Friedrich-Alexander-Universität
Erlangen-Nürnberg

Programming Techniques for Supercomputers: Introduction

Performance
Profiling
Measurement and Reporting
Benchmarks

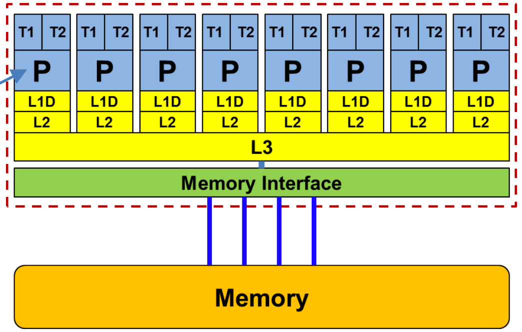
Prof. Dr. G. Wellein[a,b]

[a] Erlangen National Center for High Performance Computing
[b] Department für Informatik

University Erlangen-Nürnberg
Sommersemester 2024

One thing up front: “cycle gymnastics”

- Two time metrics are used in the lecture:
  - absolute time (seconds; s)
  - relative time on the processor (processor cycle time or cycle)

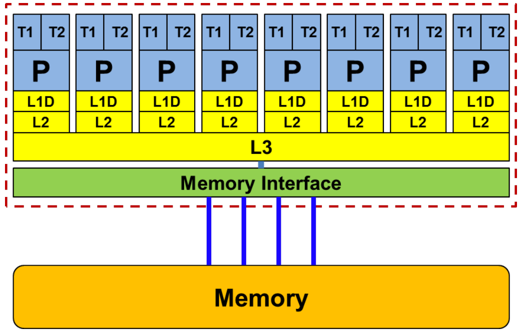


- 1 cycle [cy] = smallest unit of time on a CPU (“heartbeat”)
- 1 GHz = 10^9 cy/s ←→ 1 cy = 10^{-9} s
- Typical clock speeds (CPU): 2.0 Gcy/s,…4.0 Gcy/s (or GHz)
- Typical clock speeds (GPU): 1.0 Gcy/s,…2.0 Gcy/s (or GHz)

One thing up front: "cycle gymnastics" – Peak Performance

- Peak performance of 20-core CPU running at 2.4 GHz:

$$P_{peak} = 1536 \text{ Gflop/s} = 1.536 \text{ Tflop/s}$$

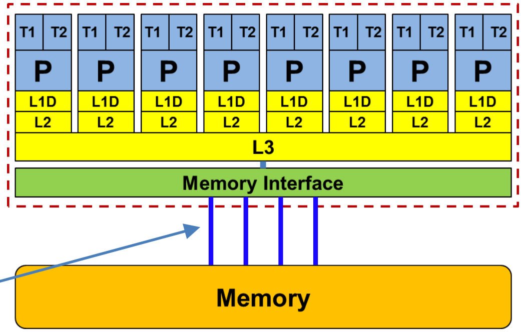


- How many Flops per cycle per core is that?

$$\frac{1536 \cdot 10^9 \frac{Flops}{s}}{20\ cores\ \cdot 2.4 \cdot 10^9 \frac{cy}{s}} = 32\ \frac{Flops}{cy \cdot core}$$

- Typical duration of a double precision multiply instruction: 4 cycles
  - How much time is that? $\frac{4\ cy}{2.4 \cdot 10^9 \frac{cy}{s}} = 1.67 \cdot 10^{-9} s = 1.67\ \mathrm{ns}$

One thing up front: “cycle gymnastics” – Memory Bandwidth



- Basic unit of traffic: Byte
- Unit of bandwidth: Bytes/s
- Typical memory bandwidth (20 cores): 160 Gbytes/s = $1.6 \cdot 10^{11}$ Bytes/s
- How many bytes per cycle is that (20 cores)? $$\frac{160 \cdot 10^9 \frac{Bytes}{s}}{2.4 \cdot 10^9 \frac{cy}{s}} = 67\ \frac{Bytes}{cy}$$
- But: $$32\ \frac{Flops}{cy \cdot core} * 20\ core = 640\ \frac{Flops}{cy}$$

Profiling

Performance

Performance: Why thoroughly measure and report it?

- Determine which computer is best suited for a given (set of) application(s)?
  - Gaming PC or Atom based Laptop?
  - Cluster or fat server? Fast CPU? Intel or AMD or GPU?
  - Which applications? Which input/data sets?

