Advanced Topics in Numerical Analysis: High Performance Computing

More Shared Memory Parallelism, Sequential Performance Demo, Libraries

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Spring 2019, Monday, 5:10–7:00PM, WWH #1302

March 11, 2019

Outline

Organization

Scheduling:

- Homework assignment #2 due tonight
- New assignment will be posted this week

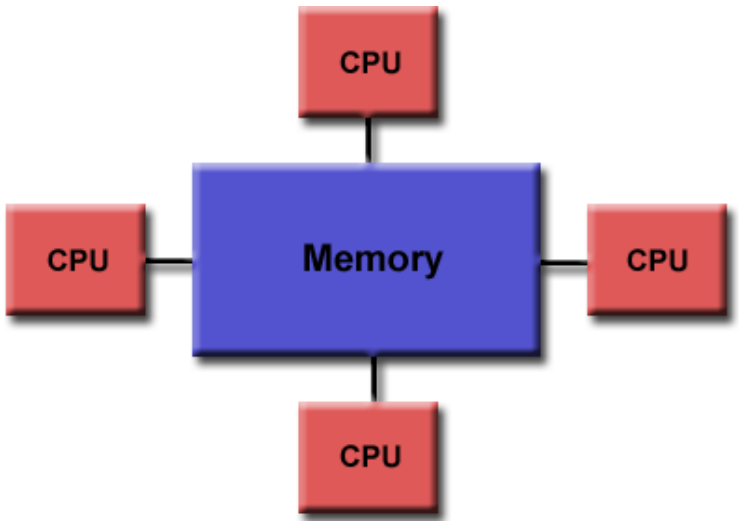
Topics today:

- Wrapping up shared memory parallelism
- Revisit sequential performance (finish demo from lecture 3)
- Libraries BLAS, LAPACK, FFTW

Outline

Shared memory programming model

- Program is a collection of control threads, that are created dynamically
- Each thread has private and shared variables
- Threads can exchange data by reading/writing shared variables
- Danger: more than 1 processor core reads/writes to a memory location: race condition



Only one process is running, which can fork into shared memory threads.

#pragma omp for schedule (static/dynamic/guided [,chunk])

- **static** divided into pieces of size chunk, and statically assigned to threads.
- **dynamic** divided into pieces of size chunk and dynamically scheduled as requested.
- **guided** size of chunk decreases over time.

