Parallel Programming (IN2147) Optimization of Sequential Programs

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New TOP500 List

And the winner is: Summit

Oak Ridge National Laboratory

2,282,544 cores - 122.3 PFlop/s - 8.8 MW 13.889 GFlops/Watt (rank 5 in Green500)

China

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM D0E/SC/Oak Ridge National Laboratory United States	2,282,544	122,300.0	187,659.3	8,806
2	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
3	Sierra - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/NNSA/LLNL United States	1,572,480	71,610.0	119,193.6	
4	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, NUDT National Super Computer Center in Guangzhou	4,981,760	61,444.5	100,678.7	18,482

Which strategy?

- First ensure scalability
- Optimizing sequential code gives constant factors
- ► Optimization is an iterative process

Programming Languages I

- Major differences in:
 - Efficiency
 - Ease of programming
 - Abstractions
- ▶ Classic HPC languages: C, Fortran
 - ▶ Rather low-level, allow for manual optimizations
 - Efficient machine code (mostly)
 - ► Rather low programming comfort

Programming Languages II

- Byte-code compiled languages: Java
 - More easy to program
 - Machine code not as efficient
- Scripting languages: Python, Perl, JavaScript, . . .
 - Very easy to program (typically)
 - Don't expect performance
- ▶ New languages: C++, Swift, Rust, Go, ...
 - ► C++: gaining traction in HPC
 - Go: Compile-time is important, runtime is not
 - ▶ Others: To be seen...

Detecting optimization potential

- Optimizing code taking 1% of total time?
 - Probably not worth the effort
- Analysis of optimization potential is important
- Profiling helps in analysis
 - Tools: perf, Gprof, etc.
- Start with part having the biggest impact on performance

Algorithms

- Last week: choose algorithms which scale
- Today: care about sequential performance
- Vectorization, super-scalarity
 - Independent parallel computations
 - Data-parallelism
- Cache efficiency
 - Regular access patterns
 - Few indirections

Abstractions

- Abstractions make (programmer's) life easier
 - No need to care about technical details
 - Increases portability
 - ► That's why they are all over the place ::
- Often, many abstractions are stacked
- Abstractions (often) introduce overhead
- Abstractions at some point leak
 - ▶ E.g. lead to strange performance effects

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Abstractions

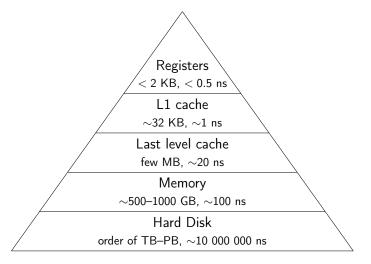
- ▶ C++ makes it easy to use complex abstractions
 - Bounds checking (indexing)
 - Hidden function calls (operator overloading)
 - Indirect function calls (vtables)
 - Many (hidden) pointer dereferences (references)
 - Random access in memory (std::list)
 - Huge code size (templates)
 - **.** . . .

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Abstractions

- Be aware of (hidden) abstractions
- Know their impact
- Use abstractions with care, avoid if possible with reasonable effort

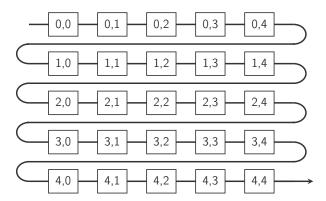
Memory Hierarchy (simplified)



Cache Optimizations

- Exploit spatial and temporal locality
- Data layout in memory
 - Row-major vs. column-major arrays hello Fortran
- Predictable, regular access pattern allows prefetching
- Prefetch instructions (use with care)
- "Blocking" in loops
- Avoid cache pollution
 - Streaming instructions don't write to the cache

Layout of Matrices in Memory



- ▶ What's better? Row-wise vs. column-wise access?
- ▶ Row-wise access > 50% faster (in C)

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Cache Optimization

- Exploit spatial and temporal locality
- Cache optimization may require large code changes
- Cache optimization can yield large speed-ups
- ► Tools may help: Cachegrind, KCachegrind
 - KCachegrind developed by Josef Weidendorfer (LRZ)

Compiler Optimizations

- Compilers generate and optimize machine code
- Compilers (usually) apply (complex) code transformations
 - Only if proven to be correct
- Compilers (usually) don't change data structures
 - Typically impossible to prove correctness automatically
- ► Compilers (usually) don't optimize maths
 - ▶ If they do, don't trust the result
 - Mathematical optimizations can change accuracy

Common Optimization Options

- -00 no optimization
- ▶ -01 "optimize"
 - Better register allocation, dead code elimination, . . .
- ▶ -02 "optimize even more"
 - More aggressive CSE, remove redundant instructions, . . .
- ▶ -03 "optimize yet more"
 - Aggressive inlining, vectorization, . . .
- -0s "optimize for size"
- -0g "optimize debugging experience"
- -Ofast "disregard strict standards compliance."
 - Floating-point optimizations
- ► -march=native (in addition) architecture tuning

Some Optimizations

- ► Loop-invariant Code Motion (LIM/LICM)
 - Statements independent of the loop moved outside
 - Avoid redundant execution of code
- Loop Unrolling
 - Loop is known to be executed 5 times
 - Copy the loop body 5 times
 - No loop overhead, but code size grows
- Inlining
 - ▶ Body of other function is copied into the caller
 - ▶ No overhead through call, calling convention, etc.

