

Maximizing performance in HPC computations

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Parallel performance - models and metrics

23.11.2015

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About me:

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About me:

- Maya Neytcheva Sofia University, University of Nijmegen, Uppsala University
- Background: Mathematical modelling
 Work experience: Design and implementation of information
- systems Interests: Iterative solution methods, preconditioning, optimal solution methods, PDEs, parallelization, parallel performance PhD thesis: 'Arithmetic and communication complexity of preconditioning methods', 1995, University of Nijmegen, The Netherlands

About you:



Research areas, represented in the group

- Groundstate of anti-ferromagnetic spin chains (Hylke Donker)
 - Cosmology (Adri Duivenvoorden)
 Beam-forming prediction for millimeter wave based on
- Beam-forming prediction for millimeter wave based on 3D simulation (Joo Gante
 - Using HPC solutions to attain real time advanced medical imaging ultrasound techniques (Joao Amaro)
 - Computer assisted image analysis (Sajith Sadanandan)
- Energy efficiency data communication with participatory sensing (Peramanathan Sathyamoorthy)
- Cut Finite Element methods for multiphase flow simulations (Thomas Frachon)
- Computer architecture, cache modeling (Moncef Mechri)
- Algorithms for the nonlinear eigenvalue problem (Giampaolo Mele)
- Data mining and recognition of historical handwritten documents (Tomas Wilkinson)
 - Computer architecture / Distributed shared memory / Coherence mechanisms (Magnus Noren)
- ୧୦୧୯ μų Large scale electronic structure calculations (Anastasia Aruchina *

About performing computer simulations/analysis:

Performing computer simulations sequential computing parallel computing data structures programing languages Solution method Num.lin.algebra: which method matrix properties data structure mputer V Num. discretization Finite diff Finite volume Boundary elements Wathematical model A set of ODEs/PDEs Integral equations Something else R Physical pheno Z

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Performing computer simulations





Performing computer simulations





Performing computer simulations: NLA





Performing computer simulations: strategy





Performing computer simulations:

implementation issues



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Parallel performance issues

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Plan of the presentation:

- Parallel performance
- Parallel performance metrics
 - time overhead
 - speedup cost
 - efficiency
 scalability
- scalability Devollet anuforment
- Parallel performance models
 Commission communication communi
- Computational and communication complexity of algorithms
 - Examples: non-optimal optimal algorithms
 - Energy efficiency models and metrics
 - Summary. Tendencies



- Parallel performance
- Parallel performance metrics
- time
 - speedup
- efficiency
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The setting:

We need to solve a problem in parallel, and as fast as possible! Several questions arise:
 There is more than one algorithm (method) which does the job. Which one to choose?

- Can we in advance (a priori) predict the performance?
- How much does the a priori estimate depend on the computer platform?
 On the implementation?
 On the compiler?
- On the MPI/OpenMP/Pthreads implementation/Cache discipline/...?
- Can we do a posteriori analysis of the observed performance? How?
- \bullet Did we do a good job? Compare what others have done always a good idea, but how to do this?
- We have to write a paper. How to present the parallel results? Why take up this issue?
- The computers change all the time, how this affect the software counterpart?

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Parallel performance

- We follow the historical development in the HPC area.
- However, a significant shift has taken place from single core to multi/many core and from homogeneous to heterogeneous computer architectures.

Are the classical approaches to view performance relevant on the new computer architectures? Computational and communication complexity: the classical approach

Basic terminology

- computational complexity W(A, p), W(A, 1) (number of arithmetic operations to perform)
- parallel machine (homogeneous), number of PE (threads) p, size of the problem N (degrees of freedom), some algorithm A
 - clock cycle
- execution time <u>serial</u>: $T(A, 1) = t_c W(A)$ <u>parallel</u>: $T(A, p) = T_s(A) + \frac{T_p(A)}{p} + T_c(A, p)$
 - FLOPS rate (peak performance: theoretical vs sustained)
- MIPS Million Instructions per second
 - Power /Watt=Joule/second)
- Energy = Power*time (Joule)

Clock cycle:

general characteristic of the speed of the processing unit. The execution of instructions is done in quantums (unit time length) called a clock cycle:

$$au(s) = rac{1}{h} = rac{1}{ ext{frequency (Hz)}}$$

Theoretical peak performance (of one core):

$$f = rac{\#instructions \ per \ cycle}{ au}$$

mega-, giga-, tera-, peta-, exa-flops performance 10^6 10^9 10^{12} 10^{15} 10^{18}

More terminology: Granularity

The term granularity is usually used to describe the complexity and type granularity of a parallel computer and granularity of computations of parallelism, inherent to a parallel system.