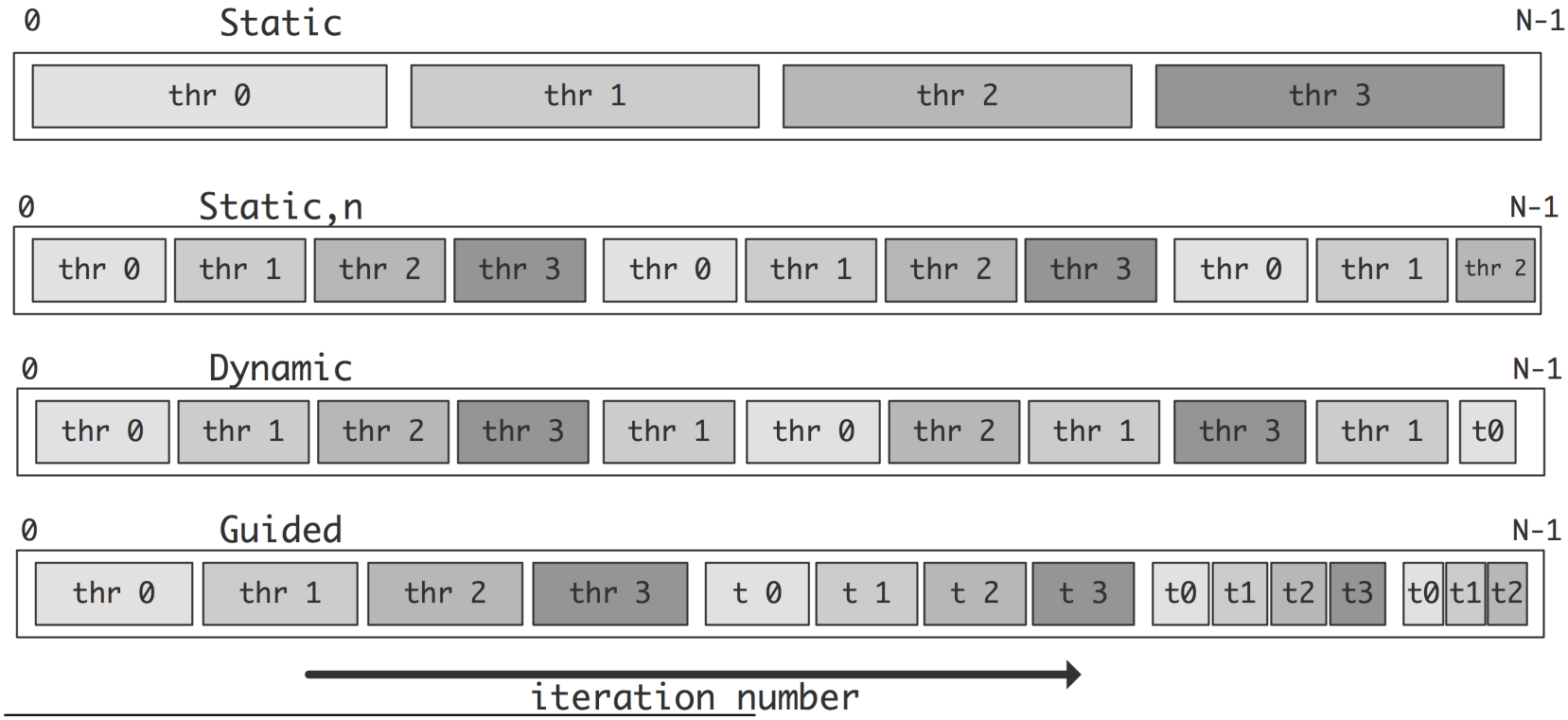


*figure from http://pages.tacc.utexas.edu/~eijkhout/pcse/html/omp-loop.html

Weak sequential consistency

```
int a = 0, b = 0;
```

Thread-1

```
a = 1;
b = 2;
```

Thread-2

```
if (b == 2)
  assert(a == 1);
```

(may fail because b may be commited before a)

Weak sequential consistency

```
int a = 0, b = 0;
```

Thread-1

```
a = 1;
#pragma omp flush(a)
b = 2;
```

Thread-2

```
if (b == 2)
  assert(a == 1);
```

Synchronization

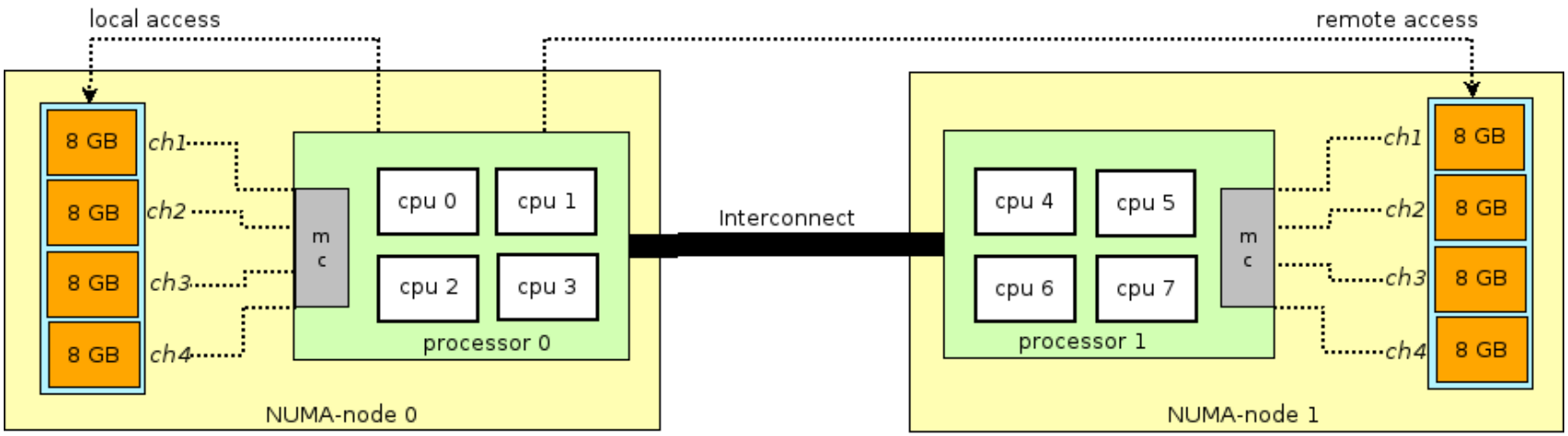
Synchronization: needed to protect access to shared data

