Software optimization in the many-core era – the CERN case

Studencki Festiwal Informatyczny, Krakow March 16th 2013

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PART 1: BACKGROUND

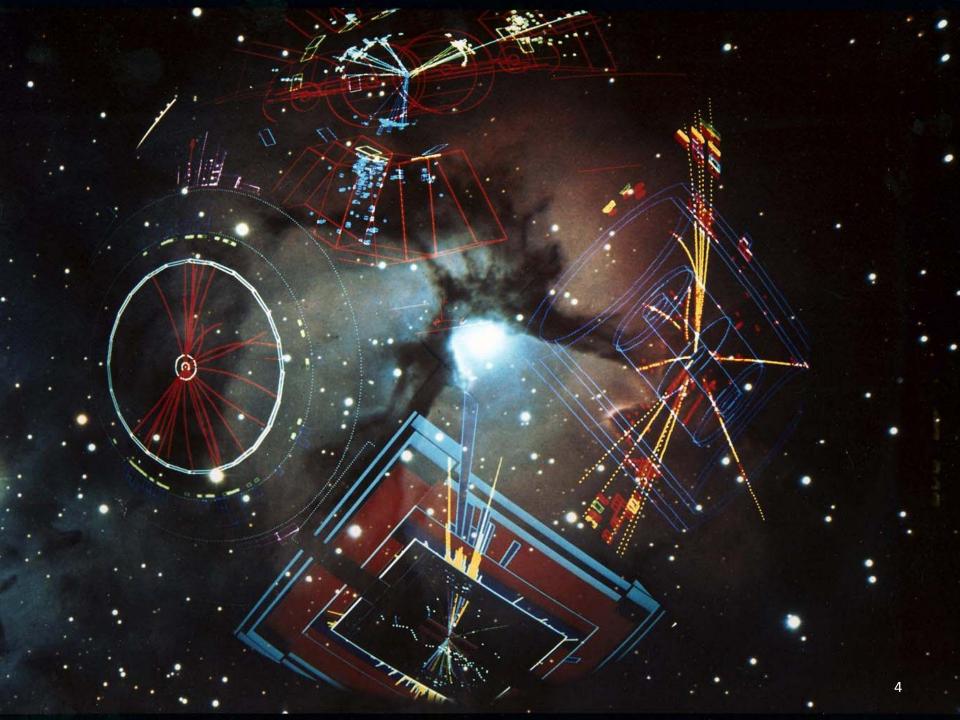


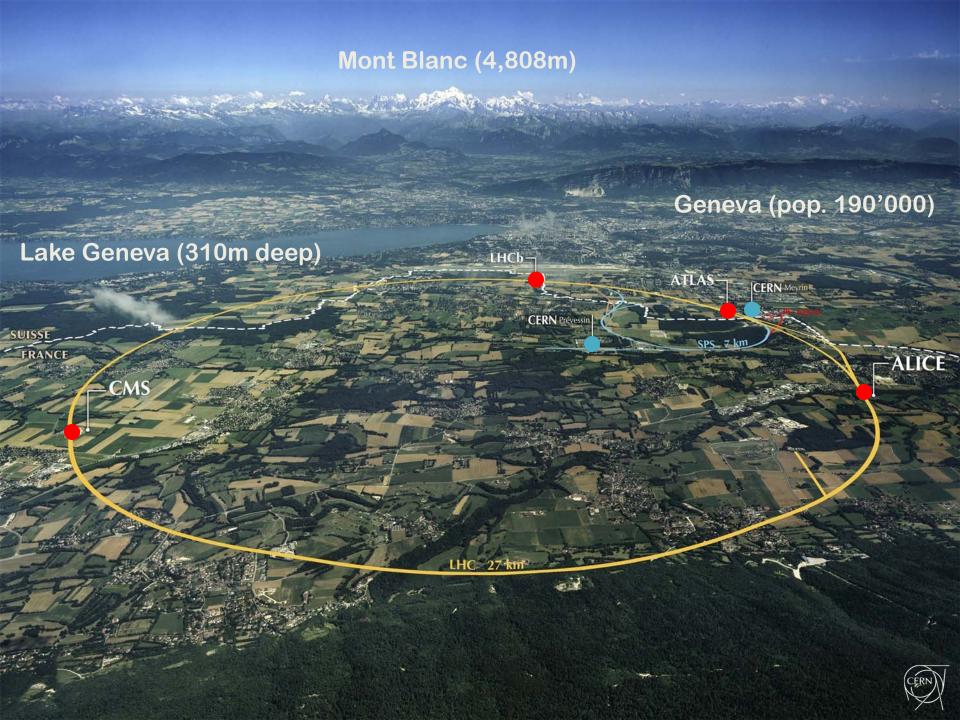
The European Particle Physics Laboratory based in Geneva, Switzerland

Founded in 1954 by 12 countries for fundamental physics research in a post-war Europe

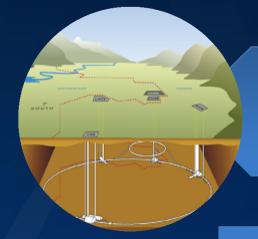
In 2013, it s a global effort of 20 member countries and scientists from 110 nationalities, working on the world's most ambitious physics experiments

~2'500 personnel, > 15'000 users ~1 bln CHF yearly budget





The Large Hadron Collider

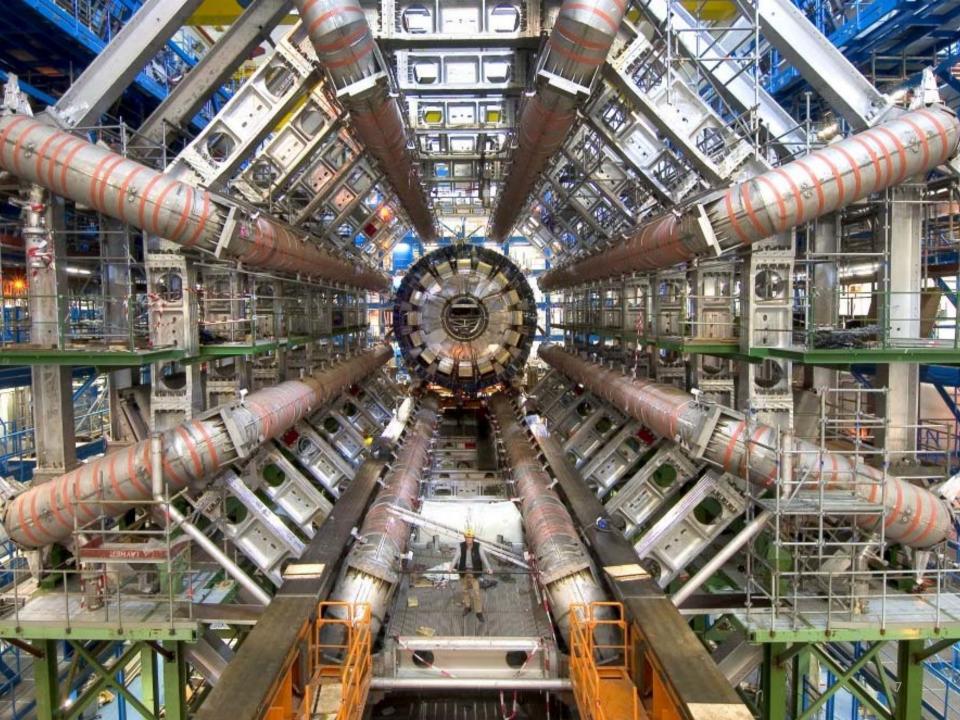


27 km underground superconducting ring – possibly the largest machine ever built by man

