

Benchmarks on Current (Dual Core) CPUs

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Application Performance

Turbulence simulation using the Lattice Boltzmann Method

Prof. Durst, Computational Fluid Dynamics FAU; P. Lammers, HLRS Teraflop-Workbench (Part of LRZ benchmark suite)

G. Wellein, P. Lammers, G. Hager, S. Donath, and Th. Zeiser, Proc. of ParCFD2005. Towards Optimal Performance for Lattice Boltzmann Applications on Terascale Computers

G. Wellein, T. Zeiser, G. Hager and S. Donath, to appear in Computer&Fluids. On the Single Processor Performance of Simple Lattice Boltzmann Kernels

Th. Pohl, F. Deserno, N. Thürey, U. Rüde, P. Lammers, G. Wellein, and T. Zeiser, in Proc. Supercomputing 2004, Pittsburgh, PA, 6.-12. Nov. 2004. *Performance Evaluation of Parallel Large-Scale Lattice Boltzmann Applications on Three Supercomputing Architectures*

TFlop/s Computing with LBM Introduction



- Performance evaluation/optimization of LBM application (BEST):
 - Fortran90
 - Push-Method (Collide-Stream) н.
 - Two Grids
 - MPI parallelisation
 - Variations:
 - Compressed Grid no performance gain
 - 1D-/3D-Blocking no performance gain
 - Temporal Blocking



A serial kernel was extracted for performance optimization

Parallel benchmark runs were done for turbulent channel flow



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TFlop/s Computing with LBM Code Structure





TFlop/s Computing with LBM Performance – Basics

- Performance unit: Mega Lattice Site Updates per Second (MLUPS)
- Per Lattice Site update we need:
 - ~ 170-250 Floating Point Ops. -> 5 MLUPS ~ 1 GFlop/s
 - ~ 40 (+20 write allocate) 8 byte transfers between CPU & Memory
- Estimate max. performance (200 Flops per Lattice Site):

	Peak Perf. [GFlop/s]	Max. MLUPS	Bandwidth [GByte/s]	Max. MLUPS	Measure 128 ³
Intel Xeon	6.8	34	5.3	11.8	5.1 (43%)
AMD Opteron	4.4	22	6.4	14.0	5.1 (36%)
Intel Itanium2	5.6	28	6.4	14.0	8.5 (61%)
CRAY X1	12.8	64	34.1	112	34.9 (55 %)
NEC SX6+	9.0	45	36.0	118	41.3 (92 %)

• Vector performance not limited by memory bandwidth!

• There is room for improvement on IA32 compatible & CRAY X1

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LBM Code tuning – Splitting innermost x-loop

- Splitting the innermost x loops in 3 separate x-loops
 - Increases number of floating point ops per lattice site (~250 Flop)
 - Increases Data transfer Cache CPU (intermediate results)
 - Reduces the pressure on the write combine buffers on IA32
 - Simplifies Instruction Scheduling for IA64

		Original	Tuned
Intel Xeon/Nocona	3.4 GHz	4.5 MLUPs	4.9 MLUPs
AMD Opteron848	2.2 GHz	2.9 MLUPs	4.7 MLUPs
AMD Opteron272*	2.2 GHz	3.6 MLUPs	5.8 MLUPs
PentiumD*	2.8 GHz	3.0 MLUPs	4.3 MLUPs
Intel Itanium2	1.4 GHz/1.5 MB L3	7.9 MLUPs	8.5 MLUPs

Dual Core Systems











• (I,J,K,0:18) best performance on all systems – except IBM Power5

• Manual fusing of the 3 spatial loops is essential on IBM Power5





LBM Scalability of SMP/ccNUMA nodes (OpenMP)

- Intel EM64T Compiler 8.1.024 (-O3 –xW): Intel & AMD
- Intel Xeon/Irwindale (3.6 GHz; 2 MB L2)
- IBM: Open Power720 (Power5): 4-fway; xlf90_r -qhot -O5 -qsmp=omp

LBM Scalability of Dual-Core CPUs (OpenMP)

Intel PentiumD: н.

