Introduction to Practical Parallel Programming

Course Overview, and The 'Big Picture'



Today's Main Goal

 Students arriving with scientific computing background should be able to leave and immediately start parallelizing codes, understand concepts involved



Schedule

9am-10:30	Basic Concepts
10:30-10:45	Break
10:45-12:45	Intro to OpenMP
12:45-1:45	Lunch
I:45-3:30	Intro to MPI
3:30-3:45	Break
3:45-5:00	Intro to MPI 2



What will we be doing doing here int mpi_bc(domain_t *d, int doi, int neigh) { /* first, uqly version which copies into a buffer double *out, *in; int count; int nx, ny, ng; int i,j,ioff,joff; int ierr: • This is a short course on parallel programming You will be doing a lot of typing and Ny; ng = d->Nguard; programming to help build skills with OpenMP, MPI. case XRIGHT DIR: otherdirn = XLEFT DIR; case XLEFT DIR: otherdirn = XRIGHT DIR;

```
case XLEFT_DIR: otherdirn = XRIGHT_DIR;
case YRIGHT_DIR: otherdirn = YLEFT_DIR;
case YLEFT_DIR: otherdirn = YRIGHT_DIR;
}
if (dirn == XRIGHT_DIR || dirn == XLEFT_DIR) {
    bufsize = ng*(ny+2*ng)*NVARS;
    out = (double *)malloc(bufsize*sizeof(dou
    in = (double *)malloc(bufsize*sizeof(dou
```



Parallel Computing

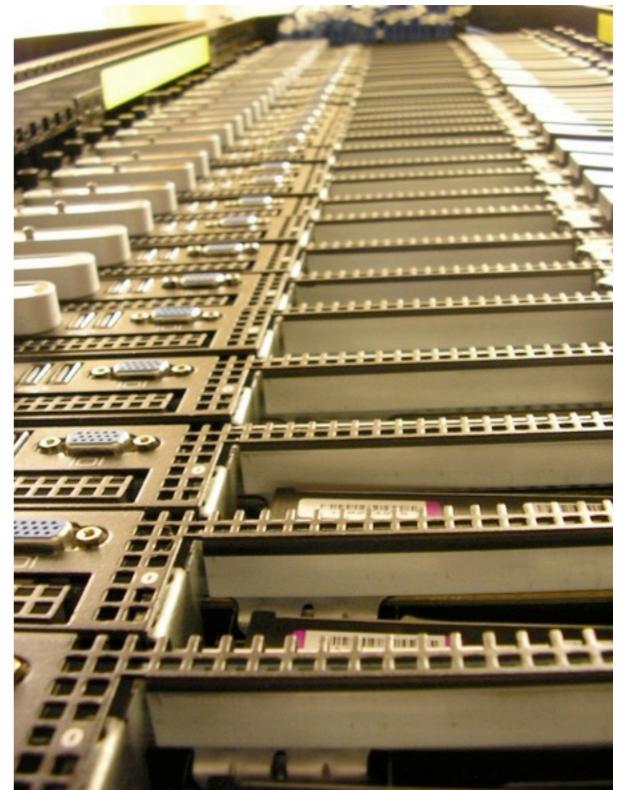
I: Concurrency, Amdahl's Law, and Locality



Why Parallel Computing?

Faster:

At any given time, there is a limit as to **how fast** one computer can compute. So use more computers!



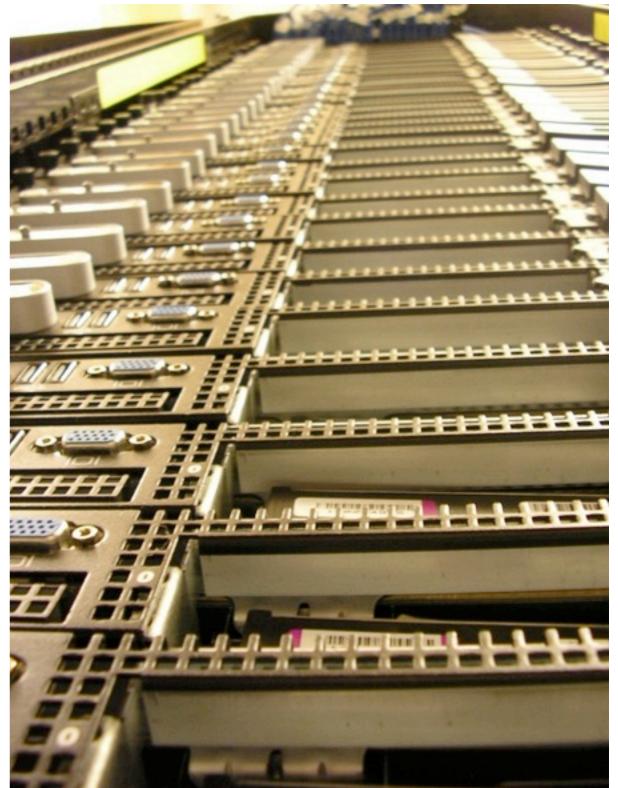


Why Parallel Computing?

Bigger:

At any given time, there is a limit as to **how much** memory, disk space, etc can be put on one computer.

So use more computers!



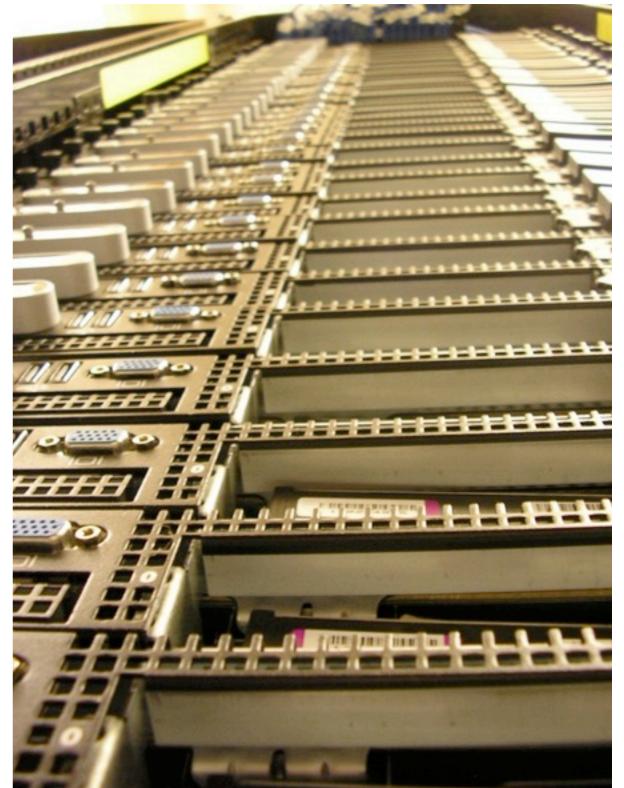


Why Parallel Computing?

More:

You have a program that runs in reasonable time one one processor but you want to run it **thousands of times**.

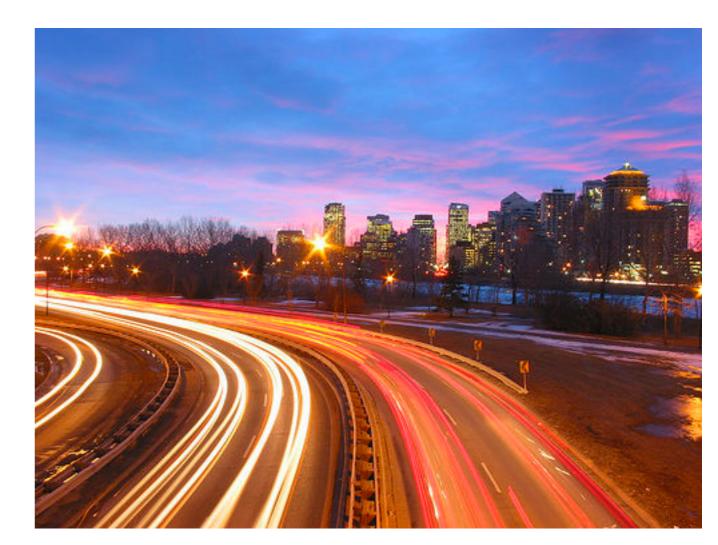
So use more computers!





Concurrency

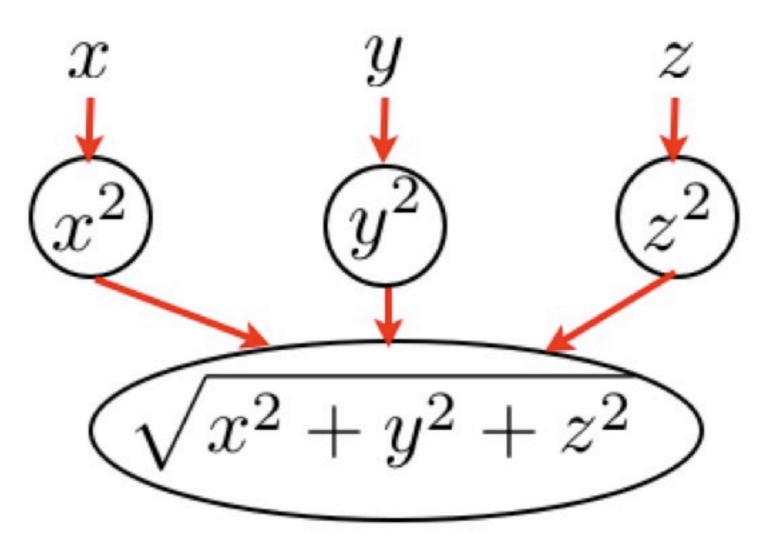
- Must be something for the 'more computers' to do.
- Must be able to find concurrency in your problems
 - Many Tasks
 - Order Unimportant



http://flickr.com/photos/splorp/



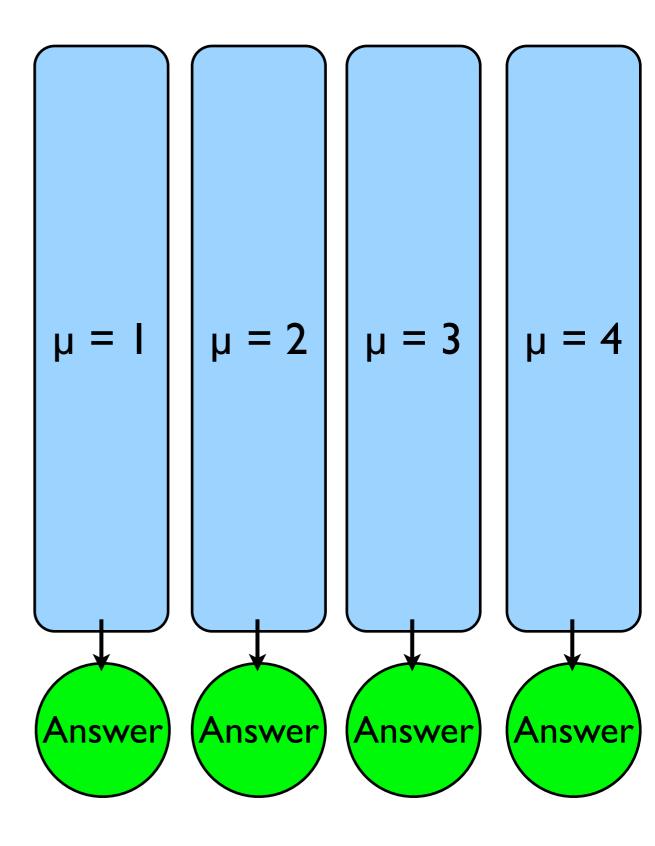
Data Dependancies Limit Concurrency





Parameter Study: Ideal case

- Want to know all results as model parameter varies
- Can run serial code on up to as many processors as parameter sets
- 'More'

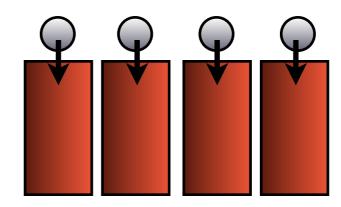




Throughput = Tasks/Time

How long it takes to process the N tasks you want done throughput $= \frac{N}{\text{time}}$ For completely independent tasks, P processors can increase throughput by factor P!





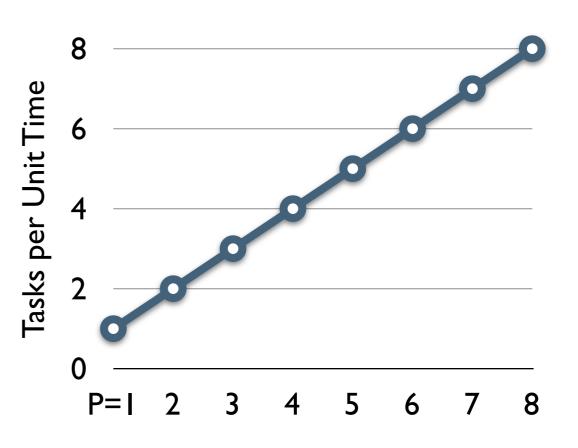
VS



Scaling with P

How a problem **scales**: how throughput behaves as processor number increases In this case, the throughput scales linearly with the number of processors

This is the best case: 'Perfect scaling'





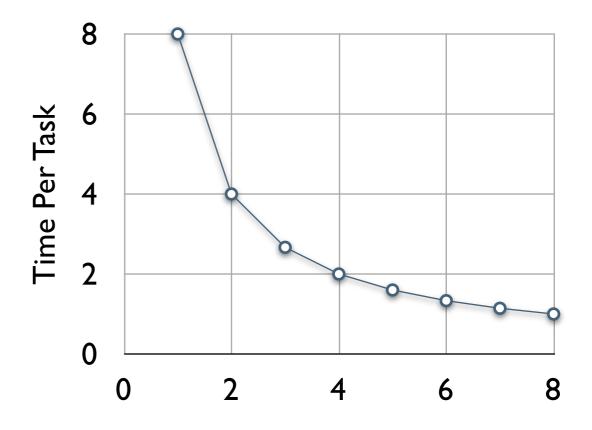
Scaling with P

Another way to look at it: time it takes to get some fixed amount of work done

More usual (and more important!)

Perfect scaling: time to completion ~ I/P

P processors - P times faster





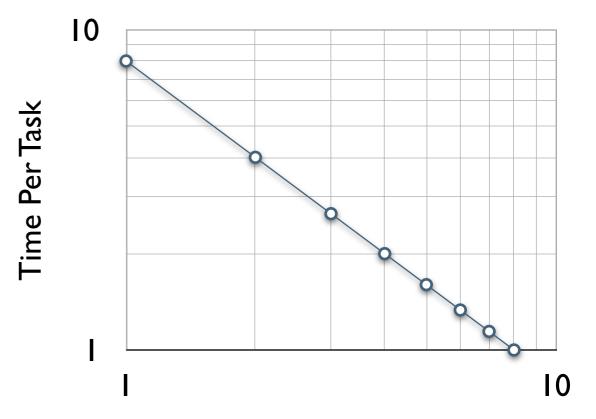
Scaling with P

Another way to look at it: time it takes to get some fixed amount of work done

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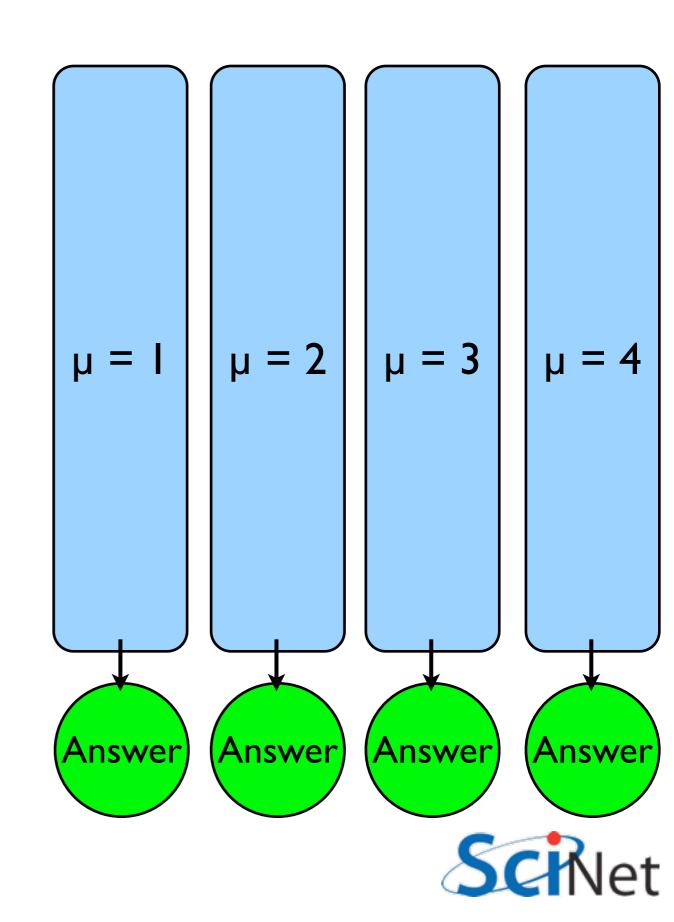
P processors - P times faster





Parameter Study: 'Embarrassingly Parallel'

- Scales perfectly up to P=N
- Speedup = P:'linear scaling', ideal case.

