A Quick Introduction to Parallel computing with MPI

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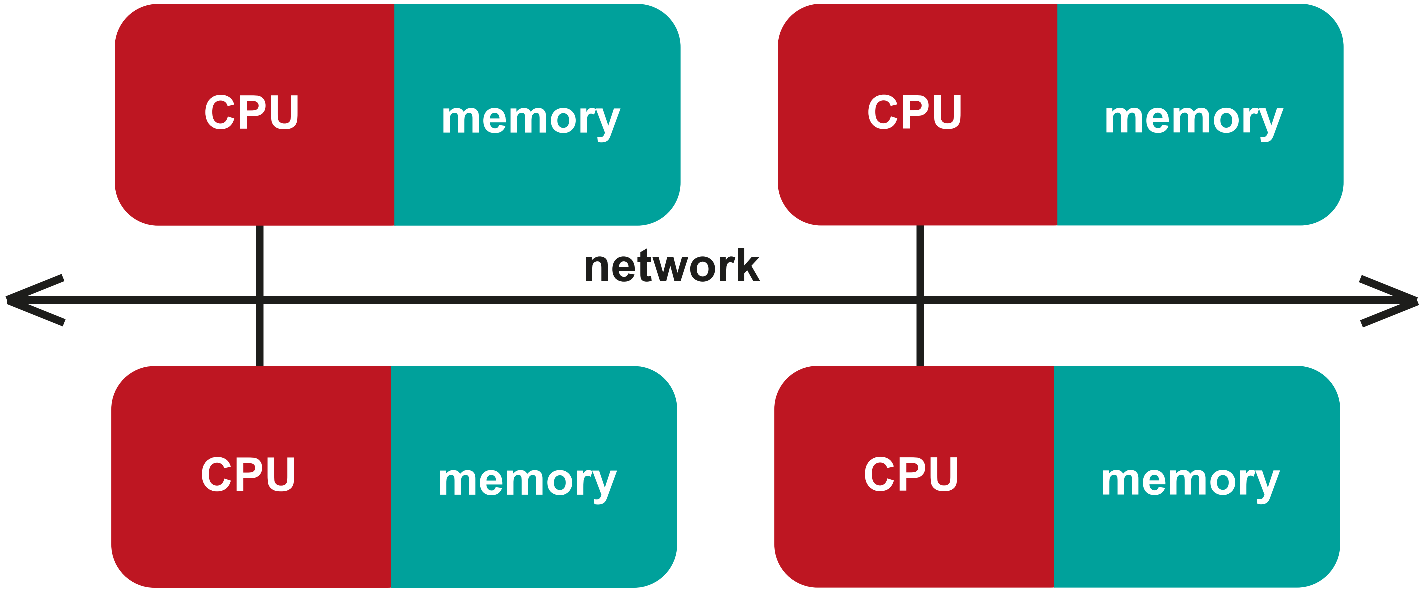
Why go parallel?

- Save time (faster rate of computation).
- Solve larger problems that don't fit on memory of single machine.
- Do different things at the same time.
- Make better use of computing resources (e.g. parallel hardware).

- Increasingly used outside of traditional physics/chemistry simulations (e.g. big data).

What is MPI?

- **Message Passing Interface** - the standard library specification for message passing programs.
- Distributed memory programming model:



- Common implementations: **OpenMPI**, MPICH, Intel MPI, …
- Usually used with C, C++ or Fortran.
- Download from: **http://www.open-mpi.org/**

Fundamentals

- All processes execute *exactly the same code*.
- Each process can access only its own memory / variables.
- Code must be specially written with this in mind.

Demo problem: 1D heat equation

- Solve

$$u_t = k u_{xx}, \qquad u(x,0) = g(x) = \mathrm{e}^{-100x^2}$$

on $D = \{ -1 < x < 1,\ t > 0 \}$.

- Discretise D with a grid

$$x_j = -1 + j\Delta x, \qquad t_n = n\Delta t, \qquad U^{j,n} = u(x_j, t_n)$$

- Use a simple explicit finite-difference scheme

$$\frac{U^{j,n+1} - U^{j,n}}{\Delta t} = k \frac{U^{j-1,n} - 2U^{j,n} + U^{j+1,n}}{(\Delta x)^2}$$

$$\Longrightarrow \qquad U^{j,n+1} = U^{j,n} + \underbrace{\frac{k\Delta t}{(\Delta x)^2}}_{\mu} \left(U^{j-1,n} - 2U^{j,n} + U^{j+1,n} \right)$$

