Programming of Parallel Computers, 2014

Course introduction

Jarmo Rantakokko
Dimitar Lukarski
Magnus Grandin
Liu Jing

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Parallel Computers

Range of parallel computers:

- Multi-core processor (2-16 cores/processor)
- Multi-processor PC (2-8 processors)
- Servers (up to 64 processors)
- PC-Cluster (multiple PCs, 100's-1000's procs)
- Integrated parallel computers (1000's procs)
- Supercomputers (100,000's procs, top10)
- GRIDs (Networks, e.g., LHC Grid 140 sites)
- Internet (1,000,000’s procs)

- SETI@home (setiathome.berkeley.edu)

Distributed computing software runs as a screensaver, making use of processor time that would otherwise be unused. Has 1,300,000 users running over 3,300,000 processors for a compute power over 1 PetaFlops (10^{15} arithmetic ops per sec)

- Folding@home
- FightMalaria@home
- DrugDiscovery@home
- Neurona@home
- etc

Parallel Computers at UU

Intel iPSC/2 (Installed 1987)

- 32 processors, Intel i386, 16 MHz
- 32 x 4 Mbyte RAM

=> 32 x 16 MFlop/s = 0.512 GigaFlop/s

Today:

Quad-Core Laptop
384 core GPU

4 core mobile

2 processor x 6-Core
1024 core GPU

Uppsala University: Tintin (2012)

- 160 nodes x 2 proc x 8 cores = 2560 cores
- QDR Inifiband interconnect (integrated network)
- AMD Opteron 6220, 3GHz
- Peak performance 30.7 TeraFlop/s
- Total memory 10.2 TeraByte RAM

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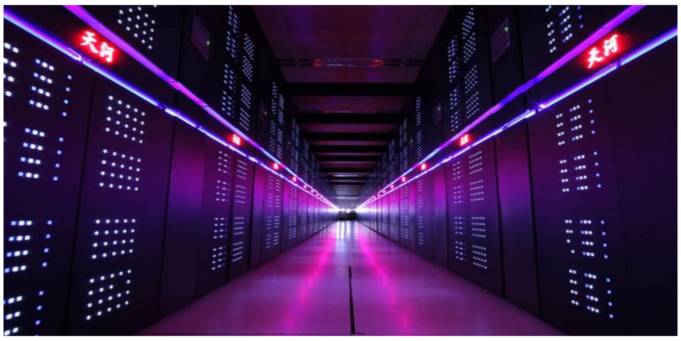
Tianhe-2 (1:st in Top 500, Nov 2013)

- National Super Computer Centre in Guangzhou, China
- 3.12 million cores, Intel Xeon processors
- Power consumption 17.8 MW (eq 6000 houses)
- 1024 TeraByte RAM
- 55 PetaFlop/s peak performance
- Cost: $390.000.000



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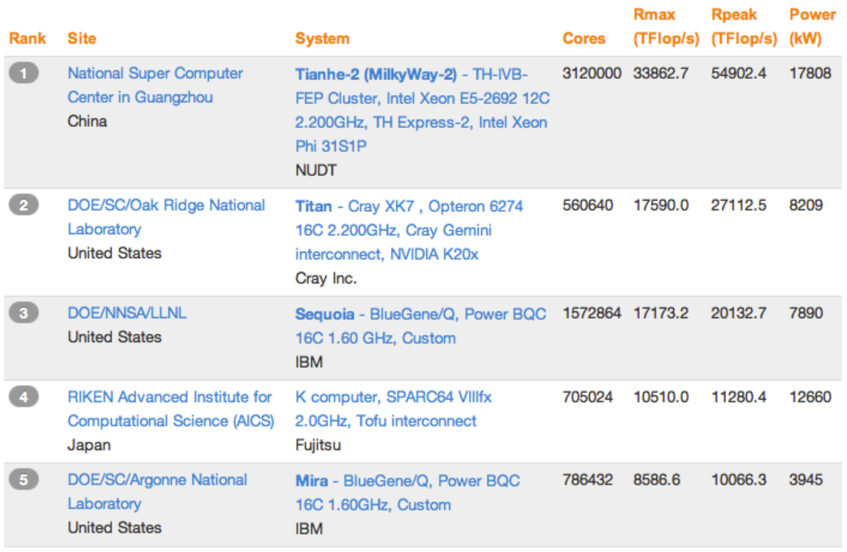
www.top500.org

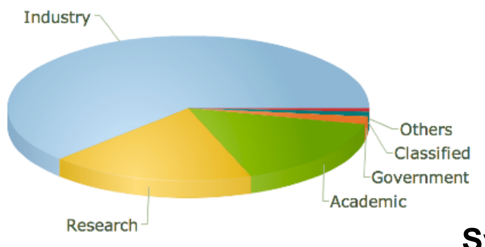


Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3120000	33862.7	54902.4	17808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560640	17590.0	27112.5	8209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1572864	17173.2	20132.7	7890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705024	10510.0	11280.4	12660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786432	8586.6	10066.3	3945