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- fine grain parallelism; fine-grained machine/algorithm;
- medium grain parallelism; medium-grained machine/algorithm;
- coarse grain parallelism; coarse-grained computer system/algorithm.



Before defining the notion: speedup curves



In practice it is much more messy...



One algorithm on three parallel computers: speedup curves

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How to measure the parallel performance?
 How to understand what we see on the performance plots?

- How to measure the parallel performance?
 How to understand what we see on the performance plots?
 - Recall some well-known stuff...

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Recall: Shared memory machines









Recall: Distrib.memory: Static interconnection networks



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Recall: Interconnection network topologies



Notes:

Virtual (logical) topologies

Notes:

Casualties of war: the machines are gone, the ideas live Once upon a time, in 1991, a computer was announced, KSR-1 (Kendal Square Research). The company went bankrupt in 1994. Why mention then?

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Notes:

- Casualties of war: the machines are gone, the ideas live Once upon a time, in 1991, a computer was announced, KSR-1 The company went bankrupt in 1994. (Kendal Square Research). Why mention then?
 - Because of the ideas!

shared virtual memory, which was physically distributed in the Novel memory architecture: the system level architecture was machine.

The memory was automatically coherent - 'All-cache', a ring The programmer or application only saw one contiguous address space, which was spanned by a 40-bit address. of rings. ୧୨୧୯ μų * |||| • ▲ ··· → ··· →
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(q) What is 'P'?



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Xeon Phi: The Knights Ferry MIC architecture board (32-core), later 72 cores, ...

Interconnection networks for multicore

- Initially employed busses and crossbar switches between the cores and cache banks
- Such solutions are not scalable to 1000 cores!
- On-chip technologies should scale close to linearly
- Scalable on-chip communication networks will borrow ideas from large-scale packet-switched networks.
- to communicate between the cores rather than cache-coherent processors on the chip and employ software-managed memory IBM Cell employ multiple ring networks to connect 9 protocols.

The road to even more parallelism in the hardware:

- Cluster with multi-socket blades: a limited number of procs have access to common pool of shared memory ī.
 - Same as before, but each proc. is a multicore unit ī.
- Add accelerators GPUs, MIC (many integrated cores)

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Performance barriers (parallel overhead)

- Startup (latency) time
- Communication overhead
- - Synchronization costs

each of these can be in the range of milliseconds, i.e., millions of flops on modern computer systems

- Redundant computation
 - load (dis-)balance
- resources system channels and CPUs) of Imbalance

0/1)

amount of work per processing unit but not so large that there is \blacklozenge Tradeoff: to run fast in parallel there must be a large enough not enough parallel work.

Parallel performance metrics

- T(A, p) is the primary metric (was?)
- ▶ speedup $S(A, p) = \frac{T(A, 1)}{T(A, p)} \le p$; relative, absolute ▶ efficiency $E(A, p) = \frac{S(A, p)}{p} \le 1$

 - redundancy W(A, p)/W(A, 1)
 - work wasted, ...
- scalability (strong, weak)

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- T(A, p)
- Not much to say we measure and observe the total time. speedup
- relative: S(A, p) = T(A,1)/T(A,p) (the same algorithm is run on one and on p PEs)
 absolute: S(A, p) = T(A,1)/T(A,p) (the performance of the parallel algorithm on p PEs is compared with the best known serial algorithm on one PE A*) ... if we dare!

Speedup:

contra: Relative speedup "hides" the possibility for $\mathcal{T}(A, 1)$ to be Measuring speedup - pros and cons: very large.