- Validate impact of new optimization / implementation / parallelization strategy and present to others
  - Results need to be interpreted and potentially reproduced by other scientists
  - Compare with other / previous work
  - Justify efficient usage of expensive resources

- Determine “attainable” capabilities of individual parts of the computer
  - E.g., data transfer / IO / computational capabilities
  - Often required to guide optimization strategies → Performance Modeling

Performance: What is a good measure/metric?

- Performance = WORK / TIME
- "Pure" metrics – basic choices for "WORK"
  - Flop/s: Floating Point Operations per Second

$$\frac{\text{number of floating-point operations executed}}{\text{TIME}}$$

(often cited for technical & scientific applications)

  - MIPS: Millions of Instructions per Second

$$\frac{\text{Number of Instructions executed}}{10^{6} \ * \ \text{TIME}}$$

(computer architect's view)

- How to determine WORK, e.g., "Floating Point Operations"?
  - Count them manually (high level code / algorithm)
  - Use CPU event counters → tools (e.g., LIKWID)

Some WORK metrics may fool the observer

- "My vector update code runs at 2,000 MFlop/s on a 2GHz processor!"
- Great – isn't it?

```
for(i=0; i<n; i++)
{
    a[i]= 3.0*c0+c1*c2 +c3*c4*a[i] -1.d0 *a[i];
}
```

→ #FLOP = 8 * n

If is `a[i]` **loaded/stored from/to main memory**:

Same execution time but…

… but my MFlop/s rate is only ¼!

```
d0 = 3.0*c0+c1*c2;
d1 = c3*c4-1.d0;

for(i=0; i<n; i++)
{
    a[i]= d0 + d1*a[i];
}
```

→ #FLOP = 2* n + 5

→ Define WORK carefully – independent of implementation issues

Performance – choices for WORK

- Iterations: Total number of loop iterations performed: WORK = n iterations (see previous slide)
  → Performance metric: Iterations / s

- Lattice Site/ Cell / Particle Updates: Often used for stencil codes or Lattice Boltzmann fluid solvers: WORK = number of sites/cells/particles to be updated/computed
  → Performance metric: Cell updates / s

- Physical simulation time: Often used in molecular dynamics codes: WORK = Physical time (e.g. nanosenconds) a system is propagated
  → Performance metric: nanoseconds / day

- Complete problem solution: WORK: “1” well-defined problem
  → Performance metric: 1 / s

Performance – TIME

- Simplest performance metric ("bestseller"): 1 / TIME
  - Measures time to solution
  - Carefully specify the "problem" you solved!
  - Best metric thinkable, but not intuitive in all situations (see later)
- Problem: Which TIME?
- LINUX / UNIX command **time** :

```
>time ./test.x
>34.650u 0.612s 0:35.28 99.9%

>time ./testwIO.x
>33.802u 0.608s 0:43.64 78.8%
```

- `> xxxu yyys  mm:ss   CPUratio%`

```
xxx → USER CPU time [s]  yyy → SYSTEM CPU time [s]
mm:ss → Elapsed time     CPUratio → (xxx+yyy)/mm:ss
```

Performance – TIME

- Stay away from CPU time – it‘s evil!
- Elapsed time (WALLTIME) is the time you wait for your result!
  (Always use dedicated resource, e.g., one node)

- WALLTIME as difference of two timestamps on UNIX(-like) systems

```
#include <stdlib.h>
#include <time.h>

double getTimeStamp() {
   struct timespec ts;
   clock_gettime(CLOCK_MONOTONIC, &ts);
return (double)ts.tv_sec + (double)ts.tv_nsec * 1.e-9; }
```

  - Replaces **`gettimeofday()`**
  - Code available in the exercise templates
  - Works fine for serial timings – due care for parallel apps is required

Profiling

Where do I spend my time?