Sweden

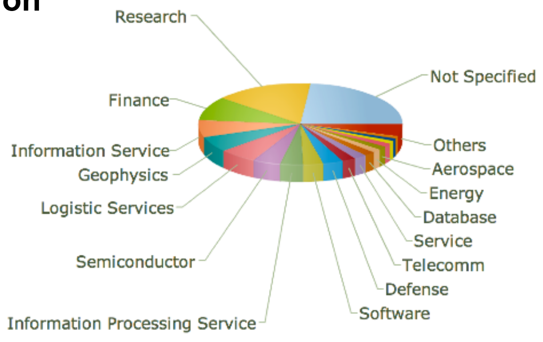
Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
79	National Supercomputer Centre (NSC) Sweden	**Triolith** - Cluster Platform SL230s Gen8, Xeon E5-2660 8C 2.200GHz, Infiniband FDR Hewlett-Packard	25,376	407.2	446.6	519
170	KTH - Royal Institute of Technology Sweden	**Lindgren** - Cray XE6, Opteron 12 Core 2.10 GHz, Custom Cray Inc.	36,384	237.2	305.6	
259	Electronic Industry Sweden	Cluster Platform 3000 BL460c Gen8, Xeon E5-2670 8C 2.600GHz, 10G Ethernet Hewlett-Packard	11,488	168.1	238.9	
398	HPC2N - Umea University Sweden	**Abisko** - Supermicro H8QG6, Opteron 6238 12C 2.600GHz, Infiniband QDR Supermicro	15,456	131.9	160.7	252.7
468	Volvo Car Group Sweden	Cluster Platform 3000 BL460c/SL250/ML350 Xeon E5-2670 8C 2.600GHz, Infiniband QDR Hewlett-Packard	6,976	123.3	145.1	

Systems per segment (top500 list)



Systems per location

Systems per area



Note:

Multi-Processor, Multi-Core PCs with powerful GPU cards are here! Number of cores are increasing in each generation, our computers are becoming more and more parallel!

⇒ Need parallel programming on all levels and applications (OS, Games, Internet servers, Data bases, Scientific applications, etc).
Impossible to do automatically, compilers can not analyze all dependencies.

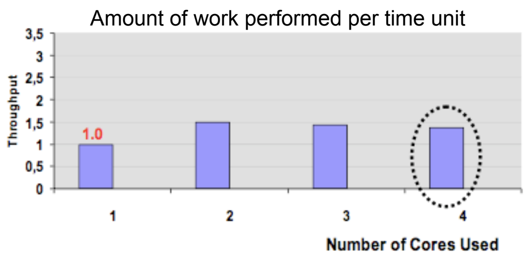
To exploit the full potential of our computers we need to explicitly parallelize our codes!

Throughput computing:

(Run P instances of the same program in parallel)

- Interfere in cache utilization (bad performance)
- Requires P times more memory
- Problems get worse with increased P

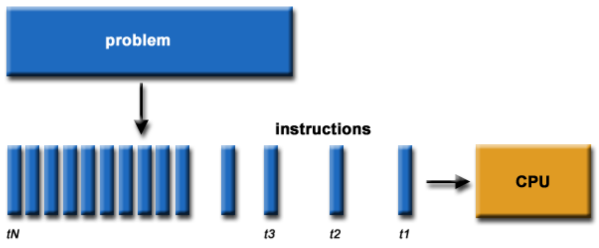
If limited by mem capacity/bandwidth go parallel



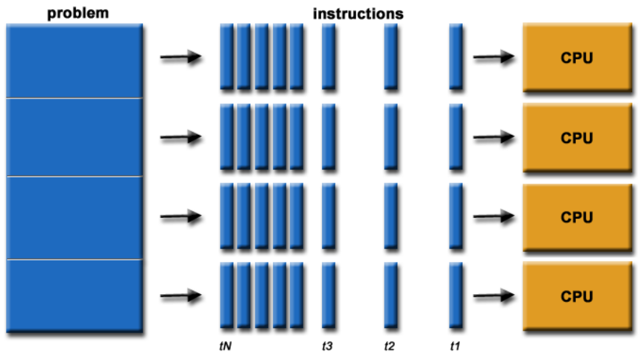
Example: "Lattice Boltzmann Method" to simulate incompressible fluids in 3D on a quad-core processor

What is Parallel Computing

Traditionally, software has been written for ***serial*** computation:
• To be run on a single computer having a single CPU.
• A problem is broken into a discrete series of instructions.
• Instructions are executed one after another.
• Only one instruction may execute at any moment in time.



In the simplest sense, ***parallel computing*** is the simultaneous use of multiple compute resources to solve a computational problem:
• A problem is broken into discrete parts that can be solved concurrently
• Each part is further broken down to a series of instructions



Parallel Programming models

Two main models (scientific computing)
1. Local name space or private memory
   C/C++/(Fortran) and **MPI**
2. Global name space or shared memory
   C/C++/(Fortran) and **OpenMP/Pthreads**

SPMD - Single Program Multiple Data
(All processors run the same program)

Parallelism through data ownership and/or branches (if MyPid==1 then)
Need to communicate and synchronize!

MPI: Message Passing Interface (1994)

Used on PC-Clusters and other large parallel computers. Each process has its own private address space => Data is shared through explicit communication calls (library).

Point-to-point : `MPI_Send - MPI_Recv`
Collective calls: `MPI_Bcast, MPI_Reduce, etc`
[Over 100 MPI function]

Need to specify exactly how to divide data and what each processor should do and who to communicate with => low-level model
But a scalable model with high performance!

Pthreads: POSIX threads

Used on multi-core machines and other shared memory computers. Shared address space model, based on threads ("*light weight process*"). All threads have access to global data.

