HPC MolSSI Stony Brook 2019:

Single core performance enhancement:

Nonintrusive way to determine the performance:

$ time hostname

Profiling tools: GNU profiler (gprof), intel VTune Amplifier, Xcode Instrument – stochatistic sampling of execution time.

Intrusive:

High-res timer around the clock block.

Microbenchmarking harnesses:

Google benchmark: github.com/google/benchmark

Hardware counters:

PAPI: icl.utk.edu/papi/

make

$ gprof ./axpy gmon.out

$ ./gemm 256 1 eigen

Statistical profiling:

All intel and apple compilers are statistical profilers.

Best to use special microbenchmarking libraries. Maybe use header libraries.

Abstract serial processor:

Instructions to execution unit to data.

How much time does processing one Op take?

Op = unit of work, i.e. instruction, kernel etc.

What are the differences between CPUs and GPUs/Accelerators?

Real processors are Abstract Data-Parallel Processor:

**Memory efficiencies:**

Registers are the fastest memory. Size is usually 1000 B. latency, cycles = 1

Level 1 cache 64 kB, latency = 3

Level 2 cache 256 kB – 12 MB, latency = 10.

Level 3 cache, latency 40.

Main memory, latency 100.

Numerical algorithms: Linear Algebra

Data in L1 cache: n = 1024.

**Arithmetic intensity**: 2/3 means there are two reads and 3 writes.

To see the system information:

$ vi /proc/cpuinfo