Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 11

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London

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Today

Further comments on f2py and timing code

Compiling and profiling fortran code

Introduction to parallel computing

Fortran timing functions

See midpoint_time.f90: timers placed around *do-loop* which computes areas of rectangles

Can use timing results to check of code is behaving "properly."

```
!timing variables
    real(kind=8) :: cpu_t1,cpu_t2,clock_time
    integer(kind=8) :: clock_t1,clock_t2,clock_rate


 call system_clock(clock_t1)
 call cpu_time(cpu_t1)
    !loop over intervals computing each interval's contribution to
integral
... Midpoint quadrature ...
 call cpu_time(cpu_t2)
 print *, 'elapsed cpu time (seconds) =',cpu_t2-cpu_t1

 call system_clock(clock_t2,clock_rate)
 print *, 'elapsed wall time (seconds)= ',
                          dble(clock_t2-clock_t1)/dble(clock_rate)
```

Fortran timing functions

- **Run midpoint_time with N=20000 and N=40000**

```
$ ./midpoint_time.exe
 elapsed cpu time (seconds) =   4.440000000000038E-004
 elapsed wall time (seconds)=    5.30000019E-04
 N=       20000
```

```
$ ./midpoint_time.exe
 elapsed cpu time (seconds) =   8.839999999999980E-004
 elapsed wall time (seconds)=    9.67999978E-04
 N=       40000
```

- **We can see the cpu time doubles (as we would hope). The wall-time shows more complicated behavior – could be related to what other background processes are running, or just the very short computation time.**

Profiling

- **Profilers give detailed information about time spent in different parts of code**
- **In python:** *run –p filename* **gives profiling info**
- **With fortran (or c), can use *gprof* utility (not available on Macs)**
- **Steps:**
  1. **Compile code with** *–pg* **flag**

```
$ gfortran –pg –o mt2.exe midpoint_time2.f90
```

Profiling

- **Profilers give detailed information about time spent in different parts of code**
- **In python:** *run –p filename* **gives profiling info**
- **With fortran (or c), can use *gprof* utility (not available on Macs)**
- **Steps:**
  1. **Compile code with** *–pg* **flag**

```
$ gfortran –pg –o mt2.exe midpoint_time2.f90
```

  2. **Run code (this will generate *gmon.out)*:**

```
$ ./mt2.exe
```

  3. **Finally, run gprof**

```
$ gprof ./mt2.exe
```

Profiling

Output looks like:

```
Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls   s/call   s/call  name
 63.67      6.25     6.25        1     6.25     9.85  MAIN__
 36.75      9.85     3.61 512000000     0.00     0.00  integrand_
```

and:

```
index % time    self  children    called     name
                6.25    3.61       1/1           main [2]
[1]    100.0    6.25    3.61       1         MAIN__ [1]
                3.61    0.00 512000000/512000000     integrand_ [3]
-----------------------------------------------
                                                 <spontaneous>
[2]    100.0    0.00    9.85                  main [2]
                6.25    3.61       1/1           MAIN__ [1]
-----------------------------------------------
                3.61    0.00 512000000/512000000     MAIN__ [1]
[3]     36.6    3.61    0.00 512000000         integrand_ [3]
-----------------------------------------------
```

Profiling

- Can get line-by-line information from other tools like, *oprof*
- The more complicated the code, the more useful profiling becomes

Notes on compiling

- **Up to now:**

```
$ gfortran –c program.f90
$ gfortran –o program.exe program.o –llapack
```

or

```
$ gfortran –o program.exe program.f90 –llapack
```

- **But typically want to turn on *optimization* -O flag:**

```
$ gfortran –O3 –c program.f90
```

- **-O3 is highest level of optimization (can also use -O1, -O2)**

Notes on compiling

- Look at midpoint_time.f90 compiled with and without -O3:

```
$ ./mt2.exe
 elapsed cpu time (seconds) =  0.3251049999999998
 elapsed wall time (seconds)=   0.326231003
 N=        25600
 sum=   3.1415926537169634
 error=   1.2717027431108363E-010

$ ./mt2_O3.exe
 elapsed cpu time (seconds) =  0.1437609999999997
 elapsed wall time (seconds)=   0.144617006
 N=        25600
 sum=   3.1415926537169634
 error=   1.2717027431108363E-010
```

