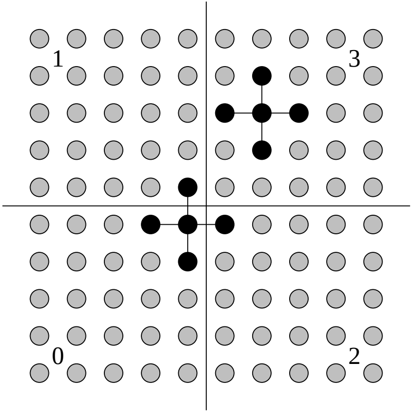


Partitioning of a rectangular 2D domain into subdomains



Each subdomain has a set of inner points, plus a set of ghost points shared with neighboring subdomains

Parallel algorithm for 2D wave equation

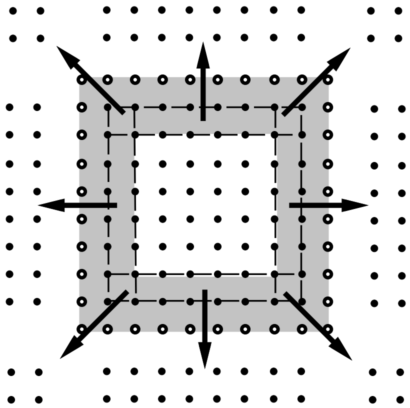


- First compute $u_{i,j}^{k+1}$ on inner points
- Then send point values to neighbors
- Then receive values at ghost points from neighbors

Python as an alternative to C for MPI programming

- MPI calls in C/Fortran are low level, easy to introduce bugs
- Python provides more high-level/Matlab-like programming
- Same logical steps as in the C code, but simpler syntax
- Python is slow, but fast enough to manage a few MPI calls

The pypar module



- Pypar (by O. Nielsen) offers a high-level interface to a subset of MPI
- Arbitrary Python objects can be sent via MPI
- Very efficient treatment of NumPy arrays
- Alternative tool: PyMPI (by P. Miller)

Python code snippets for communication

- Prepare the outgoing message:

```
upper_x_out_msg = u[nx-1,:,:]
```

  (efficient 2D array as slice reference)

- Exchange messages:

```
pypar.send(upper_x_out_msg, upper_x_neighbor_id,
           bypass=True)

pypar.receive(upper_x_neighbor_id, buffer=x_in_buffer,
              bypass=True)
```

- Extract the incoming message:

```
u[nx,:,:] = x_in_buffer
```

More detailed parallel Python code (1)

```
from RectPartitioner import partitioner  # generic!!

t = 0
while t <= tstop:
    t_old = t; t += dt

    # update all inner points (or call C/F77 for this):
    u[1:nx,1:ny] = -um2[1:nx,1:ny] + 2*um[1:nx,1:ny] +
      Cx2*(um[0:nx-1,1:ny] - 2*um[1:nx,1:ny] + um[2:nx+1,1:ny]) +
      Cy2*(um[1:nx,0:ny-1] - 2*um[1:nx,1:ny] + um[1:nx,2:ny+1]) +
      dt2*source(x[i], y[j], t_old);

    partitioner.update_internal_boundary (u)
```

More detailed parallel Python code (2)

```
def update_internal_boundary (self, solution_array):
    # communicate in the x-direction first
    if lower_x_neigh>-1:
        self.out_lower_buffers[0] = solution_array[1,:]
        pypar.send(self.out_lower_buffers[0], lower_x_neigh,
                   use_buffer=True, bypass=True)

    if upper_x_neigh>-1:
        self.in_upper_buffers[0] =
        pypar.receive(upper_x_neigh, buffer=self.in_upper_buffer[0]
                      bypass=True)
        solution_array[nx,:] = self.in_upper_buffers[0]
        self.out_upper_buffers[0] = solution_array[nx-1,:]
        pypar.send(self.out_upper_buffers[0], upper_x_neigh,
                   use_buffer=True, bypass=True)

    if lower_x_neigh>-1:
        self.in_lower_buffers[0] =
        pypar.receive(lower_x_neigh, buffer=self.in_lower_buffer[0]
                      bypass=True)
        solution_array[0,:] = self.in_lower_buffers[0]

    # communicate in the y-direction afterwards
```