- Implicit barrier synchronization at end of parallel region (noexplicit support for synch. subset of threads). Can invoke explicitly with `#pragma omp barrier`. All threads must see same sequence of work-sharing and barrier regions.
- critical sections: only one thread at a time in critical region with the same name. `#pragma omp critical [(name)]`
- atomic operation: protects updates to individual memory loc. Only simple expressions allowed. `#pragma omp atomic`
- also flush, locks, master operations

At all these (implicit or explicit) synchronization points OpenMP ensures that threads have consistent values of shared data.

Cache Coherent Non-uniform Memory Access

- **Cores:** individual processing units.
- **Sockets:** collection of cores on the same silicon die.
- Each sockets connected to its own DRAM.
- Sockets interconnected using a network: QPI (Intel), HT (AMD).
- Location of memory pages determined by first-touch policy.



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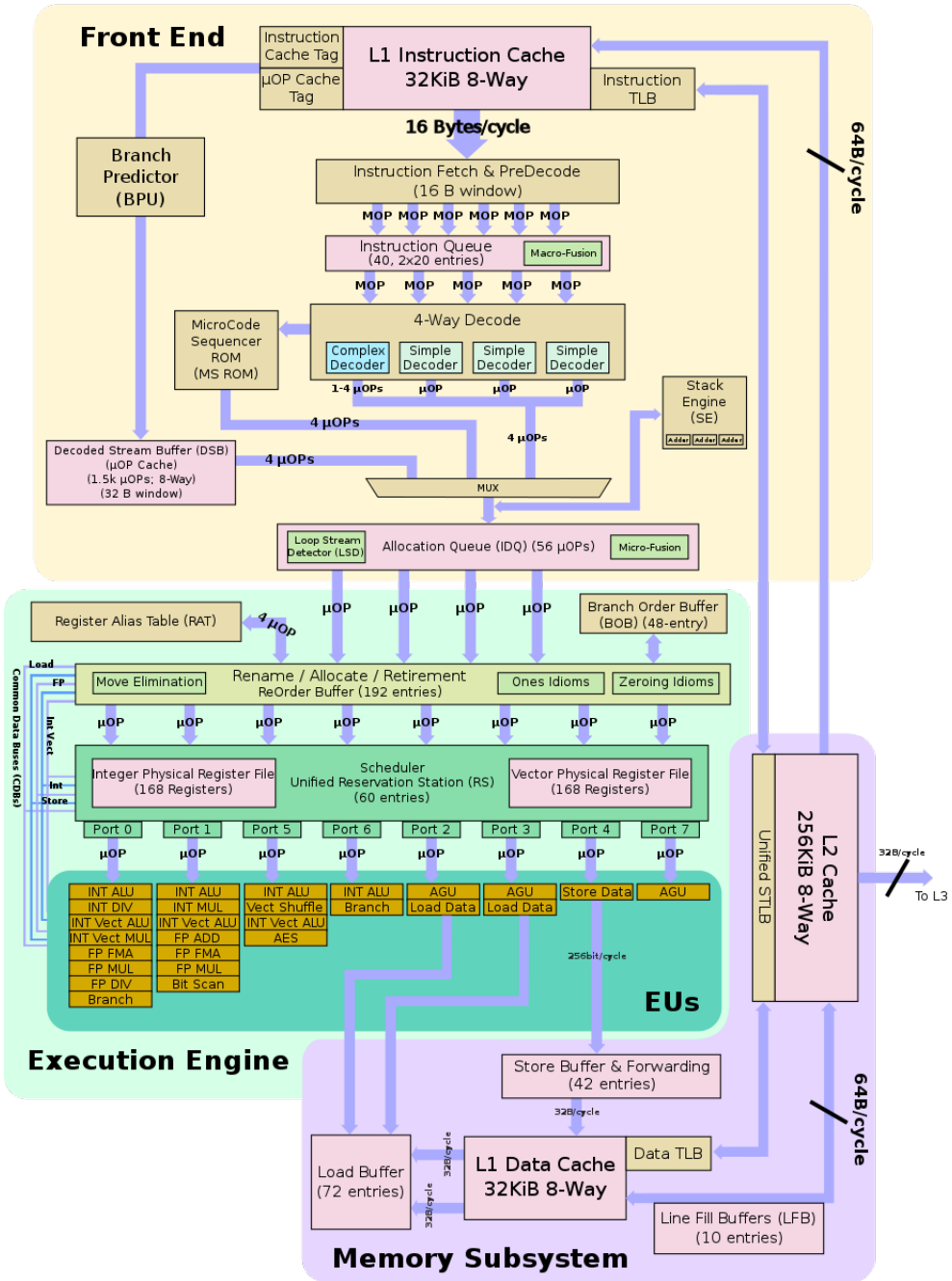
Outline