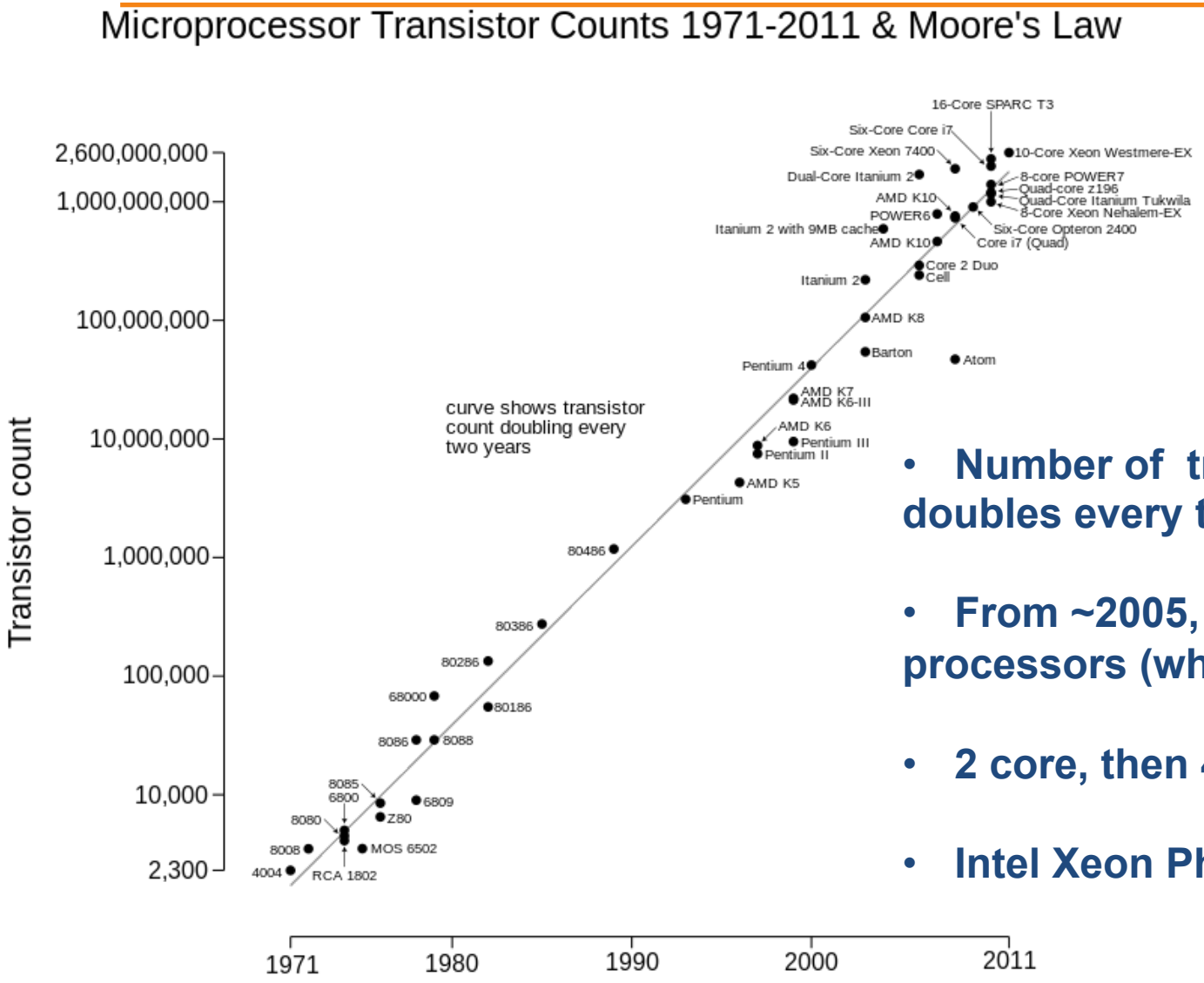
- Optimization can make a substantial difference
- f2py uses -O3 by default

Notes on compiling

- **Many other useful compiler flags, e.g.:**
  - -Wall: **“warn about all” – generates warnings about common sources of bugs**
  - -fbounds-check: **checks that array index is within bounds of an array (common problem)**