Performance: Where do I spend my time

- How do I know where my code spends most of its time?
- This is called "Profiling"
- Profiling may impact runtime (i.e., performance) → Qualitative insight
- Two kinds: instrumentation and sampling
  - Sampling
    - Application is interrupted at regular intervals while running; stack trace is recorded and all info is statistical. No recompilation required
  - Instrumentation
    - Application code is (automatically) instrumented at compile time such that runtime contributions of all subroutines, functions, etc. can be determined
- Many advanced profiling tools exist, e.g., Intel Amplifier, Oprofile, Codeanalyst – we start with simple one (gprof – instrumentation based)

Profiling with gprof

- Basic profiling tool under Linux: `gprof`
- Compiling for a profiling run (use compiler-specific flag)

```
icc -pg …… -o a.out
 ./a.out
```

- After running the binary, a file `gmon.out` is written to current directory
- Human-readable output via

```
gprof a.out
```

- Compiler inlining should be disabled for profiling
  - But then the executed code isn't what it should be…
- Profiling may (substantially) reduce overall code performance

Profiling with gprof: Example

```
tb082:/tmp> gprof ./lbmKernel-pg
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls   s/call   s/call  name
 80.05      3.17     3.17       10     0.32     0.32  relax_standard_flipped_il_2g_
 15.15      3.77     0.60        1     0.60     0.61  init_flipped_il_2g_
  3.79      3.92     0.15       10     0.01     0.01  bounceback_index_flipped_il_2g_
  0.51      3.94     0.02        2     0.01     0.01  make_bouncebacklist_
  0.25      3.95     0.01        1     0.01     0.01  obsin_
  0.25      3.96     0.01                             munmap
  0.00      3.96     0.00        2     0.00     0.00  get_time_info_
  0.00      3.96     0.00        1     0.00     3.95  MAIN__
  0.00      3.96     0.00        1     0.00     0.00  speed_info_mlups_

 %         the percentage of the total running time of the
time       program used by this function.

cumulative a running sum of the number of seconds accounted
 seconds   for by this function and those listed above it.

 self      the number of seconds accounted for by this
seconds    function alone.  This is the major sort for this
           listing.

calls      the number of times this function was invoked, if
           this function is profiled, else blank.

 self      the average number of milliseconds spent in this
ms/call    function per call, if this function is profiled,
           else blank.

 total     the average number of milliseconds spent in this
ms/call    function and its descendents per call, if this
           function is profiled, else blank.

name       the name of the function.  This is the minor sort
           for this listing. The index shows the location of
           the function in the gprof listing. If the index is
           in parenthesis it shows where it would appear in
           the gprof listing if it were to be printed.
```

Test of kernel routine:

- Initialize
- Run the 2 computational kernels 10 times

Profiling with gprof: Example

```
                     Call graph (explanation follows)


granularity: each sample hit covers 4 byte(s) for 0.25% of 3.96 seconds

index % time    self  children    called     name
                0.00    3.95       1/1           main [2]
[1]     99.7    0.00    3.95       1         MAIN__ [1]
                3.17    0.00      10/10          relax_standard_flipped_il_2g_ [3]
                0.60    0.01       1/1           init_flipped_il_2g_ [4]
                0.15    0.00      10/10          bounceback_index_flipped_il_2g_ [5]
                0.01    0.00       1/1           obsin_ [7]
                0.01    0.00       1/2           make_bouncebacklist_ [6]
                0.00    0.00       2/2           get_time_info_ [9]
                0.00    0.00       1/1           speed_info_mlups_ [10]
-----------------------------------------------
                                                 <spontaneous>
[2]     99.7    0.00    3.95                 main [2]
                0.00    3.95       1/1           MAIN__ [1]
-----------------------------------------------
                3.17    0.00      10/10          MAIN__ [1]
[3]     80.1    3.17    0.00      10         relax_standard_flipped_il_2g_ [3]
-----------------------------------------------
                0.60    0.01       1/1           MAIN__ [1]
[4]     15.4    0.60    0.01       1         init_flipped_il_2g_ [4]
                0.01    0.00       1/2           make_bouncebacklist_ [6]
-----------------------------------------------
                0.15    0.00      10/10          MAIN__ [1]
[5]      3.8    0.15    0.00      10         bounceback_index_flipped_il_2g_ [5]
-----------------------------------------------
                0.01    0.00       1/2           MAIN__ [1]
                0.01    0.00       1/2           init_flipped_il_2g_ [4]
[6]      0.5    0.02    0.00       2         make_bouncebacklist_ [6]
-----------------------------------------------
                0.01    0.00       1/1           MAIN__ [1]
[7]      0.3    0.01    0.00       1         obsin_ [7]
-----------------------------------------------
                                                 <spontaneous>
[8]      0.3    0.01    0.00                 munmap [8]
-----------------------------------------------
```

Butterfly graph

Who calls whom and how often?