Memory coherence handled by hardware but requires explicit synchronization and protection of shared variables from multiple updates.

Low-level model but easier to program as data is global to all threads (no need to explicitly create ownership and communicate data between processors). Still need to divide work manually.

OpenMP: Open specification for Multi Processing

Used on multi-core machines and other shared memory computers. Shared address space model, based on threads. All threads have access to global data. Memory coherence handled implicitly by compiler (and hardware).

Insert compiler directives for parallelization of computations => high-level model

```
#pragma omp parallel for
 for (i=1;i<N-1;i++)
    A[i]=F(B[i-1]+B[i]+B[i+1]);
```

Loop is automatically parallelized over all threads, arrays A and B are global data.

OpenMP directives:

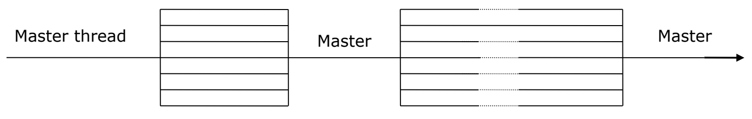
Parallel (main, fork threads)

Data sharing
- shared
- private
- firstprivate
- lastprivate
- threadprivate

Work sharing
- do/for
  - reduction
  - schedule
  - ordered
- sections
- tasks

Serial sections
- single
- master
- critical
- atomic
- ordered

Synchronization
- barrier
- flush
- nowait



Parallel region

Parallel region with single section

Example: Enumeration Sort

```
for (j=0;j<len;j++)
{
  rank=0;
  for (i=0;i<len;i++)
    if (indata[i]<indata[j]) rank++;
  outdata[rank]=indata[j];
}
```

Where is the parallelism? Identify parallel tasks!

OpenMP Solution:

```
#pragma omp parallel for private(rank,i)
for (j=0;j<len;j++)
{
  rank=0;
  for (i=0;i<len;i++)
    if (indata[i]<indata[j]) rank++;
  outdata[rank]=indata[j];
}
```

The j-loop perfectly is parallel, each iteration can be done in parallel, i.e., independently. (Impossible for compiler to analyze, you guarantee the correctness.)

Example: Quick Sort

Algorithm:
1. Select pivot element
2. Divide data into two sets (smaller or larger)
3. Sort each set with Quick Sort

Parallelism:
In each split acquire a new processor and proceed with the two lists in parallel.

=> Limited parallelism (in the first step only one processor have something to do, waste if resources)

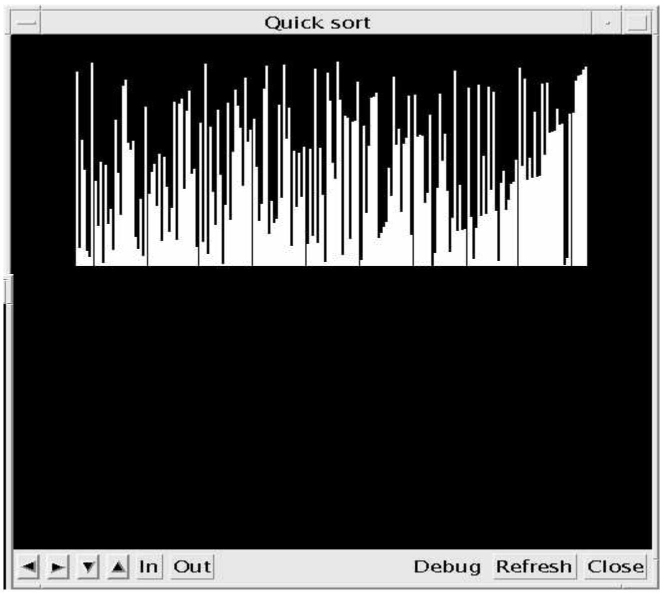
Reformulate the algorithm!

Parallel Quick Sort

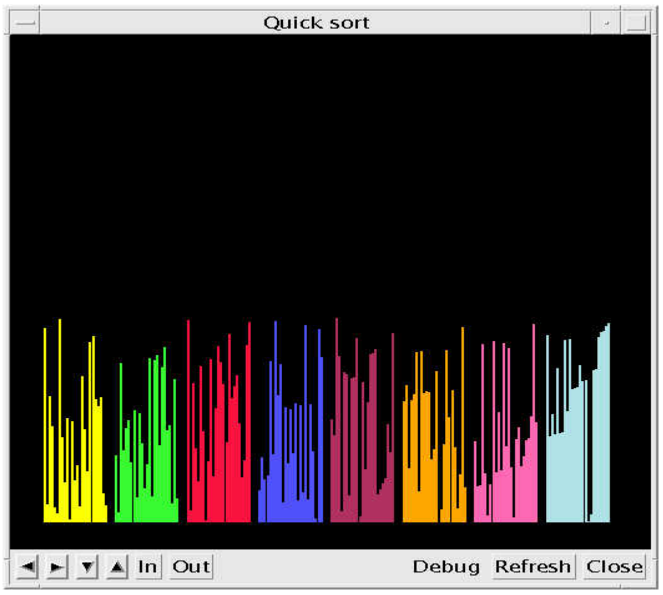
Algorithm:

1. *Divide the data into p equal parts*
2. *Sort the data locally in each processor*
3. *Perform global sort*
    - *3.1 Select pivot in each processor set*
    - *3.2 In each processor, divide the data into two sets (smaller or larger)*
    - *3.3 Split the processors into two groups and exchange data pair-wise*
    - *3.4 Merge data into a sorted list in each processor*
4. *Repeat 3.1-3.4 recursively for each processor group*

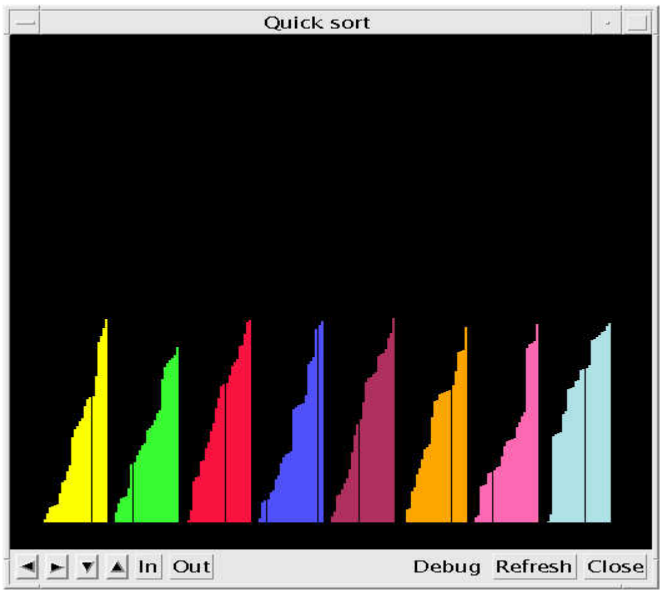
Unsorted data



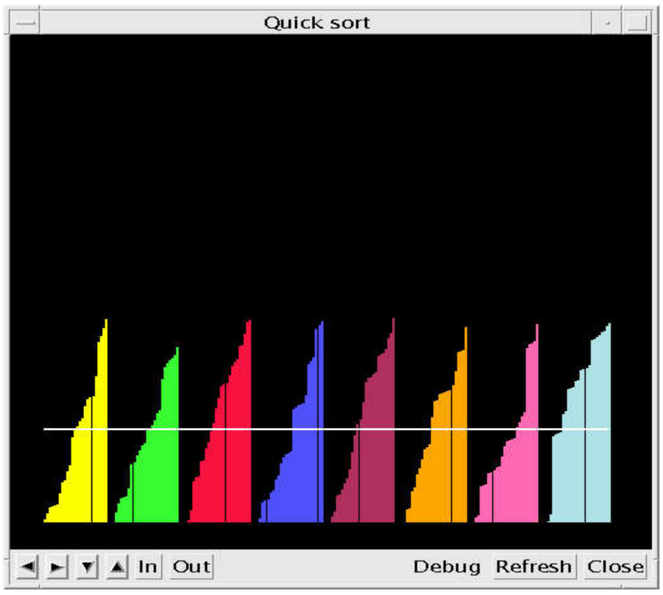
Step 1, Divide data into p equal parts



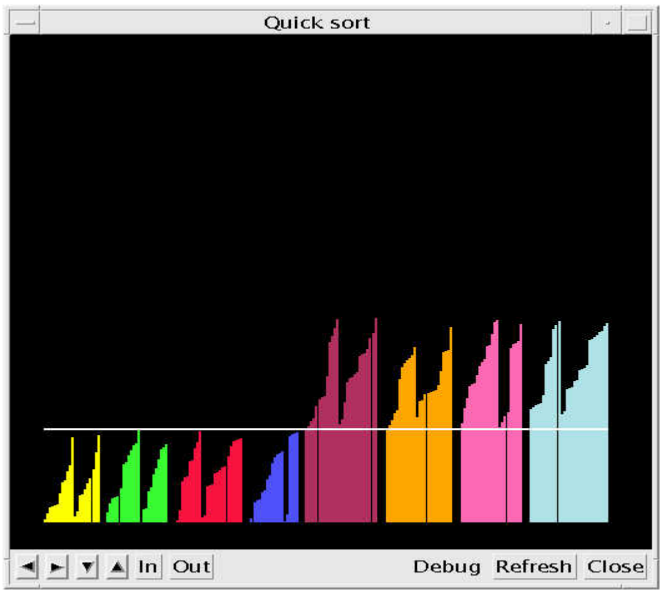
Step 2, Sort locally in each processor



Step 3.1 Select pivot



Step 3.2, 3.3 Divide and exchange



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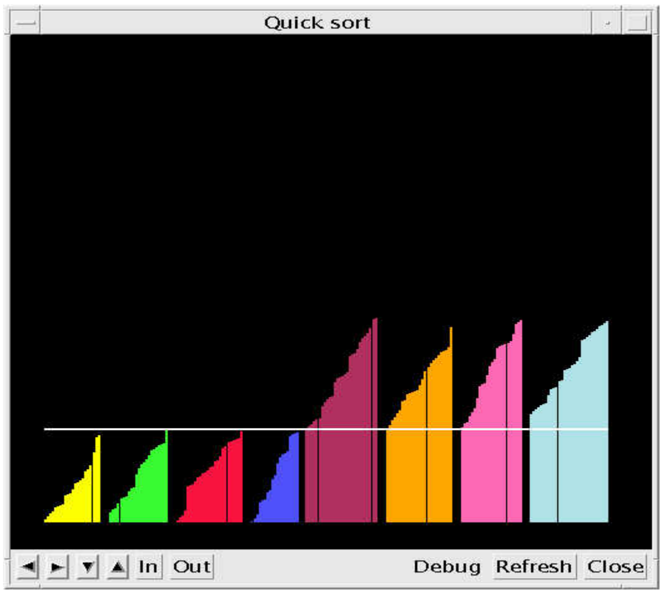
Step 3.4, Merge into a sorted list