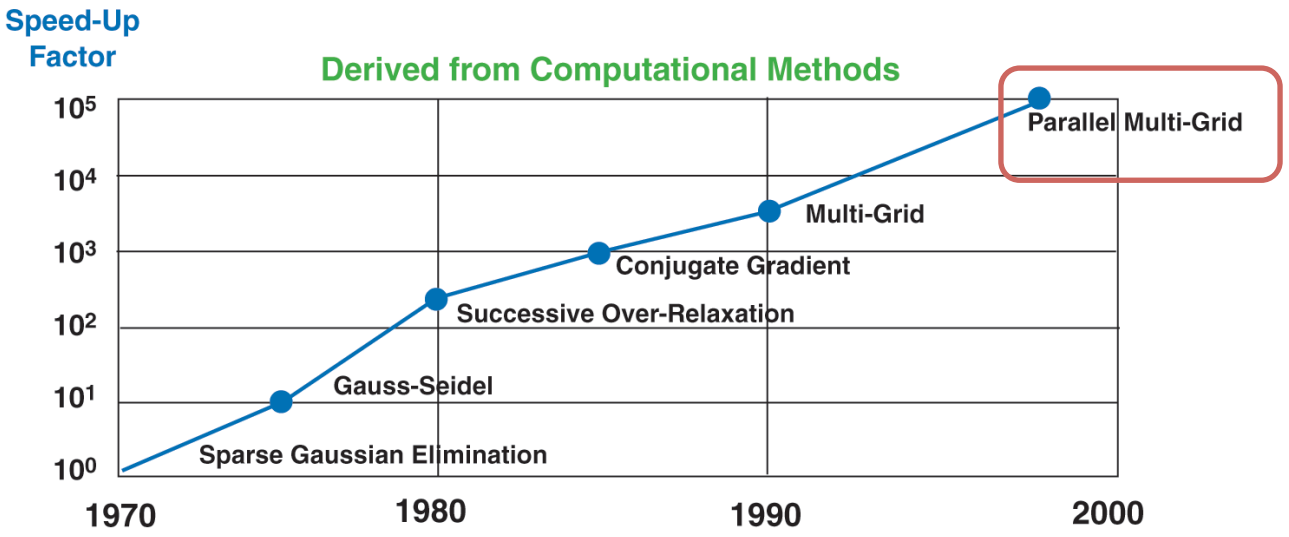
- **Comprehensive list at: https://gcc.gnu.org/onlinedocs/gfortran/Invoking-GNU-Fortran.html**

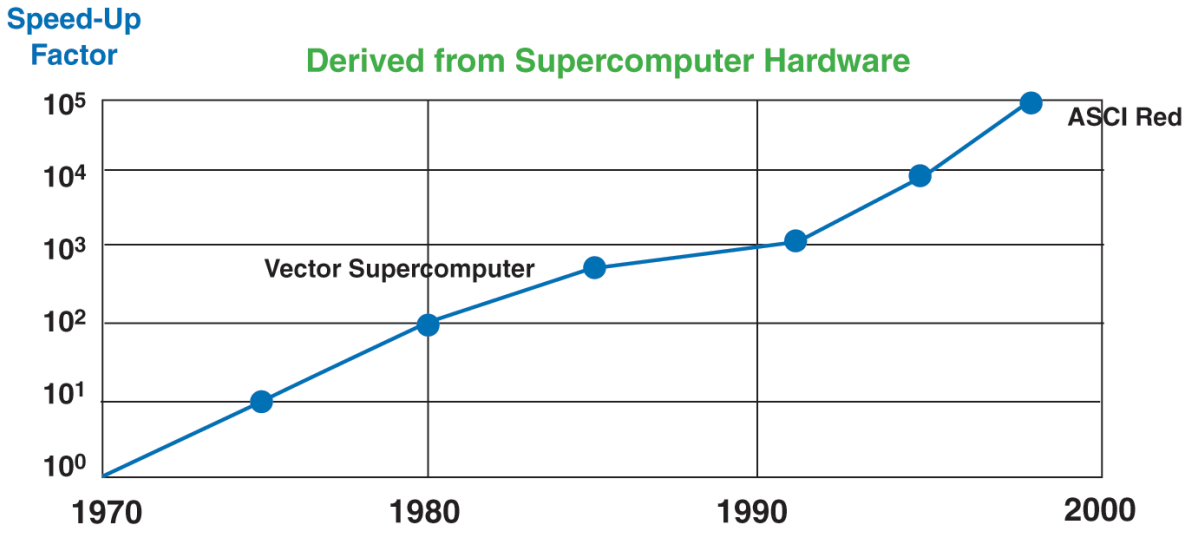
Moore's law



- **Number of transistors on chip doubles every two years**
- **From ~2005, multicore processors (why?)**
- **2 core, then 4, 6, 8, 16**
- **Intel Xeon Phi: 60+ cores!**

