

MAQAO Performance Analysis and Optimization Framework

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http://maqao.exascale-computing.eu



Performance Analysis and Optimisation

- Where is the application spending most execution time and resources?
- Why is the application spending time there?
 - Algorithm, implementation, runtime or hardware?
 - Data access or computation?
- **How much** of an application can be optimised?
 - What would the effort/gain ratio be?
- **How** to improve the situation?
 - At which step(s) of the design process?
 - What additional information is needed?





- **Pinpointing** the performance bottlenecks
- Identifying the dominant issues
 - Algorithms, implementation, parallelisation, ...
- Making the **best use** of the machine features
 - Complex multicore and manycore CPUs
 - Complex memory hierarchy
- Finding the most rewarding issues to be fixed
 - 40% total time, expected 10% speedup
 - → TOTAL IMPACT: 4% speedup
 - 20% total time, expected 50% speedup
 - → TOTAL IMPACT: **10%** speedup

=> Need for dedicated and complementary tools









Code of a loop representing ~10% walltime



Source code and associated issues:

- 1) High number of statements
- 2) Non-unit stride accesses
- 3) Indirect accesses
- 4) DIV/SQRT
- 5) Reductions
- 6) Variable number of iterations



MAQAO: Modular Assembly Quality Analyzer and Optimizer

- Objectives:
 - Characterizing performance of HPC applications
 - Guiding users through optimization process
 - Estimating return of investment (R.O.I.)



- Characteristics:
 - Modular tool offering complementary views
 - Support for Intel x86-64, Xeon Phi and AArch64 (beta version)
 - LGPL3 Open Source software
 - Developed at UVSQ since 2004
 - Binary release available as static executable



- MAQAO website: <u>maqao.exascale-computing.eu</u>
 - Mirror: <u>www.maqao.org</u>
- Documentation: <u>maqao.exascale-computing.eu/documentation.html</u>
 - Tutorials for ONE View, LProf and CQA
 - Lua API documentation
- Latest release: <u>maqao.exascale-computing.eu/downloads.html</u>
 - Binary releases (2-3 per year)
 - Core sources
- Publications: <u>maqao.exascale-computing.eu/publications.html</u>



Success stories: Optimisation of Industrial and Academic HPC Applications

- QMC=CHEM (IRSAMC)
 - Quantum chemistry
 - Speedup: > 3x
 - Moved invocation of function with identical parameters out of loop body
- Yales2 (CORIA)
 - Computational fluid dynamics
 - Speedup: up to 2,8x
 - Removed double structure indirections
- Polaris (CEA)
 - Molecular dynamics
 - Speedup: 1,5x 1,7x
 - Enforced loop vectorisation through compiler directives
- AVBP (CERFACS)
 - Computational fluid dynamics
 - Speedup: 1,08x 1,17x
 - Replaced division with multiplication by reciprocal
 - Complete unrolling of loops with small number of iterations
- Ongoing effort
 - TREX CoE project codes
 - CEA DAM codes







Partnerships

 MAQAO was funded by UVSQ, Intel (2005-2020) and CEA (French department of energy) through Exascale Computing Research (ECR) and the French Ministry of Industry through various FUI/ITEA projects (H4H, COLOC, PerfCloud, ELCI, MB3, etc...)







- Provides core technology to be integrated with other tools:
 - TAU performance tools with MADRAS patcher through MIL (MAQAO Instrumentation Language)
 - ATOS bullxprof with MADRAS through MIL
 - Intel Advisor
 - INRIA Bordeaux HWLOC
- PeXL ISV also contributes to MAQAO:
 - Commercial performance optimization expertise
 - Training and software development
 - <u>www.pexl.eu</u>





MAQAO Team and Collaborators

MAQAO Team

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- Advantages of binary analysis: What You Analyse Is What You Run
- Issues binary analysis addresses:
 - Compiler optimizations increase the distance between the executed code and the source code
 - Source code instrumentation may prevent the compiler from applying certain transformations
- Main steps:
 - Construct high level structures (CFG, DDG, SSA, ...)
 - Relate the analyses to source code using debug information
 - A single source loop can be compiled as multiple assembly loops
 - Affecting unique identifiers to loops