Generic skeleton of PDE solvers

- Nonlinear PDEs: a series of linearized problems per time step
- A time stepping scheme for the temporal discretization
- At each time step: spatial discretization on a computational mesh $\mathcal{T}$
- Explicit schemes: point-wise update (inherent parallelism)
- Implicit schemes: need to solve *linear systems* $\mathbf{Ax} = \mathbf{b}$

Direct solvers of $\mathbf{Ax} = \mathbf{b}$ are hard to parallelize, however, many iterative Solvers are well suited for parallel computing

Jacobi iteration: slow, but easy to parallelize

$$\mathbf{A} = \{a_{ij}\}, \quad x_i^k = \left(b_i - \sum_{j<i} a_{ij} x_j^{k-1} - \sum_{j>i} a_{ij} x_j^{k-1} \right) / a_{ii}$$

- A new x_i^k value only depends on old x_i^{k-1} values
- $\Rightarrow$ The values x_i^k can be updated concurrently!
- Same parallelization strategy as for the explicit PDE solvers:
  - Each processor updates all its inner points
  - Communication needed between neighbors for updating ghost boundary points

Krylov subspace solvers: Conjugate Gradients

Suitable for symmetric and positive definite matrices
$(\mathbf{A}^T = \mathbf{A},\ \mathbf{v}^T\mathbf{A}\mathbf{v} > 0,\ \forall \mathbf{v} \neq 0)$

Initially: $r = b - Ax$, $p = r$, $\pi^0_{r,r} = (r,r)$
Iterations:

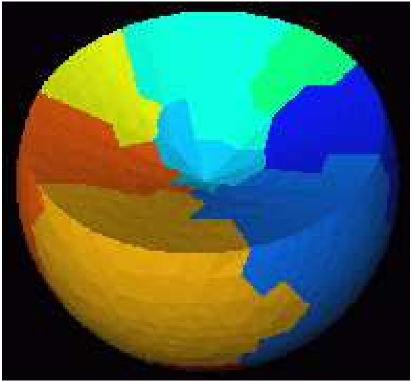
$w = Ap$	*matrix-vector product*
$M^{-1}w = w$	*solve preconditioning system*
$\pi_{p,w} = (p,w)$	*inner product*
$\xi = \pi^0_{r,r}/\pi_{p,w}$	
$x = x + \xi p$	*vector addition*
$r = r - \xi w$	*vector addition*
$\pi^1_{r,r} = (r,r)$	*inner product*
$\beta = \pi^1_{r,r}/\pi^0_{r,r}$	
$p = r + \beta p$	*vector addition*
$\pi^0_{r,r} = \pi^1_{r,r}$	

Observations

- Computational kernels of Krylov subspace solvers:
  - vector additions
  - inner products
  - matrix-vector product
- Parallelization of Krylov solvers thus needs
  - parallel vector addition
  - parallel inner product
  - parallel matrix-vector product
  - (parallel preconditioner)

Subdomain-based parallelization

Global domain $\Omega \longrightarrow \{\Omega_s\}_{s=1}^{P}$, global grid $\mathcal{T} \longrightarrow \{\mathcal{T}_s\}$, internal boundary of Ω_s: $\partial\Omega_s \backslash \partial\Omega$



Distributed matrices and vectors

- Each processor is assigned with a subdomain Ω_s and the associated subdomain mesh $\mathcal{T}_s$
- Each processor *independently* carries out spatial discretization on $\mathcal{T}_s$, giving rise to $\mathbf{A}_s$ and $\mathbf{b}_s$ (no communication needed)
- A global matrix $\mathbf{A}$ is distributed as $\{\mathbf{A}_s\}_{s=1}^{P}$
- A global vector $\mathbf{b}$ is distributed as $\{\mathbf{b}_s\}_{s=1}^{P}$
- The rows of $\mathbf{A}$ are distributed
- Each subdomain is responsible for a few rows in $\mathbf{A}$