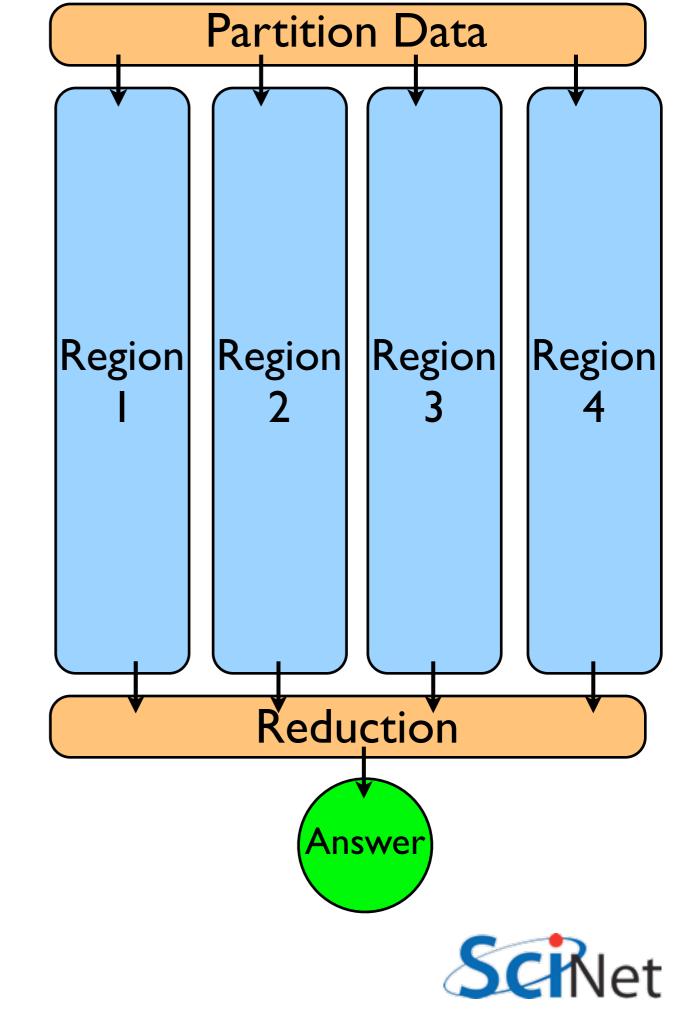


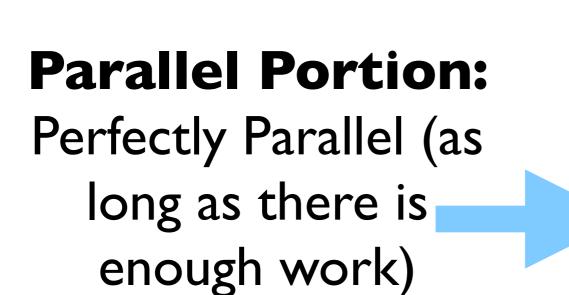
Problems Differ in amount of Concurrency

Integrate (or some other simple processing) tabulated experimental data

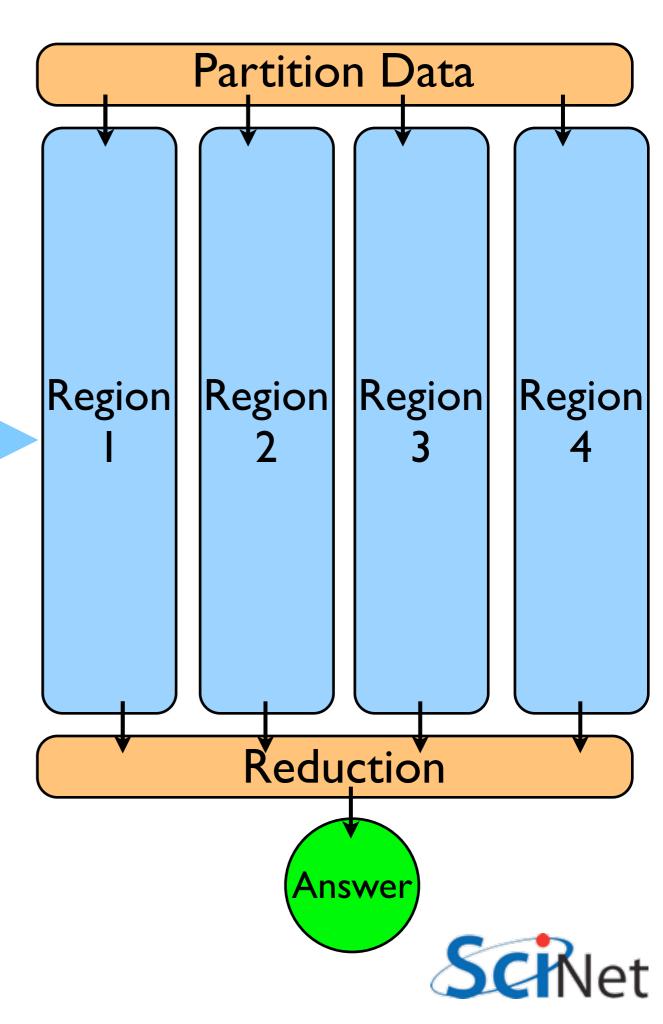
Integration of different regions can be summed by each processor

But first need to get data to processor, then bring together all the sums



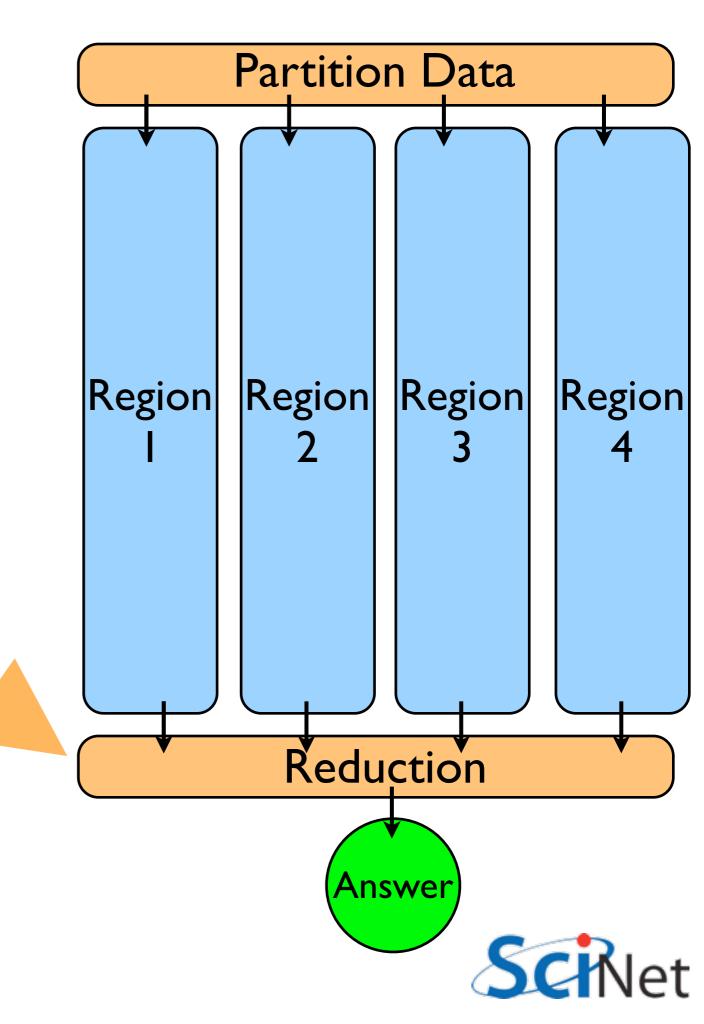


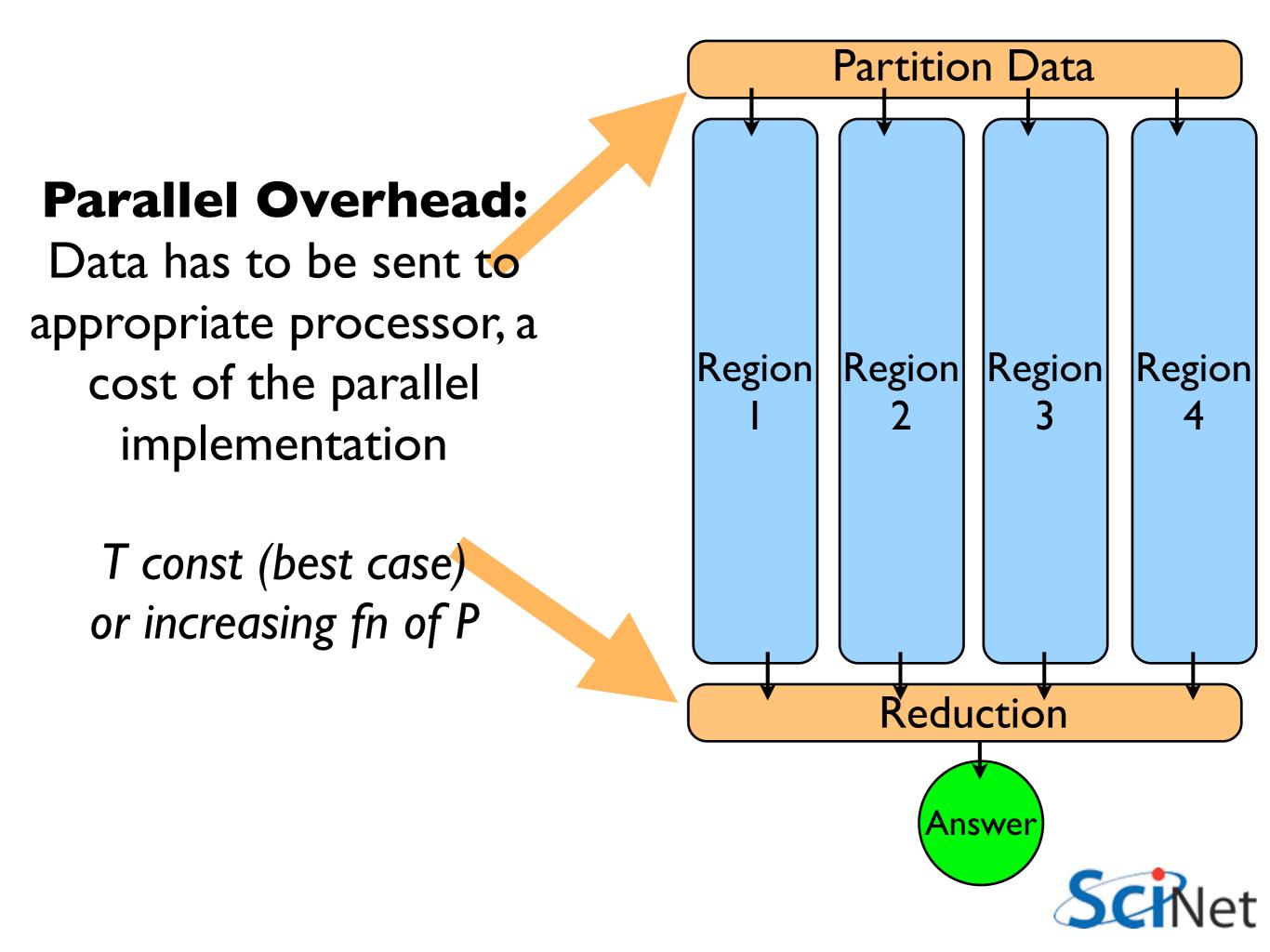
 $T \sim I/P$



Serial Portion:

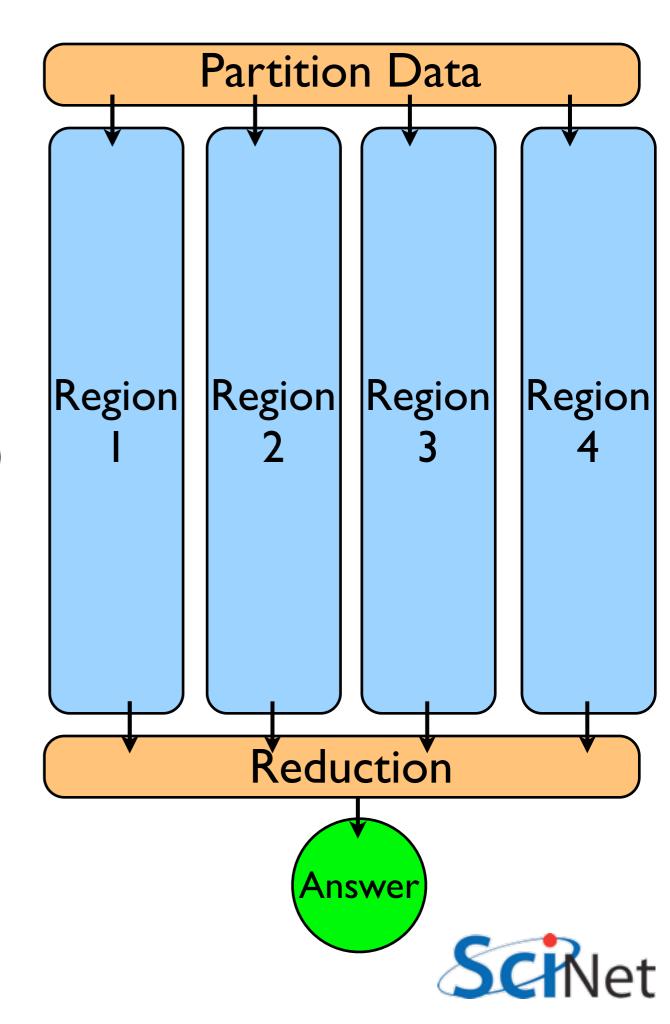
Sum has to be done; if done on one processor, just same as serial: T ~ const





Total Time: Serial + Parallel

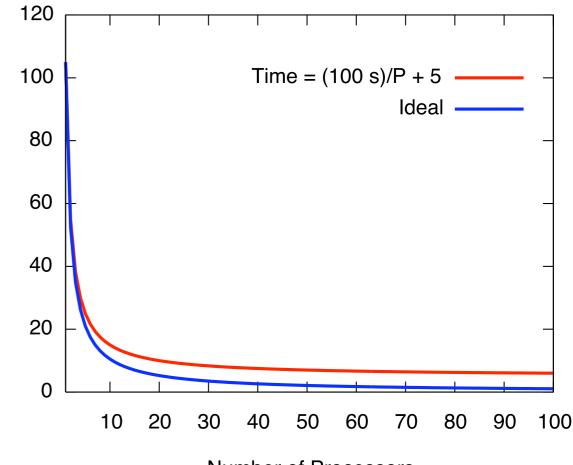
Ignoring data-moving costs (for now): time $(N, P) = \left\lfloor \frac{N}{P} \right\rfloor T_{\text{work}} + T_{\text{reduction}}(P)$ Typically linear in P (sum) Eventually, as problem becomes increasingly scaled up, serial term dominates



Timing of simple case

Ignore data transfer costs; say: 100 s in integration work 5 s in assembling the parts How does this behave on many processors?

Time (s)



Number of Processors



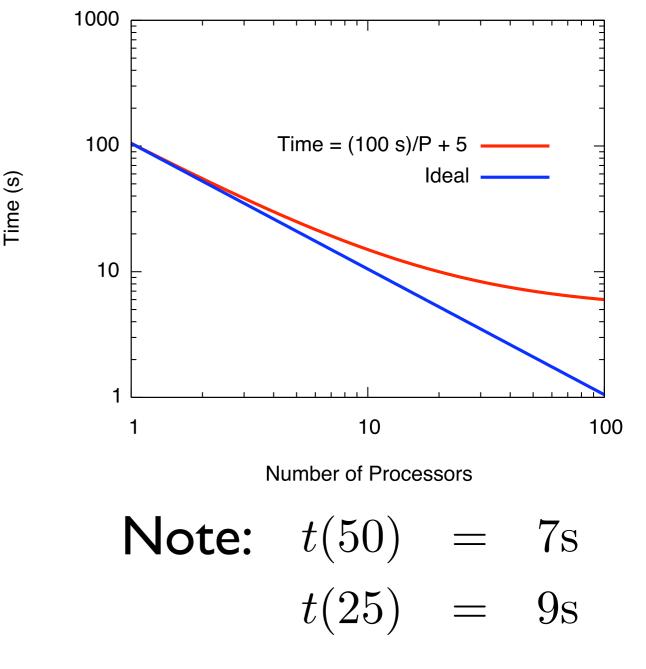
More processors per run don't always help

Given timing data, how do we choose P to run on if we have N programs to run?

Ideal case, timing goes down I/P doesn't matter

Serial part (5%!) becomes a bottleneck

Can improve **throughput** by running on *fewer* processors



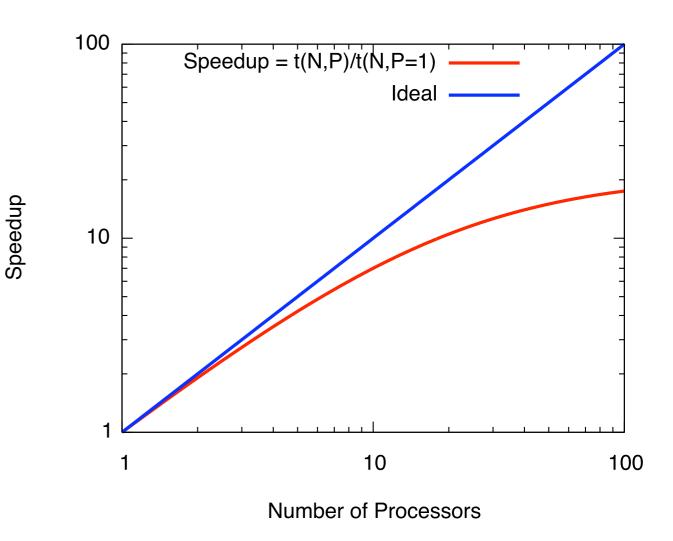
Can run 2 jobs on 25 procs each in about same time as one on 50!



Speedup: How much faster with P procs?