Algorithms and hardware





SIAM Rev (2001)

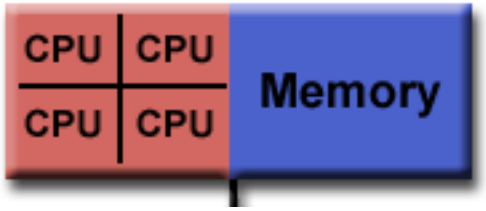
Why parallelize a code?

1. Serial (single-processor) code is too slow

   or

2 Serial code is too big

Parallel computing paradigms

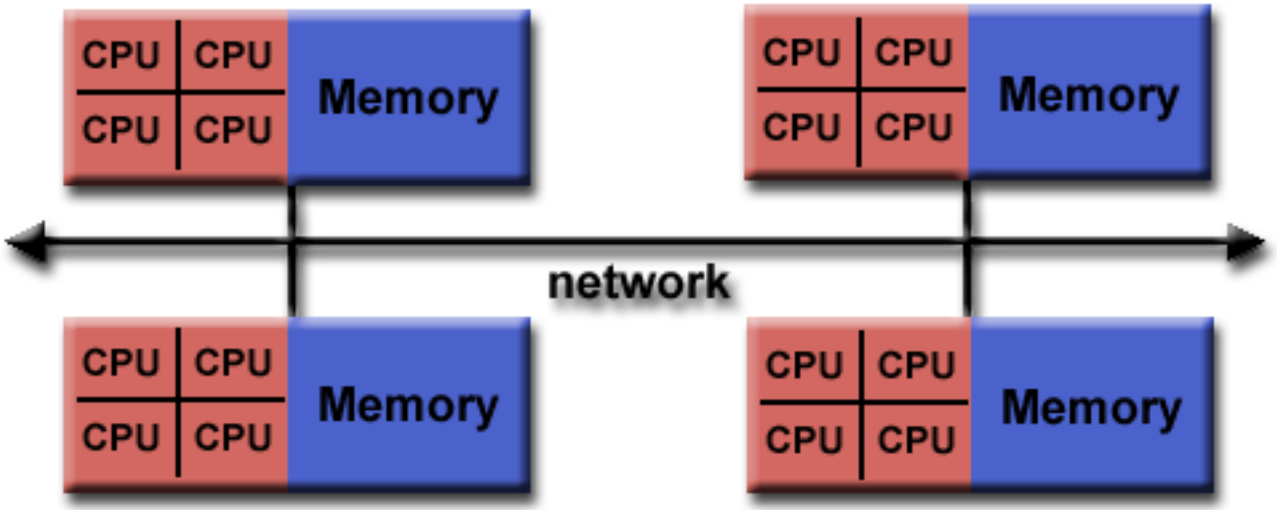


Shared memory

- One 4-core chip with shared memory (RAM)
- MPI can coordinate communication between cores
- OpenMP generally easier to use for shared-memory systems