Profiling with gprof: Example (C++)

Example with wrapped **`double`** class:

```
class D {
  double d;
public:
  D(double _d=0) : d(_d) {}
  D operator+(const D& o) {
    D r;
    r.d = d+o.d;
    return r;
  }
  operator double() {
    return d;
  }
};
```

Main program:

```
const int n=10 000 000;
D a[n],b[n];
D sum;

for(int i=0; i<n; ++i)
  a[i] = b[i] = 1.5;

double s = timestamp();
for(int k=0; k<10; ++k) {
  for(int i=0; i<n; ++i)
    sum = sum + a[i] + b[i];
}
```

Profiling with gprof: Example (C++) profiler output

- `icpc -O3 -pg perf.cc`

```
  %   cumulative   self              self     total
 time   seconds   seconds    calls  Ts/call  Ts/call  name
101.01      0.41     0.41                             main
```

- `icpc -O3 -fno-inline -pg perf.cc`

```
  %   cumulative   self              self     total
 time   seconds   seconds    calls  ns/call  ns/call  name
46.44      0.59     0.59 200000000     2.93     4.48  D::operator+(D const&)
29.63      0.96     0.37 240000001     1.56     1.56  D::D(double)
24.82      1.27     0.31                             main
```

- But where did the time *actually* go?
  - Butterfly (callgraph) profile also available
  - Real problem also with libraries
  - Sometimes you have to roll your own little profiler (timing functions within the code)

Probing hardware performance

What does the hardware do?

Probing Performance behavior

- Once a hotspot is identified → determine the hardware utilization

- Performance counters allow to monitor processor events:
  - The number and kind of instructions executed
  - The data transfers executed for each cache/memory level
  - The clock speed at which the processor runs
  - The power/energy consumption
  - …
- `likwid-perfctr` (from `likwid` toolbox) allows easy access to performance events and provides useful derived metrics, e.g., main memory bandwidth or Flop/s or cycles/instruction
  - https://github.com/RRZE-HPC/likwid

- See separate lecture → Thomas Gruber

Best Practices for Performance Measurement & Reporting

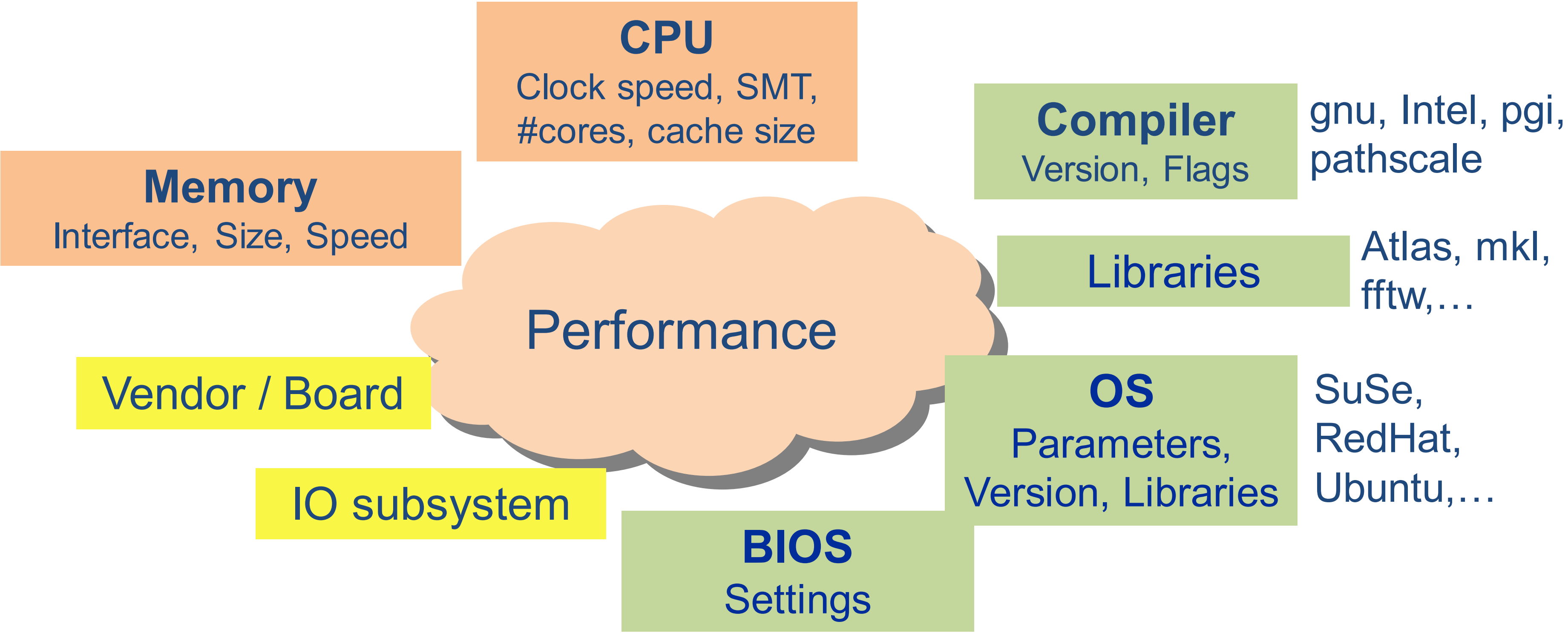
Measuring performance in a reproducible way