Distributed matrices and vectors; FDM

- Subdomains arise from dividing the mesh points
- Each subdomain owns its computational points exclusively
- Layer(s) of ghost boundary points around each subdomain
- Rows of $\mathbf{A}_s$ correspond to the computational points in Ω_s, no overlap

Distributed matrices and vectors; FEM

- Denote the global finite element mesh by $\mathcal{T}$
- Mesh partitioning distributes the elements
- Each subdomain is a subset of the elements in $\mathcal{T}$
- Rows of $\mathbf{A}_s$ may overlap between neighbors
- If there's one layer of overlapping elements between neighbors, points on the internal boundaries work as ghost points (as usual)

Parallel vector addition

Global operation:

$$\mathbf{w} = \mathbf{u} + \mathbf{v}$$

Parallel implementation:

- $\mathbf{w}_s = \mathbf{u}_s + \mathbf{v}_s$ on each subdomain
- Only distributed vectors are involved
- No communication is needed

Parallel inner product

Global operation:

$$c = \mathbf{u} \cdot \mathbf{v} = \sum u_i \, v_i \quad i \in \text{ all points in } \mathcal{T}$$

Parallel implementation:

- Partial result on subdomain Ω_s:
  $c_s = \sum u_{s,i} v_{s,i} \quad i \in$ computational points in $\mathcal{T}_s$
- Global add: $c = c_1 + c_2 + \ldots + c_P$
- All-to-all communication (`MPI_Allreduce`) $\Rightarrow$ c is available on all subdomains

Parallel matrix-vector product

Global operation:

$$\mathbf{v} = \mathbf{A}\mathbf{u}$$

Parallel implementation:

- $\mathbf{v}_s = \mathbf{A}_s\mathbf{u}_s$ on Ω_s
- Ghost points in $\mathbf{v}_s$ have to ask neighbors for values
- One-to-one communication between each pair of neighboring subdomains (`MPI_Send`/`MPI_Recv`)

Some remarks

Domain partitioning $\Rightarrow$ data decomposition $\Rightarrow$ work division $\Rightarrow$ parallelism

- Linear algebra operations in an implicit PDE solver are parallelized using subdomains
- All matrices and vectors are distributed according to the subdomain partitioning $\{\Omega_s\}$
- No global matrices and vectors are stored on a single processor
- Work on Ω_s:
  - Mostly serial operations on subdomain matrices/vectors
  - Communication is needed between chunks of serial operations

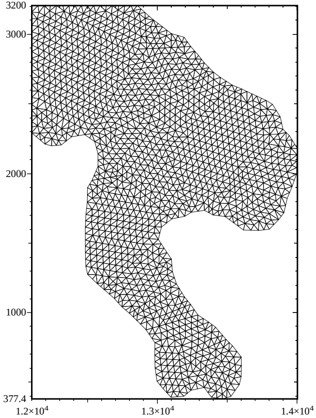
Many libraries for parallel linear algebra

Some parallel libraries for linear algebra and linear systems

- ACTS (tools collection, unified interfaces)
- ScaLAPACK (F77)
- PETSc (C)
- Trilinos (C++)
- UG (C)
- A++/P++ (C++)
- Diffpack (C++)

Finite element mesh partitioning can be easy or difficult

- When a global mesh $\mathcal{T}$ exists for Ω, domain partitioning reduces to mesh partitioning
- For *structured* global box-shaped meshes, mesh partitioning is quite easy
- For *unstructured* finite element meshes, mesh partitioning is non-trivial



Objectives for partitioning

Objectives

- Subdomains have approximately the same amount of elements and points
- Low cost of inter-subdomain communication:
  - # neighbors per subdomain is small
  - # shared points between neighbors is small