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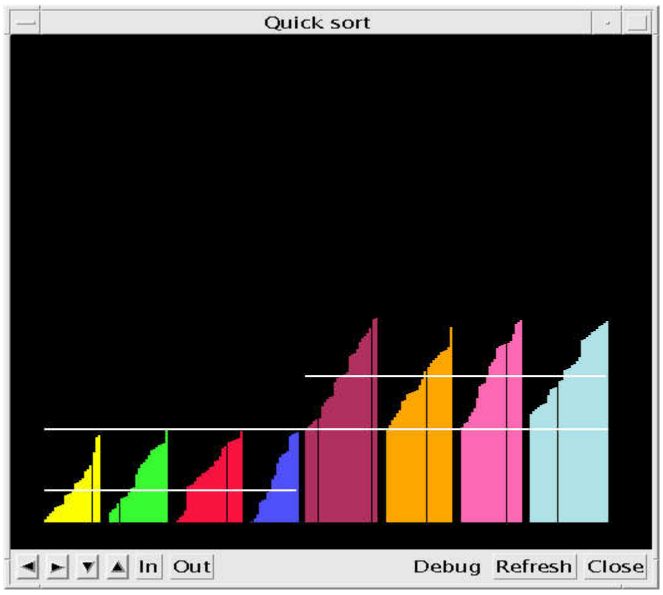
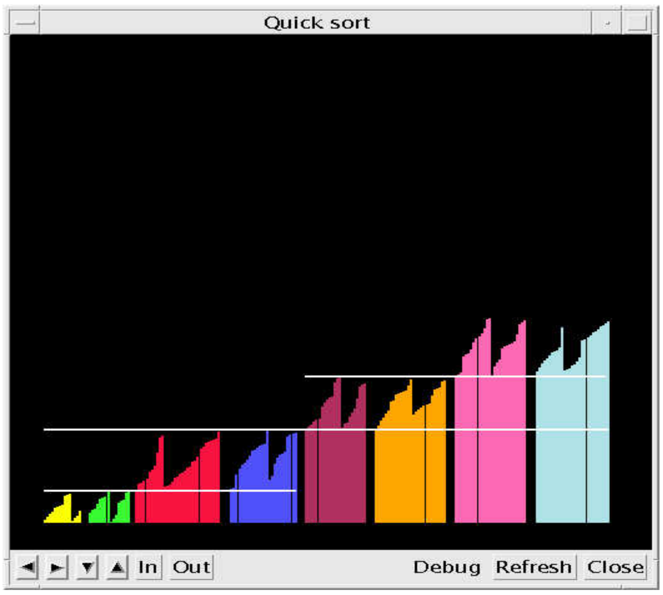
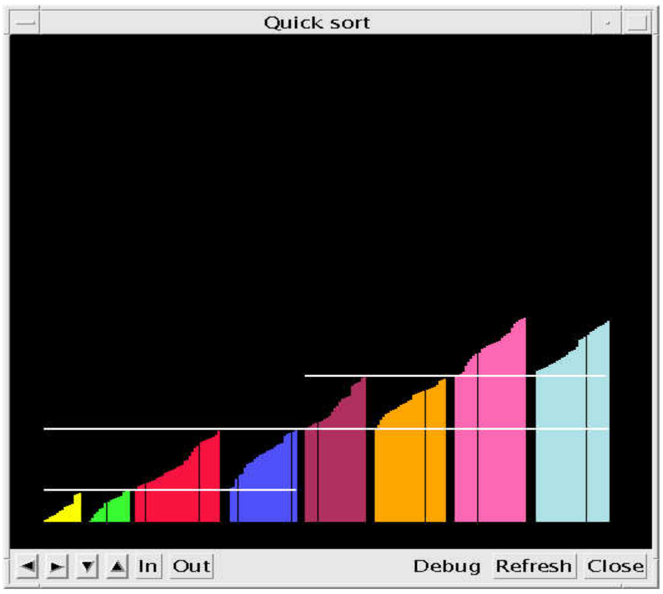
Step 3.1 Select pivot



Step 3.2, 3.3 Divide and exchange



Step 3.4, Merge into a sorted list



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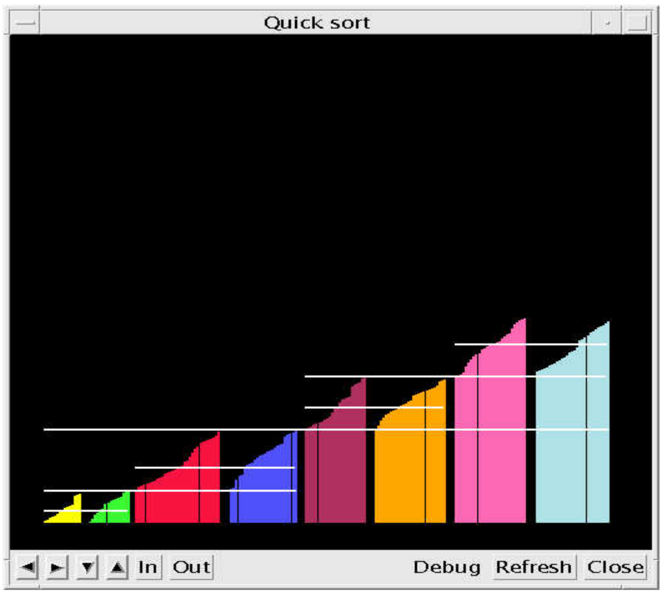
Step 3.1 Select pivot