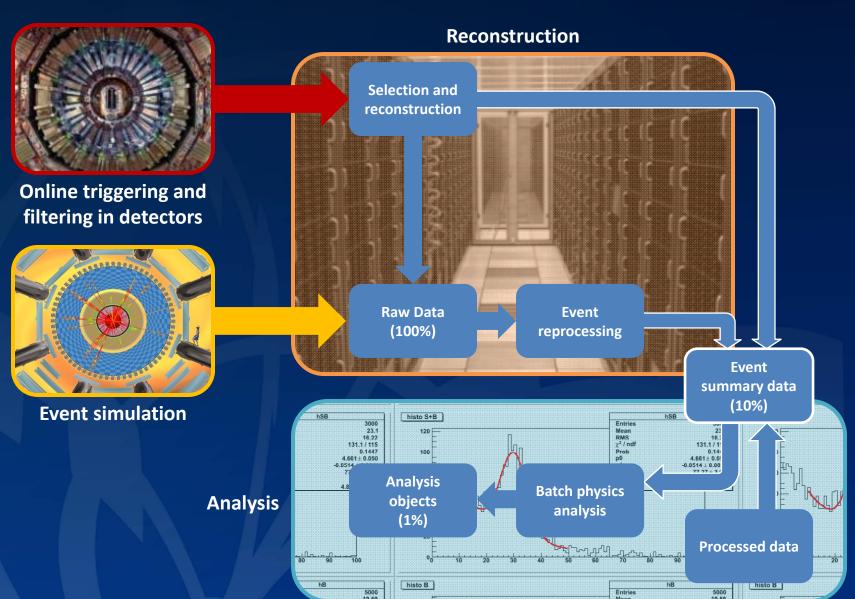
40 million collisions per second

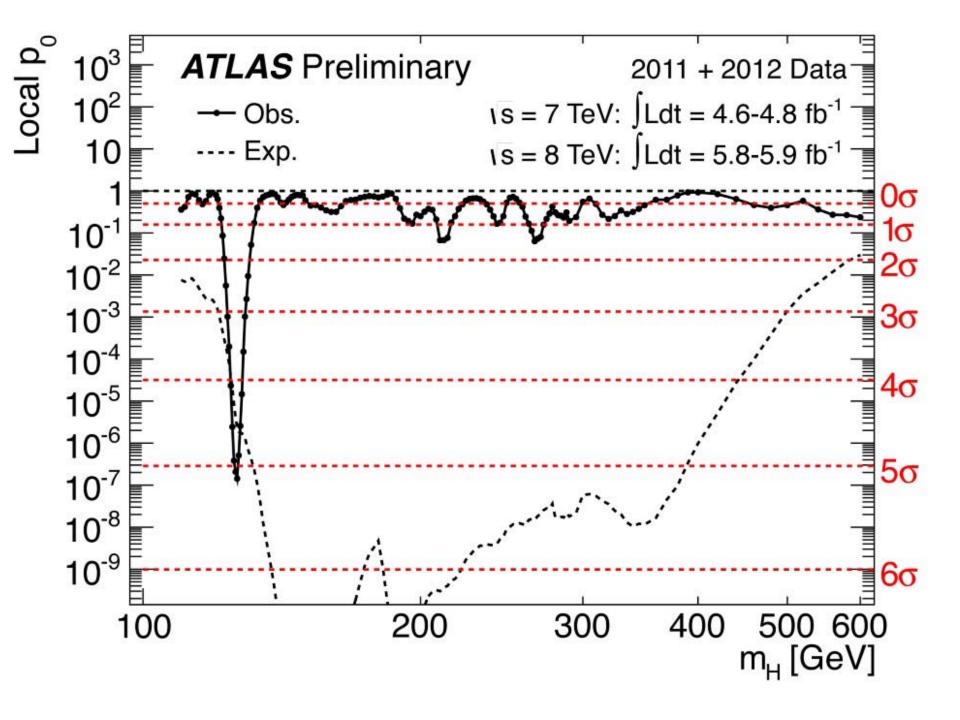


150-200 MW power consumption

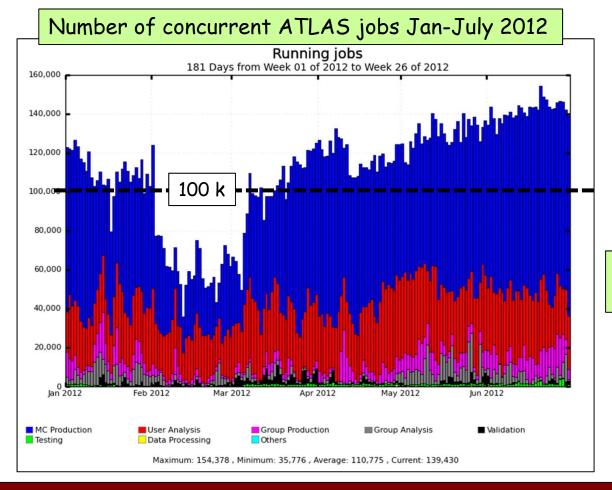


Data flow from the LHC detectors





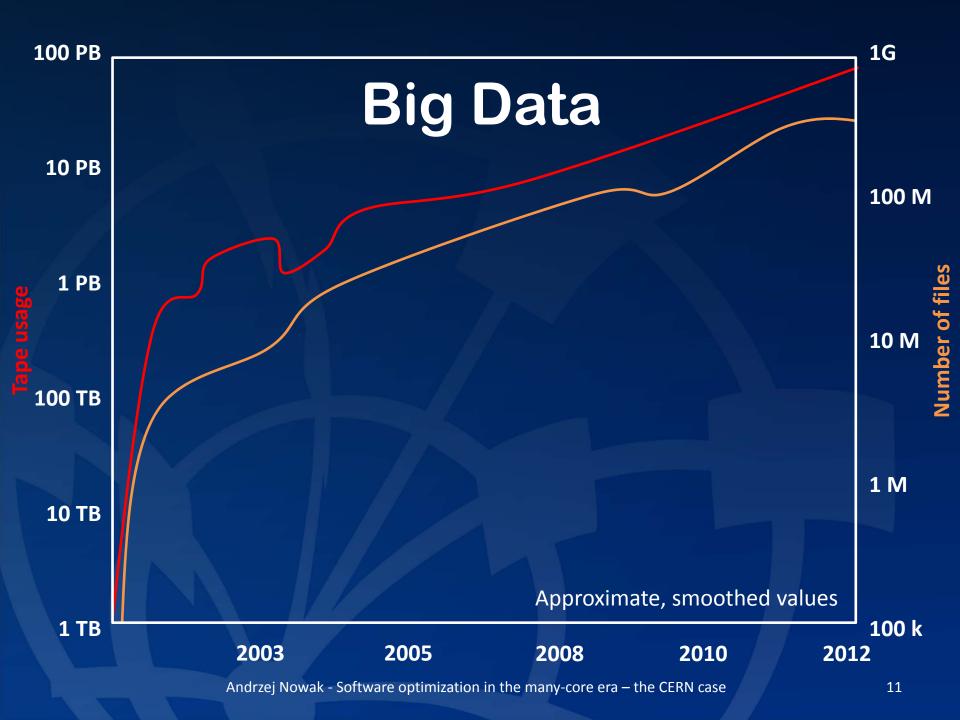
It would have been impossible to release physics results so quickly without the outstanding performance of the Grid (including the CERN Tier-0)