Performance: Impact factors

"My code runs on an Intel Xeon Sandy Bridge processor 12 times faster than the results reported for code A in [xyz]."

Performance: Impact factors

- For a given code/problem, performance may be influenced by many factors

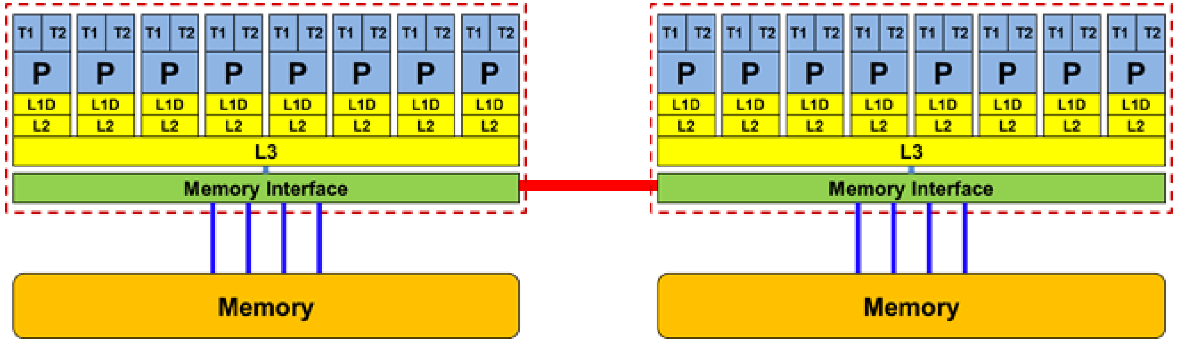


- For reproducibility of performance results:
  - All critical factors need to be reported!
  - Sensibility and stability analysis!
  - Statistics – fluctuations among several runs (min/max/median)

Important

Performance Measurement: Best Practices

- Preparation
  - Consider to automate runs with a script (shell, python, perl)
  - Reliable timing/timer granularity (minimum time which can be measured?)
  - Document code generation (flags, compiler version)
  - Document system state (clock frequency, turbo mode, memory, caches,…)