- MPI = *Message Passing Interface*
- OpenMP = *Open Multi-Processing*

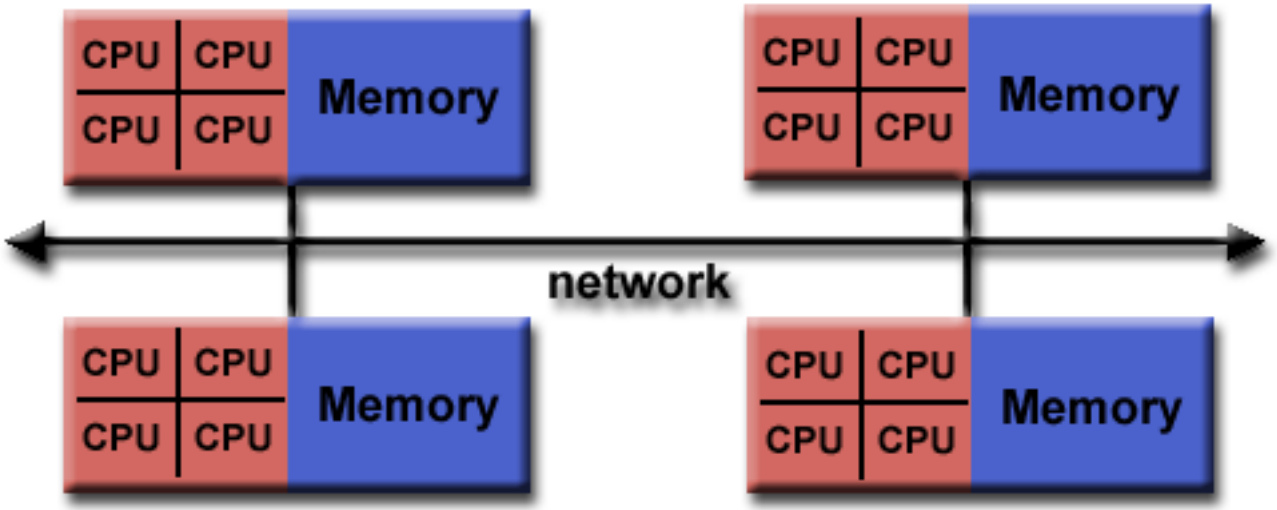
Parallel computing paradigms



Distributed memory

- Each (4-core) chip has its own memory
- The chips are connected by network ‘cables’
- MPI coordinates communication between two or more CPUs