Includes MC production, user and group analysis at CERN, 10 Tier1-s, ~ 70 Tier-2 federations → > 80 sites

> 1500 distinct ATLAS users do analysis on the GRID

- Available resources fully used/stressed (beyond pledges in some cases)
- Massive production of 8 TeV Monte Carlo samples
- □ Very effective and flexible Computing Model and Operation team → accommodate high trigger rates and pile-up, intense MC simulation, analysis demands from worldwide users (through e.g. dynamic data placement)



Innovation in computing

1989: First high bandwidth transatlantic links

1999: The Grid vision materializes

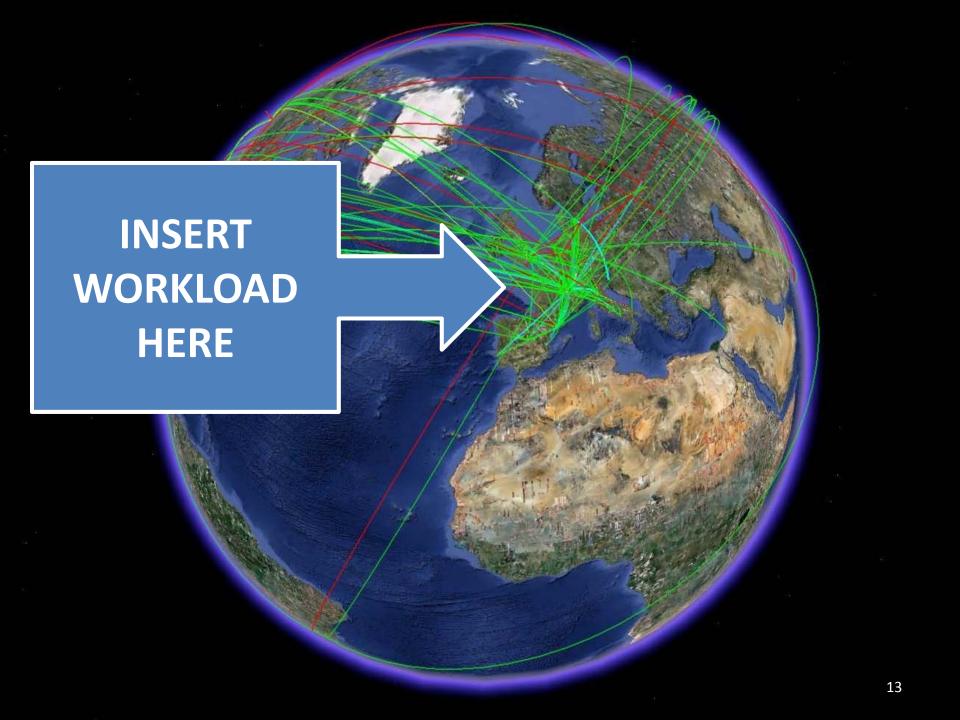
2003: Several Internet2 land speed records

2012: LHC delivering intense data challenges

1991: The World Wide Web is born at CERN

2001: CERN wins Computerworld's 21st Century Achievement Award for SHIFT

2008: The WLCG is the world's largest grid

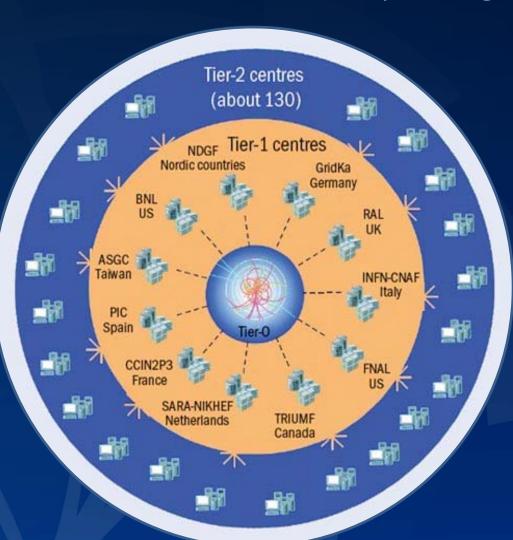


Collaboration on big data and computing The Worldwide LHC Computing Grid

Tier-0 (CERN): data recording, reconstruction and distribution

Tier-1: permanent storage, re-processing, analysis

Tier-2: Simulation, end-user analysis



nearly 160 sites

~250'000 cores

173 PB of storage

> 2 million jobs/day

Challenges in computing

Big(ger) Data

- LHC upgrades
- New paradigms, science

Exascale

- Computing evolution
- Next-gen interconnect

Society

- Scientific leadership
- Sustainable computing

Big(ger) data

Data rates at the LHC to increase by ~100x



"Sustainable computing"

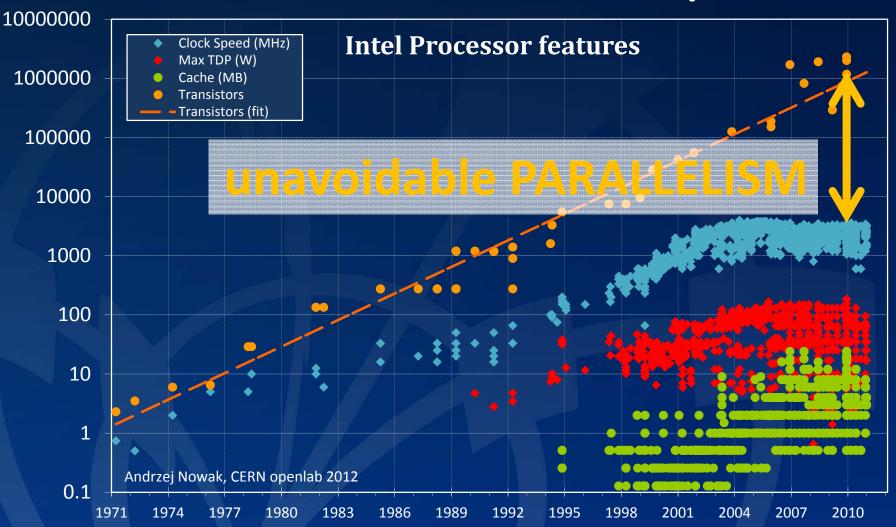
PART 2: COMPUTING LANDSCAPE

Co-design

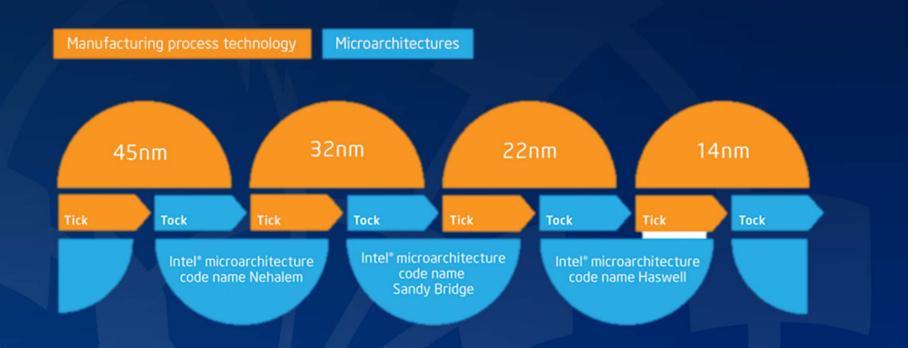
Design software independently of the hardware