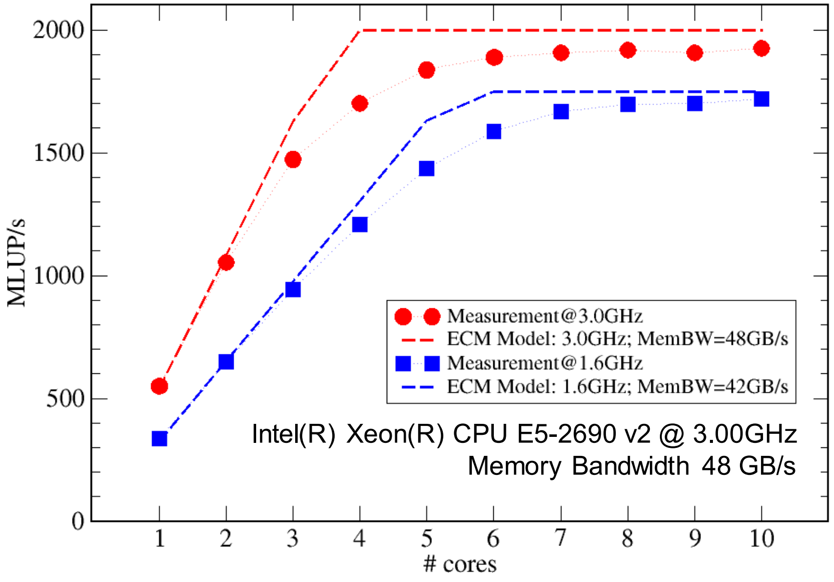
- Doing
  - Get exclusive system
  - Fix clock speed
  - Control Affinity / Topology– where does my code/threads/processes run exactly?
  - Working set size – code input parameters?!
  - Is result deterministic and reproducible → Statistics: Mean, Median, Best ??
  - Basic variations: Thread count, affinity, working set size ←→ runtime
  - Check: Are the results reasonable?

Important

Performance Measurement: Best Practices (cont.)

- Postprocessing
  - Documentation
  - Plan variations to gain more information
  - Many things can be better understood if you plot them (gnuplot, xmgrace)
  - Use statistics to report performance fluctuations
  - Try to understand and explain the result
  - Is there a (simple) model which can (qualitatively) explain the performance levels and variations?

```
  do k = 1 , Nk; do j = 1, Nj
         do i = 1, Ni
                   y(i,j,k) = const*
 $                  ( x(i-1,j,k) + x(i+1,j,k)
 $                  + x(i,j-1,k) + x(i,j+1,k)
 $                  + x(i,j,k-1) + x(i,j,k+1) )
         enddo
 enddo; enddo
```



Important

Benchmarks

Benchmarks provide insights beyond the hardware fact sheet

Benchmarks: Classification

1. Real (full) applications: Solves real world problem but includes everything and may run for hours or days on thousands of processors!

2. Proxy applications or mini-apps: Small and simplified code which allows to capture relevant performance features of real (full) scale applications, e.g., Mantevo [1], Exascale proxy applications [2], or SPEC [3]

3. Kernels: "Small" code pieces representing single steps of (proxy) applications e.g., solvers (→ LINPACK,…) or time-consuming computational steps (→ STREAM, (sparse) matrix-vector multiplication,…). Easy to port, analyze and optimize. Also very popular with vendors, easy to report (everyone knows the popular ones)

4. Toy benchmarks: Small pieces of code implementing popular algorithms (e.g. quicksort). Typically used for getting students started with programming.

5. Synthetic benchmarks (microbenchmarks): Simulate operations and data accesses of a variety of applications without having any relation to the application codes

Kernels are central for structured performance modelling!

[1] https://mantevo.github.io ; [2] https://proxyapps.exascaleproject.org ; [3] www.spec.org

Benchmarks – HPC standard benchmarks

- STREAM → Attainable main memory bandwidth (microbenchmark)
- LINPACK → Top500 Ranking / Attainable peak performance (solver)
- HPCG → Preconditioned conjugate-gradient solver (solver)
- SPEC-HPC → Industry standard (HPC proxy app suite)

Benchmarks: STREAM for memory bandwidth

- http://www.cs.virginia.edu/stream/
- Performs four “streaming” tests:
  - Copy: `A(1:N) = B(1:N)`
  - Scale: `A(1:N) = s*B(1:N)`
  - Add: `A(1:N) = B(1:N)+C(1:N)`
  - Triad: `A(1:N) = B(1:N)+s*C(1:N)`
- Results are reported in MByte/s (data transfer rate)
- No changes are allowed
- Tests the attainable main memory bandwidth