The relative speedup "favors slow processors and poorly-coded programs" because of the following observation. Let the execution times on a uni- and p-processor/core machine, and the corresponding speedup be

 $T_0(A, 1)$ and $T_0(A, p)$ and $S_0 = \frac{T_0(A, 1)}{T_0(A, p)} > 1$.

Next, consider the same algorithm and optimize its program $T(A,p) < T_0(A,p)$ but also $S < S_0$. implementation. Then usually

Thus, the straightforward conclusion is that

* Worse programs have better speedup. * Numerically inefficient methods scale better.

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A closer look:

 $\frac{S_0}{S} = rac{eta}{lpha} > 1.$ When the comparison is done via the absolute speedup formula, $T(A, p) = \beta T_0(A, p)$ for some $\beta < 1$. However, T(A, 1) is also improved, say $T(A, 1) = \alpha T_0(A, 1)$ for some $\alpha < 1$. What might very well happen is that lpha<eta . Then, of course,

T/A* 1) T/A ") 20 namely

$$\frac{S_0}{\widetilde{S}} = \frac{T(A^*, 1)}{T_0(A, p)} \frac{T(A, p)}{T(A^*, 1)} = \beta < 1$$

In this case $\mathcal{T}(A^*,1)$ need not even be known explicitly. Thus, the absolute speedup does provide a reliable measure of the parallel performance.

• Efficiency :
$$E(A, p) = \frac{T_1}{pT_p} = \frac{1}{pS_p}$$

Isoefficiency :

It has been observed (Grama, Gupta, Kumar etc.) that efficiency increases with the problem size N and decreases with increasing the number of processors p. The idea is to keep E(A, p) constant, while suitably increase N and p simultaneously. Consider efficiency based on relative speedup, given as

$$E=rac{1}{1+
horac{T(A,p)}{T(A,1)}}.$$

Since T(A, 1) is some function of N(f(N)), then $f(N) = \frac{E}{1-E} pT(A, p)$. Using some algebraic manipulations, it is possible to rewrite the latter as

$$N = \mathcal{E}(p)$$

and the function $\mathcal{E}(p)$, called the *isoefficiency function*, relates the growth of N and p so that E remains equal to a chosen constant. The isoefficiency metric – useful in the analysis of the parallel performance of various parallel systems. Both speedup and efficiency, as well as MFLOPSrate, are tools for analysis but not a goal of parallel computing. None of these alone is a sufficient criterion to judge whether the performance of a parallel system is satisfactory or not. Furthermore, there is a tradeoff between the parallel execution time and the efficient utilization of many processors, or between efficiency and speedup.

One way to observe this is to fix N and vary p. Then for some p_1 and p_2 we have the relation

$$\frac{E(A, p_1)}{E(A, p_2)} = \frac{p_2 T(A, p_2)}{p_1 T(A, p_1)}.$$

If we want $E(A, p_1) < E(A, p_2)$ and $T(A, p_1) > T(A, p_2)$ to hold simultaneously, then $\frac{p_2}{p_1} < \frac{T(A, p_1)}{T(A, p_2)}$, i.e., the possibility of utilizing more processors is limited by the gain in execution time.

which tends to one with both increasing problem size and number massively parallel computer architectures one aims at efficiency "As a realistic goal, when developing parallel algorithms for of processors/processing units/cores."

Massively parallel $\ldots ?$ We deal now with computers from 2, 4, 16, 32, to over 3000000 cores. ୧୨୧୯ jiliji

Scalability

How to define it?

* scalability of a parallel machine: The machine is scalable if it can be incrementally expanded and the interconnecting network can incorporate more and more processors without degrading the communication speed.

* <u>scalability of an algorithm</u>: If, generally speaking, it can use all the processors of a scalable multicomputer effectively, minimizing idleness due to load imbalance and communication overhead.

* scalability of a machine-algorithm pair

How to define scalability?

Definition 1: A parallel system is scalable if the performance is linearly proportional to the number of processors used.

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How to define scalability?

- Definition 1: A parallel system is scalable if the performance is linearly proportional to the number of processors used.
 BUTS: impossible to achieve in practice, 'fixed-size', 'strong' scalability.

How to define scalability?