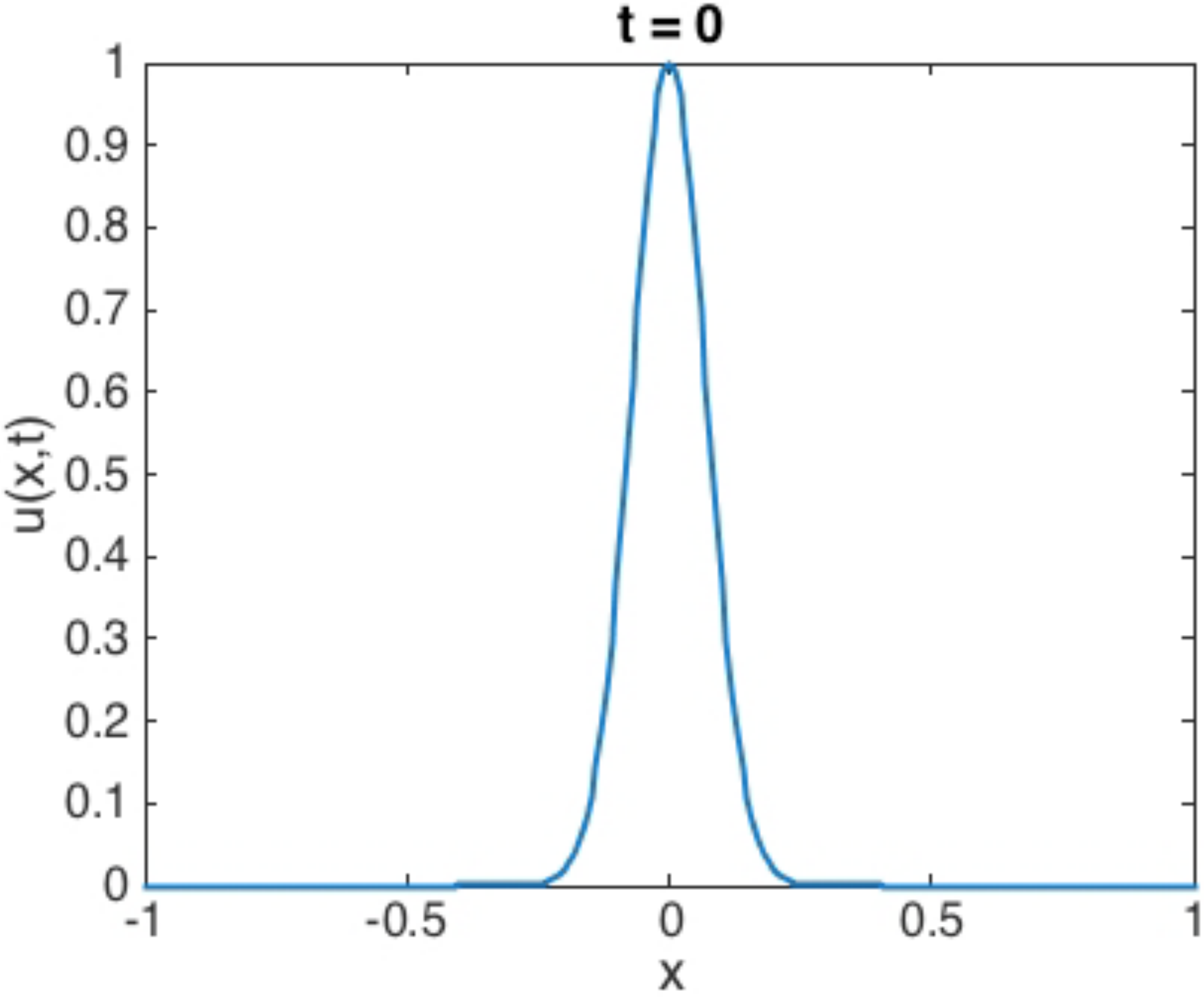
- Boundary conditions

$$U^{0,n} = U^{2,n}, \quad U^{nx+1,n} = U^{nx-1,n}$$

Exact solution

$$u(x,t) = \sqrt{\frac{a}{a+4kt}} \exp\left(-\frac{x^2}{a+4kt}\right)$$

$$a = \tfrac{1}{100}, \;\; k = 1$$



Demo code

- **`heat.cpp`** (C++) or **`heat.f90`** (Fortran 90)
- To run from a terminal:

```
> mpic++ heat.cpp              > mpif90 heat.f90
> mpirun -np 2 ./a.out         > mpirun -np 2 ./a.out
```