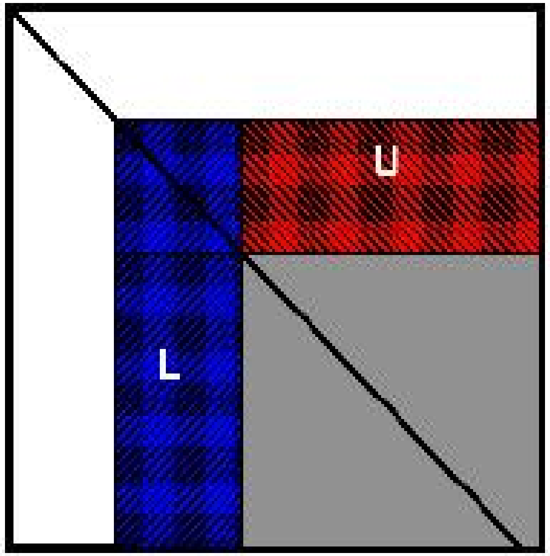
```
-------------------------------------------------------------
 Double precision appears to have 16 digits of accuracy
 Assuming 8 bytes per DOUBLE PRECISION word
-------------------------------------------------------------
 -------------------------------------------------------------
 STREAM Version $Revision: 5.6 $ common=ON
 -------------------------------------------------------------
 Array size =   33554432
 Offset     =       1024
 The total memory requirement is      768 MB
 You are running each test  10 times
 --
 The *best* time for each test is used
 *EXCLUDING* the first and last iterations
 -------------------------------------------------------------
 Number of Threads =              1
 -------------------------------------------------------------
 Printing one line per active thread....
 -------------------------------------------------------------
 Your clock granularity/precision appears to be      1 microseconds
 -------------------------------------------------------------
Function      Rate  (MB/s)  Avg time   Min time  Max time
Copy:       10758.0504     0.0499     0.0499     0.0499
Scale:      10380.3540     0.0517     0.0517     0.0518
Add:        11371.1566     0.0709     0.0708     0.0710
Triad:      11308.4169     0.0712     0.0712     0.0713
 -------------------------------------------------------------
 Solution Validates!
 -------------------------------------------------------------
tb007:/tmp>
```

- Stream & stream-like tests are used throughout the lecture

Benchmarks – LINPACK: Towards Peak Performance

- Solve large dense linear system of equations, i.e.,

$$A\,x = b$$



- with A is a dense $(N \times N)$ matrix
- Algorithm: LU factorization of A
  (+ forward/backward substitution) with
  effort $\frac{2}{3}N^3 + O(N^2)$
- Highly parallel implementations are available
- Achieves high fraction of machine peak performance (see 1st lecture)

(see http://www.netlib.org/benchmark/hpl/algorithm.html)

Benchmarks: HPCG – Something more realistic?

- HPCG: High Performance Conjugate Gradient benchmark
- Basic algorithm: Conjugate Gradient with a local symmetric Gauss-Seidel preconditioner
- Synthetic 3D sparse linear system (stencil-structure)
- Strong correlation with main memory bandwidth and STREAM benchmark
- https://www.top500.org/hpcg/

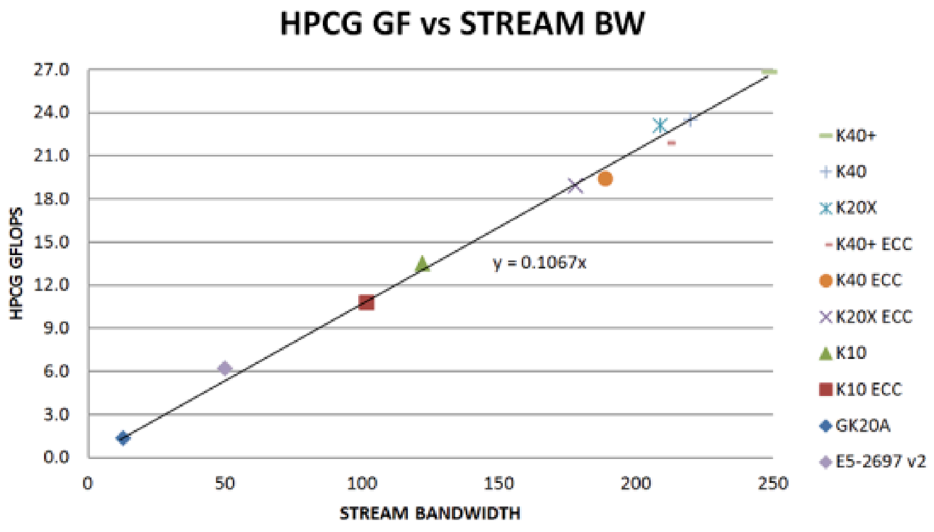


Figure from: https://devblogs.nvidia.com/parallelforall/optimizing-high-performance-conjugate-gradient-benchmark-gpus/