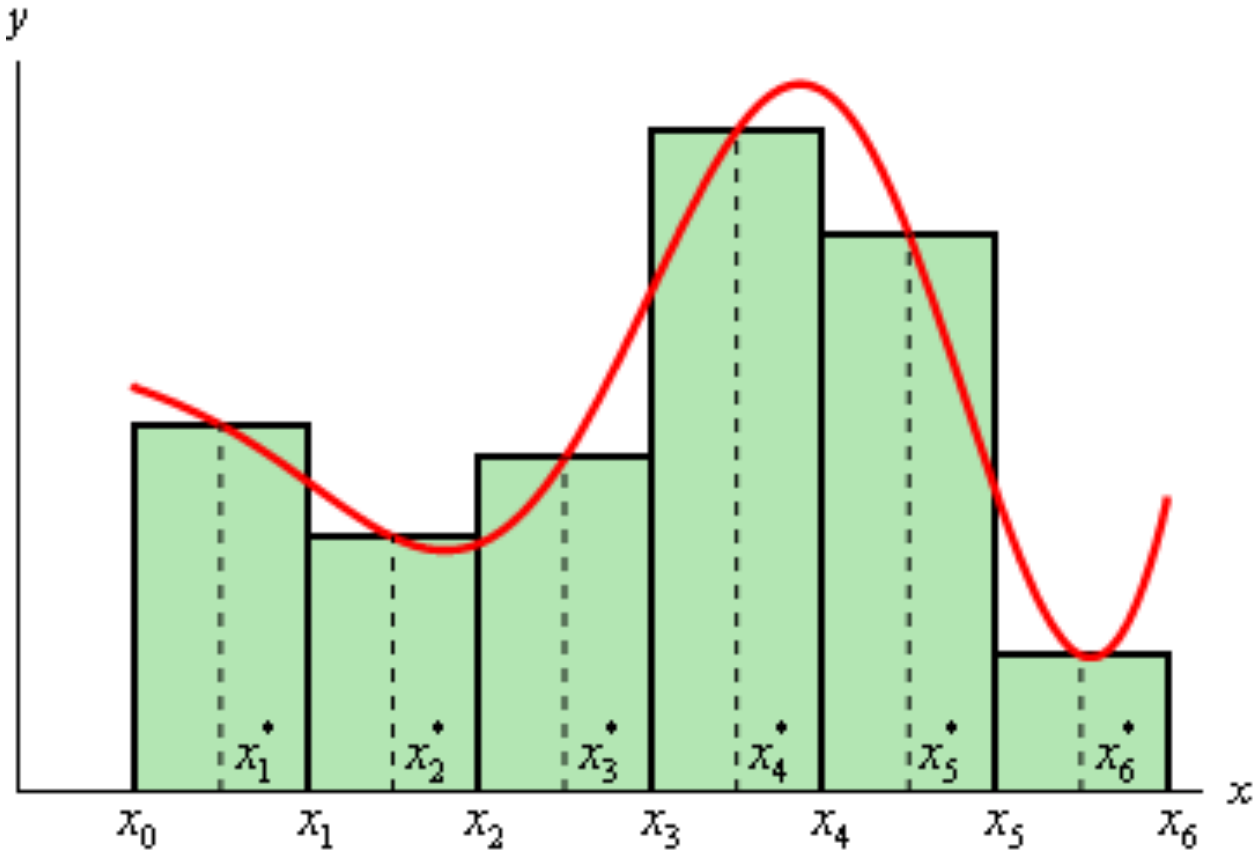
Parallel computing paradigms



Related approaches:

- Hybrid programming: mix of shared-memory (OpenMP) and distributed-memory (MPI) programming
- GPU's: Shared memory programming (CUDA or OpenCL)
- Coprocessors and co-array programming