Optimize software for the hardware

Hardware landscape



The Intel tick-tock model



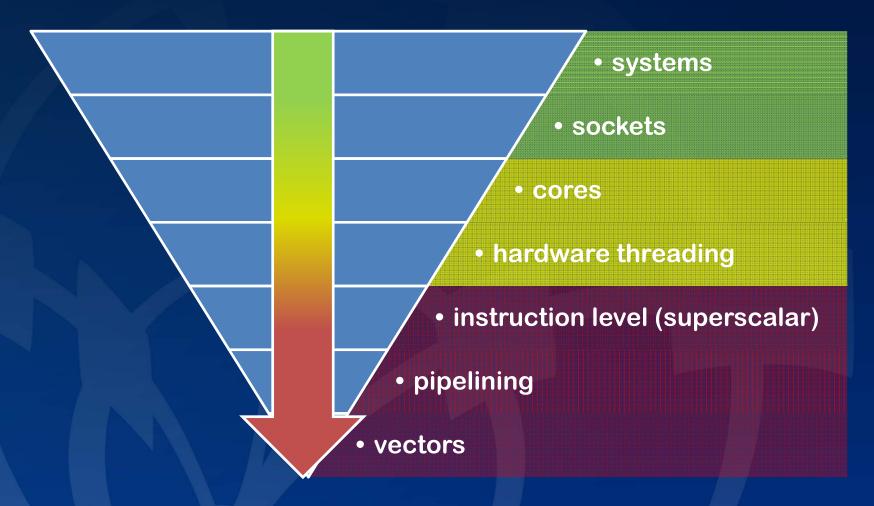
Source: Intel

A "modern" CPU that really is archaic

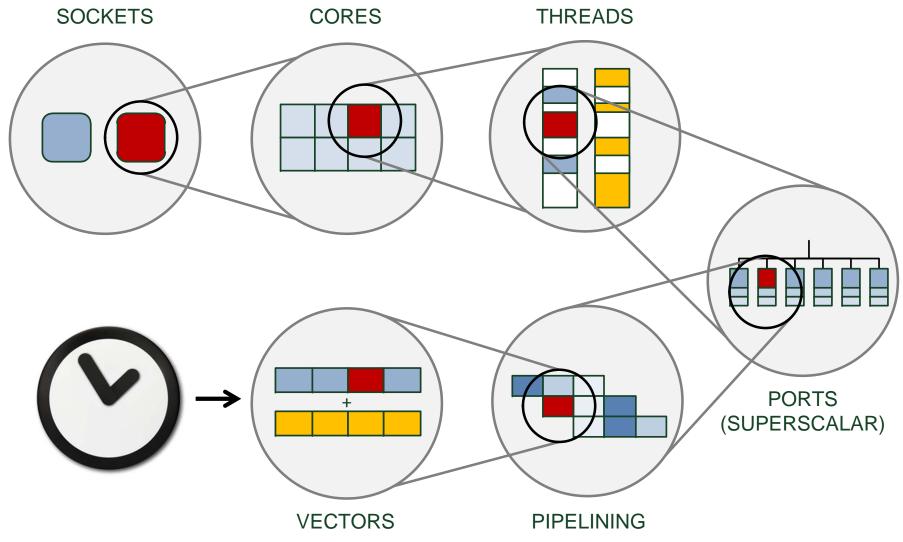


- As "stupid" as 50 years ago
- Still based on the Von Neumann architecture
- Primitive "machine language"
- Ferranti Mercury:
 - Floating-point calculations:
 Add: 3 cycles; Multiply: 5 cycles
- Today:
 - Programming for performance is the same headache as in the past

Omnipresent multiplicative parallelism



Inside a modern PC platform



Medium-term hardware trends

- Pricing follows market pressure, not technology
- IO, disk and memory do not progress at the same rate as compute power
 - bytes/FLOP decreasing
 - pJ/FLOP decreasing
- Bulk of improvements in x86 comes from Moore's Law still being in effect
- Heterogeneous architectures cross platform, cross socket, hybrid CPUs, accelerators, split into throughput and classic computing

Vector computing comes back with a vengeance





Vectors

- Comeback with a vengeance but lessons learned 20 years ago: growing substantially
 - 128-bit SSE → 256-bit AVX (designed for more)
 - AVX: new execution units
 - LRBni (Intel MIC): 512 bits, new vector instructions, FMA, 3-4op

Good news:

- can now hold 4 doubles
- only one architecture to worry about
- plenty of technologies to choose from
- compilers getting increasingly better at autovectorization (can get 2x)

Bad news:

- increasingly a key element in the performance equation
- not everything will vectorize
- iterative and auto-vectorization are promoted, but are not the "magic bullet" solution for many legacy workloads
- good vectorization requires a <u>data centric design</u> (sacrifices have to be made)
- bad past experience (before PCs)



Intel64 & ILP considerations

- x86 microarchitecture
 - steady, but limited improvements (<10% per "tock")
 - increasingly advanced features can large code benefit?
- Frequency very modest changes, if any
 - Rise of the Turbo boost
- CPI for large code is often too high, literally wasting CPU power
 - CPI figures for the major experiments hover around 0.9-1.5
- C++/OOD abuse will produce significant side-effects
 - Very frequent jumps and calls + more
 - Dynamic code has penalties x86 is already quite good at executing it but there are limits
- Pipelining not discussed explicitly as it folds into ILP

Hardware threading

- Sharing of some CPU resources
 - Little on-die overhead
 - The OS makes few distinctions between threads and cores
- A part of the solution to bad ILP
- Free money
 - Usually between +20% and +30%
 - Recommendation: use whenever possible, good for simulation
- Does not help in all cases depends on the bottleneck

Multi-core vs. many-core

- A typical modern workhorse machine has 12-16 cores
 - Some have 48 or more (AMD)
 - Major datacenters can be 1 or 2 generations behind
- # of cores "at home" grows arithmetically
 - various reasons, most linked to the way people use their computers
- # of cores in the enterprise space still grows geometrically (per platform)
- The number of cores in the datacenter grows between the two, will slow down in the long run
 - The trend is important, not the end amount
 - Is the trend sustainable? What about all these transistors?

Multiple sockets and systems

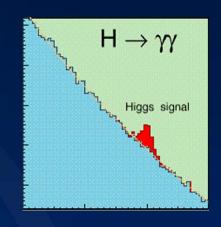
- Sockets slight growth with a limit, ultimately impacts core count per platform
- Multi-machine
 - mostly HPC
 - HTC: independent machines and processes
- Many-core is not multi-core
 - Memory hierarchy issues pop up
 - Cache coherency
 - NUMA
 - Memory bandwidth or IO paths may be constraining
 - Strong scalability tanks (need weakly scalable workloads)
- Multiprocess is a convenient model that can do the job, but it is not sustainable nor scalable

Corollary

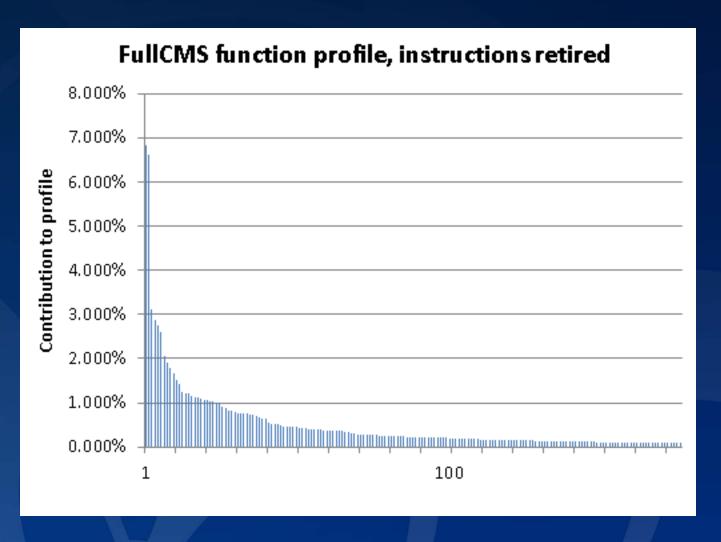
Raw platform performance is expanding in multiple dimensions simultaneously