An important concept is the speedup of a given parallel implementation t(N, P = 1)

speedup(P) =
$$\frac{t(N, P - 1)}{t(N, P)}$$





Efficiency: Speedup should be ~ P

Related concept: Parallel Efficiency (compared to serial code)

Efficiency(P) =
$$\frac{t(N, P = 1)}{Pt(N, P = 1)}$$

= $\frac{\text{speedup}(P)}{Pt(N, P = 1)}$

Efficiency

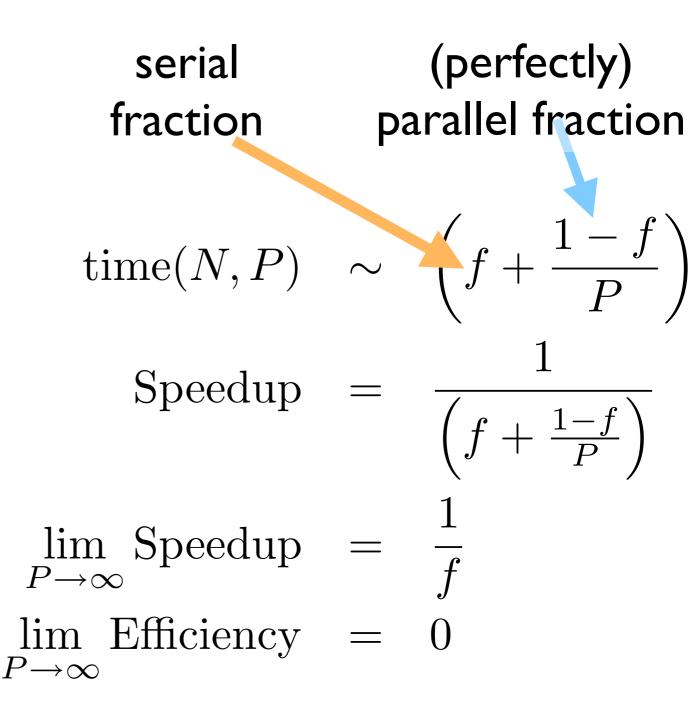
P



Amdahl's Law

Any serial part of computation will eventually dominate

If serial fraction is f, even if parallel component goes to zero, speedup can only be 1/f

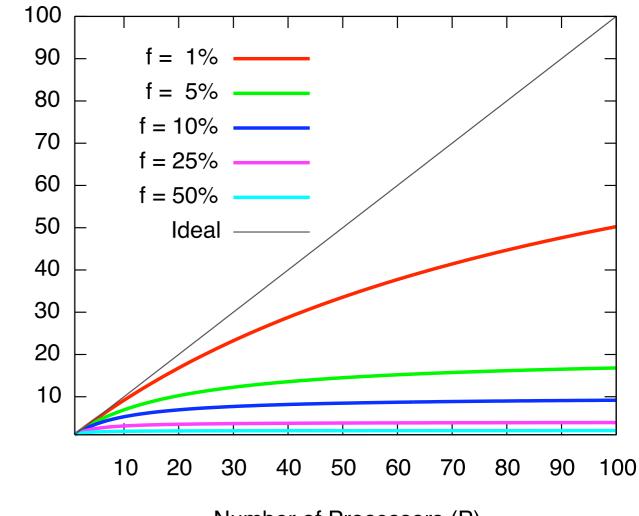




Amdahl's Law

Speedup

- Any serial part of computation will eventually dominate
- If serial fraction is f, even if parallel component goes to zero, speedup can only be 1/f

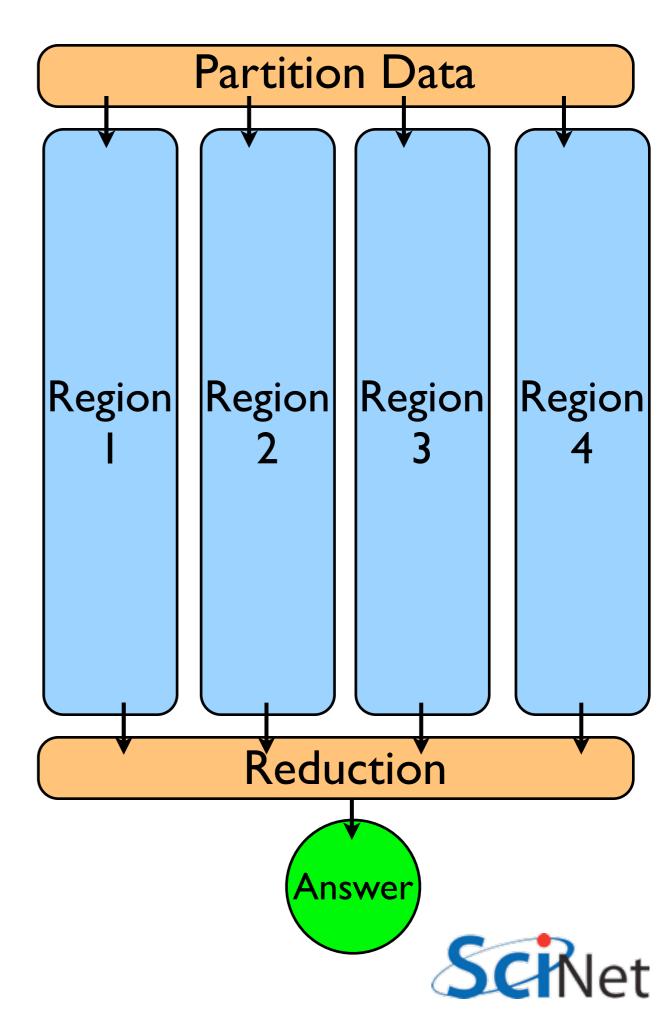


Number of Processors (P)



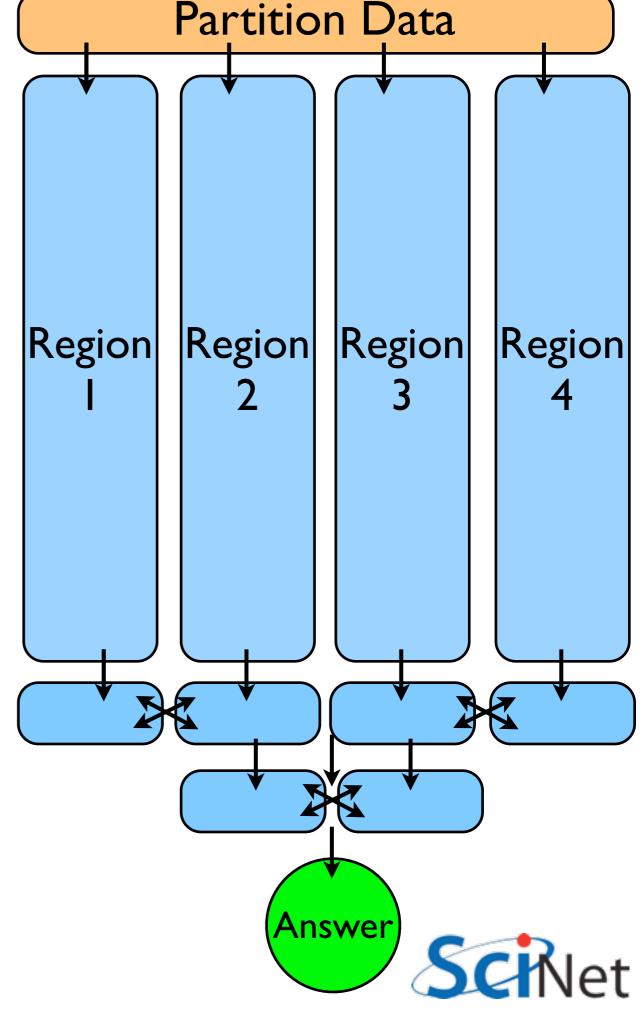
Avoiding Amdahl

In some cases, may not matter. If will run in reasonable time on some small number of processor, asymptotic arguments may not matter.



Trying to Beat Amdahl, #I

Rewrite serial portions to take into account parallelism eg, many reductions can be done in parallel that will cost log₂(P) (not I, but much better than serial = P...)



Big Lesson #1

Optimal **Serial** Algorithm for your problem may not be the $P \rightarrow I$ limit of your optimal **Parallel** algorithm



Trying to Beat Amdahl, #2 -Upsize

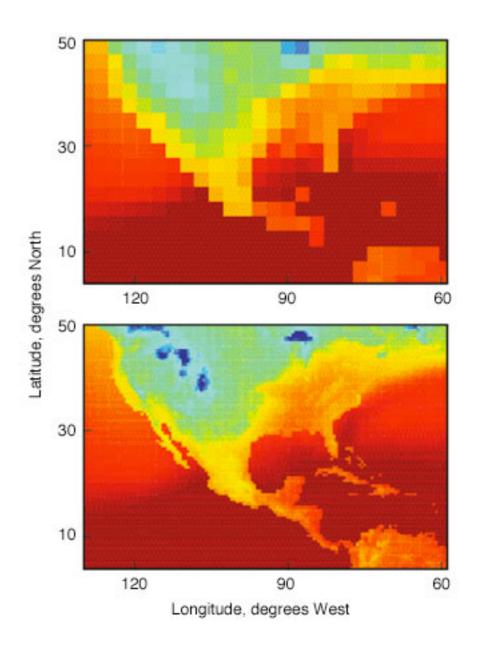
Desktop problem isn't a supercomputer problem!

Reason to run on big machines is size as well as speed

Amdahl's law assumes constant size problem

More work; f goes down.

Gustafson's law: any sufficiently large problem can be efficiently parallelized.



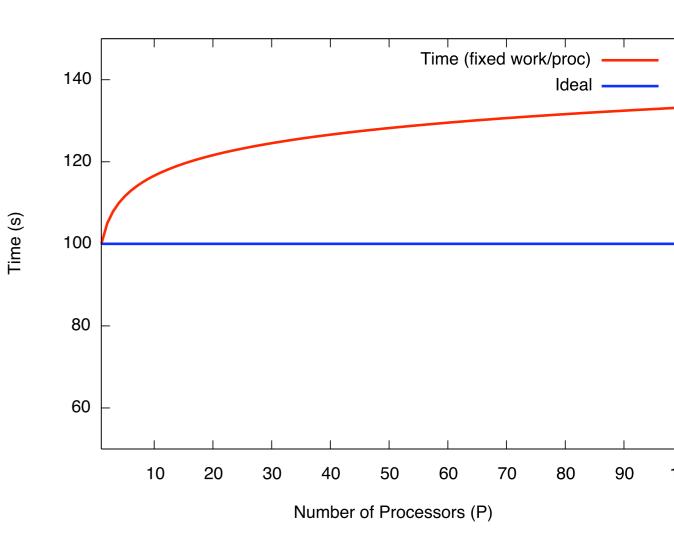


Weak Scaling

How does problem behave if you expand problem size as number of processors?

Strong Scaling - on how many processors can you efficiently run given problem

Weak Scaling - how large a problem can you efficiently run





More on Concurrency

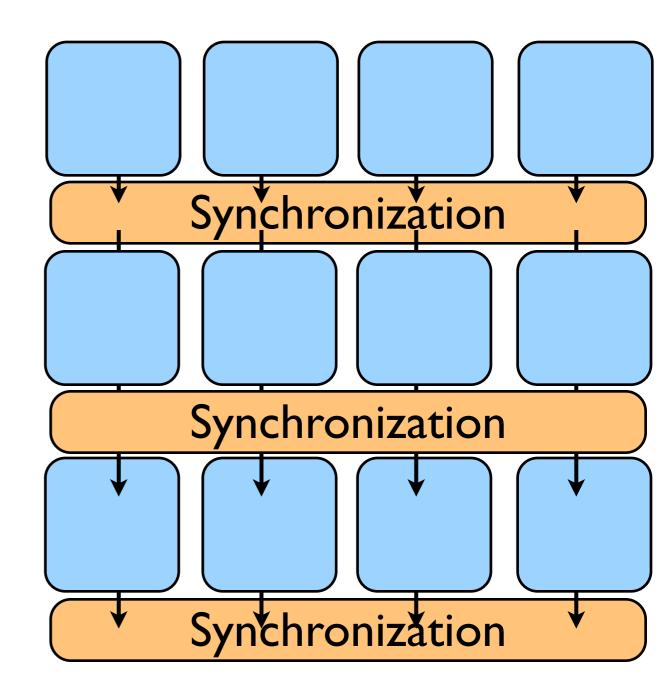
Most problems are not pure concurrency

Some level of synchronization, exchange of information needed between tasks

This needs to be minimized

Increases Amdahl's 'f'

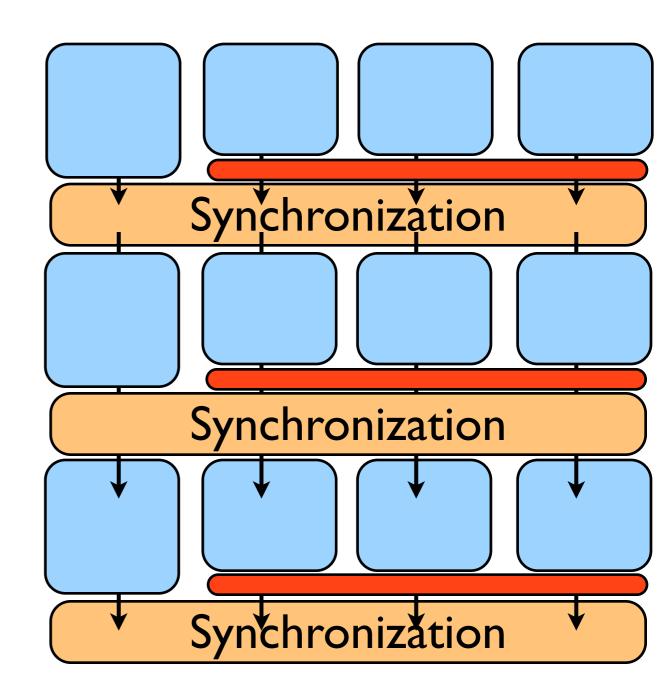
Are themselves costly





Concurrency

Makes possible lots of wasted time ('load balancing', about which more later)





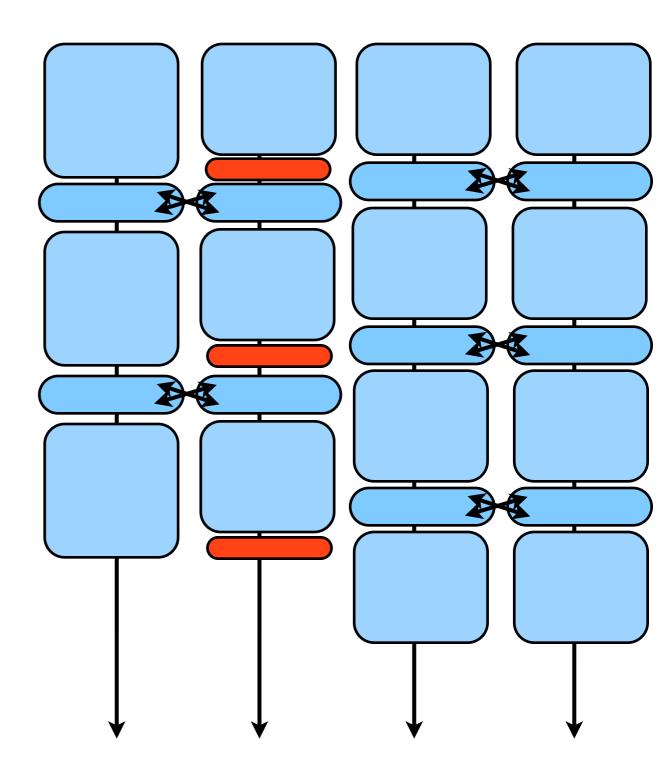
Locality

Information needed by the task should be as local as possible.

When tasks do need to interact, best that those interactions be as local as possible, and with as few others as possible

Communications cost lower

Fewer processes have are locked up during the necessary synchronization





Big Lesson #2

Parallel algorithm design is about finding as much concurrency as possible, and arranging it in a way that maximizes locality.

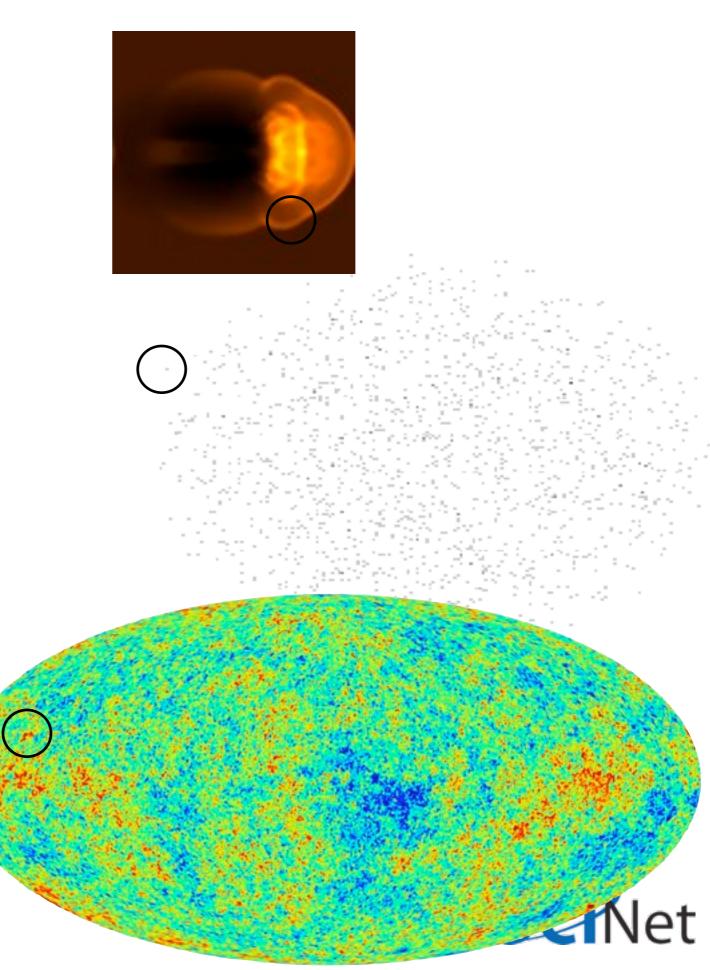


Finding Concurrency

Identify tasks that can be done independently, order doesn't matter

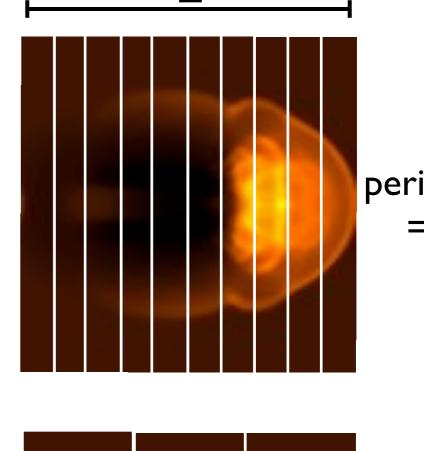
PDEs: parts of domain

N-body: particles (or interactions)

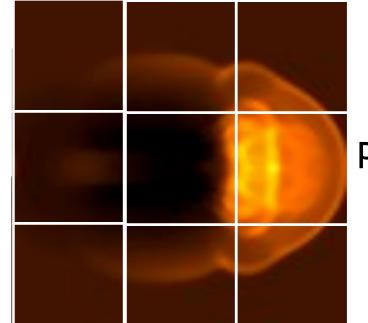


Maintaining Locality

Now have to lump the concurrent bits into tasks Choosing that re-aggregation can greatly effect locality.