- Binary layer
 - Builds internal representation from binary
 - Allows patching through binary rewriting
- Profiling
 - LProf: Lightweight sampling-based Profiler
 - VProf: Instrumentation-based Value Profiler
- Static analysis
 - CQA (Code Quality Analyzer): Evaluates the quality of the binary code and offers hints for improving it
 - UFS (Uops Flow Simulator): Cycle-accurate CPU engine simulator
- Dynamic analysis
 - DECAN (DECremental Analyzer): Modifies the application to evaluate the impact of groups of instructions on performance
- Performance view aggregation module
 - ONE View: Invokes the modules and produces reports aggregating their results



MAQAO Main Structure





MAQAO Methodology

• Decision tree





SIMD/Vectorization/Data Parallelism

a[i] = b[i] + c[i]

- Scalar pattern (C):
- Vector pattern (FORTRAN): a(i, i + 8) = b(i, i + 8) + c(i, i + 8)
- Benefits : increases memory bandwidth and IPC
- Implementations:
 - x86 : SSE, AVX, AVX512
 - ARM : Neon, SVE
- FMA/MAC: (the core operation of LinAlg/DSP algorithms)
 - Fused-Multiply-Add
 - Multiply-Accumulate







Scalar addition



Vector addition

MAQAO Performance Analysis and Optimization Tool



Compiler optimisations

- Compiler flags:
 - Loop unrolling: -funroll-loops
 - Reduce branches
 - Fill the pipeline (more instructions per iteration)
 - Increases memory bandwidth and IPC
 - Function inlining: -finline-functions
 - Vectorization: -ftree-vectorize, -ftree-slp-vectorize, ...
 - Target micro-architectures: -march or -mtune or -xHOST
- Compiler directives:
 - OpenMP directives: #pragma omp simd, #pragma omp parallel for, ...
 - Intel compiler specific: #pragma simd, #pragma unroll, #pragma inline, ...
- Compiler/language keywords/features:
 - Using restrict for pointers aliasing in C/C++
 - Using inline for function inlining in C
 - Using array sections in FORTRAN



- Computations are, in general, faster than memory accesses
- Alignment/Contiguity of memory (x86) : posix_memalign, aligned_alloc, ...
- Are caches (L1, L2, L3) used properly?
- Memory performance \rightarrow Maximum bandwidth





MAQAO LProf: Lightweight Profiler

- **Goal**: Localization of application hotspots
- Features:
 - Lightweight
 - Sampling based
 - Access to hardware counters
 - Analysis at function and loop granularity
- Strengths:
 - Non intrusive: No recompilation necessary
 - Low overhead
 - Agnostic with regard to parallel runtime

ght-click on a line to display the associated load balancing. buble click on a loop to display its analysis details.					
Name	Module	Coverage (%)	Time (s)	Nb Threads	Deviat
 binvcrhs 	bt-mz.C.16	23.19	13.66	64	1.7
▼ y_solve	bt-mz.C.16	13.09	7.71	64	1.0
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▼ Loop 205 - y_solve.f:54-407 - bt-mz.C.16		12.84	7.56		
▼ Loop 207 - y_solve.f:54-398 - bt-mz.C.16		12.84	7.56		
 Loop 211 - y_solve.f:145-307 - bt-mz.C.16 		7.06	4.16		
 Loop 213 - y_solve.f:55-137 - bt-mz.C.16 		4.43	2.61		
 Loop 206 - y_solve.f:394-398 - bt-mz.C.16 		0.88	0.52		
 Loop 209 - y_solve.f:337-360 - bt-mz.C.16 		0.33	0.19		
 Loop 210 - y_solve.f:145-307 - bt-mz.C.16 		0.09	0.05		
 Loop 212 - y_solve.f:55-137 - bt-mz.C.16 		0.05	0.03		
x_solve	bt-mz.C.16	12.49	7.35	64	1.
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mp_into", int, int, int, void")					
• matmul_sub	bt-mz.C.16	11.95	7.04	64	0.
Z_Solve	bt-mz.C.16	8.03	4.73	64	0.
compute_rns	bt-mz.C.16	7.69	4.53	64	0.
matvec_sub	Dt-mz.C.16	3.33	1.96	64	0.
MPDI_CH3I_Progress	libmpi.so.12.0	1.85	1.09	16	1.
b binvins	bt-mz.C.16	0.49	0.29	64	0.
• institut	Dt-mz.C.16	0.45	0.26	64	0.
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sverat chark	SYSTEM CALL	0.14	0.08	64	0
	libiomp5 so	0.13	0.07	57	0
>	SYSTEM CALL	0.13	0.08	64	0
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• exact solution	ht-mz C 16	0.12	0.07	64	0.
update curr	SYSTEM CALL	0.12	0.07	64	0
audit syscall entry	SYSTEM CALL	0.12	0.07	64	0
schedule	SYSTEM CALL	0.12	0.07	63	0
task tick fair	SYSTEM CALL	0.1	0.06	64	0
• copy v face#omp loop 0	bt-mz.C.16	0.1	0.06	64	0
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- mer_powe_and	SYSTEM CALL	0.00	0.00	64	