Sequential Performance



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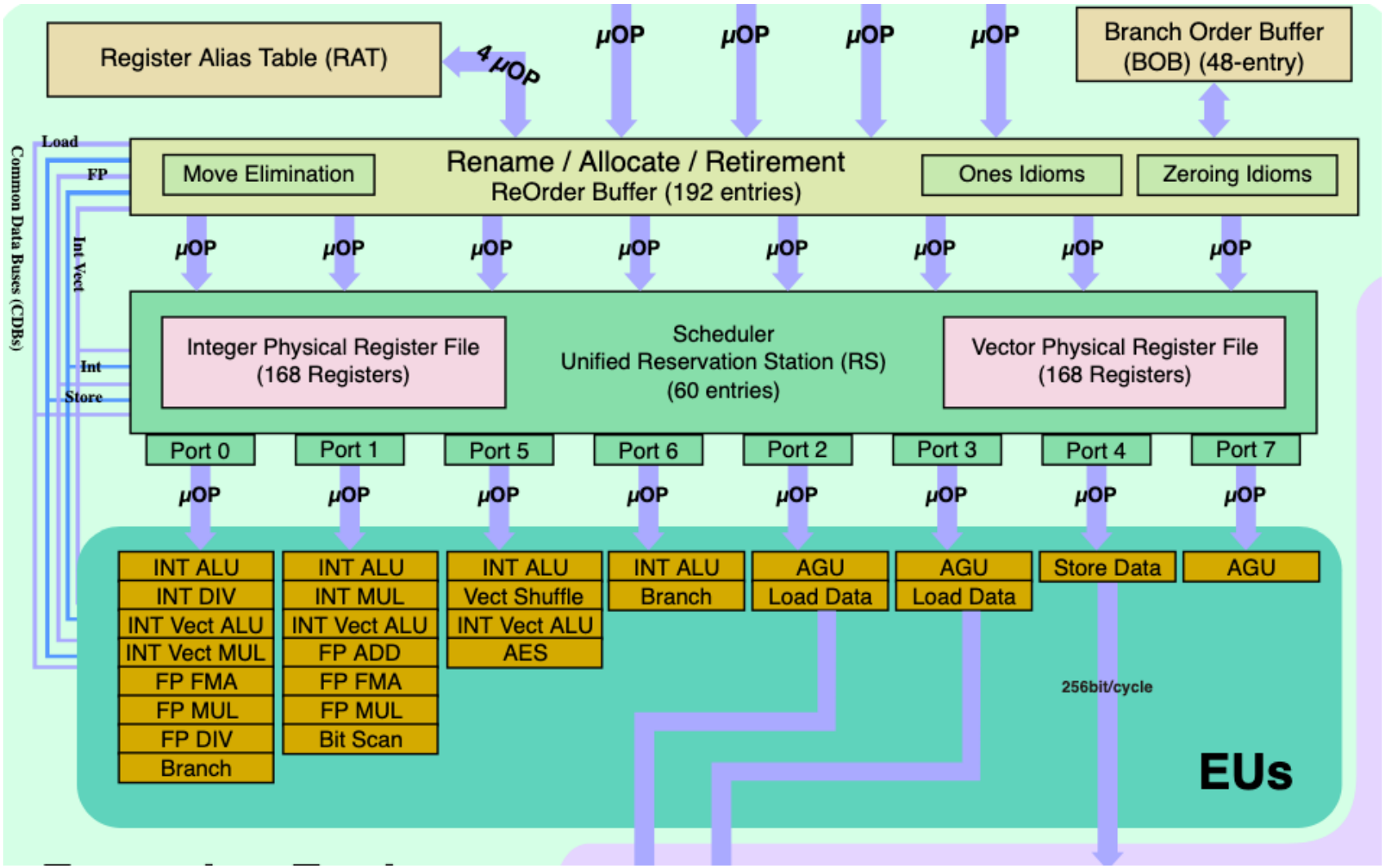