perimeter = 9L



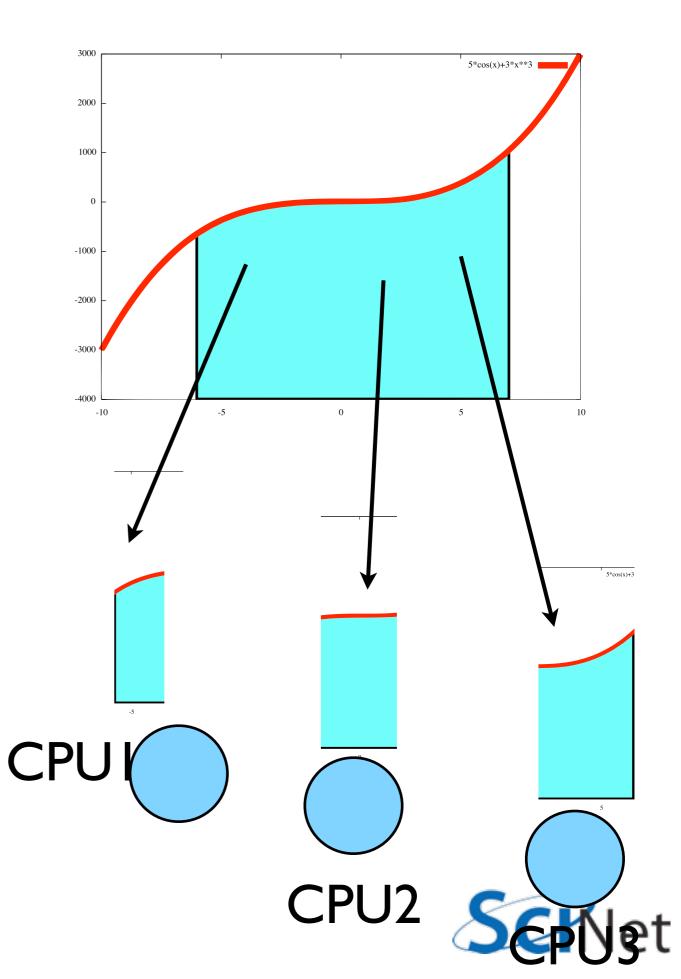
perimeter = 4L



Example: I d integration

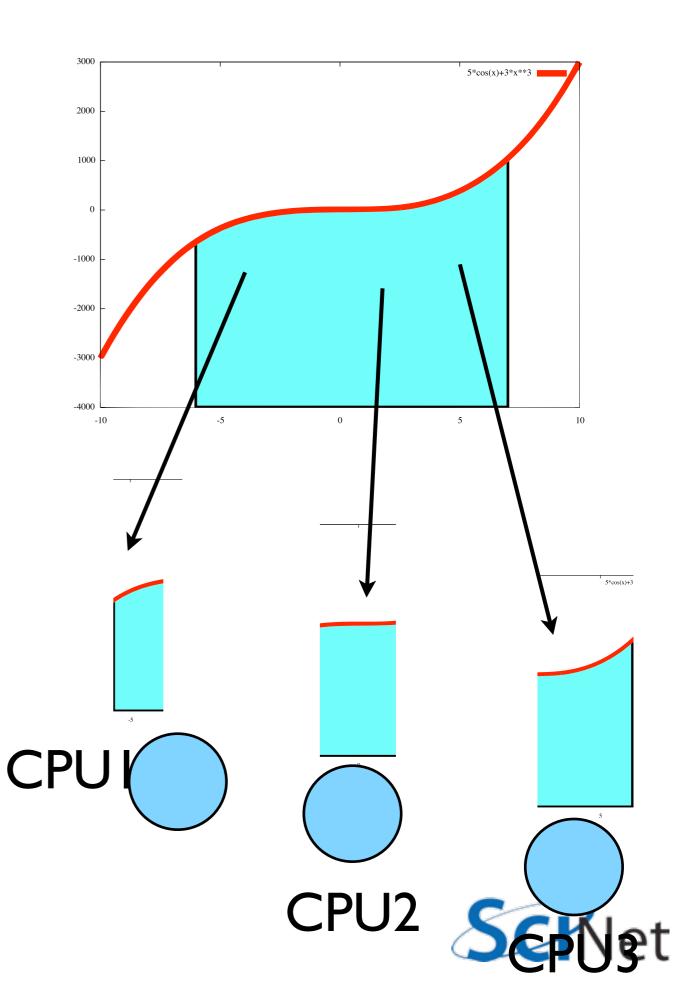
Integrate a 1d function with (say) Simpson's rule, with N points.

Concurrency: can do each of the points independently, then sum. Locality: have each do a chunk



Example: Id integration

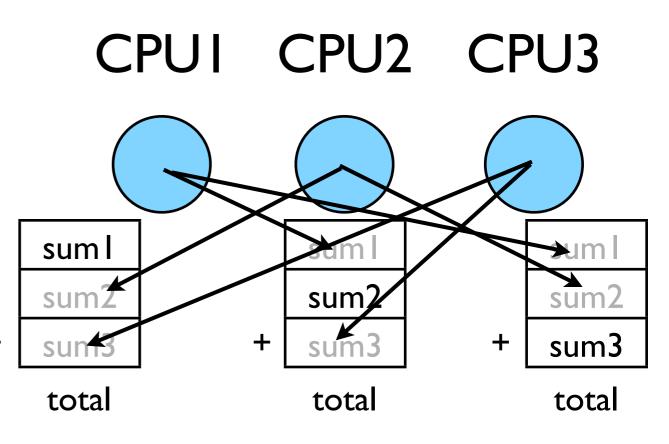
Each processor gets N/P points to do Total compute time for one process: $mp = \left(\frac{N}{P}\right) N_{SR}C_{comp}$ Now how to do sums? $T_{\rm comp} = I$



Example: I d integration

Each processor sends partial sums to others, then all can do + total Each processor sends its result (P-1) times and receives (P-1) results

$$T_{\rm comm} = 2(P-1)C_{\rm comm}$$

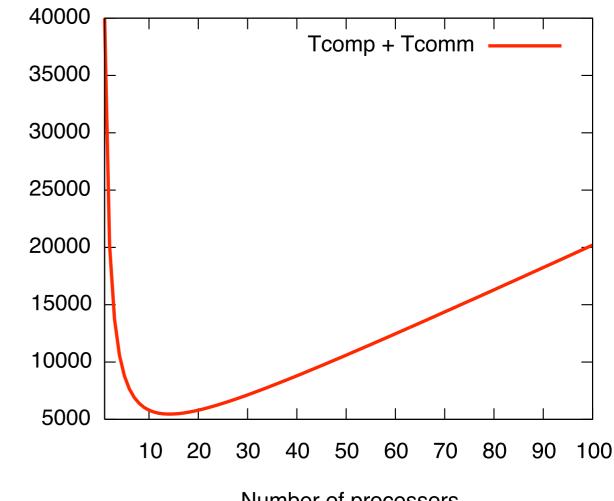




Integration with parallel costs:

Time (some units)

Can actually get worse with P! Communication cost increases with P



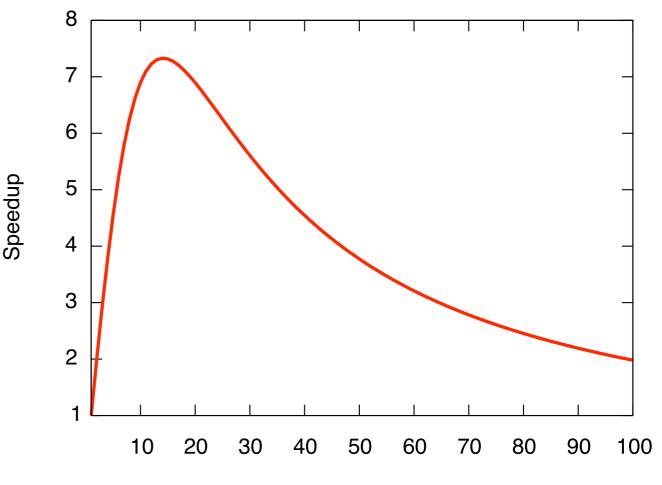
Number of processors

 $N = 10000, N_{sr} = 4,$ $C_{comm}/C_{comp} = 100$



Integration with parallel costs:

Can actually get worse with P! Communication cost increases with P



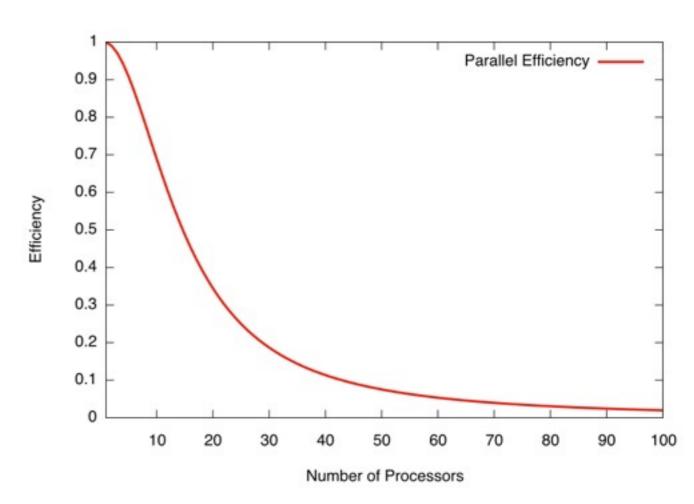
Number of processors

 $N = 10000, N_{sr}=4, C_{comm}/C_{comp} = 100$



Integration with parallel costs:

Can actually get worse with P! Communication cost increases with P



 $N = 10000, N_{sr}=4, C_{comm}/C_{comp} = 100$



Communication -to-Computation ratio

We want this to be (ideally) constant in P, or at least grow slowly; otherwise as we scale up, we spend more time sending messages than computing.

$$= \frac{2(P-1)C_{\text{comm}}}{\frac{N}{P}N_{SR}C_{\text{comp}}}$$
$$= \frac{2P(P-1)}{N}\frac{1}{N_{SR}}\frac{C_{\text{comm}}}{C_{\text{comp}}}$$
$$\sim P^2$$

If $N_{SR} \sim 4$, $C_{comm} \sim 1000 C_{comp}$, N = 10000, then $T_{comm}/T_{comp} \sim 1.2$ for P=16

(Advanced: this even matters for serial computation, due to memory bandwidth limitations. "Arithmetic Intensity")

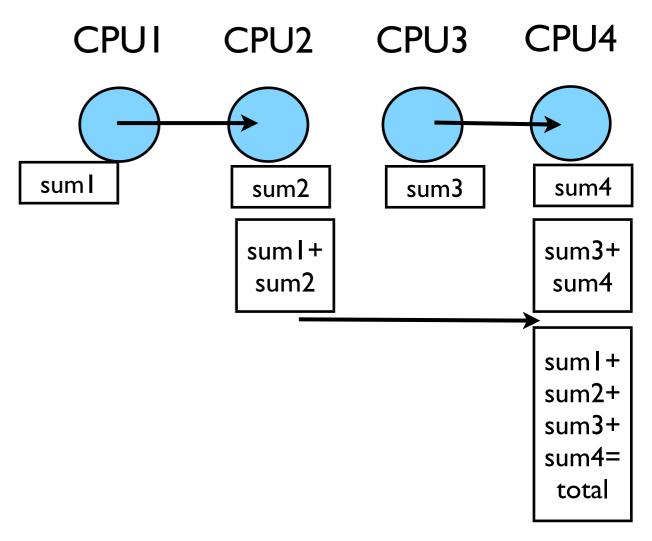
 $T_{\rm comm}$

 $T_{\rm comp}$

Better Summing

Pairs of processors; send partial sums Max messages recieved log₂(P) Can repeat to send total back

 $T_{\rm comm} = 2\log_2(P)C_{\rm comm}$

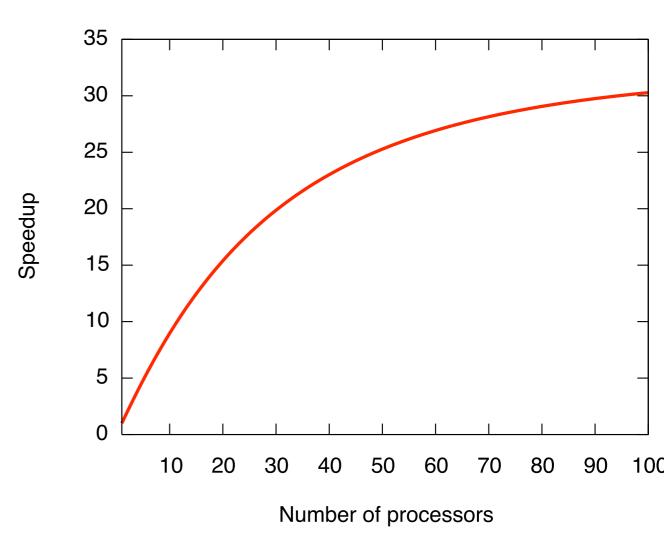


Reduction; works for a variety of operators (+,*,min,max...)



Speedup with reduction

Very good! Efficiency still falling off past 20 or so processors (But integrating 10,000 numbers...)

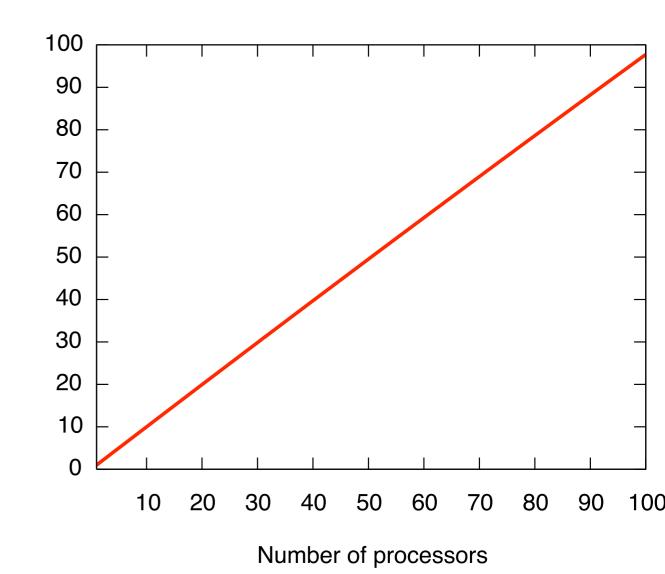




Speedup with reduction

with 1,000,000 numbers...

Speedup





$\frac{T_{\rm comm}}{T_{\rm comp}} = \frac{2\log_2(P)C_{\rm comm}}{\frac{N}{P}N_{SR}C_{\rm comp}}$ $2P \log_2(P) \quad 1 \quad C_{\text{comm}}$ Communication \overline{N} $N_{\rm SR} C_{\rm comp}$ $\sim P \log_2(P)$ -to-**Computation** ratio If $N_{SR} \sim 4$, $C_{comm} \sim 100 C_{comp}$, N Much better! = 10000, then As number of processors goes $T_{\text{comm}}/T_{\text{comp}} \sim 0.08$ for P=16 up, relative cost of

communications goes up only

logarithmically.



Parallel Computing

II: Parallel Computers





Home + Lists + June 2009

TOP500 List - June 2009 (1-100)

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description. Power data in KW for entire system

Rank	Site	Computer/Year Vendor	Cores	R _{max}	R _{peak}	Power
1	DOE/NNSA/LANL United States	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband / 2008 IBM	129600	1105.00	1456.70	2483.47
2	Oak Ridge National Laboratory United States	Jaguar - Cray XT5 QC 2.3 GHz / 2008 Cray Inc.	150152	1959.00	1381.40	6950.60
3	Forschungszentrum Juelich (FZJ) Germany	JUGENE - Blue Gene/P Solution / 2009 IBM	294912	825.50	1002.70	2268.00

Top500.org:

List updated every 6 months of the worlds 500 largest supercomputers.

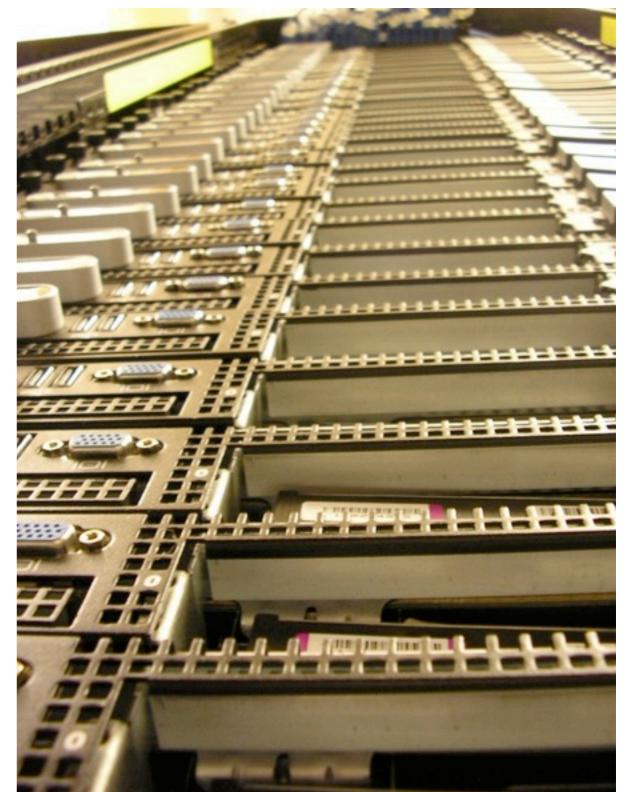
Info about architecture, ...

Petaflop (10¹⁵ flop/s); 126,600 cores



Computer Architectures

How the computers work shape how best to progam them Shared Memory vs Distributed Memory. Vector computers...