MAQAO CQA: Code Quality Analyzer

- Goal: Assist developers in improving code performance
- Features:
 - Static analysis: no execution of the application
 - Allows cross-analysis of/on multiple architectures
 - Evaluate the **quality** of compiler generated code
 - Proposes hints and workarounds to improve quality / performance
 - Loop centric
 - In HPC loops cover most of the processing time
 - Targets compute-bound codes

Static Reports

CQA Report

The loop is defined in /tmp/NPB3.3.1-MZ/NPB3.3-MZ-MPI/BT-MZ/z_solve.f:415-423

▼ Path 1

2% of peak computational performance is used (0.77 out of 32.00 FLOP per cycle (GFLOPS @ 1GHz))

gain potential hint expert

Code clean check

Detected a slowdown caused by scalar integer instructions (typically used for address computation). By removing them, you can lower the cost of an iteration from 65.00 to 57.00 cycles (1.14x speedup). Workaround

- Try to reorganize arrays of structures to structures of arrays
- Consider to permute loops (see vectorization gain report)
- To reference allocatable arrays, use "allocatable" instead of "pointer" pointers or qualify them with the
 "contiguous" attribute (Fortran 2008)
- For structures, limit to one indirection. For example, use a_b%c instead of a%b%c with a_b set to a%b before this loop

Vectorization

Your loop is not vectorized. 8 data elements could be processed at once in vector registers. By vectorizing your loop, you can lower the cost of an iteration from 65.00 to 8.12 cycles (8.00x speedup).

Workaround

• Try another compiler or update/tune your current one

- use the vec-report option to understand why your loop was not vectorized. If "existence of vector dependences", try the IVDEP directive. If, using IVDEP, "vectorization possible but seems inefficient", try the VECTOR ALWAYS directive.
- Remove inter-iterations dependences from your loop and make it unit-stride:
 - If your arrays have 2 or more dimensions, check whether elements are accessed contiguously and, otherwise, try to permute loops accordingly: Fortran storage order is column-major: do i do j a(i,j) = b(i,j) (slow, non stride 1) => do i do j a(i,j) = b(i,j) (fast, stride 1)

Execution units bottlenecks

Found no such bottlenecks but see expert reports for more complex bottlenecks.



- Applications only exploit at best 5% to 10% of the peak performance
- Main elements of analysis:
 - Peak performance
 - Execution pipeline
 - Resources/Functional units



- Key performance levers for core level efficiency:
 - Vectorisation
 - Avoiding high latency instructions if possible (e.g. DIV/SQRT)
 - Guiding the compiler code optimisation
 - Reorganizing memory and data structures layout



- Compiler can be driven using flags, pragmas and keywords:
 - Ensuring full use of architecture capabilities (e.g. using flag -xHost on AVX capable machines)
 - Forcing optimization (unrolling, vectorization, alignment...)
 - Bypassing conservative behaviour when possible (e.g., 1/X precision)
- Hints for implementation changes
 - Improve data access patterns
 - Memory alignment
 - Loop interchange
 - Change loop stride
 - Reshaping arrays of structures
 - Avoid instructions with high latency (SQRT, DIV, GATHER, SCATTER, ...)