- Definition 1: A parallel system is scalable if the performance is linearly proportional to the number of processors used.
- **Definition 2:** A parallel system is scalable if the efficiency E(A, p) can become bigger than some given efficiency $E_0 \in (0, 1)$ by increasing the size of the problem, i.e., E(A, p) stays bounded away from zero when N increases (efficiency-conserving model).

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- remains constant when the number of processors p increases linearly with the size of the problem N (time-bounded model). Definition 3: A parallel system is scalable if the parallel execution time
- ► BUTS: too much to ask for since there is communication overhead.

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- Definition 4: A parallel system is scalable if the achieved average speed of the algorithm on the given machine remains constant when increasing the number of processors, provided that the problem size is increased properly with the system size.

Strong vs weak scalability

Fixed size speedup (strong scalability):

Compare scalability figures when the problem size is kept fixed and the number of PEs is increased.

Scaled speedup (weak scalability):

Compare scalability figures when problem size and number of PEs are increased simultaneously in a way that the load per individual PE is kept large enough and approximately constant. 、
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Scalability example:

The parallelization of the summation problem $A = \sum_{i=1}^{N} a_i$ has been floating point additions that can be done in the time it takes to proportionality that can be interpreted as the the number of modeled for a broadcast medium to have an execution time proportional to $N/P + (\gamma + 1)P$, where γ is a constant of send one word.

Choosing P as a function of N can yield arbitrarily large speedup in apparent contradiction to Amdahl's Law. For the summation problem,

$$E_{P} = \left(1 + (\gamma + 1)rac{P^{2}}{N}
ight)^{-1}$$

For fixed N, this implies that the efficiency goes to zero as P goes to infinity.

 ୧୦୧୯ case of a fixed N. For example, suppose P and N are related by the equation $P = \sqrt{N}$. Then the efficiency is constant \Rightarrow , \Rightarrow , \Rightarrow , \Rightarrow obtain an efficiency that does not go to zero, as it would for the But if we choose P as a function of N as N increases, we can

Presuming an algorithm is parallelizable, i.e., a significant part of it can be done concurrently, we can achieve large speed-up of the computational task using

- (a) well-suited architecture;
- (b) well-suited algorithms;
- (c) well-suited data structures.

A degraded efficiency of a parallel algorithm can be due to either the computer architecture or the algorithm itself:

- (i) lack of a perfect degree of parallelism in the algorithm;
- (ii) idleness of cores/processing units due to synchronization and load imbalance;
- (iii) due to the parallel algorithm itself;
- (iv) communication delays.

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cost More on measuring parallel performance:

of solving a problem in parallel is proportional to the execution time Definition: A parallel system is said to be cost-optimal if the cost of the fastest-known sequential algorithm on a single processor.

The cost is understood as the product ρT_{ρ} , i.e.

 $pT_p \sim T_{bestserial}$

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- Parallel performance metrics Parallel performance ٠ .
 - time

 - speedup
 efficiency
- scalability
- Parallel performance models

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- Computational and communication complexity of algorithms .

 - Examples: nonoptimal optimal algorithms Energy efficiency models and metrics • •
 - Summary. Tendencies

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Born on Nov 11, 1922, 93 years old. Gene Amdahl, 1965

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Gene Amdahl, March 13, 2008

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Gene Amdahl:

organization of a single computer has reached its limits and that truly significant advances can be made only by interconnection of a multiplicity Overhead alone would then place an upper limit on throughput on five to seven times the sequential processing rate, even if the housekeeping were The nature of this overhead (in parallelism) appears to be sequential so that it is unlikely to be amendable to parallel processing techniques. of computers in such a manner as to permit cooperative solution... For over a decade prophets have voiced the contention that the done in a separate processor.

done in a separate processor... At any point in time it is difficult to foresee how the previous bottlenecks in a sequential computer will be effectively overcome.