The CERN case: physics jobs

- Independent events (collisions of particles)
 - trivial (read: pleasant) parallel processing
- Bulk of the data is read-only
- Very large aggregate requirements:
 - computation, data, input/output
- Chaotic workload
 - research environment physics extracted by iterative analysis:
 Unpredictable, Unlimited demand
- Compute power scales with combination of SPECint and SPECfp
 - Good double-precision floating-point (10%-20% of total) is important!
 - Good transcendental math libraries needed
- Key foundation: Linux together with GNU C++ compiler



Large jobs – profile fragmentation



Where is High Energy Physics code now?

- Large C++ frameworks with millions of lines of code
 - Thousands of shared libraries in a distribution, gigabytes of binaries
 - Low number of key players but high number of brief contributors
- Large regions of memory read only or accessed infrequently
- Characteristics:
 - Significant portion of double precision floating point (10%+)
 - Loads/stores up to 60% of instructions
 - Unfavorable for the x86 microarchitecture (even worse for others)
 - Low number of instructions between jumps (<10)
 - Low number of instructions between calls (several dozen)
- For the most part, code won't fit accelerators in its current shape
- Intensive upgrade efforts underway

How does High Energy Physics use hardware now?

- Very limited vectorization
 - Bad conditions to vectorize
- Sub-optimal instruction level parallelism (CPI at >1)
- Hardware threading introduced
 - Memory constriants
- Cores used well through multiprocessing bar the stiff memory requirements
 - However, systems put in production with tender related delays
- Sockets used well
- Multiple systems used well
- Relying on in-core improvements and # cores for scaling

Where are we now?

	SIMD	ILP	HW THREADS	CORES	SOCKETS
ТОР	4	4	1.35	8	4
OPTIMIZED	2.5	1.43	1.25	8	2
UNOPTIMIZED	1	0.80	1	6	2

	SIMD	ILP	HW THREADS	CORES	SOCKETS
ТОР	4	16	21.6	172.8	691.2
OPTIMIZED	2.5	3.57	4.46	35.71	71.43
UNOPTIMIZED	1	0.80	0.80	4.80	9.60

Using a low single digit percentage of raw machine power available today

Write your percentage here

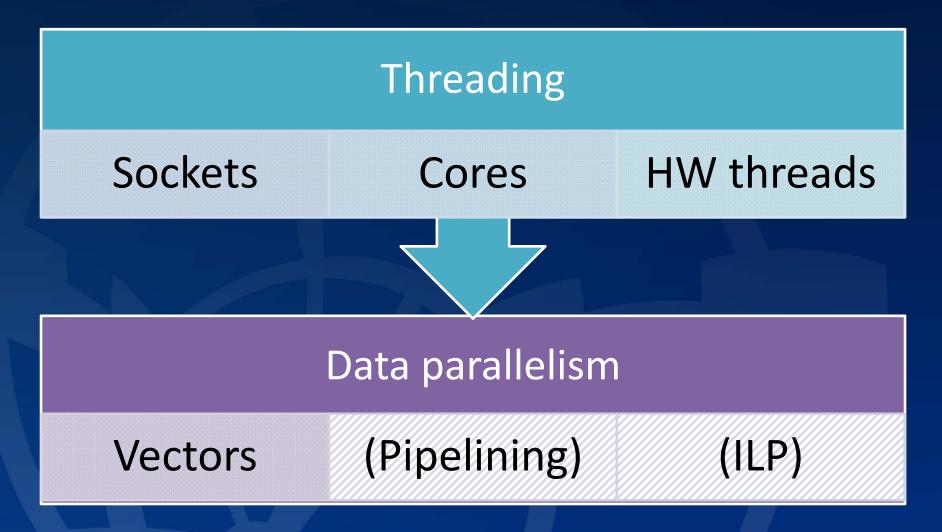
Corollary

Need to program for tomorrow's hardware today

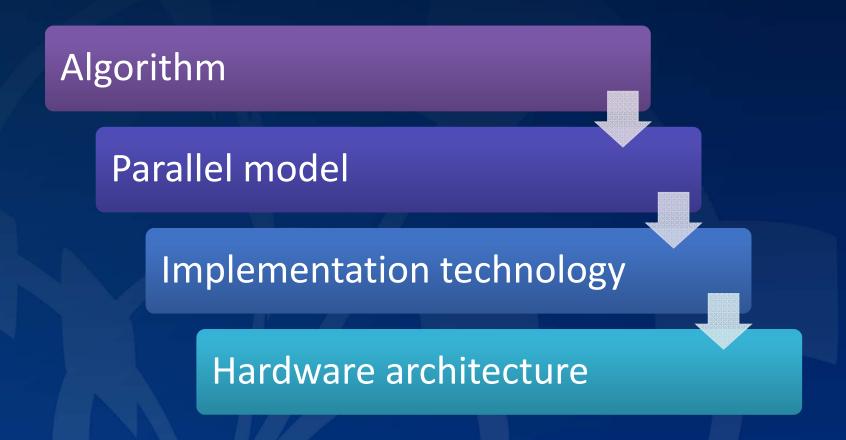


PART 3: EFFICIENT CODE

SW performance dimensions



The parallel technology stack



AVX data layout



Programming with vectors

- Classical tradeoff: code manageability vs. speed
- AoS vs. SoA
 - SoA favored
- Available levels of abstraction
 - Assembly
 - Intrinsics (C/C++)
 - Auto-vectorization (C/C++)
 - High level and interpreted code
- Data-centric design is key

Auto-vectorization and vector notations

- Compilers are becoming increasingly effective in autovectorization
 - ICC leading the effort, GCC is behind but pushing forward
 - Numerous caveats and dependencies: need to align data, use pragmas, restrict keywords etc.
- Array notations gaining popularity (CEAN etc)

```
Example: FIR Scalar Code

for (i=0; i<M-K; i++){
    s = 0
    for (j=0; j<K; j++){
        s+= x[i=j] * c[j];
    }
    y[i] = s;
}

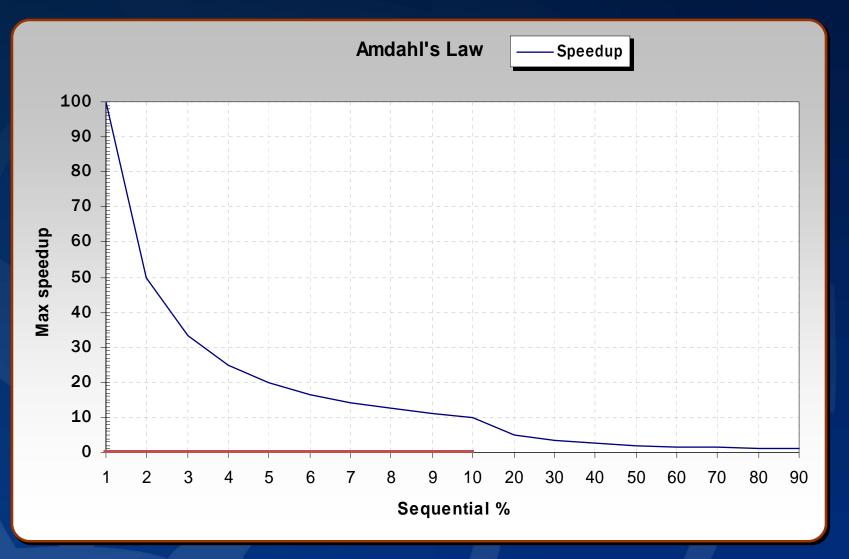
Example: FIR Inner Loop Vector

for (i=0; i<M-K; i++){
    y[i] = __sec_reduce_add(x[i:K] * c[0:K]);
}

Example: FIR Outer Loop Vector

y[0:M-K] = 0;
    for (j=0; j<K; j++){
    y[0:M-K]+= x[j:M-K] * c[j];
}</pre>
```