MAQAO CQA Advanced Features Vector Efficiency

- Ex: vectorized SSE code on AVX machine
- Compiler: "LOOP WAS VECTORIZED"
- In reality 50% vectorization speedup loss
- CQA:
- vectorization ratio: 100% ("all instructions vectorized")
- vec. efficiency ratio: 50% ("but using only half vector width")
- hint: "recompile with –xHost" (on Intel compilers)

128 bits	256 bits					
vectorized:	vectorized:					
<i>Vec. ratio = 100%</i>	<i>Vec. ratio = 100%</i>					
ADDPD (xmm)	VADDPD (ymm)					
MULPD (xmm)	VMULPD (ymm)					
etc	etc					
50%	100%					



MAQAO CQA Application to Motivating Example

Issues identified by CQA



CQA can detect and provide hints to resolve most of the identified issues:

- 1) High number of statements
- 2) Non-unit stride accesses
- 3) Indirect accesses
- 4) DIV/SQRT
- 5) Reductions
- 6) Variable number of iterations
- 7) Vector vs scalar



MAQAO CQA: Code Quality Analyzer Application to motivating example





- Goal: Automating the whole analysis process
 - Invoke multiple MAQAO modules
 - Generate aggregated performance views
 - Reports in HTML or XLS format





MAQAO ONE View: Performance View Aggregator

- Main steps:
 - Invokes LProf to identify hotspots
 - Invokes CQA and other modules on loop hotspots
- Available results:
 - Speedup predictions
 - Global code quality metrics
 - Hints for improving performance
 - Detailed analyses results
 - Parallel efficiency analysis

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tion C file	Aj ategoriz	ation	z, solve z, solve Functions	mp.f 5.7 mp.f 5.7 τ.	0.87	1126 Topology 055	1		8 10.1 10.1 10.1 0 8 3 3 8 3 8 4 4 6 8 8 8 8 8 8 8 8 8 8 8 8 4 4 8 10.67 7.2 8
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ioop cop ilobal izatic	Ar ategoriz	ation	z, zołwo	7 T		11.06	1		8 10.1 10.1 10.1 0 8 3 3 8 0 4 0 8 8 8 8 8 8 8 8 8 8 8 8 8



- ONE VIEW ONE
 - Requires a single run of the application
 - Profiling of the application using LProf
 - Static analysis using CQA
- ONE VIEW TWO (includes analyses from report ONE)
 - Requires 3 or 4 runs on average
 - Value profiling using VProf to identify loop iteration count
 - Decremental analysis for L1 projection using DECAN
- ONE VIEW THREE (includes analyses from report TWO)
 - Requires 20 to 30 runs
 - Decremental analyses using all DECAN variants
 - Collects hardware performance events
- Comparison mode
 - Comparison of multiple runs (iso-binary or iso-source)
 - Allows to evaluate scalability or compare performance across different datasets, compilers, or hardware platforms



- ONE View execution
- Provide all parameters necessary for executing the application
 - Parameters can be passed on the command line or as a configuration file

\$ maqao oneview -R1 ./myexe

\$ maqao oneview --create-report=one --executable=./myexe --mpi_command="mpirun -n 16"

\$ maqao oneview --create-report=one --config=my_config.lua"

- Analyses can be tweaked if necessary
- ONE View can reuse an existing experiment directory to perform further analyses
- Results available in HTML format by default
 - XLS spreadsheets and textual output generation are also available
- Online help is available:

```
$ maqao oneview --help
```



Analysing an application with MAQAO

MAQAO modules can be invoked separately for advanced analyses

- LProf
 - Profiling

\$ maqao lprof xp=exp_dir --mpi-command="mpirun -n 16" -- ./myexe

Display functions profile

\$ maqao lprof xp=exp_dir -df

Displaying the results from a ONE View run

\$ maqao lprof xp=oneview_xp_dir/lprof_npsu -df

• CQA

\$ maqao cqa loop=42 myexe

Online help is available:

\$ maqao lprof --help

\$ maqao cqa --help



Thanks for your attention

QUESTIONS ?