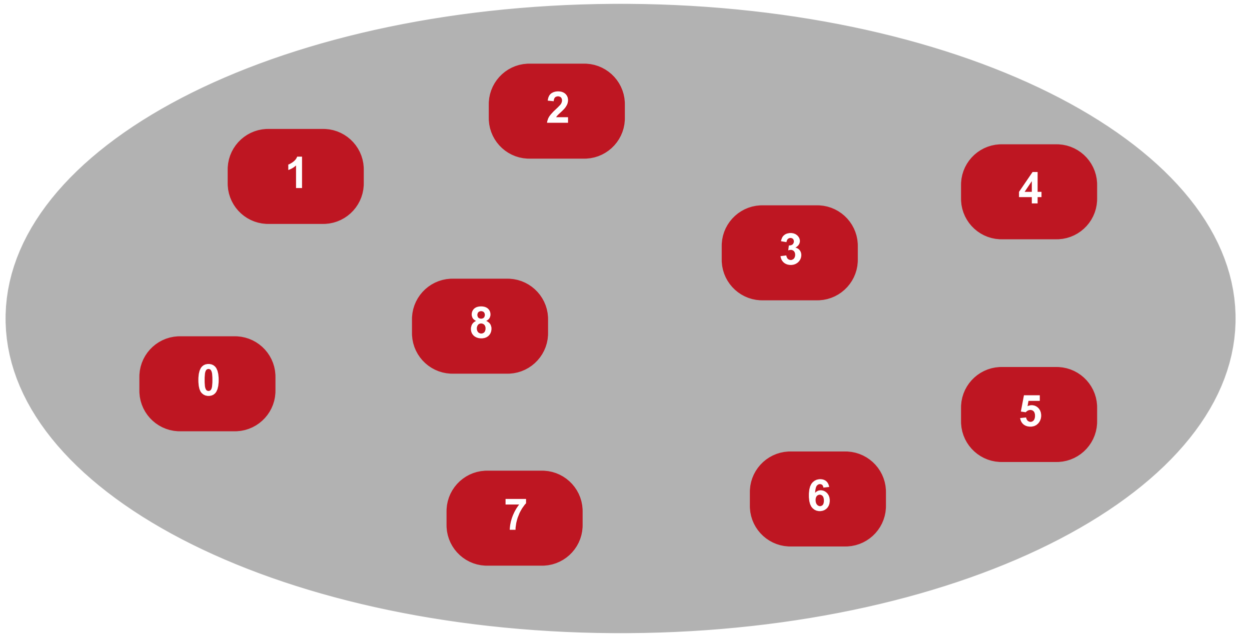
- On the maths network, the path is `/usr/lib64/openmpi/bin/`

- Main differences between MPI in C++ and Fortran:

  1. C++ is case sensitive (e.g. `MPI_Comm_size`).
  2. Fortran subroutines all have an extra output argument `ierr`.
  3. Special types like `MPI_Comm` are all just `integer` in Fortran.
  4. Some arguments need to be *references* in C++.
  5. Some defined constants like `MPI_DOUBLE` are different.

Initialising MPI

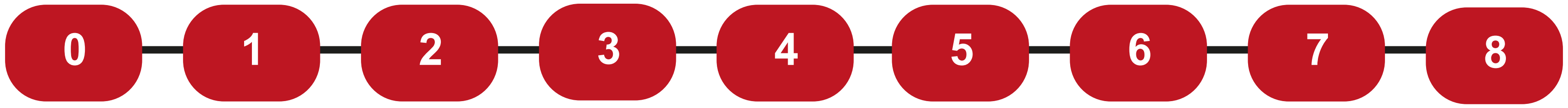
- **`#include <mpi.h>`** - include file, always required.
- **`MPI_Init`**`(NULL, NULL)` - always required, call first and only once.
- **`MPI_Finalize()`** - must be last MPI call.



- **`MPI_Comm_size`**`(MPI_COMM_WORLD, &nProcs)` - returns the number of processes in the global “communicator”.
- **`MPI_Comm_rank`**`(MPI_COMM_WORLD, &myRank)` - returns the “rank” of the current process. - *this tells you your identity.*