- 1 socket; 2 cores (2.8 GHz, 1 MB L2)
- AMD Opteron272: н.
 - 2 sockets; 2 cores (2.2 GHz; 1 MB L2) (SUN V20Z)
- AMD Opteron875:
- 4 sockets; 2 cores (2.2 GHz; 1 MB L2) (transtec) 2 sockets; 2 cores (IBM Power5 1.65 GHz)
- OpenPower 720: (Performance in MLUPs)

	1 socket		2 sockets		4 sockets	
threads/ socket	1	2	1	2	1	2
PentiumD	4.3	6.3				
Opteron275	5.7	7.7	11.4	15.1		
Opteron875	5.6	7.3	10.9	14.5	21.1	27.9
OPower720	n.a.	n.a.	n.a.	13.2		

Speed-Up of 2nd core ~ 30%

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LBM Scalability of Dual-Core / SMP systems (OpenMP)

- AMD Opteron275:
- 2 sockets; 2 cores (2.2 GHz; 1 MB L2) (SUN V20Z)
 - 2 sockets; 2 cores (IBM Power5 1.65 GHz) OpenPower 720: (Performance in MLUPs)

	Clock	Bandwidth	1 thread	2 threads	4 threads
Intel Prestonia	2.66 GHz	4.2 GB/s	2.6	3.0	
Intel Nocona	3.4 GHz	5.3 GB/s	4.8	5.5	
Intel Irwindale	3.6 GHz	5.3 GB/s	5.0	6.0	
PentiumD	2.8 GHz	6.4 GB/s	4.3	6.3	
Opteron275	2.2 GHz	12.8 GB/s	5.7	7.7	15.1
OPower720	1.65 GHz	~20 GB/s	n.a.	n.a.	13.2

LBM Remote Memory access via ccNUMA

- **FFZE**
- Place data and compute thread on different nodes to measure the potential of the ccNUMA interconnect

```
taskset -c i numactl -m k ./lbmkernel
i=0 N 1:k=0 (N /2) 1
```

- i=0,...,N_{CPU}-1 ; k=0,...,(N_{CPU}/2) -1
- AMD Opteron275 (SUN V20z): HT-1000 (4 GB/s per direction)
- AMD Opteron848 (4-way)
- SGI Altix3700 Bx2 (32-way): NUMALink4 (3.2 GB/s per direction)

	-m 0	-m 1	-m 2	-m 3
AMD 275	5.8	4.6		
AMD 848	4.7	4.0	4.0	3.5
Altix	7.9	6.0	5.5 (-m 7)	5.5 (-m 15)

TFlop/s Computing with LBM Parallel Performance - Basics

 Strong Scaling: Total problem size (e.g. N³) is fixed. Amdahl's law limits speed-up (s: Serial fraction; P: processors)

 Weak Scaling: Total problem size (e.g. N³) increases linearly with processor count (Gustafsson`s law)
 S_P = S + (1-S) * P

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HPC

New LRZ system >1.25 GFlop/s per CPU -> Total performance > 6 TFlop/s VK HLRS/RRZE/ZIH 20.10.2005

HPC

Plenty of bandwidth within the node - Scales perfectly

1 node (8 CPUs) ~ 13 GFlop/s ~ 10 SGI Altix CPUs

Large gap between theoretical and sustainable bandwidth on IBM systems...

TFlop/s Computing with LBM: Weak Scaling: Vector vs. the rest of the world ?!

Vector systems are still a class of their own for LBM codes

Full HLRS system (576 SX8-CPUs): 32.000 MLUPS (5.5 TFlop/s)

Assuming weak scaling, this is equivalent to

 Cluster of ~ 7.000 AMD Opteron 	[12:1]
• ~14.000 Intel Xeon CPUs	[24:1]
	F4.4.41

- SGI Altix with ~6.500 Intel Itanium2 CPUs [11:1]
- IBM BG/L with ~ 32.000 CPUs (cf. next slide) [60:1]

So far "microprocessor/-friendly" test case has been considered (empty channel):

- No indirect addressing
- Contiguous memory access

LBM application performance: Price Performance

CPUs MLUPS Performance Price (K€) MLUPS/K€ **NEC SX8** 1 66.8 11.8 GFlop/s (74%) 50 1.34 1 Opteron 2.4GHz/IB 4.3 1.1 GFlop/s (23 %) 2.2 GFlop/s (23 %) Opteron 2.4GHz/IB 2 8.5 6 1.42 Xeon 3.2 GHz/IB 1 4.7 1.2 GFlop/s (19 %) Xeon 3.2 GHz/IB 2 4.8 1.2 GFlop/s (10 %) 4.5 1.07 1 SGI Altix/1.6 GHz 8.3 2.1 GFlop/s (33 %) SGI Altix/1.6 GHz 2 9.7 2.4 GFlop/s (19 %) 10 0.97 IBM BG/L 2 ~2* ~0.5 GFlop/s (9%) ?? ??