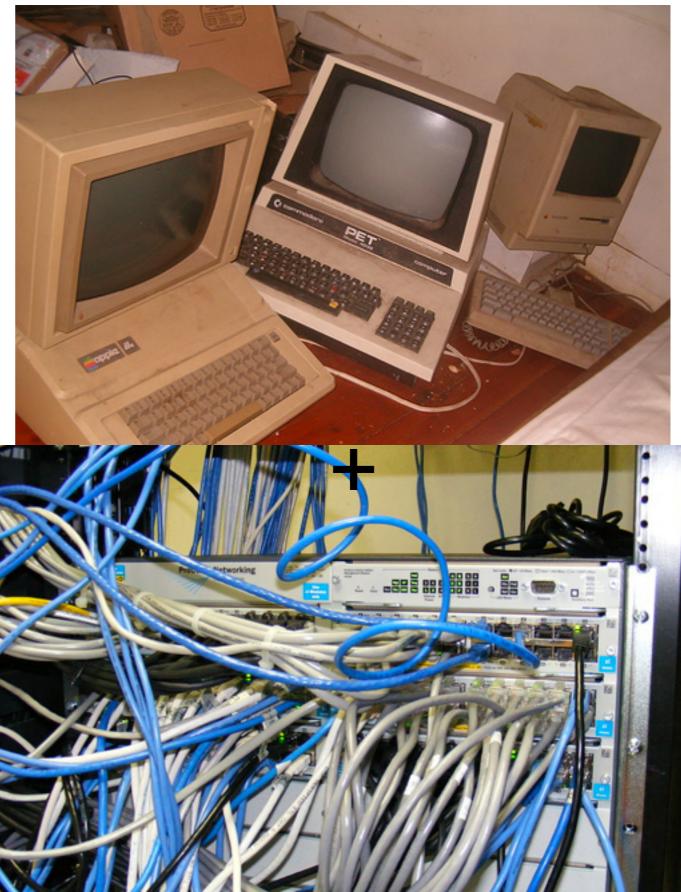




Distributed Memory: Clusters

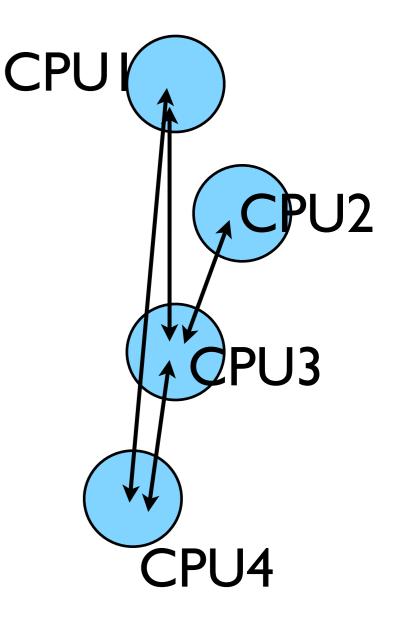
- Simplest type of parallel computer to build
- Take existing powerful standalone computers
- And network them

http://flickr.com/photos/eurleif/



Each Node is Independent

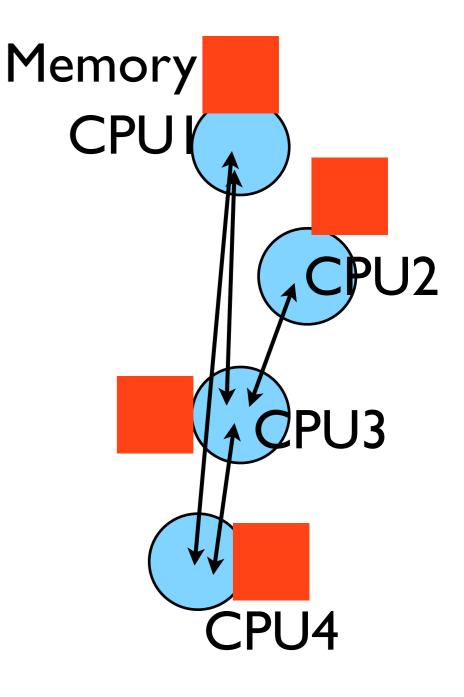
Parallel code consists of programs running on separate computers, communicating with each other *Could* be entirely different programs





Each node has independent memory

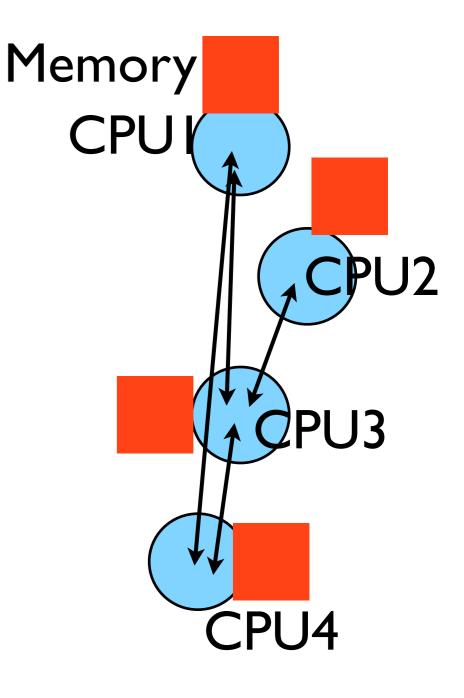
Locally stores its own portion of problem Whenever it needs information from another region, requests it from appropriate CPU Usual model: 'message passing'





Clusters +Message Passing

HW: Easy to build (harder to build *well*) HW: Can build larger and larger clusters relatively easily SW: Every communication has to be hand coded -- hard to program





	Latency	Bandwidth
GigE	~10 µs (10,000 ns)	I Gb/s (~60 ns/double)
Infiniband	~2 µs (2,000 ns)	2-10 Gb/s (~10 ns/double)

Processor speed: I FLOP ~ few ns or less

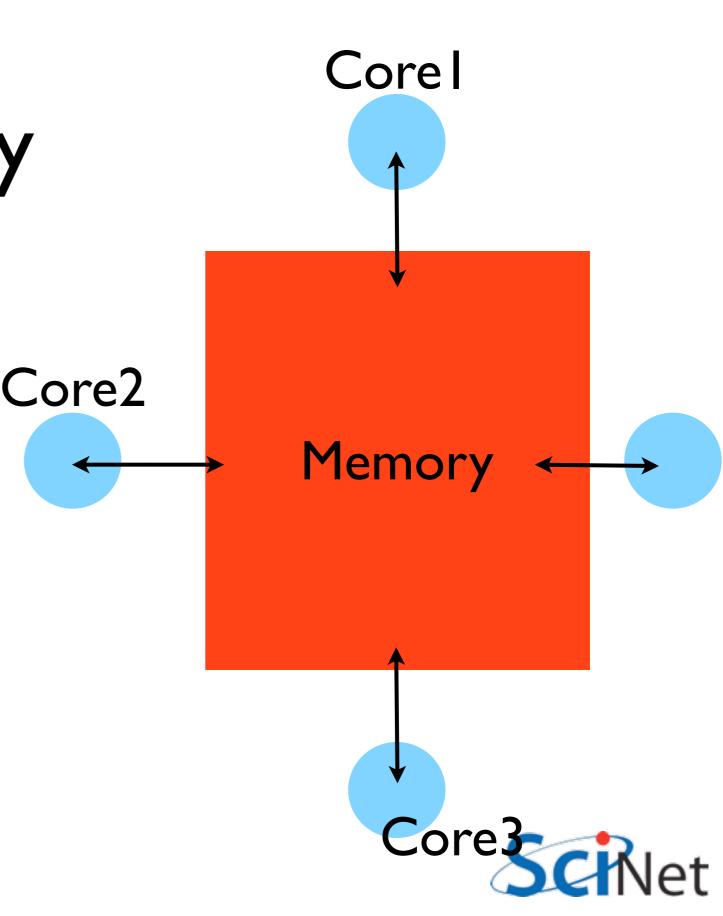


Shared Memory

One large bank of memory, different computing cores acting on it. All 'see' same data

Any coordination done through memory.

Could do like before, but why? Each core is assigned a *thread of execution* of a single program that acts on the data



Thread Vs. Process

Processes: Independent tasks with their own memory, resources

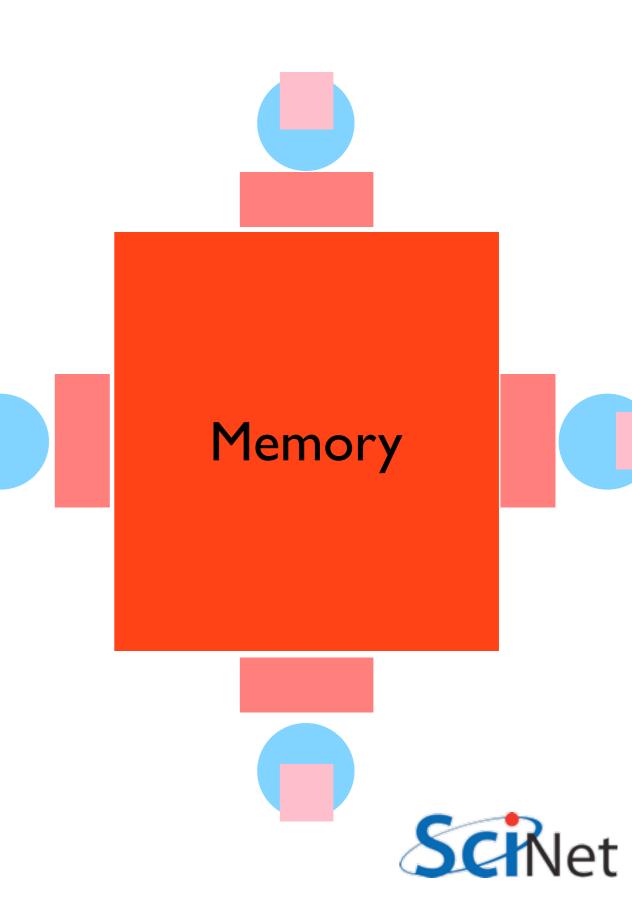
Threads: Threads of execution within one process, 'seeing' the same memory, etc.

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		150 t 191 USER	sotal, Reus, 0 72k tot 0k tot PR 25 25	0.0% al, al, NI 0 0	sy, 0 2801 VIRT 187m 187m	172k 0k RES 5504 5512	used, used, SHR 3484 3492	1 S R R	361070 %CPU 100.2 100.2	0k fr 0k fr MEM 0.0 0.0	ee, 2568 ee, 22685688 TIME+ COM 0:05.45 d: 0:05.46 d:	0.0%si, 0.0 k buffers k cached MMAND iffusion-mp: iffusion-mp:
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	Cpu (s Men Swa P10 P30 8395 18397 18392	: 150 t):100.0 1918 USER USER	otal, Reus, 0 72k tot 0k tot PR 25 1 25 1 25 1 25	0.0% al, al, NI 0 0 0 0	5y, 0 2801 VIRT 187m 187m 187m 187m	172k 0k RES 5504 5512 5508 5580	used, used, 3484 3492 3488 3556	1 R R R R	361070 %CPU 100.2 100.2 100.2 99.9	0k fr 0k fr 0.0 0.0 0.0 0.0 0.0	ee, 2568 ee, 22685688 0:05.45 d: 0:05.46 d: 0:05.46 d: 0:05.46 d:	0.0%si, 0.0 k buffers k cached MMAND iffusion-mp: iffusion-mp: iffusion-mp: ffusion-mpi
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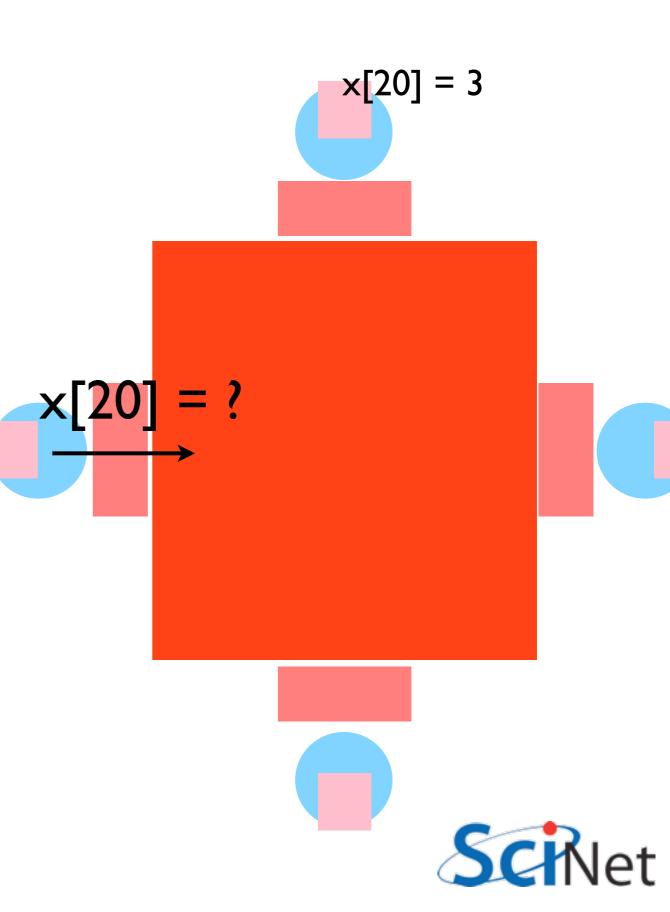
Shared Memory:NUMA

Complicating things: each core typically has some of its own memory Non-Uniform Memory Access Locality still matters Cores have cache, too. Keeping this memory *coherent* is extremely challenging



Coherency

The different levels of memory imply multiple copies of some regions Multiple cores mean can update unpredictably Very expensive hardware Hard to scale up to lots of processors, very \$\$\$ Very simple to program!!



	Latency	Bandwidth		
GigE	~10 µs (10,000 ns)	I Gb/s (~60 ns/double)		
Infiniband	~2 µs (2,000 ns)	2-10 Gb/s (~10 ns/double)		
NUMA Shared Mem	~0.1 µs (100 ns)	10-20 Gb/s (~4 ns/double)		

Processor speed: I FLOP ~ ns or less



Big Lesson #3

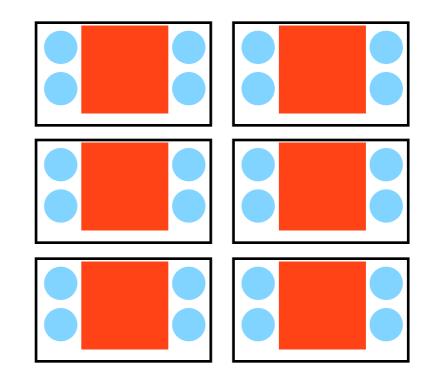
The best approach to parallelizing your problem will depend on both details of your problem and of the hardware available.



Hybrid Architectures

Almost all of the biggest computers are now clusters of shared memory nodes

Generally just use message passing across all cores, but as P(I node) goes up, hybrid approaches start to make sense.





- cp -R ~ljdursi/intro-ppp ~/
- source ~/intro-ppp/setup
- cd ~/intro-ppp/ gettingstarted/

Before we start with OpenMP:

- make omp_hello_world
 - ./omp_hello_world
 - make mpi_hello_world
 - mpirun -np 8
 ./mpi_hello_world
 - qsub -I -X into your reserved node as per instruction sheet and ensure this works



An introduction to OpenMP

OpenMP

- For Shared Memory systems
- Add Parallelism to functioning serial code
- Add compiler directives to code
- http://openmp.org tonnes of useful info





OpenMP

- Compiler, run-time environment does a lot of work for us
- Divides up work
- But we have to tell it how to use variables, where to run in parallel





OpenMP

- Mark off parallel regions

 in those regions, all
 available threads do
 same work
- Markup designed to be invisible to non-OpenMP compilers; should result in working serial code





```
C: omp-hello-world.c
gcc -fopenmp <u>-o omp-hello-world omp-hello-world.c -lgomp</u>
```

F90: omp-hello-world.f90 gfortran -fopenmp -o omp-hello-world omp-hello-world.f90 -lgomp





```
$ export OMP_NUM_THREADS=1
$ ./omp-hello-world
...
$ export OMP_NUM_THREADS=32
$ ./omp-hello-world
...
```

```
$ ./omp-hello-world
```

```
$ export OMP_NUM_THREADS=8
```

```
or
$ gfortran -o omp-hello-world omp-hello-world.f90 -fopenmp -lgomp
```

```
$ gcc -o omp-hello-world omp-hello-world.c -fopenmp -lgomp
or
```

```
gpc-f102n084-$ gcc -o omp-hello-world omp-hello-world.c -fopenmp -lgomp
qpc-f102n084-$ export OMP NUM THREADS=8
gpc-f102n084-$ ./omp-hello-world
At start of program
Hello, world, from thread 0!
Hello, world, from thread 6!
Hello, world, from thread 5!
Hello, world, from thread 4!
Hello, world, from thread 2!
Hello, world, from thread 1!
Hello, world, from thread 7!
Hello, world, from thread 3!
gpc-f102n084-$ export OMP NUM THREADS=1
gpc-f102n084-$ ./omp-hello-world
At start of program
Hello, world, from thread 0!
gpc-f102n084-$ export OMP NUM THREADS=32
gpc-f102n084-$ ./omp-hello-world
At start of program
Hello, world, from thread 11!
Hello, world, from thread 1!
Hello, world, from thread 16!
. . .
```



What did happen?

- OMP_NUM_THREADS threads launched
- Each print "Hello world..."
- In seemingly random order
- Only one 'At start of program'

gpc-f102n084-\$ gcc -o omp-hello-world omp-hello-world.c -fopenmp -lqomp gpc-f102n084-\$ export OMP NUM THREADS=8 gpc-f102n084-\$./omp-hello-world At start of program Hello, world, from thread 0! Hello, world, from thread 6! Hello, world, from thread 5! Hello, world, from thread 4! Hello, world, from thread 2! Hello, world, from thread 1! Hello, world, from thread 7! Hello, world, from thread 3! gpc-f102n084-\$ export OMP NUM THREADS=1 gpc-f102n084-\$./omp-hello-world At start of program Hello, world, from thread 0! gpc-f102n084-\$ export OMP NUM THREADS=32 gpc-f102n084-\$./omp-hello-world At start of program Hello, world, from thread 11! Hello, world, from thread 1! Hello, world, from thread 16! . . .