Example: computing an integral



- **Estimate integral with midpoint rule,**

$$I = \int_{x_0}^{x_6} f(x)dx$$

1. **Compute:**

$$f(x_1^*), f(x_2^*), \ldots$$

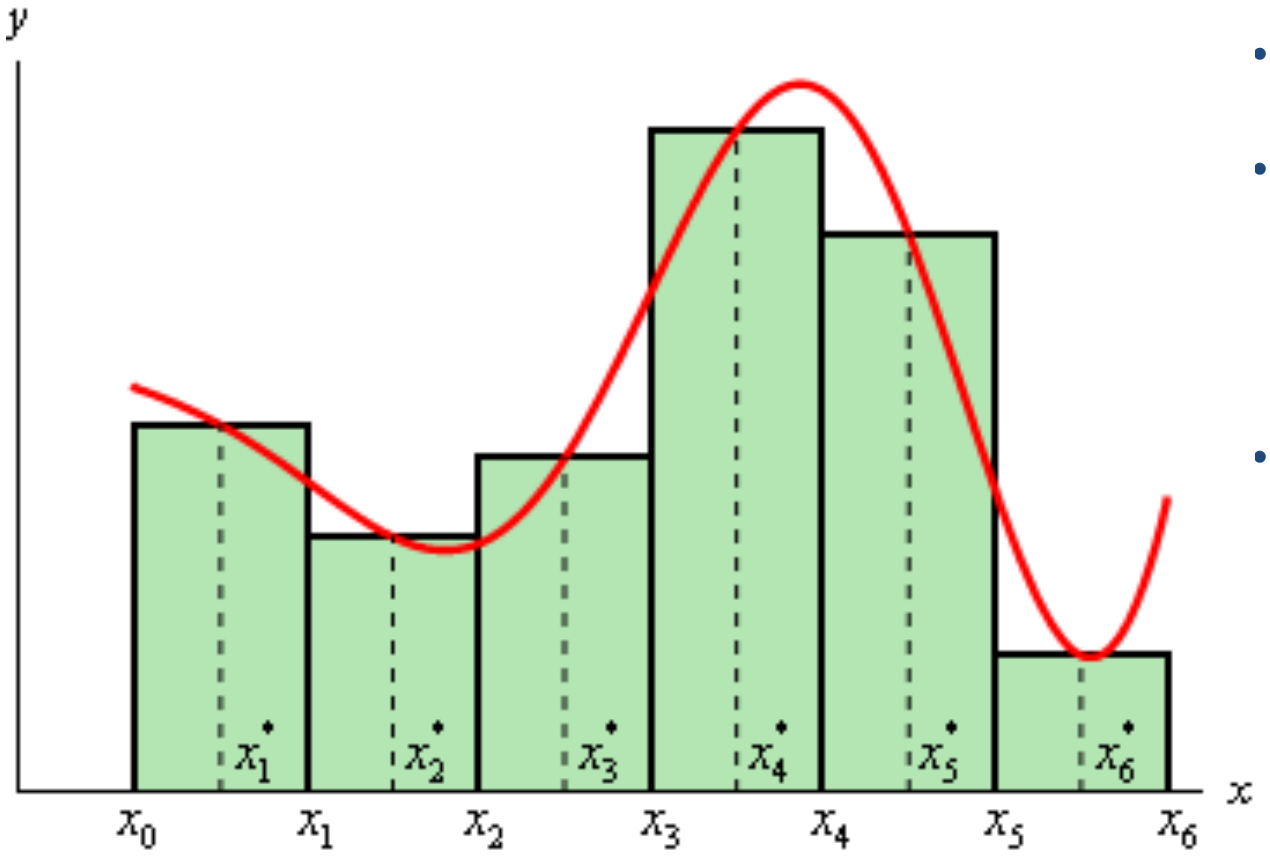
2. **Compute areas of rectangles:**

$$I_1 = (x_1 - x_0) * f(x_1^*)$$

3. **Sum areas:**

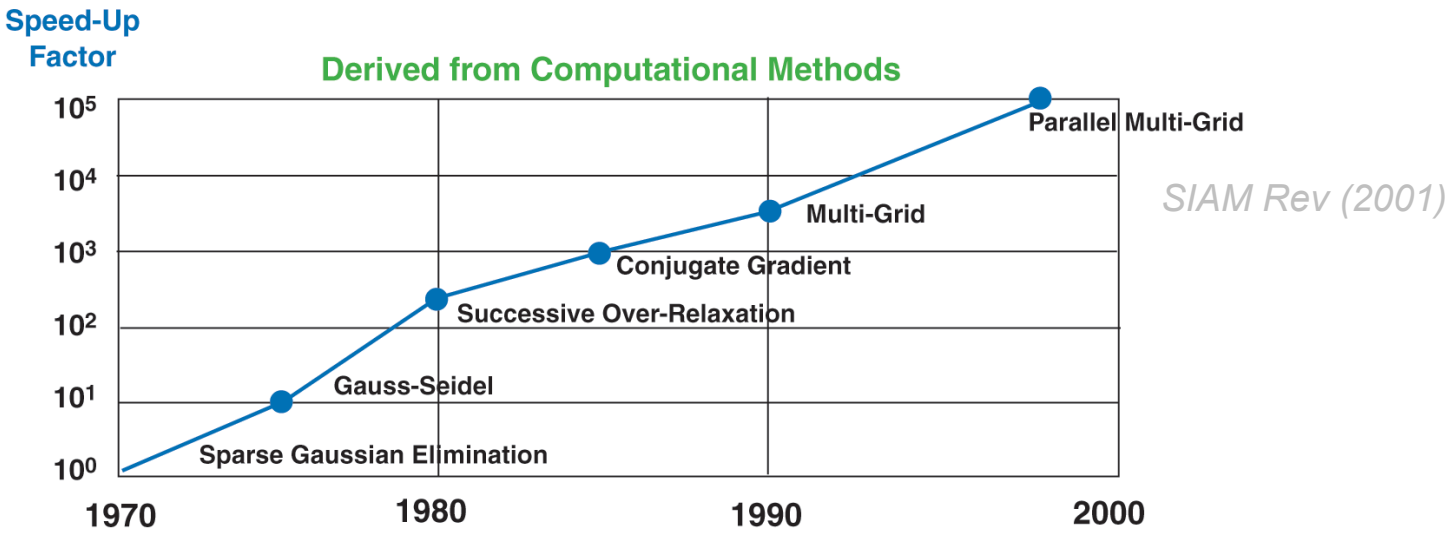
$$I \approx I_1 + I_2 + I_3 + \ldots$$

Example: computing an integral



- How to parallelize?
- With three processors, can compute areas of two rectangles on each processor
- Not practical for small calculations, but could split 1e7 rectangles across, say, 10 processors