Amdahl's Law



Gustafson's Law

- Often when the problem size increases, the sequential portion remains constant
- Therefore, as the problem size increases, so do the opportunities for parallelization
- Let a(n) be the sequential portion function of the program, diminishing as n approaches infinity

Speedup =
$$a(n) + N(1 - a(n))$$

 As n approaches infinity, the speedup approaches the number of processors N

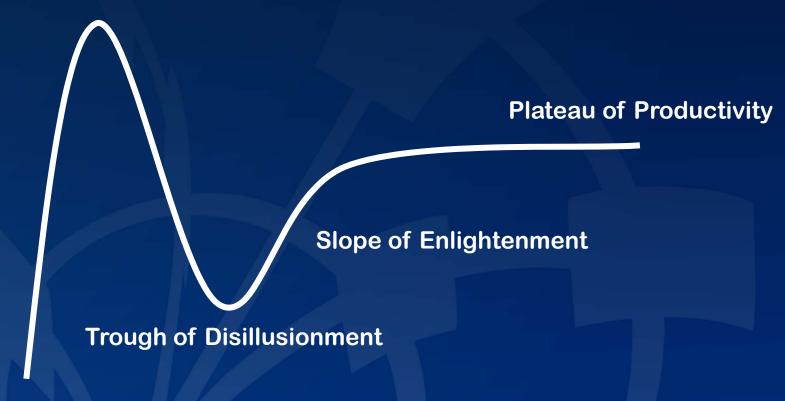
A plethora of options for parallelism (subset)

- OpenMP
- CUDA
- pthreads
- MPI
- Cilk
- Ct/RapidMind/ArBB
- TBB
- OpenCL
- Boost threads
- Concurrent Collections

- Less mainstream:
 - Axum
 - Co-array Fortran
 - UPC
 - Go
 - Chapel
 - Fortress
 - X10
 - Erlang
 - Linda
 - Haskell

The Hype Cycle

Peak of Inflated Expectations



Technology Trigger

Modeled after Gartner Inc.

Tradeoffs in software development (with focus on hardware)

- Flexibility and programmability vs. performance
 - Impacts the choice of the programming language, technologies etc
- Revamp vs. iterative improvement
- Homogeneous vs. heterogeneous processing model
- Single/multi process vs. multi-threaded
- Data-centric software design or not?
- Kernels vs. heavy code
- Program for specific architectures or not?

Key aspects in any choice



C++ specific issues

- Key performance related aspects of the C++ language:
 - the compiler is particularly important
 - memory allocation
 - virtual mechanisms
 - small and temporary objects
- Large projects in C++ produce extreme optimization challenges
 - Highly fragmented profiles, few instructions/jump, few instructions/call
 - Difficult without collaboration from domain experts

STL Container Efficiency

With material from A. Lazzaro

Container	Stores	Overhead	[]	Iterators	Insert	Erase	Find	Sort
list	Т	8	n/a	Bidirect'l	С	С	N	N log N
deque	Т	12	С	Random	C at begin or end; else N/2	C at begin or end; else N	N	N log N
vector	Т	0	С	Random	C at end; else N	C at end; else N	N	N log N
set	T, Key	12	n/a	Bidirect'l	log N	log N	log N	С
multiset	T, Key	12	n/a	Bidirect'l	log N	d log (N+d)	log N	С
map	Pair, Key	16	log N	Bidirect'l	log N	log N	log N	С
multimap	Pair, Key	16	n/a	Bidirect'l	log N	d log (N+d)	log N	С
stack	Т	n/a	n/a	n/a	С	С	n/a	n/a
queue	Т	n/a	n/a	n/a	С	С	n/a	n/a
priority_ queue	Т	n/a	n/a	n/a	log N	log N	n/a	n/a
slist	Т	4	n/a	Forward	С	С	N	N log N

Other C++ tips (1)

- Avoid virtual functions and classes extra memory, indirections, compiler optimizations prevented
 - Use C++ templates where possible
- dynamic_cast can be expensive
- Conditions are evaluated from left to right
- Switch statements prevent branch prediction
 - Avoid unless absolutely necessary
- Use STL with caution

With material from A. Lazzaro

Other C/C++ tips (2)

- Dynamic memory allocation will suffer from fragmentation
 - Use pools
 - Pass arguments by reference
 - Reuse objects instead of creating new ones
 - Avoid temporary variables
- Data locality matters
- Code locality matters in large code
- Align data for vectorization
- Pay attention to floating point math
- Always help the compiler

With material from A. Lazzaro

The complexity of a large software project

- Strategy and hardware-related requirements are a must when the hardware is a variable
- Hard to plan for unknowns, but easier to plan for changes
- Requirements management
- Software middle-men threaten scalability
- Long time to produce and stabilize
 - Consequently: faraway targets should be considered, not current

PART 4: OPTIMIZATION

Performance optimization is:

Fair benchmarking

Workload characterization

Problem identification

Performance monitoring

Bottleneck elimination

Performance tuning

Benchmarking tips

- Be objective
- Be in control
 - Especially: PIN YOUR JOBS (CPU and memory)
- Choose representative, stable, correct benchmarks
- Choose good metrics
 - Throughput, latency, scalability, etc...
- Repeatability
- Keep a log

Benchmarking control

- Benchmarking a modern PC has become a complex issue:
 - CPU frequency
 - Number of cores
 - Number and configuration of sockets
 - Vector and floating point usage
 - Cache
 - Memory size and layout
 - BIOS and firmware version
 - Hardware threading on or off
 - Turbo mode on or off
 - Power consumption
 - Virtualization
 - Operating system version, kernel, libraries
 - Compiler version and flags
 - Pinning to cores and to NUMA memory

Tuning – reality check

Level	Potential gains	Estimate		
Algorithm	Major	~10x-1000x		
Source code	Medium	~1x-10x		
Compiler level	Medium-Low	~10%-20% (more possible with autovec or parallelization)		
Operating system	Low	~5-20%		
Hardware	Medium	~10%-30%		

Performance monitoring



Measuring performance

- The most common performance measurement unit is time
 - Wall clock time "how long do I have to wait for it to be done?"
 - CPU time "for how long is the computer busy?"
 - Latency "how long do I have to wait to get an answer?"
 - Throughput "how much of X in a period of time?"
- Minimizing time/latency is not the same as maximizing throughput
 - and vice versa i.e. see Amdahl's and Gustafson's laws
- 1 second: 9,192,631,770 periods of specific radiation of ¹³³Cs
 - 1 second is just 1 event, composed of individual events (oscillations)
- What if there could be a different "event" to define performance? Or a whole set of them?