Creating a virtual topology

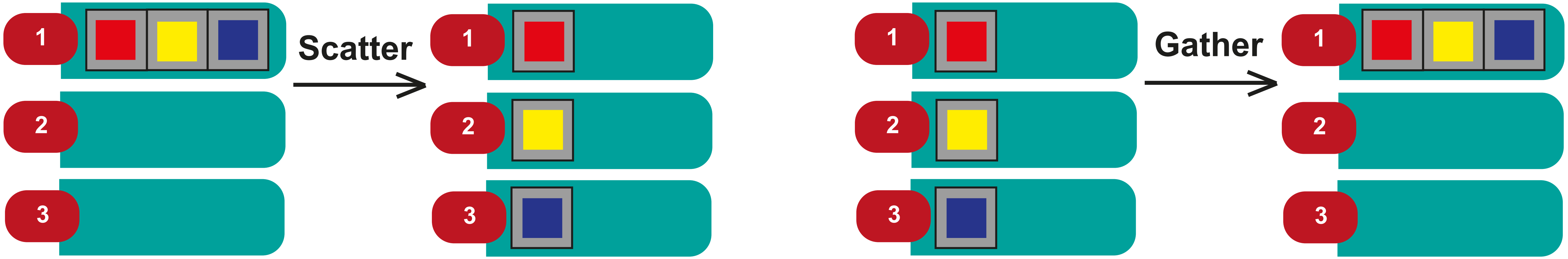
- A “communicator” is a group of processes that can communicate with each other. We use it to define a “virtual topology”.



- **MPI_Cart_create**`(MPI_COMM_WORLD,n,dims,periods,`
  `reorder,&comm)`
  - make a *Cartesian* communicator `comm` with `n` directions, where:
    - `dims` - number of processes in each direction;
    - `periods` - whether periodic boundaries in each direction;
    - `reorder` - whether ranking may be reordered.
- **MPI_Comm_rank**`(comm,&myRank)` - get rank *in this communicator*.
- **MPI_Cart_shift**`(comm,dirn,displ,&prvRank,&nxtRank)`
  - return the ranks of nearby processes in the coordinate direction `dirn`, at distance `displ` away.

Collective communications

- Each process needs different initial conditions: we create a global `xGlob` array in process 0, then distribute chunks to the others.
- **`MPI_Scatter`**`(&sendbuf, sendcnt, sendtype, &recvbuf,recvcnt,recvtype,root,comm)`
  - `root` is the rank of the sender, `sendbuf` is the global array, `recvbuf` is the local one.



- **`MPI_Gather`**`(&sendbuf, sendcnt, sendtype, &recvbuf,recvcnt,recvtype,root,comm)`
  - the inverse of `MPI_Scatter`: we use it at the end to output `u`.

Point-to-point communications

- **MPI_Send**`(&buf,count,datatype,dest,tag,comm)` - send from the buffer `buf` (with `count` values) to rank `dest`.

- **MPI_Recv**`(&buf,count,datatype,source,tag,comm,&stat)` - receive `count` values in the buffer `buf` from rank `source`.

  - These are “blocking” operations:
    - `MPI_Send` returns when `buf` is ready for re-use. (This doesn’t mean that the message has been received; it may be stored in a “system buffer”.)
    - `MPI_Recv` returns when the requested data has reached the receiving `buf` and can be used.

Point-to-point communications

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- a message can only be received if its `tag` (an integer) matches that in the `MPI_Recv` statement (or if it is set to `MPI_ANY_TAG`).

- the structure `stat` contains the source of the message and the tag: `stat.MPI_SOURCE` and `stat.MPI_TAG`.

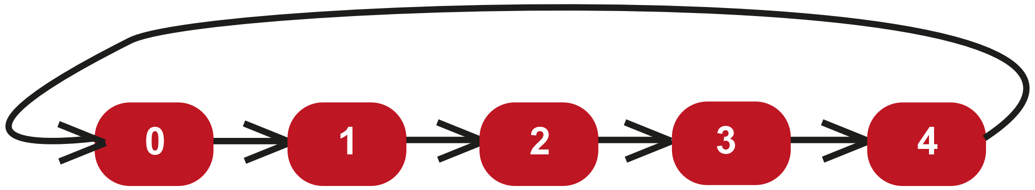
Things to be aware of

- There is no requirement that each `MPI_Send` is matched by an equivalent `MPI_Recv` (or alternative command).
  - There is *no overtaking*: if two messages are send from the same sender to the same destination, and both match an `MPI_Recv` statement, then the first message to be sent will be received first.
  - If two processes A and B both send messages to process C that match a single receive statement, then *only one* of the sends will complete.
- A process can get *stuck* on an `MPI_Recv` if no corresponding message is sent.

Deadlock!

