CMSC 714
Lecture 19
Autotuning

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Notes

- Midterm exam is on Thursday, Nov. 16
  - on readings through previous week
- Group Project interim report due Nov. 13
- Email me about whether you are interested in a tour of Zaratan on Nov. 27 or 29

Autotuning for HPC Applications

- Overall goal is *performance portability*
  - Across diverse HPC architectures
  - Which has not been achievable through languages and compilers
- Involves "automatic generation of a search space of possible implementations of a computation that are evaluated through models and/or empirical measurement to identify the most desirable implementation"
- Search space is a set of code variants functionally equivalent
  - Paper says to an original implementation, but could be to a specification (e.g., an API)

Autotuning

- Empirical autotuners
  - Execute each code variant
  - Measure runtime (or another objective function)
  - Evaluate performance of each variant
  - Run the best performing variant
  - Need intelligent search methods and models to prune a potentially very large search space
  - Can also use runtime prediction models, esp. for long-running kernels
- Code variants
  - Different code organization, data structures, algorithms, low-level implementation details
  - Parallelization strategies
  - Memory hierarchy optimization (data placement, blocking/tiling, tile size)
- Can be applied offline, or online while the application is running, or even incrementally

Tools

- Libraries
  - Isolate performance critical functions behind a standard API
  - Examples include Atlas (linear algebra), SPIRAL (digital signal processing), Sparsity (sparse matrix computations), FFTW (fast Fourier transforms)
- Compilers and code generators
  - Generate a collection of architecture-specific codes from same high-level input
  - Examples include CHiLL (USC, Utah, UMD), Orio (Oregon, Ohio State), POET (Georgia Tech, LLNL)
  - Can include parallelization – SIMD pragmas, OpenMP directives, CUDA, etc.
  - And various loop optimizations – tiling, unrolling, permutation, fusion, distribution, prefetching, software pipelining, …
    - And what order to apply them

Application-level tools

- Tools allow expressing tunable parameters and code variants representing alternate implementations
  - Can select code variant based on problem size, to target different levels of memory hierarchy or parallelism
  - Must be done at runtime if depends on input dataset
    - Active Harmony (UMD) and Adapt (Purdue) can create, link, test new variants in parallel with execution during iterative computations
- Disadvantage is that each application developer has to specify autotuning
- New frameworks like RAJA (LLNL) and Kokkos (SNL) can specialize high level code using C++ template abstractions around loops and data structures
- Domain specific languages (DSLs) for some application areas – e.g., Halide for image processing, others for stencil computations (PDEs)

Search

- Evaluate points in the search space (parameter values, code variants) to find optimal solution
- Complete enumeration
  - Doesn’t scale since there can be too many points in the search space
- Two ways to limit search space to a subset
  - Model-free – global or local search
    - Global includes simulated annealing, genetic algorithms, particle swarm optimization – guaranteed to find global optimum if given long enough search time, but in practice stop earlier
    - Local includes Nelder-Mead simplex, orthogonal search, variable neighborhood search – move from current to nearby point in search space, so can terminate in a local optimum
  - Model-based
    - Use performance prediction metrics (analytical or empirical models)
    - Limited by accuracy of models

Software Engineering Challenges

- Offline autotuning makes compilation slow
  - Many variants need to be compiled and executed
- Empirical autotuning makes developer manage the tuning process
- Build process for autotuning can be complex
  - Can be different while autotuning vs. running autotuned code (library, application, etc.)
- Package management systems (e.g., Spack) help
  - Can wrap compilers to generate autotuning variants
- Debugging autotuned code can be difficult
  - You may be running automatically generated code!
  - But the generated code is more likely than yours to be correct …

ATLAS

- Automatically Tuned Linear Algebra Software
  - Library produced by autotuning – they call it automated empirical optimization of software (AEOS)
- Start from well-known, widely used API for linear algebra core operations
  - BLAS – basic linear algebra subroutines
  - For linear algebra, need to characterize parameters that vary across machines – biggest one is blocking factor for blocked LA algorithms, which affects cache utilization
  - Can also try different source code implementations
    - Multiple implementations or code generation
- To produce highly tuned code, not enough to understand the hardware
  - Because of complex interactions between hardware features, compiler, OS, …
  - So we're back to an empirical process – try code variants, parameter values, etc. to find the best implementation on a specific machine

ATLAS

- Goal is portable, efficient implementation of BLAS
  - BLAS are building blocks for performing vector and matrix operations
    - Level 1 is vector-vector
    - Level 2 is matrix-vector
    - Level 3 is matrix-matrix
  - Level 1 has no possible memory reuse, so not addressed
  - Level 2 memory blocking allows for reuse of vector operands, but not matrix
    - Reduces movement of vector operands from $O(N^2)$ to $O(N)$
    - Allows for modest speedups – 10-300%
  - Level 3 blocking allows for reuse of both operands
    - Blocking reduces $O(N^3)$ fetch costs to $O(N^2)$
    - Also better optimizes $O(N^3)$ computation costs than many compilers (run on non-blocked code)
    - Can give orders of magnitude performance improvements

ATLAS

- Level 3 BLAS mainly targets generalized matrix multiplication (GEMM)
  - $C \leftarrow \alpha op(A) op(B) + \beta C , op(X) = X \text{ or } X^{\mathsf{T}}$
  - *C* is an *MxN* matrix, *op(A)* and *op(B)* are *MxK* and *KxN*
- Uses both parameterized adaptation and code generation to adapt to a new machine
  - To generate L1 cache-contained matrix multiply kernel
- Most of the paper goes into the details of how to generate the MM kernel that fits into L1 cache
  - All sorts of decisions need to be made about copying matrices, which matrix is in the outermost loop, writing output to *C* or to an output temporary matrix, choosing loop structure to help with L2 cache reuse
  - ATLAS determines size of L1 data cache, but not L2 (instead computes a value that represents the amount usable for its blocking)

ATLAS

- Other optimizations
  - Instruction cache reuse – fit code into L1 instruction cache
  - Floating point instruction ordering – to hide pipeline latencies (if no fused multiply-add) – modern processors do out-of-order execution in hardware, so this is not needed
  - Reduce loop overhead by loop unrolling
  - Expose instruction-level parallelism – for floating point computations and for memory fetches
- Search heuristic uses a code generator coupled with a timer routine
  - Start with some initial good guesses, then try different loop unrolling and latency hiding strategies to find the best performing variant and parameter values
- Performance results show that ATLAS produces code that is as good as vendor BLAS implementations and much better than what a compiler can do
  - For 500x500 matrices
- Paper also discusses Level 2 BLAS optimization process
  - More complex in some ways than Level 3!