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
                                           Include definitions
                                              for OpenMP
   printf("At start of program\n");
#pragma omp parallel
                                           supporting library
       printf("Hello world from thread %d!\n"
                                      (omp_get_thread_num())
               omp_get_thread_num());
   return 0;
program omp helle world
use omp lib
implicit none
print *, 'At start of program'
!$omp parallel
   print *, 'Hello world from thread ', &
              omp get thread num(), '!'
!$omp end parallel
end program omp hello world
```



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
   printf("At state of program\n");
#pragma omp parallel
       printf("Hello world from thread %d!\n",
               omp get thread num());
                                          Program starts normally
    return 0;
                                               (Single thread of
                                                  execution)
program omp hello world
use omp lib
implicit none
print *, 'At start of program'
!$omp parallel
   print *, 'Hello world from thread ', &
              omp get thread num(), '!'
!$omp end parallel
end program omp hello world
```



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
   printf("At start of program\n");
#pragma omp parallel
       printf("Hello world from thread %d!\n"At start of parallel
               omp_get_thread_num());
                                                  section,
   return 0;
                                        OMP NUM THREADS
                                         threads are launched,
program omp hello world
use omp lib
                                       each execute same code.
implicit none
print *, 'At start of program'
!$omp parallel
   print *, 'Hello world from thread ', &
              omp get thread num(), '!'
!$omp end parallel
end program omp hello_world
```



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
   printf("At start of program\n");
#pragma omp parallel
       printf("Hello yerld from thread %d!\n",
               omp_get_thread_num());
                                            At end of parallel
    return 0;
                                        section, the threads join
                                       back up and back to serial
program omp hello world
                                                 execution
use omp lib
implicit none
print *, 'At start of program'
!$omp parallel
   print *, 'Hello world from thread ', &
              omp get thread num(), '!'
!$omp end parallel
end program omp hello world
```



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
   printf("At start of program\n");
#pragma omp parallel
       printf("Hello world from thread %d!\n",
               omp_get_thread_num());
                                          Special OMP function
                                        called to find the thread
   return 0;
                                       number of current thread
program omp hello world
                                                 (first = 0)
use omp lib
implicit none
print *, 'At start of program'
!$omp parallel
   print *, 'Hello world from thread ', &
              omp_get_thread_num(), '!'
!$omp end parallel
end program omp hello world
```



Turn OpenMP on in compiler (default off; incantation varies from compiler to compiler. Intel: -openmp). Always needed for OpenMP code.

- \$ gcc -o omp-hello-world omp-hello-world.c -fopenmp -lgomp
 or
- \$ gfortran -o omp-hello-world omp-hello-world.f90 -fopenmp -lgomp



Link in OpenMP libraries; normally only needed if you use functions like omp_get_num_threads(). Only at link time.

\$ gcc -o omp-hello-world omp-hello-world.c -fopenmp -lgomp
or

\$ gfortran -o omp-hello-world omp-hello-world.f90 -fopenmp -lgomp



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
    printf("At start of program\n");
#pragma omp parallel
        printf("Hello world from thread %d of %d!\n",
                omp get thread num(),
                omp get num threads());
    }
    return 0;
```

(Advanced: can set num_threads (but not thread_num), too.)



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

```
int main(int argc, char **argv) {
    printf("At start of program\n");
#pragma omp parallel
        printf("Hello world from thread %d!\n",
                omp get thread num());
    }
    printf("There were %d threads.\n",
            omp_get_num_threads() );
    return 0;
```



Variables in OpenMP

- Need to put a variable in the parallel section to store the value
- But variables in parallel sections are a little tricky.



C: omp-vars.c gcc -fopenmp -o omp-vars omp-vars.c -lgomp

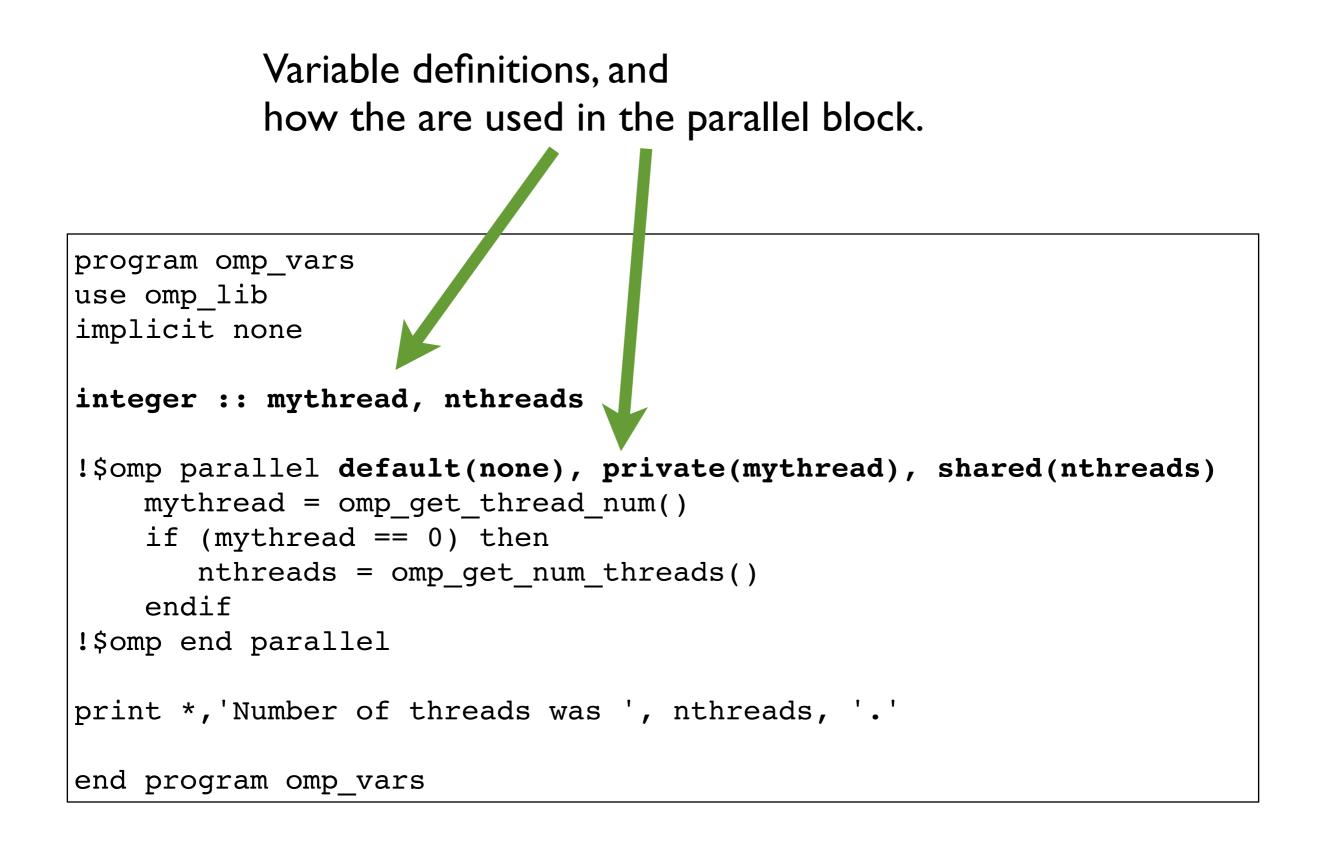
```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
    int mythread, nthreads;
#pragma omp parallel default(none), shared(nthreads), private(mythread)
    {
        mythread = omp_get_thread_num();
        if (mythread == 0)
            nthreads = omp_get_num_threads();
        }
        printf("Number of threads was %d.\n",nthreads);
        return 0;
}
```



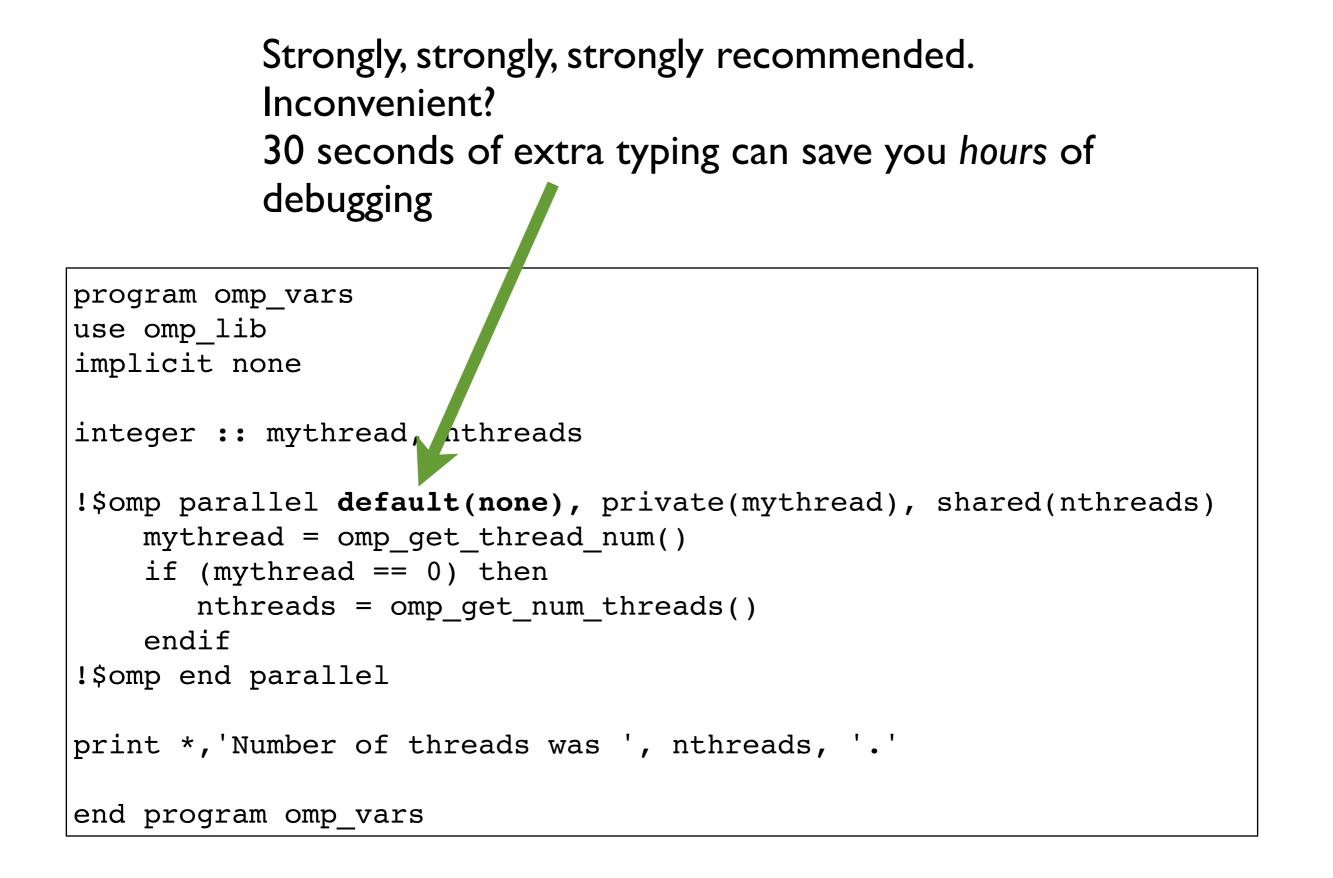
FORTRAN: omp-vars.f90 gfortran -fopenmp -o omp-vars omp-vars.f90 -lgomp

```
program omp vars
use omp lib
implicit none
integer :: mythread, nthreads
!$omp parallel default(none), private(mythread), shared(nthreads)
    mythread = omp get thread num()
    if (mythread == 0) then
       nthreads = omp get num threads()
    endif
!$omp end parallel
print *, 'Number of threads was ', nthreads, '.'
end program omp vars
```







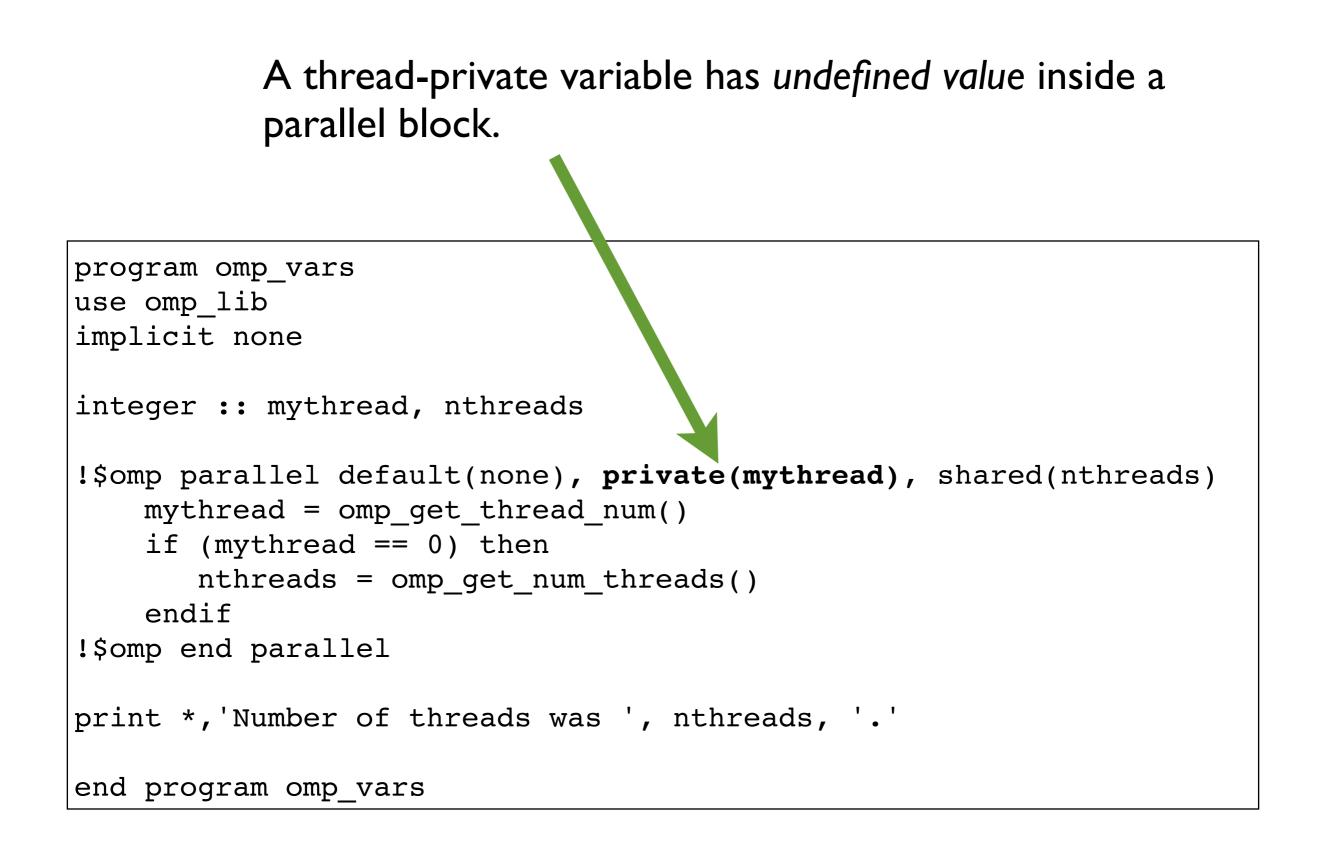




Each thread gets its own private copy of mythread to do with as it pleases. No other thread can see, modify.

```
program omp vars
use omp lib
implicit none
integer :: mythread, nthreads
!$omp parallel default(none), private(mythread), shared(nthreads)
    mythread = omp get thread num()
    if (mythread == 0) then
       nthreads = omp get num threads()
    endif
!$omp end parallel
print *, 'Number of threads was ', nthreads, '.'
end program omp vars
```





(Advanced: firstprivate, lastprivate - copy in/out.)



Everyone can see (ok), modify (danger! danger!) a shared variable. Keeps its value between serial/parallel sections

```
program omp vars
use omp lib
implicit none
integer :: mythread, nthreads
!$omp parallel default(none), private(mythread), shared(nthreads)
    mythread = omp get thread num()
    if (mythread == 0) then
       nthreads = omp get num threads()
    endif
!$omp end parallel
print *, 'Number of threads was ', nthreads, '.'
end program omp vars
```



Variables in OpenMP

- Program runs, launches threads.
- Each thread gets its own copy of mythread
- Only thread 0 writes to nthreads
- Outputs number of threads
- What would mythread be if we printed it?

```
program omp_vars
use omp_lib
implicit none
integer :: mythread, nthreads
!$omp parallel default(none), private(mythread), shared
(nthreads)
    mythread = omp_get_thread_num()
    if (mythread == 0) then
        nthreads = omp_get_num_threads()
    endif
!$omp end parallel
print *,'Number of threads was ', nthreads, '.'
end program omp_vars
```



For C folks:

```
#include <stdio.h>
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
    int nthreads;
#pragma omp parallel default(none), shared(nthreads)
    {
        int mythread;
        mythread = omp_get_thread_num();
        if (mythread == 0)
            nthreads = omp_get_num_threads();
    }
    printf("Number of threads was %d.\n",nthreads);
    return 0;
}
```

Local definitions are powerful, and avoid lots of bugs! Variables defined in a parallel block are automatically thread private.



Single Execution in OpenMP

- Do we care that it's thread 0 in particular that updates nthreads?
- Why did we pick 0?
- Often we just want the first thread through to do something, don't care who.

```
program omp_vars
use omp_lib
implicit none
integer :: mythread, nthreads
!$omp parallel default(none), private(mythread), shared
(nthreads)
    mythread = omp_get_thread_num()
    if (mythread == 0) then
        nthreads = omp_get_num_threads()
    endif
!$omp end parallel
print *, 'Number of threads was ', nthreads, '.'
end program omp_vars
```



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
    int nthreads;
#pragma omp parallel default(none), shared(nthreads)
#pragma omp single
        nthreads = omp_get_num_threads();
    printf("Number of threads was %d.\n",nthreads);
    return 0;
}
```

```
program omp vars
use omp lib
implicit none
integer :: nthreads
!$omp parallel default(none), shared(nthreads)
!$omp single
    nthreads = omp get num threads()
!$omp end single
!$omp end parallel
print *, 'Number of threads was ', nthreads, '.'
end program omp vars
```



Loops in OpenMP

- Now let's try something a little more interesting
- copy one of your omp programs to omp_loop.c (or omp_loop.f90) and let's put a loop in the parallel section



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
    int i, mythread;
#pragma omp parallel default(none) XXXX(i) XXXX(mythread)
    {
        mythread = omp_get_thread_num();
        for (i=0; i<16;i++) {
            printf("Thread %d gets i=%d\n",mythread,i);
        }
        return 0;
}</pre>
```

```
program omp_loop
use omp_lib
implicit none
integer :: i, mythread
!$omp parallel default(none) XXXX(i) XXXX(mythread)
    mythread = omp_get_thread_num()
    do i=1,16
        print *, 'thread ', mythread, ' gets i=', i
    enddo
!$omp end parallel
end program omp loop
```



Worksharing constructs in OpenMP

- We don't generally want tasks to do exactly the same thing
- Want to partition a problem into pieces, each thread works on a piece
- Most scientific programming full of work-heavy loops
- OpenMP has a worksharing construct: omp for (or omp do)

```
program omp_loop
use omp_lib
implicit none
integer :: i, mythread
!$omp parallel default(none) XXXX(i) XXXX(mythread)
    mythread = omp_get_thread_num()
    do i=1,16
        print *, 'thread ', mythread, ' gets i=', i
        enddo
!$omp end parallel
end program omp_loop
```

(Advanced: Can combine parallel and for into one omp line.)



```
#include <stdio.h>
#include <omp.h>
int main(int argc, char **argv) {
    int i, mythread;
#pragma omp parallel default(none) XXXX(i) XXXX(mythread)
    ł
        mythread = omp get thread num();
#pragma omp for
        for (i=0; i<16;i++) {</pre>
            printf("Thread %d gets i=%d\n",mythread,i);
        }
    }
    return 0;
program omp loop
use omp lib
implicit none
integer :: i, mythread
!$omp parallel default(none) XXXX(i) XXXX(mythread)
    mythread = omp get thread num()
!$omp do
    do i=1,16
        print *, 'thread ', mythread, ' gets i=', i
    enddo
!$omp end parallel
end program omp loop
```



Worksharing constructs in OpenMP

- omp for / omp do construct breaks up the iterations by thread.
- If doesn't divide evenly, does the best it can.
- Allows easy breaking up of work!