1 NEC SX8 CPU ~ 60 BG/L CPUs

* Own estimation based on Read/Modify/write bandwidth of 1 BG/L CPU ~ 0.5 Opteron (cf. "A Performance and Scalability Analysis of the BlueGene/L Architecture", K. Davis et al. Proc. SC2004)

C

Application LESOCC from TFlops-Workbench: Method

- LESOCC (Large Eddy Simulation On Curvilinear Coordinates)
- Navier-Stokes solver (incompressible fluid)
- 3-D finite volume approach
 - Curvilinear body-fitted coordinate system
 - Non-staggered (cell-centered) grid arrangement
 - Block-structured grids
- Spatial discretization
 - Viscous fluxes: central differences
 - Convective fluxes: five different schemes, central diff. CDS-2
- Temporal discretization
 - Predictor step (moment. eqns.): low-storage Runge-Kutta scheme, O(Δt²)
 - Corrector step (pressure correction equation): SIP solver (ILU)
- Pressure-velocity coupling: Momentum interpolation of Rhie & Chow
- High-performance computing techniques
 - Highly vectorized
 - Parallelized by domain decomposition and explicit message passing
 - Vector-parallel computers and SMP-clusters (Hitachi, NEC-SX, SR8k-F1)

By courtesy of PD Dr. Breuer, LSTM

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Application performance LESOCC

- LESOCC is being used for more than 10 years
- SIP solver vectorization in 1980's

Sustained performance of LESOCC over time (qualitative numbers)
NEC SX-4: 1 GFlop/s (50% Peak)

- Fujitsu VPP 700 (1996-2004): 0.92 GFlop/s (41% Peak)
- Itanium2 (1.3 GHz) (2003-2008): 1 CPU of VPP 700
- Intel Xeon (2.66 GHz): ~0.5 GFlop/s
- Hitachi SR 8000 (1 node):
- Hitachi SR 8000 (16 node): 41 GFlop/s (Parallel Eff.: ~86%)

3 GFlop/s

First Measurements on NEC SX6+ / SX8 (simple test case)

- NEC SX6+ (1 CPU): 4.7 GFlop/s Same Executable: Speed-Up ~ 1.77
- NEC SX8 (1 CPU): 8.3 GFlop/s 🞺

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CFD kernel: SIP-Solver

(Part of LRZ benchmark suite)

 Solving A x = b for finite volume methods can be done by Strongly-Implicit-Procedure (SIP) according to Stone

SIP-solver is widely used:

- LESOCC, FASTEST, FLOWSI (Institute of Fluid Mechanics, Erlangen)
- STHAMAS3D (Crystal Growth Laboratory, Erlangen)
- CADiP (Theoret. Thermodynamics & Transport Processes, Bayreuth)
- SIP-Solver: 1) Incomplete LU-factorization
 2) Series of forward/backward substitutions
- Basic toy program available at: ftp.springer.de in /pub/technik/peric (M. Peric)
- Highly Optimized kernels for various architectures

CFD kernel: SIP-solver Data-dependencies & Implementations

- Data-locality (Caches !)
- Shared memory parallelization: Pipeline parallel processing
- Comp. intensity: 1.3 Flop/Word -> Max. Performance: 1 GFlop/s at 6.4 GByte/s bandwidth

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SIP-solver: Resolving Data Dependencies With Hyperplanes

Define Hyperplane: i+j+k=const

- non-contiguous memory access
- shared memory parallelization /vectorization of innermost loop

do l=1,hyperplanes n=ICL(1) do m=n+1,n+LM(1) ijk=IJKV(m) RES(ijk)=(RES(ijk)-\$ LB(ijk)*RES(ijk-ijMax)-\$ LW(ijk)*RES(ijk-1)-\$ LS(ijk)*RES(ijk-1)-\$ \$ *LP(ijk) enddo

enddo

CFD kernel: SIP-solver Data-dependencies & Implementations

It's hard to reproduce these numbers on production systems

CFD kernel: SIP-solver Pipeline Parallel Processing

- Split up j-loop in chunks of equal size for each thread
- Split up k-direction in blocks of equal chunks
- Pipelining in k-direction: Only one k-Index is active at a fixed time
- Efficient parallelisation if kMax, jMax >> #Threads

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CFD kernel: SIP-solver Pipeline Parallel Processing using OpenMP

CFD kernel: SIP-solver Pipeline Parallel Processing using OpenMP

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Application Performance

Density Matrix Renormalization Group computations for Highly Correlated Quantum Systems

Prof. H. Fehske, Theoretical Physics, Univ. Greifswald Dipl. Phys. G. Hager, Dr. G. Wellein, RRZE, Erlangen

(Part of LRZ benchmark suite)

G. Hager, E. Jeckelmann, H. Fehske, and G. Wellein, J. Comp. Phys., 194-2, 795-808 (2004). Parallelization strategies for density-matrix renormalization group algorithms on shared-memory systems

Quantum Physics Application: DMRG (C++ & OpenMP)

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Quantum Physics Application: DMRG (C++ & OpenMP)

OpenPower 720

Excerpts from RRZE benchmark report

G. Hager, T. Zeiser, G. Wellein RRZE

OpenPower 720 triads - serial

GHz)