Parallel performance models

The fundamental principle of computer performance; Amdahl's law (1967) Given: N operations, grouped into k subtasks N_1, N_2, \cdots, N_k , which must be done sequentially, each with rate R_i .

$$T = \sum_{i=1}^{k} t_i = \sum_{i=1}^{k} \frac{N_i}{R_i} = \sum_{i=1}^{k} \frac{f_i N}{R_i}; \quad \overline{R} = \frac{T}{N} N / \sum (f_i N / R_i) = \frac{1}{\sum_{i=1}^{k} f_i / R_i}$$

Hence, the average rate $\overline{R}(=N/R)$ for the whole task is the weighted harmonic mean of R_1, R_2, \ldots, R_k . For the special case of only two subtasks - f_p (parallel) and $1 - f_p$ - serial,

then

$$\overline{R}(f_p) = \frac{1}{\frac{f_p}{R_p} + \frac{1-f_p}{1-F_p}} \quad \text{and} \quad S = \frac{p}{f_p + (1-f_p)p} \leq \frac{1}{1-f_p}.$$

Thus, the speedup is bounded from above by the inverse of the serial fraction.

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Example:



If we drive 125 km/h on the highway, then the total time would

So, why bother to drive fast on the highway?! increase with only 15%.

Gustafson-Barsis law (1988):

Perhaps, the first breakthrough of the Amdahl's model is the result achieved by the 1988 Gordon Bell's prize winners - a group from Sandia Laboratories.

On a 1024 processor nCUBE/10 and with f_p computed to be in the range of (0.992, 0.996) they encountered a speedup of 1000 while the Amdahl's law prediction was only of the order of 200 ($S=1024/(0.996+0.004*1024)\approx 201$).

$$\begin{array}{lcl} T(A,1) &=& (1-f_p)+f_p p \\ T(A,p) &=& (1-f_p)+f_p = 1 & \text{properly scaled problem} \\ S &=& T(A,1) = p-(p-1)(1-f_p) \end{array}$$

An example:

32 cores, 1% serial part and 0.99% parallel part Amdahl's law: $S \le 1/(0.01 + 0.99/32) = 24.43$ Gustafson's law: $S \le 32 - 31 * 0.01 = 31.69$



Let $f_p = 0.5$.

No.S PEsAmdahl'sGustafsson-Barsis'2 $S = \frac{1}{0.5+0.5*2} = 1.33$ S = 2 + 0.5(2 - 1) = 1.54 $S = \frac{1}{0.5+0.5*4} = 1.6$ S = 4 + 0.5(4 - 1) = 2.5

► What has happened to the computer hardware since 1988?

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- What has happened to the computer hardware since 1988?
 - What has happened to the computer hardware since 1993?
 1993 2010
 2003 2011
 2006 2012
 2015

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Top 500, June 1993

- Los Alamos Nat.Lab., CM-5/1024 Fat tree SuperSPARC I 32 MHz (0.128 GFlops) Hypercube, tree ----
 - Minnesota Supercomputer Center CM-5/544 Fat tree 2 6 4 9
 - NCSA United States CM-5/512 Fat tree
- National Security Agency CM-5/512 Fat tree NEC Japan SX-3/44R NEC NEC 400 MHz (6.4 GFlops) Multi-stage crossbar

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Top 500, November 2003

- The Earth Simulator Center Japan Earth-Simulator NEC NEC 1000 ----
 - 3 5
 - MHz (8 GFlops), Multi-stage crossbar Los Alamos Nat. Lab., ASCI Q AlphaServer SC45, 1.25 GHz HP Virginia Tech X 1100 Dual 2.0 GHz Apple G5/Mellanox Infiniband 4X/Cisco GigE Self-made NCSA Tungsten PowerEdge 1750, P4 Xeon 3.06 GHz, Myrinet 4
- Dell ഹ
 - Pacific Northwest National Laboratory Mpp2 Cluster Platform 6000 rx2600 Itanium2 1.5 GHz, Quadrics HP
- Lawrence Livermore National Laboratory ASCI White, SP Power3 375 MHz IBM, SP Switch (clusters - faster) ∞