Scaling and performance



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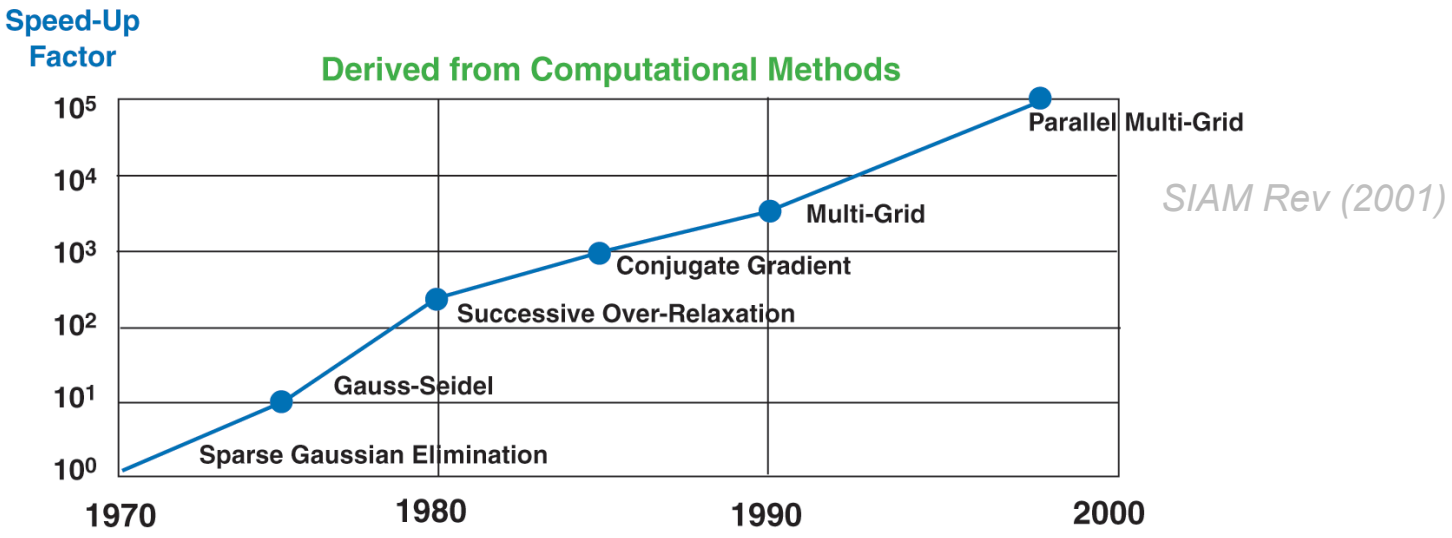
- How do we measure performance of a parallel code?
- Serial code: Optimize the *efficiency* → cost required to obtain a certain level of accuracy

Scaling and performance



SIAM Rev (2001)

- How do we measure performance of a parallel code?
- Serial code: Optimize the *efficiency* → cost required to obtain a certain level of accuracy
- Parallel code: Also optimize *scaling* or *speedup*: how much faster is the calculation when the number of procs is increased?

Speedup

- Speedup = Computation time on one proc/time on N procs = Ts/Tp
- Ideal: N = 10 processors, speedup = N = 10

Speedup

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- Ideal: N = 10 processors, speedup = N = 10
- Real life: Speedup will be less than N (possibly much less) Why?
  - Startup costs
  - Communication
  - Only part of the algorithm parallelizes
- Typically interested in performance of large problems running on large number of processors
  - Workstation: N= 16, 32
  - Imperial HPC (cx2): N = 256+
  - UK HPC (Archer): N = 1e3, 1e4, …
- Ahmdal's law provides guidance

Ahmdal's law

- Usually only part of a computation can be parallelized
  - One processor: T(1) = s + p
  - Two processors: T(2) = s + p/2
  - N processors: T(N) = s + p/N

    p is the part of the code that can be parallelized

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    p is the part of the code that can be parallelized

So, if only half the code can be parallelized (s = p = 0.5), Then the maximum speedup T(1)/T(N → inf) = (s+p)/(s) = 2

It is important for p to be much larger than s!

Ahmdal's law

Speedup T(1)/T(N) = (s+p)/(s+p/N)

Example: s = 0.1, p = 0.9

Number of processors	Speedup
1	1
2	1.8
4	3.1
8	4.7
16	6.4
32	7.8
256	9.7

Ahmdal's law

Speedup T(1)/T(N) = (s+p)/(s+p/N)

Example: s = 0.1, p = 0.9

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1	1
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Waste of resources to use N=256!

Strong and weak scaling

- **Strong scaling: Time needed to solve a problem of fixed size as number of processors increases**
- **Weak scaling: Time needed for problem with *fixed size per processor***