Partitioning an unstructured finite element mesh is a nontrivial load balancing problem

Overview of partitioning algorithms

- Geometric algorithms (using mesh point coordinates):
  - Recursive bisections
  - Space-filling curve approaches
- Graph-based algorithms (using connectivity info):
  - Greedy partitioning
  - Spectral partitioning
  - Multilevel partitioning
- Best choice: multilevel graph-based partitioning algorithms (Metis/ParMetis package)

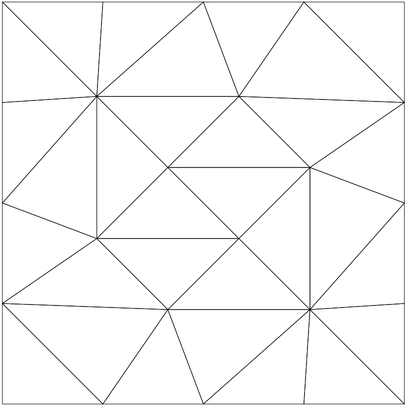
Graph-based partitioning algorithms

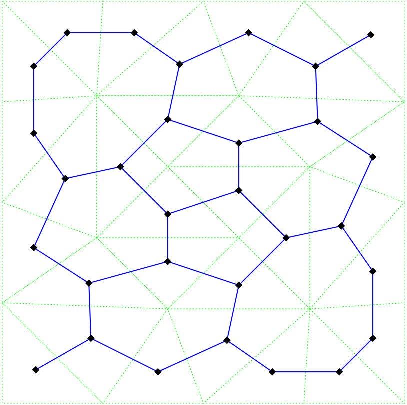
- Graph partitioning is a well-studied problem, many algorithms exist
- Mesh partitioning is similar to graph partitioning (However, not identical!)
- Easy to translate a mesh to a graph
- The graph partitioning result is projected back to the mesh to produce the subdomains

The graph partitioning problem

- A graph $G = (V, E)$ is a set of vertices and a set of edges, both with individual weights, one edge connects two vertices
- P-way partitioning of G: divide V into P subsets of vertices, V_1, V_2, ..., V_P, where
  - all subsets have (almost) the same summed vertex weights
  - summed weights of edges that stride between the subsets—**edge cut**—is minimized

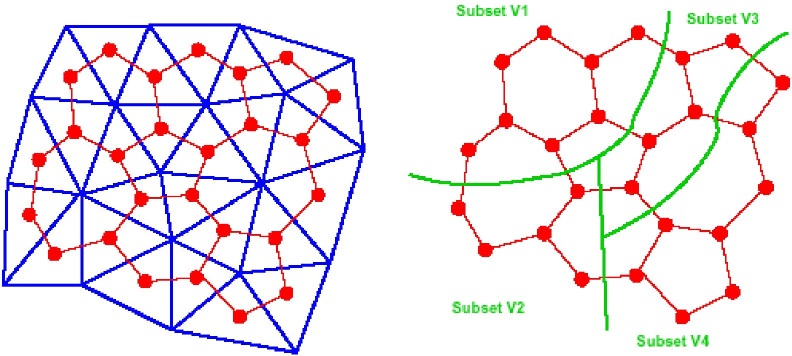
From a mesh to a graph





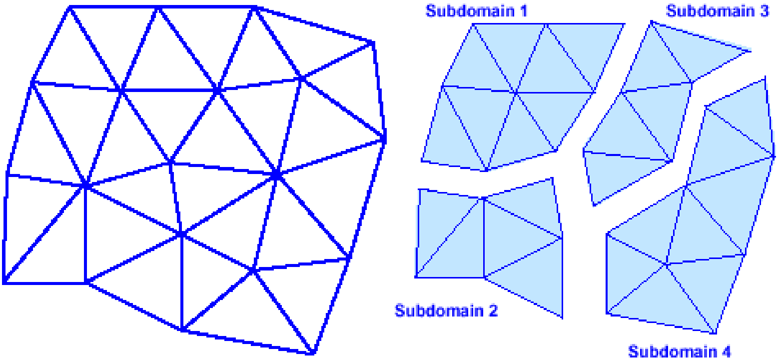
Each element becomes a vertex in the resulting graph. Whether or not an edge between two vertices depends on "neighbor-ship",

A partitioning example



A dual graph is first built on the basis of the mesh. The graph is then partitioned.