An OS abuses your trust

- 100% CPU utilization in "top"? Awesome.
 Aren't we done here?
- Maybe not:
 - Spinlocks
 - Pointless iterations
 - Floating point side effects
 - Memory traffic
 - etc etc
- Use performance counters to obtain an accurate image

Performance monitoring in hardware

- Most modern CPUs are able to provide real-time statistics concerning executed instructions via a Performance Monitoring Unit (PMU)
- The PMU is spying in real time on your application (and everything else that goes through the CPU)
- Limited number of "sentries" (counters) available, but they are versatile
- Counters monitor events as they happen
- Recorded occurrences are called samples or counts
- Typically on modern Intel CPUs:
 - 2-4 universal counters per HW thread: #0, #1 (#2, #3)
 - 3 specialized counters: #16, #17, #18
 - Additional 8 "uncore" counters

Performance events

- Many events in the CPU can be monitored
 - A comprehensive list is dependent on the CPU and can be extracted from the manufacturer's manuals or from relevant tools
 - Examples: cache misses, instructions, cycles, loads, vector ops
- On some CPUs (e.g. Intel Core), some events have bitmasks which limit their range, called "unit masks" or "umasks"
 - Example: instructions retired: "ALL" or "only LOAD" or "only STORE"
- Extensive information: Intel Manual 248966-023a
 - Intel Manual 248966-023a "Intel 64 and IA-32 Architectures Optimization Reference Manual"
- AMD CPU-specific manuals
 - i.e. "BIOS and Kernel Developer's Guide for AMD Family 10h
 Processors" or "Software Optimization Guide For AMD Family 10h and 12h Processors"

The CPI figure and its meaning

- CPI cycles per instruction
 - Thanks to multiple execution ports (superscalar architecture), more than one instruction can be executed per cycle
 - In modern Intel CPUs, CPI can go as low as 0.25 = 4 instructions per cycle
 - CPI above 1.0 is generally not impressive
- The ratio of the number of CPU cycles spent on a program to the number of program instructions retired by the CPU
 - CYCLES / INSTRUCTIONS
- Lower CPI often means better efficiency
 - This figure illustrates the CPU usage efficiency in an indirect way, and, like all ratios, can be tricky to interpret

Simple CPI demo

1.25



instructions

Simple cache miss demo

- 50 cycles of work (incl. L1 consultations/misses)
- 50 cycles of work with one L2 cache miss
- 50 cycles of no work



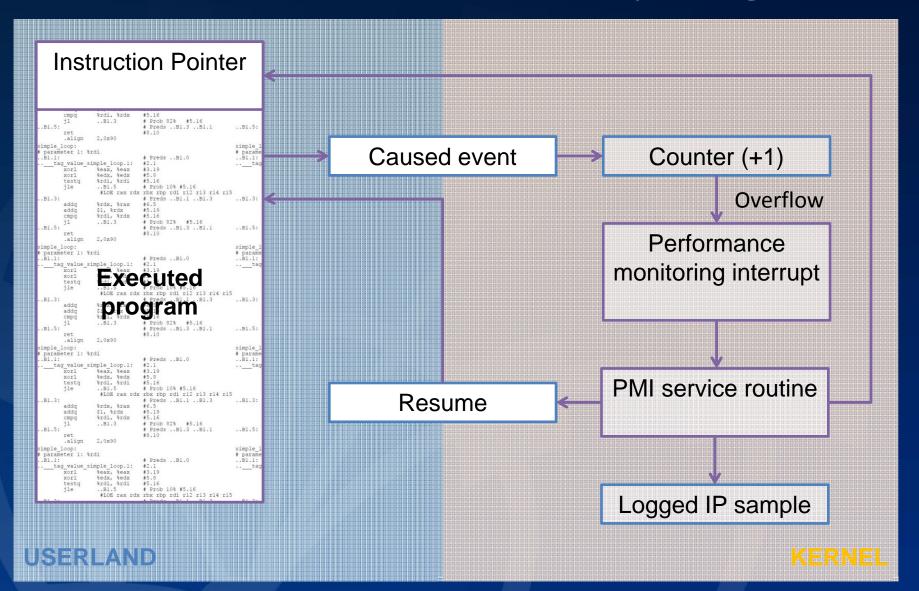
Assuming 20% of the instructions are loads and 3% of L2 misses...

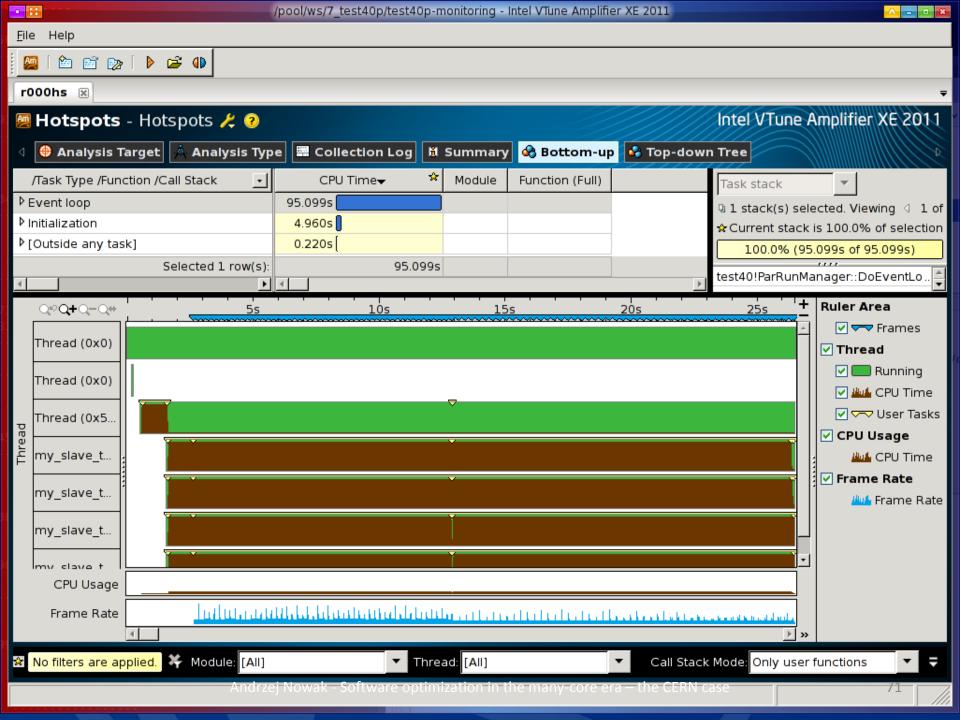
~35% cycles wasted, program runs ~60% slower!