Sequential Performance

Instruction Level Parallelism (ILP)

- **Out of order execution** re-order instructions
- **Pipelining** "assembly line" parallelism
- **Superscalar architecture** multiple execution units
- **Branch prediction** speculative execution

Compilers and processors already very good at this part!
How can we help?

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New Instruction Set Architectures (ISA)

- **MMX** 2-wide float
- **SSE** 4-wide float, 2-wide double
- **AVX** 8-wide float, 4-wide double
- **New instructions** FMA (fused multiply accumulate)

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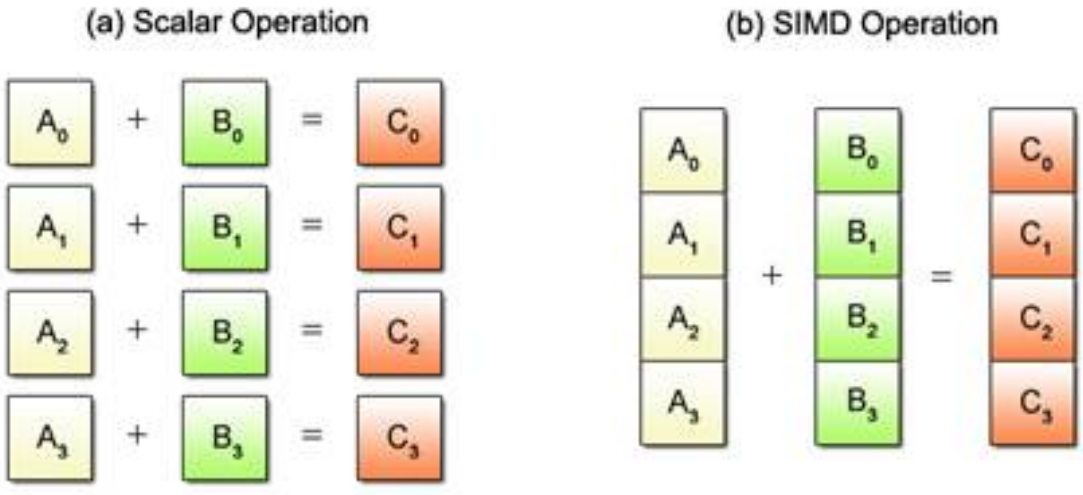
Many ways of doing this!