A partitioning example (cont'd)



The graph partitioning result is mapped back to the mesh and gives rise to the subdomains.

Multilevel graph partitioning

Efficient and flexible with three phases:

- Coarsening phase: a recursive process that generates a sequence of subsequently coarser graphs $G^0, G^1, \ldots G^m$
- Initial partition phase: the coarsest graph G^m is divided into P subsets
- Uncoarsening phase: the partitions of G^m is projected backward to G^0, while the partitions are adjusted for improvement along the way

Examples of public-domain software: `Jostle` & `Metis`

List of Topics

About parallel PDE solvers

- Programming a new PDE solver can be relatively easy
  - start with partitioning the global mesh $\Rightarrow$ subdomain meshes
  - parallel discrtetization $\Rightarrow$ distributed matrices/vectors
  - use parallel linear algebra libraries (PETSc, Trilinos, etc.)
- Parallelizing an existing serial PDE can be hard
  - low-level loops may not be readily parallelizable
- Special numerical components may also be hard to parallelize
  - not available in standard parallel libraries

Need a user-friendly parallelization for the latter two situations

Programming objectives

A general and flexible programming framework is desired

- extensive reuse of serial PDE software
- simple programming effort by the user
- possibility of hybrid features in different local areas

Mathematical methods based on domain decomposition

- Global solution domain is decomposed into subdomains:

$$\Omega = \cup_{s=1}^{P} \Omega_s$$

- Solving a global PDE on $\Omega \Rightarrow$ iteratively and repeatedly solving the smaller subdomain problems on Ω_s, $1 \leq s \leq P$
- The artificial condition on the internal boundary of each Ω_s is updated iteratively
- The subdomain solutions are "patched together" to give a global approximate solution

More on mathematical DD methods

- Efficient methods for solving PDEs
- Flexible treatment of local features in a global problem
- Many variants of mathematical DD methods
  - overlapping DD
  - non-overlapping DD
- Work as both stand-alone PDE solver and preconditioner
- Well suited for parallel computing

Alternating Schwarz algorithm

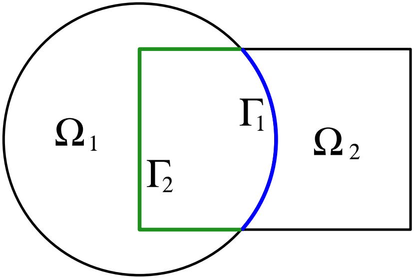
The very first DD method for

$$
\begin{aligned}
-\nabla^2 u &= f \quad \text{in } \Omega = \Omega_1 \cup \Omega_2 \\
u &= g \quad \text{on } \partial\Omega
\end{aligned}
$$

For $n = 1, 2, \ldots$ until convergence

$$
\begin{aligned}
-\nabla^2 u_1^n &= f_1 \quad \text{in } \Omega_1, \\
u_1^n &= g \quad \text{on } \partial\Omega_1 \backslash \Gamma_1, \\
u_1^n &= u_2^{n-1}|_{\Gamma_1} \quad \text{on } \Gamma_1.
\end{aligned}
$$

$$
\begin{aligned}
-\nabla^2 u_2^n &= f_2 \quad \text{in } \Omega_2, \\
u_2^n &= g \quad \text{on } \partial\Omega_2 \backslash \Gamma_2, \\
u_2^n &= u_1^n|_{\Gamma_2} \quad \text{on } \Gamma_2.
\end{aligned}
$$