MAQAO Performance Analysis and Optimization Tool



NAVIGATING ONE VIEW REPORTS

MAQAO Performance Analysis and Optimization Tool



MAQAO ONE View Global Summary

- Experiment summary
 - Characteristics of the machine where the experiment took place
- Global metrics
 - General quality metrics derived from MAQAO analyses
 - Global speedup predictions
 - Speedup prediction depending on the number of vectorised loops
 - Ordered speedups to identify the loops to optimise in priority





- Global metrics
 - General quality metrics derived from MAQAO analyses
 - Global speedup predictions
- Potential speedups
 - Speedup prediction depending on the number of optimised loops
 - Ordered speedups to identify the loops to optimise in priority
- Global Speedup = $\sum_{loops} coverage * potential speedup$
- LProf provides coverage of the loops
- CQA and DECAN provide speedup estimation for loops
 - Speedup if loop vectorised or without address computation
 - All data in L1 cache



MAQAO ONE View: Functions Profiling

M Func

Identifying hotspots

- Exclusive coverage
- Load balancing across threads
- Loops nests by functions •



MA⊕AO Global	Application	Functions	Loops	Topology				
Functions and Loops								0
► Filters								?
	Name			Module	Coverage	Time (s)	Nb Threads	Deviation (coverage)
 gomp_team_barrier_wait_end binvcrhs z_solveomp_fn.0 matmul_sub V_Loop 114 - y_solve.f.4.398 - bt- Loop 115 - y_solve.f.4.398 - bt- Loop 116 - y_solve.f.4.398 - bt- Loop 116 - y_solve.f.4.398 - bt- Loop 117 - y_solve.f.4.398 - bt- Loop 116 - y_solve.f.334.33 Loop 117 - y_solve.f.337.36 x_solve_omp_fn.0 gomp_barrier_wait_end compute_rhsomp_fn.0 gomp_barrier_solve. binsint opal_progress coop_y_faceomp_fn.0 binvrhs ompi_coll.libnbc.progress copy_y_faceomp_fn.0 opal_timer_linux_get_cycles.sys_ exat_solution copy_r.faceomp_fn.3 copy_y_faceomp_fn.3 copy_y_faceomp_fn.3 	mz.C.16 ht-mz.C.16 J& -bt-mz.C.16 F - bt-mz.C.16 J& -bt-mz.C.16 o - bt-mz.C.16 ess			libgomp.so.1.0.0 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 libgomp.so.1.0.0 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16 bt-mz.C.16	(%) 21.34 16.06 9.84 9.52 9.99 9.88 8.82 8.82 8.85 1.77 0.12 8.68 8.62 2.73 0.54 0.35 0.335 0.335 0.335 0.13 0.13	3.26 2.45 1.5 1.45 1.35 1.35 0.89 0.27 0.02 1.32 1.26 1.16 0.55 0.42 0.08 0.06 0.05 0.05 0.05 0.05 0.04 0.02 0.02	64 64 64 64 64 64 64 16 64 64 16 64 64 16 64 16 64	(coverage) 4.47 1.10 0.68 0.68 0.68 0.68 0.68 0.68 0.68 0.6
o exat_rhsomp_fn.0 o opal_progress@plt ininitalizeomp_fn.0 o ompi.request_default_wait_all o gomp_thread_start Unknown kernel region most ween	Coverage 			y_solve	28104 282	50 2222		
	20102	20209 20283	20108	MAOAO thread rank	20104 282	20202	20200 281	~~



- Identifying loop hotspots
- Vectorisation information
- Potential speedups by optimisation
 - Clean: Removing address computations
 - FP Vectorised: Vectorising floating-point computations
 - Fully Vectorised: Vectorising floating-point computations and memory accesses