OpenPower 720 triads - OpenMP

OpenPower 720 triads – NUMA effects

OpenPower 720 triads – architectures

Aktuelle Experimente mit Compilern

G. Hager RRZE

Compilerversionen im Einsatz am RRZE

- Intel 9.0-02X + 8.1-02X auf IA32/EM64T/x86_64/IA64
 - stabile Situation, wenig Bugs
 - Probleme mit Optimierungen unter OpenMP (nur bei C++?)
- PGI 6.0-5
 - Unter OpenMP besser als IA64-Compiler aber schlechter als EM64T-Compiler
- Pathscale 2.2.1
 - Testlizenz mittlerweile abgelaufen, Beschaffung läuft
 - gut bei Standard-Code, schlägt sich gut bei OpenMP
 - etwas buggy, Abhängigkeit von GCC
- MIPSPro 7.41 (IRIX/MIPS)
 - einfach nur cool.
- Stepanov-Test?

cx HPC

C++-Triade mit STL und OpenMP

V1


```
#pragma omp parallel for schedule(static)
for(i=0; i<len; ++i)
        a[i] = b[i] + c[i] * d[i];
...</pre>
```

vector<double>::iterator ai = a.begin(); vector<double>::const_iterator bi = b.begin();

```
V2 ···
#pragma omp parallel for schedule(static)
for(i=0; i<len; ++i)
    ai[i] = bi[i] + ci[i] * di[i];</pre>
```

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C++-Triade: Penalties (out of cache)

	STL + operator[]	STL + iterator	STL + operator[] + OMP (V1)	STL + iterator + OMP (V2)	double[] + OMP
Intel V9 IA64*	0.50	0.99	0.25	0.28	0.98
Intel V9 EM64T	0.78	0.80	0.64	0.79	1.00
PGI x86_64	0.53	0.90	0.47	0.68	0.79
Pathscale x86_64 [§]	0.87	0.87	0.81	0.87	1.00
MIPSPro MIPS	0.78	1.00	0.84	0.95	1.00

* #pragma ivdep vor Schleife verhindert OMP-Parallelisierung

§

Probleme


```
Pathscale 2.2.1 (Forts.): In class NUMA_Allocator<T>:
pointer allocate(size_type numObjects, const void *lh=0) {
       size_type ofs,len = numObjects * sizeof(value_type);
       void *m = malloc(len); char *p = static cast<char*>(m);
 25
 26
       int i,pages = len >> PAGE_BITS;
 27 #pragma omp parallel for schedule(static) private(ofs)
       for(i=0; i<pages; ++i) {</pre>
 28
         ofs = static_cast<size_t>(i) << PAGE_BITS;</pre>
 29
 30
         p[ofs]=0;
       }
 31
       return static_cast<pointer>(m);
     }
  GCC 3.3: nalloc.h: In member function `T*
            NUMA_Allocator<T>::allocate(long unsigned int,
               const void*)':
            nalloc.h:26: error: parse error before `;' token
            nalloc.h:27: error: parse error before `;' token
  GCC 3.4: kein Problem!
```


Experience with the latest VTune releases

T. Zeiser, G. Hager RRZE

Intel VTune

- Released versions
 - Intel VTune 3.0 Linux
 - Command line version (CLI)
 - Command line version with GUI
 - Eclipse GUI (only 32-bit)
 - Intel VTune 7.2 Windows
 - Native for MS Windows
 - Remote data collection (RDC) => Linux
- New beta version
 - Intel VTune 8.0 beta Linux (beta program: 08/2005...12/2005)
 - Command line version (CLI)
 - Command line version with GUI
 - Eclipse GUI (only 32-bit)
 - Remote data collection (RDC with access control)
- VTune = Linux kernel module + database services + user tools

Intel VTune 3.0 / 7.2

- Kernel modules and modules compatible between Windows and Linux versions
- Updated versions of the kernel modules unofficially available
- Only very limited support for kernel 2.6
- No access control for RDC; port 50000 open for everybody
- Typical problems:
 - Modules (programs) not found => Other32/Other64
 - Source code information not found
 - Severe dependence on kernel, glibc, compiler, ... versions

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New features of Intel VTune 8.0 beta Linux

- Better support for kernel 2.6
- Access control now supported for RDC (via PAM)

Typical problems:

- Still sometimes modules (programs) not found => Other32/Other64
- Still some dependence on compiler versions
- Iocale must have appropriate value, i.e. "C" instead of iso*/*UFT*
- => otherwise sometimes segfault or similar non-specific errors when running user commands
- CLI sensitive to certain stacksize limits
- Parallel installation of Linux beta and old Windows-compatible RDC possible but requires much manual activity during installation
- General remarks
 - Eclipse GUI still not usable (slow, unstable, ...)
 - Collected data must be stored on a local directory not NFS