\$./omp_loop			
thread	3	gets i=	7
thread	3	gets i=	8
thread	4	gets i=	9
thread	4	gets i=	10
thread	5	gets i=	11
thread	5	gets i=	12
thread	6	gets i=	13
thread	6	gets i=	14
thread	1	gets i=	3
thread	1	gets i=	4
thread	0	gets i=	1
thread	0	gets i=	2
thread	2	gets i=	5
thread	2	gets i=	6
thread	7	gets i=	15
thread	7	gets i=	16
\$			

(Advanced: can break up work of arbitrary blocks of code with "omp task" construct.)



DAXPY

- multiply a vector by a scalar, add a vector.
- (a X plus Y, in double precision)
- Implement this, first serially, then with OpenMP
- daxpy.c or daxpy.f90
- make daxpy or make fdaxpy

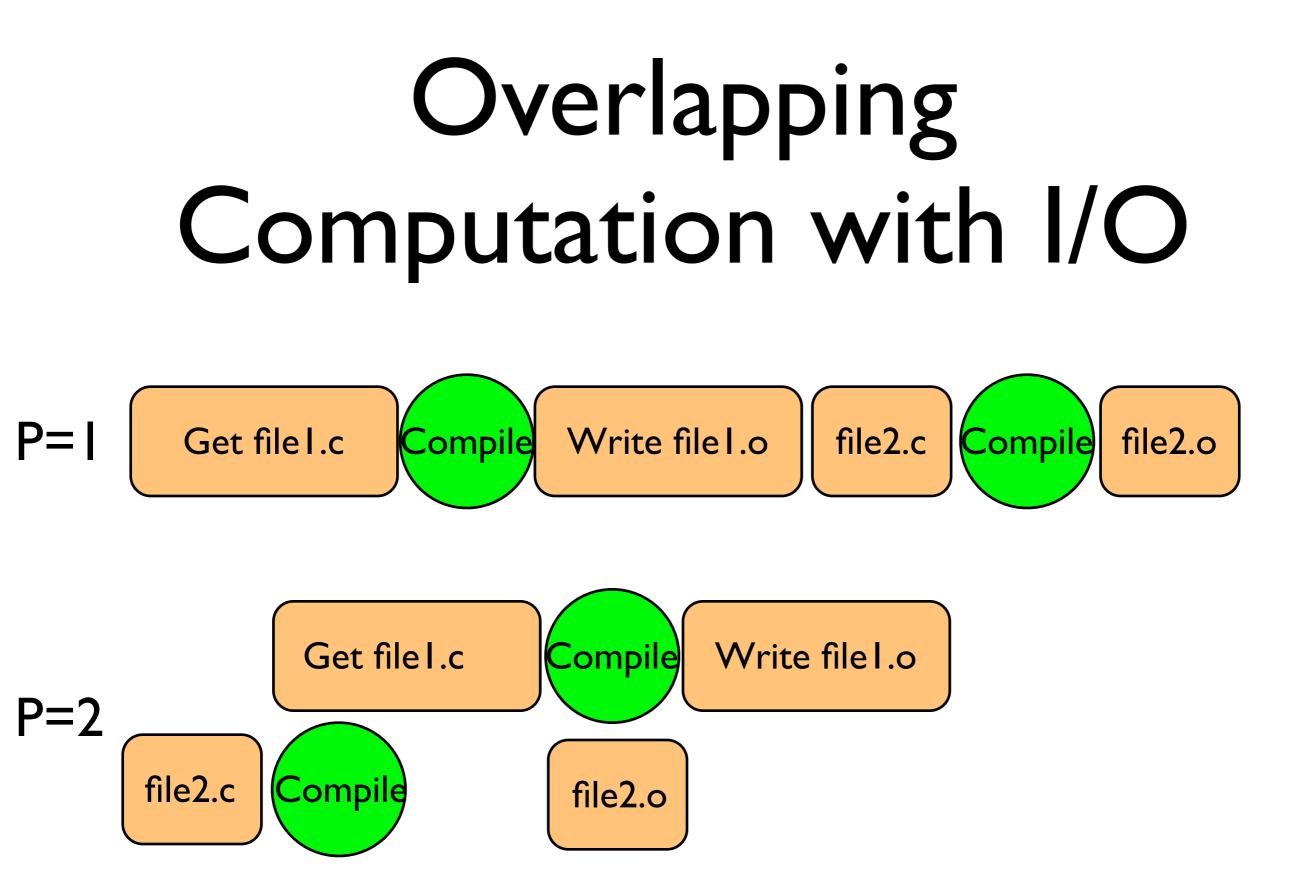
$$\hat{z} = a\hat{x} + \hat{y}$$



make

- Make builds an executable from a list of source code files and rules
- Many files to do, of which order doesn't matter for most
- Parallelism!
- make -j N launches N processes to do it
- make -j 2 often shows speed increase even on single processor systems

\$ make \$ make -j 2 \$ make -j



```
#include <stdio.h>
#include "pca utils.h"
                            NType *x, NType *y, NType *z)
void daxpy(int n, NType
{
    for (int i=0; i<n; i++) {</pre>
        x[i] = (NType)i*(NType)i;
        y[i] = ((NType)i+1.)*(NType)i-1.);
    }
    for (int i=0; i<n; i++)</pre>
                                         Utilities for this course; NType is a
        z[i] += a * x[i] + y[i];
                                         numerical type which can be set to sir
}
                                         or double precision
int main(int argc, char *argv[]) {
    int n=1e7;
    NType *x = vector(n);
    NType *y = vector(n);
    NType *z = vector(n);
    NType a = 5./3.;
    pca time tt;
    tick(&tt);
    daxpy(n,a,x,y,z);
    tock(&tt);
    free(z);
    free(y);
    free(x);
```

```
#include <stdio.h>
#include "pca utils.h"
void daxpy(int n, NType a, NType *x, NType *y, NType *z)
{
    for (int i=0; i<n; i++) {</pre>
                                                  Fill arrays with
        x[i] = (NType)i*(NType)i;
                                                  calculated values
        y[i] = ((NType)i+1.)*((NType)i-1.);
    }
    for (int i=0; i<n; i++)</pre>
        z[i] += a * x[i] + y[i];
}
int main(int argc, char *argv[]) {
    int n=1e7;
    NType *x = vector(n);
    NType *y = vector(n);
    NType *z = vector(n);
    NType a = 5./3.;
    pca time tt;
    tick(&tt);
    daxpy(n,a,x,y,z);
    tock(&tt);
    free(z);
    free(y);
    free(x);
```

```
#include <stdio.h>
#include "pca utils.h"
void daxpy(int n, NType a, NType *x, NType *y, NType *z)
{
    for (int i=0; i<n; i++) {</pre>
        x[i] = (NType)i*(NType)i;
        y[i] = ((NType)i+1.)*((NType)i-1.);
    }
    for (int i=0; i<n; i++)</pre>
                                        Do calculation
        z[i] += a * x[i] + y[i];
}
int main(int argc, char *argv[]) {
    int n=1e7;
    NType *x = vector(n);
    NType *y = vector(n);
    NType *z = vector(n);
    NType a = 5./3.;
    pca time tt;
    tick(&tt);
    daxpy(n,a,x,y,z);
    tock(&tt);
    free(z);
    free(y);
    free(x);
```



```
#include <stdio.h>
#include "pca utils.h"
void daxpy(int n, NType a, NType *x, NType *y, NType *z)
{
    for (int i=0; i<n; i++) {</pre>
        x[i] = (NType)i*(NType)i;
        y[i] = ((NType)i+1.)*((NType)i-1.);
    }
    for (int i=0; i<n; i++)</pre>
        z[i] += a * x[i] + y[i];
}
int main(int argc, char *argv[]) {
    int n=1e7;
    NType *x = vector(n);
    NType *y = vector(n);
    NType *z = vector(n);
    NType a = 5./3.;
                                                    here).
    pca time tt;
    tick(&tt);
    daxpy(n,a,x,y,z);
    tock(&tt);
    free(z);
    free(y);
    free(x);
```

Driver - do timings, etc. (nothing needs to be changed in here).



OpenMPing DAXPY

- How do we OpenMP this?
- Try it (~5-10 min)

```
#include <stdio.h>
#include "pca utils.h"
void daxpy(int n, NType a, NType *x, NType *y, NType *z)
{
    for (int i=0; i<n; i++) {</pre>
        x[i] = (NType)i*(NType)i;
        y[i] = ((NType)i+1.)*((NType)i-1.);
    }
    for (int i=0; i<n; i++)</pre>
        z[i] += a * x[i] + y[i];
}
int main(int argc, char *argv[]) {
    int n=1e7;
    NType *x = vector(n);
    NType *y = vector(n);
    NType *z = vector(n);
    NType a = 5./3.;
    pca time tt;
    tick(&tt);
    daxpy(n,a,x,y,z);
    tock(&tt);
    free(z);
    free(y);
    free(x);
    return 0;
```



```
void daxpy(int n, NType a, NType *x, NType *y, NType *z)
{
#pragma omp parallel default(none) shared(n,x,y,a,z) private(i)
{
#pragma omp for
    for (int i=0; i<n; i++) {
        x[i] = (NType)i*(NType)i;
        y[i] = ((NType)i+1.)*((NType)i-1.);
    }
#pragma omp for
    for (int i=0; i<n; i++)
        z[i] += a * x[i] + y[i];
}
</pre>
```



```
$ ./daxpy
Tock registers 2.5538e-01 seconds.
[...add OpenMP...]
$ make daxpy
gcc -std=c99 -g -DPGPLOT -I/home/ljdursi/intro-ppp//util/ -I/scinet/gpc/
Libraries/pgplot/5.2.2-gcc -fopenmp -c daxpy.c -o daxpy.o
gcc -std=c99 -g -DPGPLOT -I/home/ljdursi/intro-ppp//util/ -I/scinet/gpc/
Libraries/pgplot/5.2.2-gcc -fopenmp daxpy.o -o daxpy /home/ljdursi/intro-
ppp//util//pca utils.o -lm
$ export OMP NUM THREADS=8
$ ./daxpy
Tock registers 6.9107e-02 seconds.
$ export OMP NUM THREADS=4
$ ./daxpy
Tock registers 1.0347e-01 seconds.
$ export OMP NUM THREADS=2
$ ./daxpy
Tock registers
                  1.8619e-01 seconds.
```



\$./daxpy Tock registers 2.5538e-01 seconds. [...add OpenMP...] \$ make daxpy gcc -std=c99 -g -DPGPLOT -I/home/ljdursi/intro-ppp//util/ -I/scinet/gpc/ Libraries/pgplot/5.2.2-gcc -fopenmp -c daxpy.c -o daxpy.o gcc -std=c99 -g -DPGPLOT -I/home/ljdursi/intro-ppp//util/ -I/scinet/gpc/ Libraries/pgplot/5.2.2-gcc -fopenmp daxpy.o -o daxpy /home/ljdursi/introppp//util//pca utils.o -lm \$ export OMP NUM THREADS=8 \$./daxpy 3.69x speedup, 46% efficiency Tock registers 6.9107e-02 seconds. \$ export OMP NUM THREADS=4 \$./daxpy 2.44x speedup, 61% efficiency Tock registers 1.0347e-01 seconds. \$ export OMP NUM THREADS=2 ./daxpy \$ 1.86x speedup, 93% efficiency 1.8619e-01 seconds. Tock registers



```
void daxpy(int n, NType a, NType *x, NType *y, NType *z)
ł
#pragma omp parallel default(none) shared(n,x,y,a,z) private(i)
#pragma omp for
    for (int i=0; i<n; i++) {</pre>
       x[i] = (NType)i*(NType)i;
       y[i] = ((NType)i+1.)*((NType)i-1.);
    }
#pragma omp for
    for (int i=0; i<n; i++)</pre>
        z[i] += a * x[i] + y[i];
                                                     Why is this safe?
}
                                                     Everyone's modifying x,y,z
!$omp parallel default(none) private(i) shared(a,x,b,y,z)
!$omp do
         do i=1,n
             x(i) = (i)*(i)
             y(i) = (i+1.)*(i-1.)
         enddo
!$omp do
         do i=1,n
             z(i) = a * x(i) + y(i)
         enddo
!$omp end parallel
```

Dot Product

- Dot product of two vectors
- Implement this, first serially, then with OpenMP
- ndot.c or ndot.f90
- make ndot or make ndotf
- Tells time, answer, correct answer.

$$n = \hat{x} \cdot \hat{y} \\ = \sum_{i} x_{i} y_{i}$$

\$./ndot
Dot product is 3.3333e+20
(vs 3.3333e+20) for n=10000000.
Took 5.3578e-02 seconds.



```
...main program...
 print *, 'Dot product is ', res, '(vs ', ans,') for n = ',n,'.
Took ', time, 'sec.'
 deallocate(x,y)
 contains
  double precision function calc ndot(n, x, y)
      implicit none
      integer, intent(in) :: n
      double precision, dimension(n) :: x
      double precision, dimension(n) :: y
      double precision :: ndot
      integer :: i
      ndot = 0.
      do i=1,n
          ndot = ndot + x(i)*y(i)
      enddo
      calc ndot = ndot
  end function calc_ndot
```

How to OpenMP this?



```
double precision function calc_ndot(n, x, y)
                                                fomp_ndot_race.f90
       implicit none
                                                omp_ndot_race.c
       integer, intent(in) :: n
       double precision, dimension(n) :: x
       double precision, dimension(n) :: y
       double precision :: ndot
       integer :: i
!$omp parallel default(none) shared(ndot,x,y,n) private(i)
       ndot = 0.
       do i=1,n
           ndot = ndot + x(i)*y(i)
       enddo
!$omp end parallel
       calc ndot = ndot
   end function calc ndot
```



```
double precision function calc_ndot(n, x, y)
                                                fomp_ndot_race.f90
       implicit none
                                                omp_ndot race.c
       integer, intent(in) :: n
       double precision, dimension(n) :: x
       double precision, dimension(n) :: y
       double precision :: ndot
       integer :: i
!$omp parallel default(none) shared(ndot,x,y,n) private(i)
       ndot = 0.
       do i=1,n
           ndot = ndot + x(i)*y(i)
       enddo
!$omp end parallel
       calc ndot = ndot
   end function calc ndot
```

\$./ndotf

Dot product is 3.33333283333717098E+020 (vs 3.33333363469873840E+020)
for n = 10000000. Took 5.0000007E-02 sec.
\$ export OMP_NUM_THREADS=8
\$./fomp_ndot_race
Dot product is 6.06898061003712922E+019 (vs 3.3333363469873840E+020)
for n = 10000000. Took 0.16300000 sec.

Wrong answer - and slower!



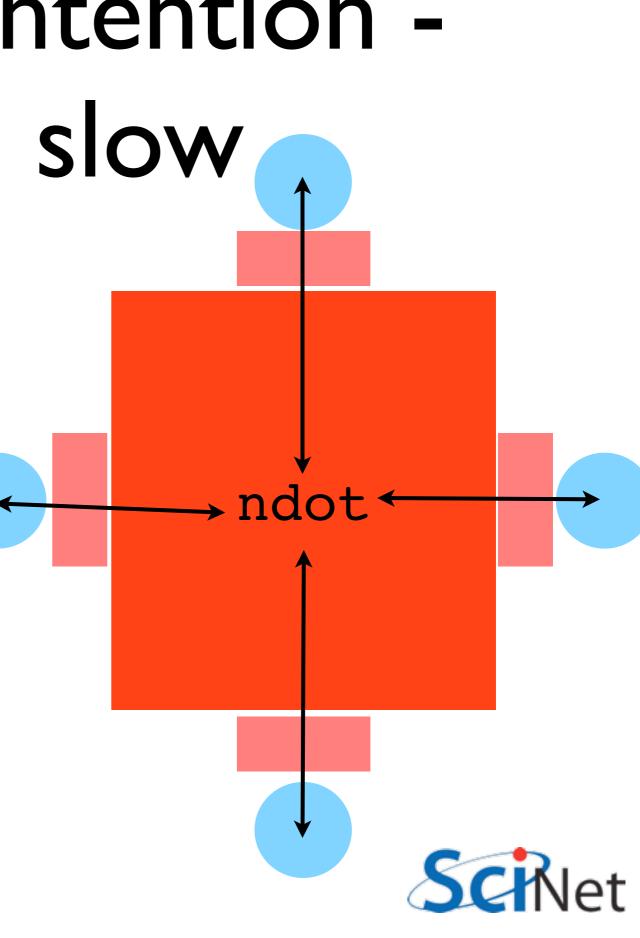
Race Condition - why it's wrong N Classic parallel bug ndot = 0.

- Multiple writers to some shared resource
- Can be very subtle, and only appear intermittently
- Your program can have a bug but not display any symptoms for small runs!
- Primarily a problem with shared memory

Thread 0: add I	Thread I: add 2
read ndot (=0) into register	
reg = reg + I	read ndot (=0) into register
store reg (=1) into ndot	reg = reg + 2
	store reg (=2) into ndot
ndot =2	

Memory contention - why it's slow

- Multiple cores repeatedly trying to read, access, store same variable in memory
- Not (such) a problem for constants (read only); but a big problem for writing.
- Sections of arrays -- better.