Additive Schwarz method

- One particular overlapping DD method for many subdomains
- Original PDE in Ω: $L_\Omega u_\Omega = f_\Omega$ (i.e., $u_\Omega = L_\Omega^{-1} f_\Omega$)
- Additive Schwarz iterations $\Rightarrow$ concurrent work all Ω_s:

$$u_{\Omega_s}^{k+1} = L_{\Omega_s}^{-1} f_{\Omega_s}(u_\Omega^k) \text{ in } \Omega_s,$$

$$u_{\Omega_s}^{k+1} = u_\Omega^k \text{ on } \partial\Omega_s,$$

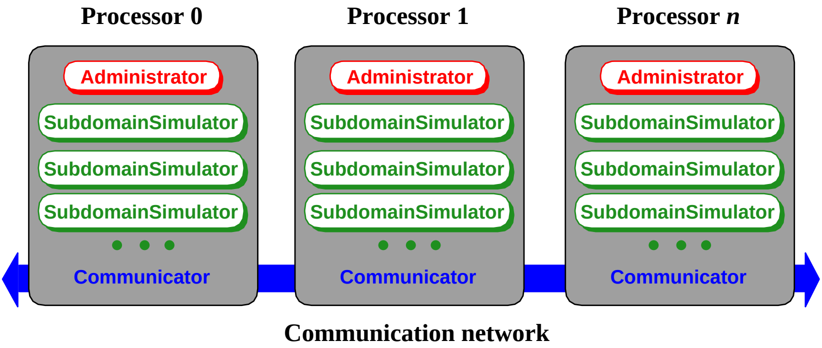
where u_Ω^k is a "global composition" of latest subdomain approximations $\{u_{\Omega_s}^k\}$

  - during each iteration a subdomain independently updates its local solution
  - exchange of local solutions between neighboring subdomains at end of each iteration

More on additive Schwarz

- Simple algorithmic structure
- Straightforward for parallelization
  - serial local discretization on Ω_s
  - serial subdomain solver on Ω_s
  - communication needed to compose the global solution
- The numerical strategy is *generic*
- Can be implemented as a parallel library
- Possibility of having different features among subdomains
  - different mathematical models
  - different numerical methods
  - different mesh types and resolutions
  - different serial code

A generic software framework



- Object-oriented programming
- `Administrator`, `SubdomainSolver` and `Communicator` are programmed as generic classes *once and for all*
- Re-usable for parallelizing many different PDE solvers
- Can hide communication details from user

Parallelizing a serial PDE solver in C++

- An existing serial PDE solver as `class MySolver`
- New implementation work task 1:
  `class My_SubdSolver : public SubdomainSolver, public MySolver`
  - Double inheritance
  - Implement the generic functions of `SubdomainSolver` by calling/extending functions of `MySolver`
  - Mostly code reuse, little new programming
- New implementation work task 2:
  `class My_Administrator : public Administrator`
  - Extend `Administrator` to handle problem-specific details
  - Mostly "cut and paste", little new programming
- Both implementation tasks are small and easy

Summary on programming parallel PDE solvers

- Subdomains give a natural way of parallelizing PDE solvers
- Discretization is embarrasingly parallel $\Rightarrow$ distributed matrices/vectors
- Linear-algebra operations are easily parallelized
- Additive Schwarz approach may be useful if
  - special parallel preconditioners are desired, and/or
  - high-level parallelization of legacy PDE code is desired, and/or
  - a parallel hybrid PDE solver is desired
- Most of the parallelization work is generic
- Languages like C++ and Python help to produce user-friendly parallel libraries

Concluding remarks

- Distributed memory is present in most parallel systems
- Message passing is used to program distributed memory
  - full user control
  - good performance
  - however many low-level details
- Use existing parallel numerical libraries if possible
- High-level parallelization is achievable
- Hybrid parallelism is possible by using SMP/Multicore for each subdomain