Vectorization

SIMD: Single Instruction Multiple Data



Steps

- Start thinking in vectors instead of scalars (float, double)
- Re-organize computations as vector operations
- Tell the compiler it is safe to use SIMD instructions

Implicit Vectorization

- **Auto-Vectorisation:** Loop unrolling, inlining, compiler flags (-O3, -march=native) and hints
  - Compiler specific extensions, not portable and no guarantee of vecorizing
  - #pragma ivdep (tell GCC to ignore vector dependency)
  - __builtin_assume_aligned(a, 32) (tell GCC array is aligned)
  - __assume_aligned(a, 32) (tell Intel compiler array is aligned)
  - -fopt-info-vec-optimized (vectorization report with GCC)
  - -qopt-report=2 (vectorization report with Intel)

Explicit Vectorization

- **OpenMP 4.0: SIMD pragma**
  - #pragma omp simd [clauses] (vectorize for loops)
  - clause: safelen(len) (vectors of length len are safe)
  - clause: aligned(v1,v2:alignment) (vectors are aligned)

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- **Vector Intrinsics (the C++ way)**
  - Vector objects, overloaded operatos (+, -, *, ||, && etc)
  - See file "intrin-wrapper.h" in https://github.com/NYU-HPC19/lecture3
  - Other implementations https://www.agner.org/optimize/#vectorclass
  - Similar proposals for future C++ standard library https://en.cppreference.com/w/cpp/experimental/simd

Vector Intrinsics

https://software.intel.com/sites/landingpage/IntrinsicsGuide/

- **Aligned memory allocation:** reading from aligned arrays is faster, un-aligned reads require multiple instructions. Allocate arrays using,
  - void* aligned_malloc(int); (for dynamic memory)
  - alignas(64) char double[128]; (for static arrays)
- **Basic Vector Operations (AVX only)**
  - Vector type: __m256d (vector of 4-doubles)
  - Load aligned: _mm256_load_pd(double const *)
  - Load unaligned: _mm256_load_pd(double const *)
  - Store aligned: _mm256_store_pd(double const *, __m265d)
  - Store un-aligned: _mm256_store_pd(double const *, __m265d)
  - Vector Addition: _mm256_add_pd(__m265d, __m265d)
  - Vector Multiplication: _mm256_mul_pd(__m265d, __m265d)
  - Vector FMA: _mm256_fmadd_pd(__m265d, __m265d, __m265d)
  - Other intrinsics to know: permutation, comparison, bitwise operations, streaming reads/writes, prefetch instructions etc.

Special Functions

- Special functions like div, mod, $\exp$, $\sqrt{x}$, $\sin$, $\cos$ computed in software or special hardware units.
- Require $\mathcal{O}(10)$ or $\mathcal{O}(100)$ cycles to compute.
- Example: division requires 10 cycles and has latency of 38 cycles.
- Specialized algorithms for some computations (fast inverse sqrt used in Quake III)

Outline

Basic Linear Algebra Subprograms (BLAS)

Specification for basic linear algebra operations

- Level 1: vector-vector operations (dot-product, norm, axpy)
- Level 2: matrix-vector operations (generalized matrix-vector multiplication: gemv)
- Level 3: matrix-matrix operations (generalized matrix-matrix multiplication: gemm)

Many implementations available

- Open-source: GotoBLAS (Kazushige Goto), OpenBLAS, ATLAS (Automatically Tuned Linear Algebra Software)
- Intel Math Kernel Library (MKL)

GEMM (sgemm, dgemm)

Function declaration:

```
extern "C" { // from C++
void dgemm_(char* TRANSA, char* TRANSB,
    int* M, int* N, int* K, double* ALPHA,
    double* A, int* LDA, double* B, int*
    LDB, double* BETA, double* C, int* LDC);
}
```

Linking:

```
g++ MMult.cpp -lblas
icpc MMult.cpp -mkl
```

(for linking to MKL using non-Intel compilers: https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor)

Other Useful Libraries

Linear Algebra Package (LAPACK)

- Linear solvers, LU factorization, QR factorization, singular value decomposition (SVD)
- Built on top of BLAS
- Many implementations available (also included in MKL)

Fastest Fourier Transform in the West (FFTW)
http://www.fftw.org

- Optimized FFT implementation, open source.