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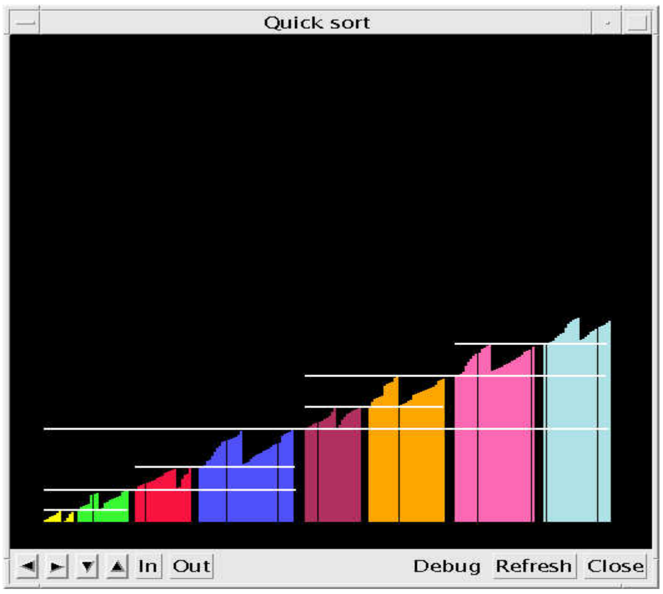
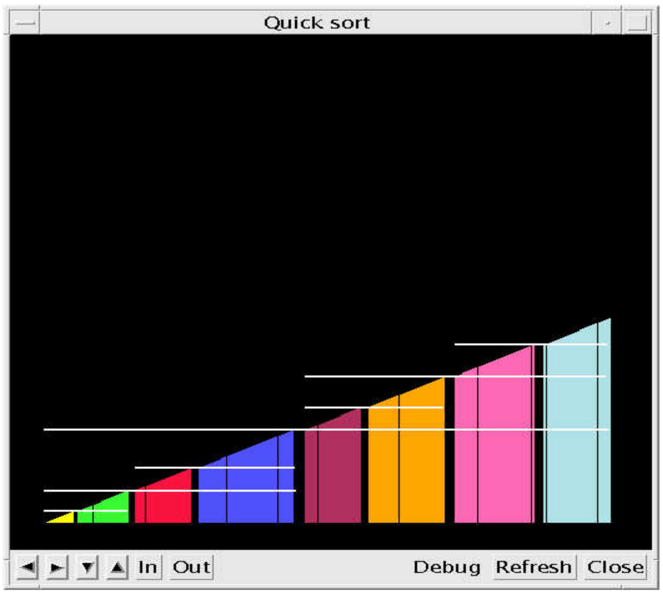
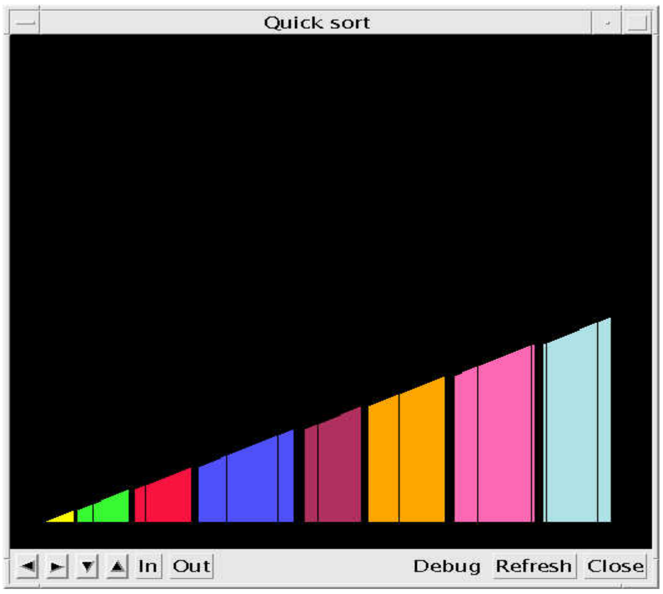
Step 3.2, 3.3 Divide and exchange