OpenMP critical

construct

- Defines a "critical region"
- Only one thread can be operating within this region at a time
- Keeps modifications to shared resources safe
- #pragma omp critical or !\$omp critical / !\$omp end critical

```
NType ndot_critical(int n, NType *x, NT
```

```
NType tot=0;
#pragma omp parallel for shared(x,y,n,t
for (int i=0; i<n; i++)
#pragma omp critical
        tot += x[i] * y[i];
    return tot;
```

OpenMP atomic construct

- Most hardware has support for atomic (indivisible - eg, can't get interrupted) instructions
- Small subset, but load/add/store usually one
- Not as general as critical
- Much lower overhead
- Better -- 'only' 18x slower than serial! Still some overhead, still memory contention.

\$./ndot		
Dot product is 3.3333e+20		
(vs 3.3333e+20) for n=10000000.		
Took 5.3570e-02 seconds.		
\$./omp_ndot_atomic		
Dot product is 3.3333e+20		
(vs 3.3333e+20) for n=10000000.		
Took 9.7981e-01 seconds.		



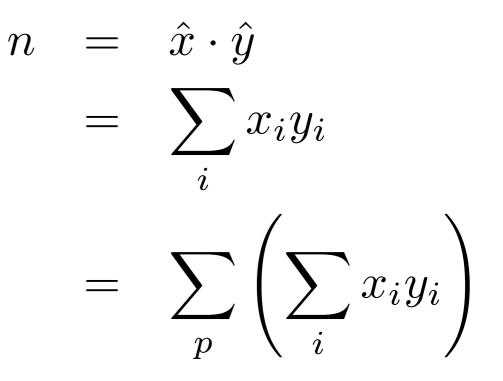
How should we fix this?

$$n = \hat{x} \cdot \hat{y} \\ = \sum_{i} x_{i} y_{i}$$



How should we fix this?

- Local sums
- Each processor sums its local value (10⁷/P additions)
- And then sums to ntot (only P additions) with critical, or atomic..
- Try this (5-10 min)
- cp one of the omp_ndot.c's or fomp_ndot.c's to omp_ndot_local.c (or fomp_ndot_local.f90)





Local variables:

```
#pragma omp parallel shared(x,y,n,tot)
    private(mytot)
  {
```

```
mytot = 0;
#pragma omp for
for (int i=0; i<n; i++)
    mytot += x[i] * y[i];
```

```
#pragma omp atomic
tot += mytot;
```

}

```
$ ./ndot
Dot product is 3.3333e+20
(vs 3.3333e+20) for n=10000000.
Took 5.3570e-02 seconds.
```



OpenMP Reduction Operations

sum

- This is such a common operation, there is something built into OpenMP to handle it
- "reduction" variables like shared or private
- Can support several types of operations - +, *...
- omp_ndot_reduction.c, fomp_ndot_reduction.f90

Reduction; works for a variety of operators (+,*,min,max...)

CPU4

sum4

sum3+

sum4

sum +

sum2+

sum3+

sum4=

total

sum3

sum2

sum I+

sum2

OpenMP Reduction Operations

```
NType ndot_atomic(int n, NType *x, NType *y)
{
    NType tot=0;
#pragma omp parallel shared(x,y,n), reduction(+:tot)
{
    #pragma omp for
    for (int i=0; i<n; i++)
        tot += x[i] * y[i];
}
    return tot;
}</pre>
```



OpenMP Reduction Operations

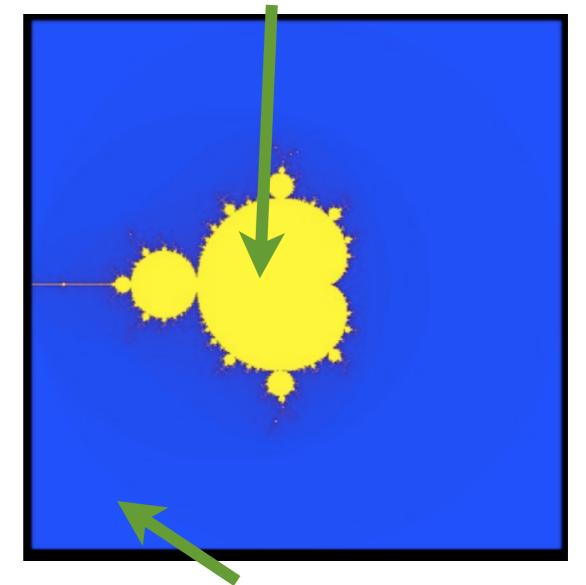
```
double precision function calc ndot(n, x, y)
implicit none
integer, intent(in) :: n
double precision, dimension(n) :: x
double precision, dimension(n) :: y
double precision :: ndot
integer :: i
ndot = 0.
!$omp parallel default(none) shared(n,x,y) reduction(+:ndot) private(i)
!$omp do
    do i=1,n
        ndot = ndot + x(i)*y(i)
    enddo
!$omp end parallel
calc ndot = ndot
```

end function calc_ndot



Lots of work

- So far, every iteration of the loop has had the same amount of work:
- Not always the case
- make mandel; ./mandel
- Plots a function at every pixel with different amount of work - in fact, amount of work is basically the plotted color.

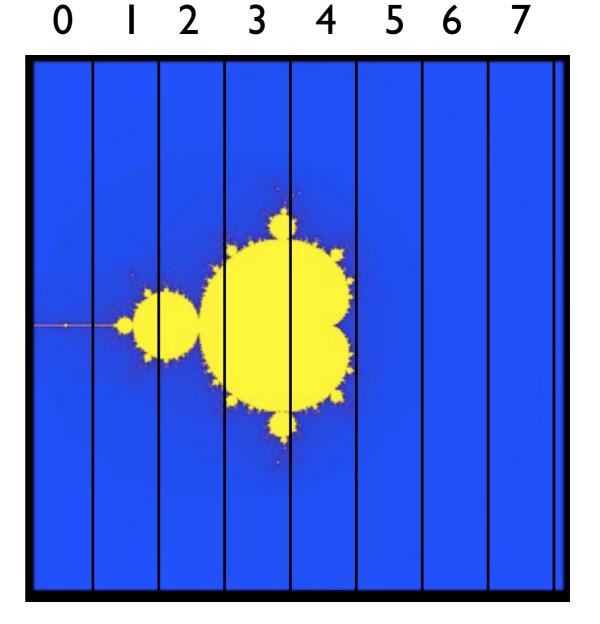






0

- Default work sharing breaks N iterations into ~N/nthreads contiguous chunks and assigns them to threads
- But now threads 7, 6, 5 will be done and sitting idle while threads 3,4 work alone...

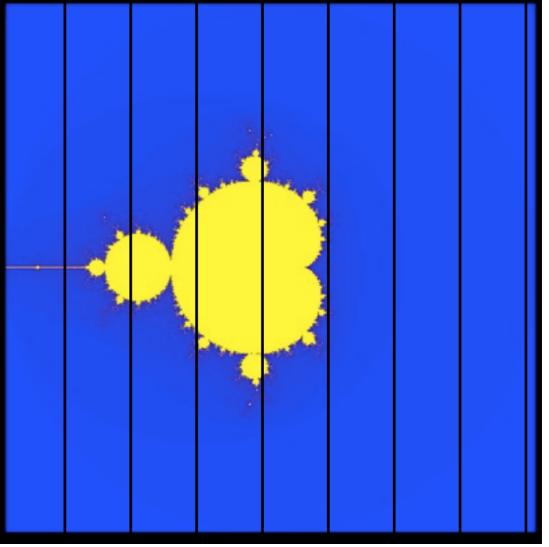


Inefficient use of resources



0

Serial 0.63s Nthreads=8 0.29s Speedup 2.2x 27% Efficiency



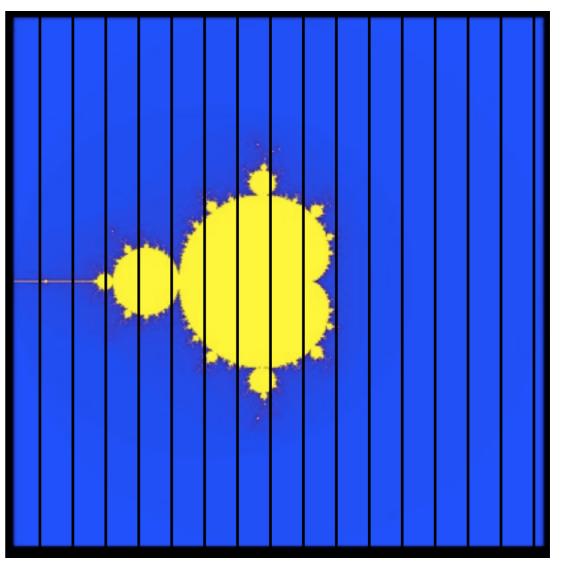
I 2 3 4 5 6 7

800x800 pix; N/nthreads ~ 100x800

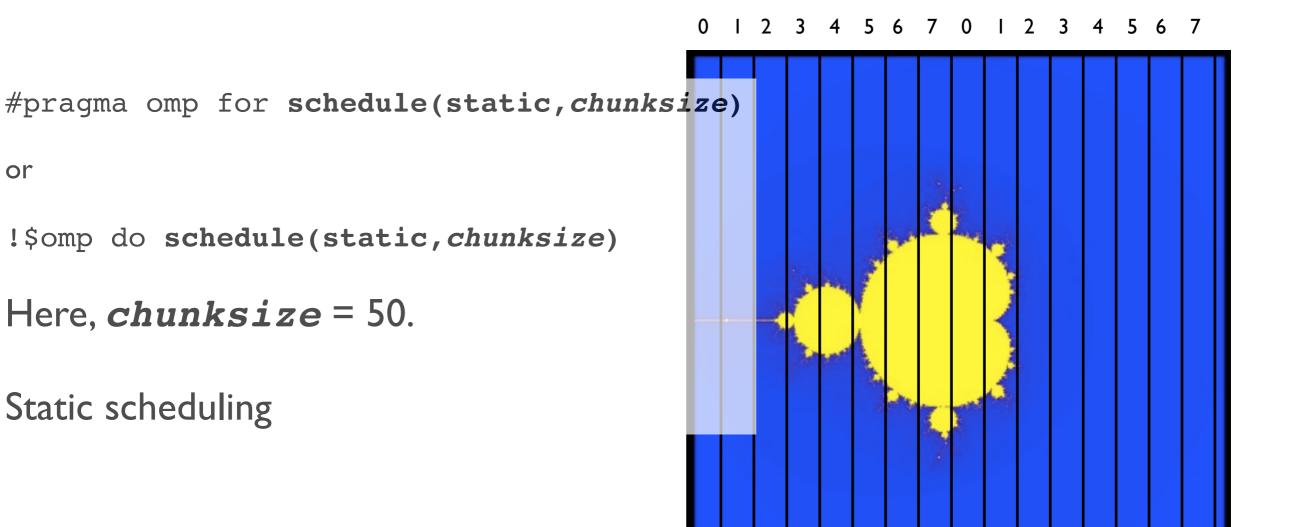


- Can change the `chunk size' from ~N/nthreads to arbitrary number
- In this case, more columns - work distributed a bit better
- Now, for instance, chunk size ~ 50, and thread 7 gets both a big work chunk and a little work chunk.

I 2 3 4 5 6 7 0 I 2 3 4 5 6 7





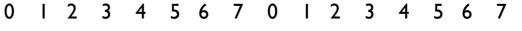


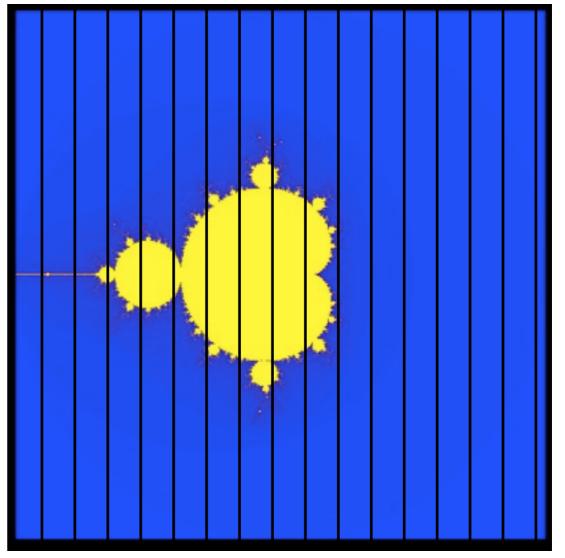
or



schedule(static,50)

Serial	0.63s
Nthreads=8	0.15s
Speedup	4.2x
Efficiency	52%

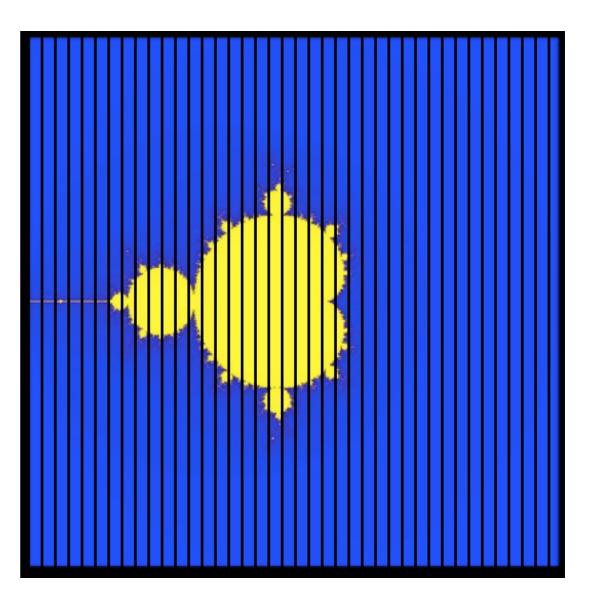






schedule(dynamic)

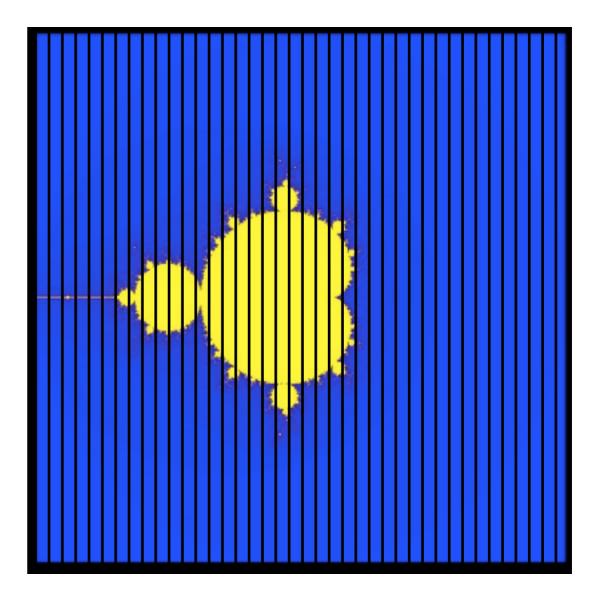
- Still another choice is to break it up into many pieces and hand them to threads when they are ready
- dynamic scheduling
- Has increased overhead, but can do a very good job
- can also choose chunksize for dynamic





schedule(dynamic)

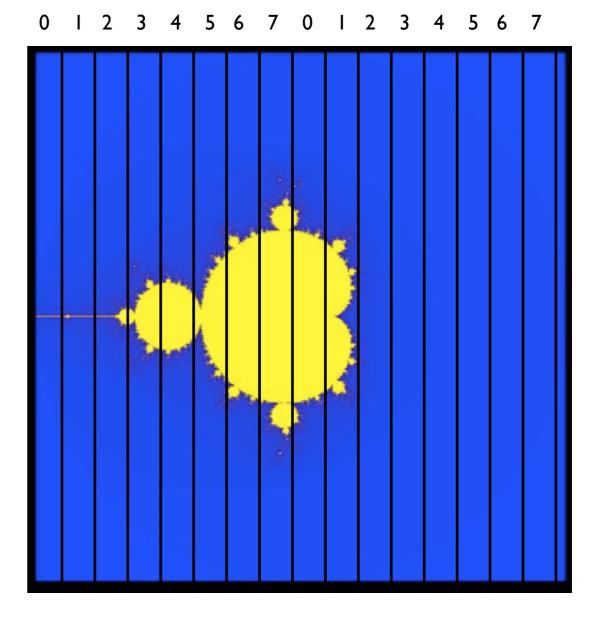
Serial	0.63s
Nthreads=8	0.10
Speedup	6.3x
Efficiency	79%





Tuning

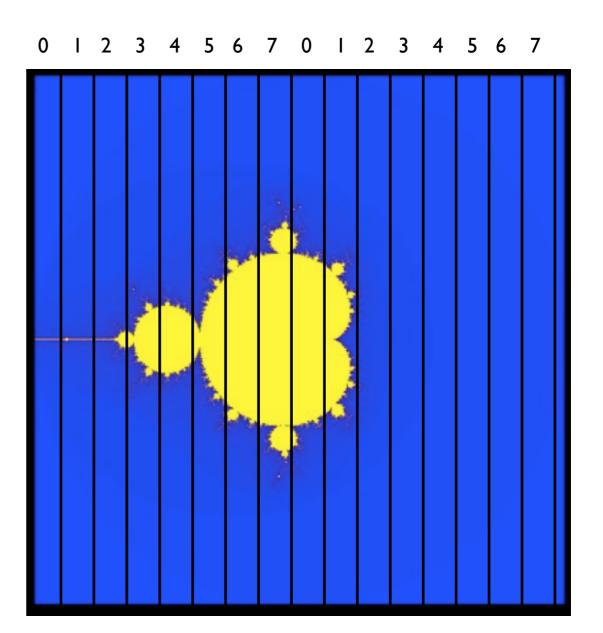
- schedule(static) (default) or schedule(dynamic) are good starting places
- To get best performance in badly imbalanced problems, may have to play with chunk sizes will depend on your problem, and hardware.





Tuning

(static,4)	(dynamic, I 6)
0.084s	0.099s
7.6x	6.4x
95%	80%





Two-level loops

 In scientific code, we usually have nested loops where all the work is.

```
#pragma omp for schedule(static,4)
for (int i=0;i<npix;i++)
for (int j=0;j<npix;j++) {
   double x=((double)i)/((double)np
   double y=((double)j)/((double)np
   double complex a=x+I*y;
   mymap[i][j]=how_many_iter_real(a
  }</pre>
```

 Almost without exception, want the loop on the *outside-most* loop. Why?

mandel.c



Summary

- omp parallel
- omp single
- shared/private/reduction variables
- omp atomic, omp critical
- omp for