- It is possible to reach "deadlock" where two (or more) processes are each waiting for the other to send or receive.
- For example, suppose there is a *circular* topology and we call:

```
 …
MPI_Send(&a,1,MPI_INT,nxtRank,comm);
MPI_Recv(&b,1,MPI_INT,prvRank,comm,&stat);
…
```



- This is unsafe; if the system buffer runs out of memory (not under our control), then all of the processes could be stuck waiting to send.
- We can see this if we use the "synchronous send" `MPI_Ssend`, which waits until the destination process has started to receive the message before returning.

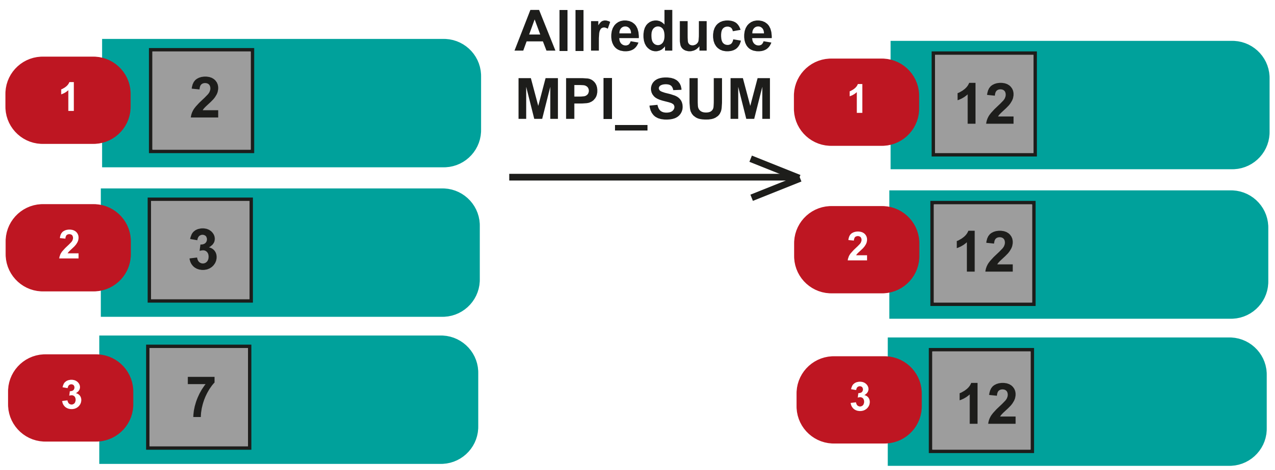
Collective computations

- MPI has routines for collective computation, or "reduction".
- **MPI_Allreduce**(&sendbuf,&recvbuf,count,datatype,
  op,comm)

  - perform the global operation op using sendbuf from each process, and broadcast the overall result to every recvbuf.

- Operations include MPI_SUM, MPI_PROD, MPI_MAX, MPI_MIN, …

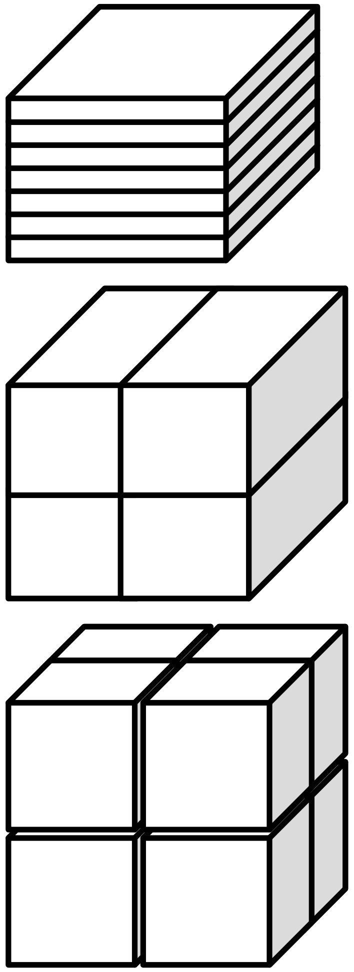
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-1}^{1} u\,\mathrm{d}x = \int_{-1}^{1} k u_{xx}\mathrm{d}x = k\left[u_x\right]_{-1}^{1} = 0$$



Timing

- `MPI_Wtime()` - returns wall-clock time on the individual processor.

- **Improving speed/scaling with number of processors:**
  - increase fraction of program that can be parallelized;
  - balance the workload;
  - minimize communication time (decrease both amount of data and number of calls);
  - use collective communications wherever possible.



Further reading

- A useful tutorial and reference for other commands:
  https://computing.llnl.gov/tutorials/mpi/
- Another tutorial (more advanced topics) with examples:
  http://mpitutorial.com
- The official standard:
  http://mpi-forum.org/docs/docs.html