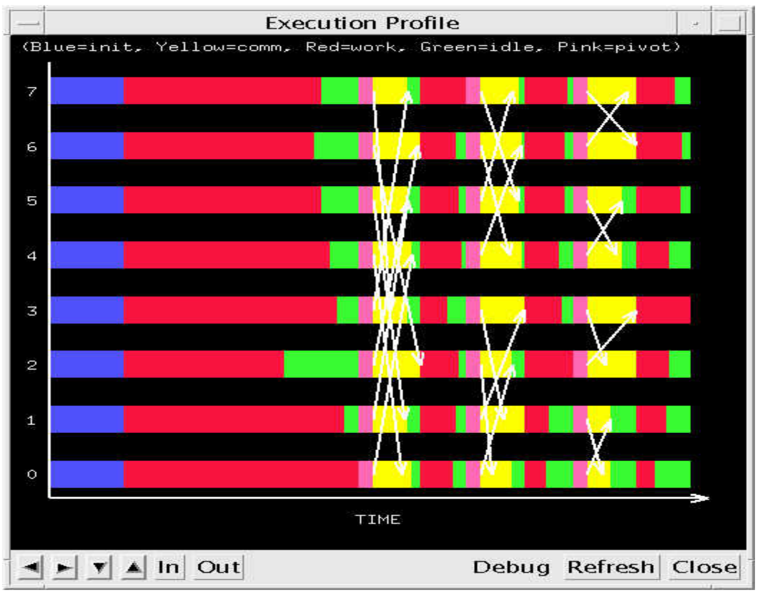
Step 3.4, Merge into a sorted list



Final state



Execution profile, second view



Performance obstacles:

- **Communication**
  -Use asynchronous comm and message probing
- **Load balance**
  - Choose pivot carefully, different strategies
- **Synchronization**
  - Split communicator (topology) in each step to avoid global synchronization

Example: Numerical PDE Solver

Consider the Hyperbolic PDE:

$$u_t + u_x + u_y = F(t,x,y) \quad 0 \le x \le 1, 0 \le y \le 1$$

$$\begin{cases} u(t,0,y) = h_1(t,y) & 0 \le y \le 1 \\ u(t,x,0) = h_2(t,x) & 0 \le x \le 1 \end{cases} \quad \textit{Boundary Conditions}$$

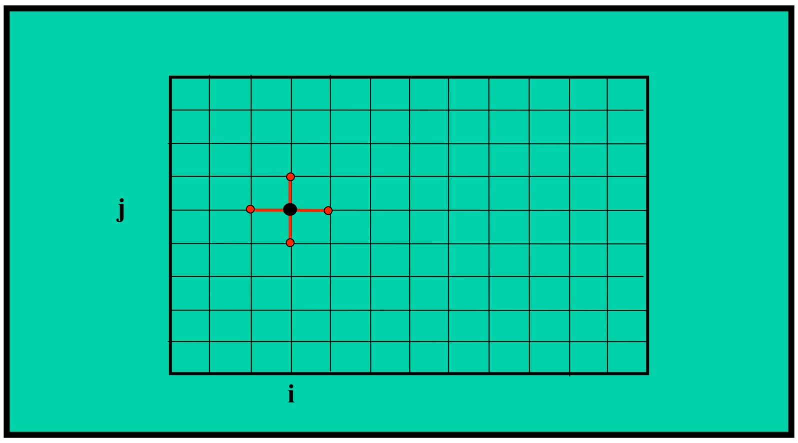
$$u(0,x,y) = g(x,y) \quad \textit{Initial Conditions}$$

Solve with explicit finite difference method, for example Leap-Frog

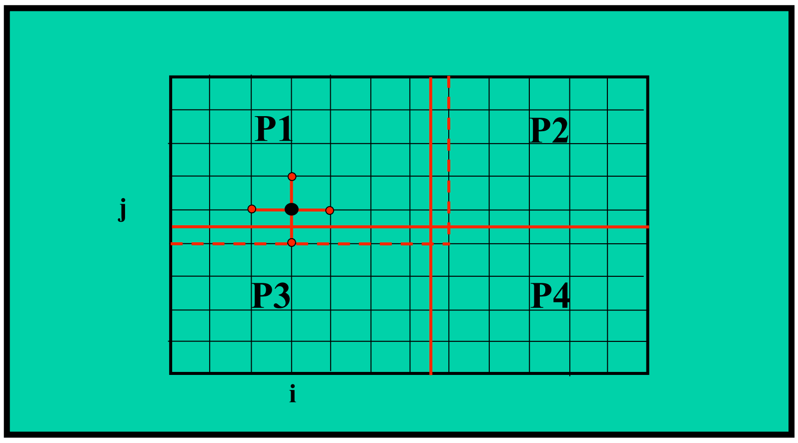
Core of the computations:

```
do k=2,Nt
   t=k*dt; Uold=U; U=Unew;
   do j=1,Ny-1
      do i=1,Nx-1
        x=i/Nx; y=j/Ny
        Unew(i,j)=Uold(i,j)+2*dt*(F(t,x,y)-
                (U(i+1,j)-u(i-1,j))/(2*dx)-
                (U(i,j+1)-U(i,j-1))/(2*dy))
      end do
   end do
end do
```

Computational stencil:



Parallelization, partition grid:

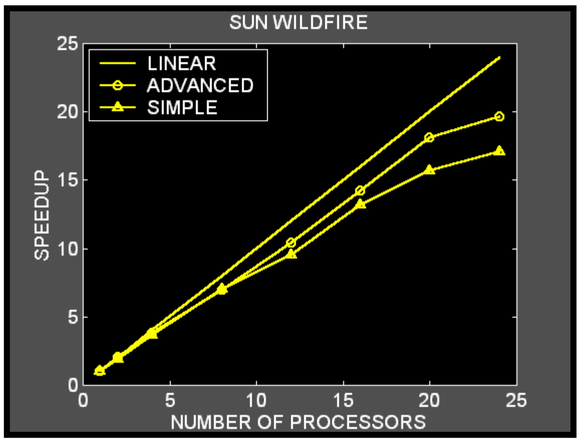


Message Passing Version:

```
do k=2,Nt
   t=k*dt; Uold=U; U=Unew;
   update partition boundary - communicate
   do j=j1,j2
      do i=i1,i2
         x=i/Nx; y=j/Ny
         Unew(i,j)=Uold(i,j)+2*dt*(F(t,x,y)-
                 (U(i+1,j)-u(i-1,j))/(2*dx)-
                 (U(i,j+1)-U(i,j-1))/(2*dy))
      end do
   end do
end do
```

```
Compute 'left, right, up, down' node

! Send and receive left-right
if ('not at left boundary')
   call mpi_send(left, ... )
end if

if ('not at right boundary')
   call mpi_recv(right, ... )
   call mpi_send(right, ... )
end if

if ('not at left boundary')
   call mpi_recv(left, ... )
end if

! Send and receive up-down
...
```

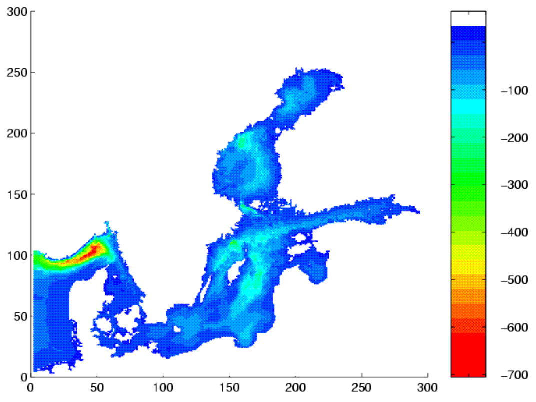
Performance, 256x256 grid:



Hands-on session: Study implementation details and measure parallel performance

Real world example:

- Irregular shape
- Irregular work load (due to sea depth)



Oceanographic model from SMHI

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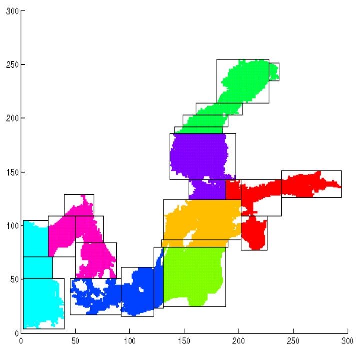
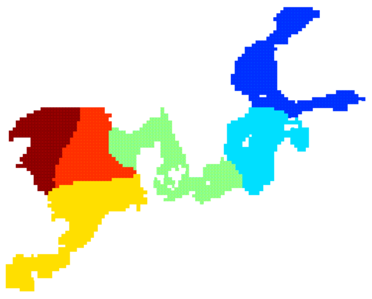
Need to use *data partitioning algorithms* to:
- optimize load balance
- minimize communication



Block-structured partitioning


Unstructured graph partitioning

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Summary:

Parallel computers are here, ranging from laptops to supercomputers. Need parallel programming in all programs and applications.

When writing parallel programs need to:
- think about algorithm (parallelism)
- optimize load balance (equal work load)
- minimize communication (parallel OH)

The topics are interdependent which makes it very hard (impossible) for a compiler to create efficient code.

Course content:

- Parallel computer architecture
- Programming with message passing, **MPI**
- Programming with threads, **Pthreads**
- Programming with compiler directives, **OpenMP**
- Algorithms in linear algebra
- Algorithms in sorting
- Performance analysis
- Load balancing and data partitioning
- Programming of GPUs, **CUDA**
- Other programming models, e.g., **UPC, Matlab**

Aim of the course: To give skills in parallel programming with MPI, Pthreads and OpenMP! Examination is to a large extent through programming assignments.

Schedule:

Lecture	Theme
21/1	Introduction (JR)
23/1, 24/1	Lab C-Programming (optional) (MG)
24/1	Parallel Computer Architecture (JR)
27/1	MPI, 1 (DL)
29/1	MPI, 2 (DL)
30/1	Lab MPI (JR, DL, LJ)
31/1	MPI, 3 (DL)
3/2	Parallel Algorithms, Algebra (LJ)
4/2	Parallel Algorithms, Algebra (LJ)
5/2	Parallel Algorithms, Sorting (JR)

Lecture	Theme
6/2	Performance analysis (JR)
7/2	Data partitioning,load balancing (JR)
12/2	Pthreads 1 (JR)
13/2	Pthreads 2 (JR)
14/2	Lab Pthreads (JR, DL, LJ)
17/2	OpenMP 1 (JR)
18/2	OpenMP 2 (JR)
19/2	Lab OpenMP (JR,DL)
21/2	OpenMP 3 (JR)
27/2	UPC, Matlab (JR)
3/3	GPU programming 1 (DL)
5/3	GPU programming 2 (DL)
12/3	Lab GPU (DL, LJ)

Examination:

- Four labs (MPI, Pthreads, OpenMP, GPU)
- Three programming assignments
  Can be done in groups of 2-3 students

Then chose:

- Project work (grade 3)
- Written exam (grade 3, 4 or 5)

- Project work + written exam (3, 4 or 5)
  Project work can raise your exam grade

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Project work:

- Individual assignment
- *You* formulate a problem that you want to parallelize, write a project proposal
- Hand in project proposal to me
- If approved you get an account on Uppmax systems, e.g., Tintin.
- Perform the project and write a report.