False Sharing

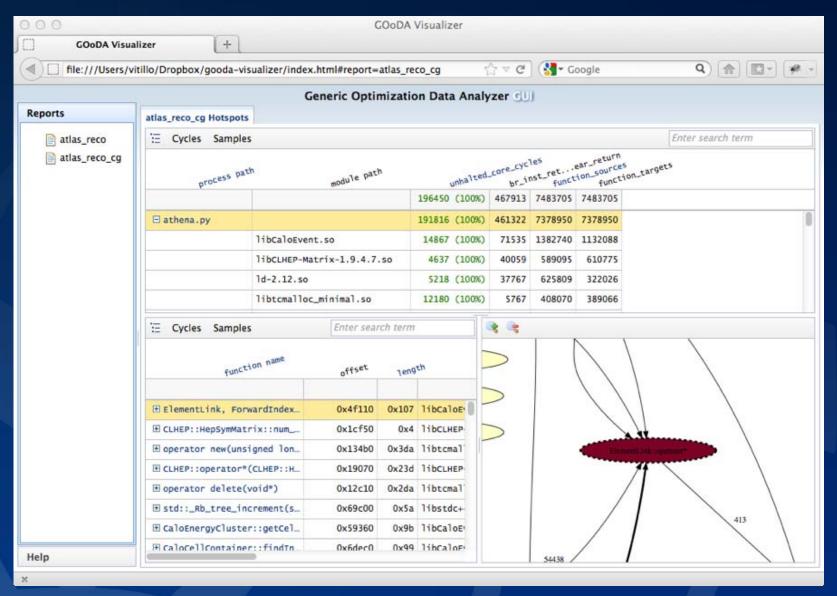


Event Based Sampling





Google GOODA



Optimization tips (1)

Unimpressive CPI / stalls

- Doing too many operations?
- Large latency instructions in the code?
- Using vector instructions?
- Do a stall analysis to see where and why you're stalling

Cache misses, false sharing

- Memory access characteristics
- Data structures and their layout
- Does your program fit in the cache?
- Help the hardware prefetcher!
- Do a cache analysis to see which data (and where) is not serviced properly

Optimization tips (2)

Many mispredicted branches

- Is there a way to restructure the code?
- Is there a way to make the "ifs" more predictable?
- Rearranging conditions and loops
- Too many jumps / function calls?
- Sample with branch events (e.g. in perfmon2 or PTU) to locate offending pieces of code

Excessive floating point operations

- Does everything need to be calculated?
- Are you running in loops?
- Could some results be reused?
- Do you really need that much precision?

Additional tips

Pay special attention to memory access patterns

- How does your programming language, compiler and allocator lay out your structures and variables? Is it better to leak or to "free()"?
- What is the temporal and spatial locality of your data?
 - Temporal locality: accesses to the same data in a short time frame
 - Spatial locality: accesses to nearby data in a short time frame
- Consider your memory usage model
 - Data set
 - Data organization
 - Data access patterns
- This area will only grow in complexity in the upcoming years

The Pareto (80/20) principle

- Sometimes adapted to "90/10"
- Might suggest that improving 20% of code will give you 80% of your results
- Might also suggest that 90% of the time is spent in 10% of the code Is it true for large applications with their C++ fragmentation and large codebases?

Relating to design

- Choose best available algorithms
 - Re-implementing an algorithm is usually the last thing you will want to do when "it" finally works
- Choose the appropriate programming language
 - Managed and VM languages are not performance friendly; optimizing properly is often impossible
 - Common tradeoff: an object oriented language values form over performance, and C or Fortran the other way around
- Make informed decisions. The optimal method of doing something isn't always the fastest one, but you need to know why

Common misconceptions

On hardware

- Myth: "Performance is a hardware issue"
- Reality: See the slides on Moore's Law

On responsibility

- Myth: "Performance should be handled by the compiler and libraries"
- Reality: no compiler and libraries will fix poorly written code (remember the elephant)

On premature optimization

- Myth: "Premature optimization is the root of all evil"
- Reality: an often misunderstood quote, referring to not optimizing bottlenecks that are not yet apparent – not to "any optimization" as a whole

On "GOTO programming"

- Myth: GOTO programming is entirely bad
- Reality: It's a tradeoff see the assembly "jmp" instruction

True pitfalls

- The rule of diminishing returns
 - The amount of benefits that you can get with a relatively small effort is limited; each additional investment will yield less results
- Not knowing your limits and not knowing when to stop
- Over-optimization can do damage
 - Especially if you optimize for a certain processor family: consider placing highly optimized routines in CPU-specific libraries
- Double-check your results
 - Flukes aren't common they're frequent! Consider this talk for an idea of the hardware complexity you have to deal with
- Wrong or overlapping optimizations can do damage
 - Optimize when the time is right, but design with optimization in mind
 - Premature micro-optimizations (of unquantifiable benefit) can reduce the readability / comprehension / maintainability of the code and threaten correctness
 - DO NOT wait until the end of the project to optimize
- Under-optimization is not worth the time
 - Do it right and remember that the penalty for abandoning the benefits of new platforms or techniques can be very high!

Tuning summary

Get the right tools for the job

Master the 7 performance dimensions

Scalable designs and high performance are friends

PART 5: FUTURE CHALLENGES

The CERN openlab

A unique research partnership of CERN and the industry Objective: The advancement of cutting-edge computing solutions to be used by the worldwide LHC community

- Partners support manpower and equipment in dedicated competence centers
- openlab delivers published research and evaluations based on partners' solutions – in a very challenging setting
- Created robust hands-on training program in various computing topics, including international computing schools; Summer Student program
- Past involvement: Enterasys Networks, IBM, Voltaire, F-secure, Stonesoft, EDS; Future involvement: Huawei
- Now in phase IV: 2012-2014

http://cern.ch/openlab



The Platform Competence Center

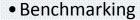
Focus on efficient computing

Technology monitoring



- Analysis
- Forecasting

Research and experimentation



- Parallelization
- Optimization

Results and dissemination

- Recommendations
- Papers, conferences
- Education

Close collaboration with the Physics department at CERN

PCC - particular interests

- Compute optimization
 - Absolute, per CHF, per Watt
 - Optimization tools
- Compilers
- Parallelization
 - x86 compatible technologies spanning the whole range from OpenCL to MPI
- Accelerators
 - Intel MIC, limited interest in GPUs, combos
- Storage
- Next phase V in 2015-2018 (Exascale era)

Intel MIC at openlab

Early access

- Work since MIC alpha (under RS-NDA)
- ISA reviews in 2008

Results

 3 benchmarks ported from Xeon and delivering results: ROOT, Geant4, ALICE HLT trackfitter

Expertise

- Understood and compared with Xeon
- Post-launch dissemination

MTG4 on MIC – example profile

Function / Call Stack	CLK %	INST %
sqrt	14.35%	22.16%
ехр	6.47%	9.47%
atan2	4.22%	6.31%
CLHEP::RanluxEngine::flat	3.24%	5.60%
G4ElasticHadrNucleusHE::HadronNucleusQ2_2	3.01%	2.41%
G4PhysicsVector::Value	2.76%	0.95%
log	2.22%	2.85%
G4VoxelNavigation::LevelLocate	2.05%	0.66%
G4VoxelNavigation::ComputeStep	1.64%	1.10%
G4ClassicalRK4::DumbStepper	1.59%	2.96%
G4SteppingManager::DefinePhysicalStepLength	1.54%	1.39%
G4Navigator::ComputeStep	1.40%	1.01%

Teaching

- International computing schools
- Workshops
 - 10 workshops in 2012
 - >350 participants





ICE-DIP

- EU Framework Program 7 project looking for (amongst other things) efficient methods of accelerator/co-processor use
- Focus on data taking past 2016
- Of particular interest
 - Getting data into the platform
 - Getting data into the accelerator/co-processor
 - Efficient processing
 - Efficient distribution of results
- What role for software?
- Are you interested?
 We will employ 5 PhD students to work on Si Photonics, FPGAs, networks, many-core

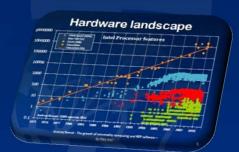


Possible future directions

- Software replacing hardware
 - Programmability replaces rigid structures
- Intensive compute
 - Local farms must have much higher processing capacity
- Accelerators
 - Experiments with Intel MIC and GPUs
- Silicon photonics







THANK YOU Q & A



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