Vectorization

- Auto-Vectorization...
 - Works well for simple cases
 - High overhead for complex code (if vectorized at all)
 - May require restrict keyword
- Manual vectorization can yield high performance improvement
 - Even compared to the Intel compiler
- Manual vectorization is target-dependent
 - Portability? Development time?

Floating-point Optimizations

- ► IEEE-754 defines floating-point numbers and operations
- ▶ Possible to optimize $x + 0 \rightarrow x$? **No!**
 - Signed zeros, (-0) + (+0) = (+0)
- ▶ Possible to optimize $x x \rightarrow 0$? **No!**
 - ▶ If x is NaN, result is NaN
- Options for relaxing IEEE semantics
- Trade-off: performance vs. accuracy
- ▶ Note: enabling -ffast-math can make code slower

Compilers: Miscellaneous

- Providing Hints
 - restrict keyword
 - Pointers don't overlap each other
 - inline keyword
 - __attribute__((aligned(32)))
- Intrinsics (see lecture on SIMD)
- Inter-procedural Optimization
 - Compile and link with -flto
 - Unified builds (combined with -fwhole-program)
- ▶ In doubt, analyze generated assembly code

Hand-written Assembly Routines

Should you write assembly by hand?

NO (unless you have a good reason)

- ▶ Possible reasons for writing assembly routines:
 - ▶ Hot code that compiler *really* fails to optimize
 - Intrinsics don't yield intended effect
 - "Research Code"

Time Measurement

- Preferred functions: MPI_Wtime or clock_gettime(CLOCK_MONOTONIC_RAW, ...)
- Common pitfalls:
 - Measured time too short
 - No repetitions to exclude external influences
 - Measurement of I/O or other syscalls (unless you want to measure I/O)
 - ▶ Wrong clock, e.g. CPU time instead of wall-clock time

Ongoing Research

Research: Dynamic Code Generation

- Limitations of classic compile-execute model: Overhead through indirections and missing runtime data
 - Input data/Configuration
 - Previous computations
 - Data distribution, scheduling
 - Highly irregular data structures
 - **•** . . .
- ▶ Idea: Incorporate data in machine code

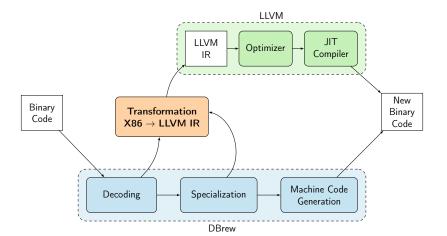
Dyn. Code Gen.: Approaches

- Dedicated languages failed 20 years ago
- ► LLVM: full-featured compilation framework
- LIBXSMM: generate code for matrix multiplications and convolutions
 - Developed by Intel
 - Generates highly tuned code
- DBrew: dynamic binary rewriting
 - Developed at CAPS, TUM
 - Specialize existing compiled functions at runtime

DBrew

- Library for binary rewriting at runtime
- Operates on functions, producing drop-in replacements
- Targets x86-64
- Specialization by fixing parameters and memory regions
- Very simple optimizations only (fast code generation)
- Advanced optimizations available via LLVM

DBrew: Overview

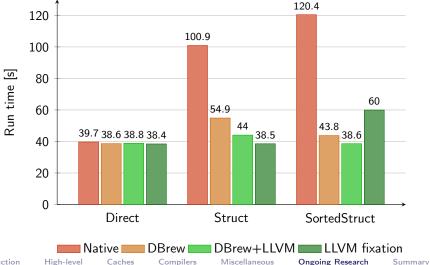


DBrew: Example

```
Rewriter* r = dbrew_new(fn);
dbrew_const_param(r, 0, 42);
dbrew_const_mem_nested(r, stencil, sizeof(Stencil));
Func new_fn = dbrew_rewrite(r);
```

▶ Possible to approach "native" performance (?)

Results when specializing Stencil



Summary

- Care about scalability first
- ► Choice of programming languages, algorithms, data structures has high impact on performance
- Complex abstractions slow down
- Cache optimization can bring high constant factors
- Compilers do technical optimizations only
- Code generation at runtime can improve performance, new techniques are under research

Thank you!