MA	AQAO	Global	Application	Functions	Loops	Topolog	ıy							
Show In	Show Innermost Profile Open Expert Summary													
Loop	Loops Index													
► Fi	▶ Filters									?				
	⊘Coverage (%) ②Level ⊘Time (s) ⊘Vectorization Ratio (%) ⊘Speedup If Clean ⊘Speedup If FP Vectorized ⊘Speedup If Fully Vectorized ⊘Speedup If Data in L1 □Select none													
Loc	Source	Location		Source Fur	oction		Coverage (%)	Level	Time (s)	Vectorization Ratio (%)	Speedup If Clean	Speedup If FP Vectorized	Speedup If Fully Vectorized	Speedup If Data in L1
184	D3 qmcpack:Mult	iBsplineValue.h	qmcplusplus::BsplineSet >::evaluate			26.71	Innermost	3.61	100	1	1	1	8.25	
260	27 gmcpack:cma	th:261-464	qmcplusplus::Sc	aDistanceTableAA:	:moveOnSphere		12.01	Single	1.62	100	1	1	1	1.03
184	24 qmcpack:Mult pp:187-207	iBsplineVGLH.h	ILH.h gmcplusplus::BsplineSet >::evaluate 10.81				10.81	Innermost	1.46	100	1.06	1	1	4.15
184	74 qmcpack:Mult pp:187-207	dmcpack:MultiBsplineVGLH.h qmcplusplus::BsplineSet >::evaluate_notranspose 4.84 Innermost 0.65 100 1.06 1 1 4						4.52						
260	26 qmcpack:cma	th:261-464	qmcplusplus::SoaDistanceTableAA::evaluate				2.78	Single	0.38	100	1	1	1	1.05
260	28 qmcpack:cma	th:261-464	qmcplusplus::SoaDistanceTableAA::move			2.64	Single	0.36	100	1	1	1	1.03	
875	4 qmcpack:Cou 425-427	lombPBCAA.cpp	qmcplusplus::CoulombPBCAA::evalSR			1.57	Innermost	0.21	0	1.64	2.59	7.67	1.01	
127	11 qmcpack:Bsp 0-695	ineFunctor.h:69	qmcplusplus::J2	OrbitalSoA >::ratio0	irad		1.41	Innermost	0.19	0	1.3	1	16	1.08
185	on dmcpack:Spli h:325-373	neC2RAdoptor.	void qmcpluspli ector, std::alloca	us::SplineC2RSoA::ator > > >	assign_vgl >, qmcplus	splus∷V	1.22	Single	0.16	100	1.01	1	1	3.51

MAQAO Performance Analysis and Optimization Tool



- Coverage per category
 - Comparison of categories for each run
- Coverage per parallel efficiency
 - $Efficiency = \frac{T_{sequential}}{T_{parallel*N_{threads}}}$
 - Distinguishing functions only represented in parallel or sequential
 - Displays efficiency by coverage

	pplication	Functio	ons Loop	ps Topol	ogy		
Application Categorization	? Sc	alability -	Coverage per (Category			
Scalability - Coverage per Category Scalability - Time per Category	2	100.000					
Scalability - Coverage per Parallel Efficien	сү 2	71.429					
Detailed Loop Based Profile	? (%) =	57.143			-		
	Coverag	42.857					
		28.571					
		14.286					
		0.000	1-1	1-2 Configuration	1-4 (Processes MPI - Three	1-8 ids OpenWP)	1-16





BACKUP SLIDES

MAQAO Performance Analysis and Optimization Tool

MAQAO History

- 2004: Begun development
 - Focusing on Intel Itanium architecture
 - Analysis of assembly files
- 2006: Transition to Intel x86-64
- 2009: Binary analysis support
 - First version of decremental analysis
- 2012: Support of KNC architecture
- 2014: Profiling features
- 2015: First version of ONE View
- 2017: Prototype support of ARM architecture
- 2018: Scalability mode
- 2020: Comparison mode
- 2022: Support of ARM (beta)