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Computer no 1: The ES: a highly parallel vector supercomputer system of distributed-memory type. Consisted of 640 processor nodes (PNs) connected by 640×640 single-stage crossbar switches. Each PN is a system with a shared memory, consisting of 8 vector-type arithmetic processors (APs), a 16-GB main memory system (MS), a remote access control unit (RCU), and an I/O processor. The peak performance of each AP is 8Gflops. The ES as a whole consists of 5120 APs with 10 TB of main memory and the theoretical performance of 40 Tflop. 、
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- DOE/NNSA/LLNL BlueGene/L eServer Blue Gene Solution IBM PowerPC 440 700 MHz (2.8 GFlops), 32768 GB
 - 2 NNSA/Sandia Nat.Lab., Red Storm Sandia/ Cray Red Storm, Opteron 2.4 GHz dual core Cray Inc.
- IBM Thomas J. Watson Research Center BGW eServer Blue Gene Solution IBM \mathfrak{c}
 - 4 DOE/NNSA/LLNL ASCI Purple eServer pSeries p5 575 1.9 GHz IBM
 - 5 Barcelona Supercomputing Center MareNostrum BladeCenter JS21 Cluster, PPC 970, 2.3 GHz, Myrinet IBM

Computer no 1:

The machine was scaled up from 65,536 to 106,496 nodes. Each Blue Gene/L node is attached to three parallel communications networks:

 a 3D toroidal network for peer-to-peer communication between compute nodes,

- a collective network for collective communication,

- a global interrupt network for fast barriers.

communication with the world via an Ethernet network. The I/O nodes Finally, a separate and private Ethernet network provides access to any also handle the filesystem operations on behalf of the compute nodes. The I/O nodes, which run the Linux operating system, provide node for configuration, booting and diagnostics. し、
 <li

- National Supercomputing Center in Tianjin, China, Tianhe-IA NUDT TH MPP, X5670 2.93 GHz 6C, NVIDIA GPU, FT-1000 8C NUDT -
 - 2 DOE/SC/Oak Ridge Nat.Lab., Jaguar Cray XT5-HE Opteron 6-core 2.6 GHz
- 3 National Supercomputing Centre in Shenzhen (NSCS) China Nebulae - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU Dawning
- GPU Dawning GSIC Center, Tokyo Institute of Technology, Japan TSUBAME 2.0 HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows NEC/HP 4
 - 5 DOE/SC/LBNL/NERSC Hopper Cray XE6 12-core 2.1 GHz
- 9 Forschungszentrum Juelich, Germany, JUGENE Blue Gene/P IBM

Computer no 1: Peta-flop machine Configuration of the system: Computing node: 2560 in total * Each computing node is equipped with 2 Intel Xeon EP CPUs (4 cores), 1 AMD ATI Radeon 4870x2 (2GPUs, including 1600 Stream Processing Units -SPUs), and 32GB memory

* Each operation node is equipped with 2 Intel Xeon CPUs (4 cores) and 32GB Operation node: 512 in total memory

Interconnection subsystem:

* Infiniband QDR * The point-to-point communication bandwidth is 40Gbps and the MPI latency is 1.2 μs

Programming framework for hybrid architecture - adaptive task partition and streaming data access. **୬**୯୯ jiliji . ılılı ▼ ▲ |||| ▼ • © • .

- nect / 2011 Fujitsu, 705024 cores, 10.51 PetaFlops National Supercomputing Center in Tianjin China, 186368 RIKEN Advanced Institute for Computational Science (AICS) Japan, K computer, SPARC64 VIIIfx 2.0GHz, Tofu intercon-----
- cores \sim
 - States, DOE/SC/Oak Ridge National Laboratory United 224162 cores \mathfrak{c}

Tokyo and Tsukuba, Japan, November 18, 2011 - A research group from RIKEN, the Univ. Tsukuba, the Univ. Tokyo, and Fujitsu Ltd announced that research results obtained using the "K computer" were awarded the ACM Gordon Bell Prize.

The award-winning results, revealed the electron states of silicon nanowires, which have attracted attention as a core material for next-generation semiconductors.

quantum-mechanical computations were performed on the electron states of a nanowire with approx. 10^5 atoms (20 νm in diameter and 6 νm long), close to transport characteristics will change depending on the cross-sectional shape of the actual size of the materials, and achieved execution performance (*2) of nanowires, comprised of 10,000 to 40,000 atoms, clarified that electron The results of the detailed calculations on the electron states of silicon To verify the computational performance of the K computer, 3.08 PFLOPS (representing execution efficiency of 43.6%).

the nanowire.

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- Cray Gemini interconnect, NVIDIA K20x, 560 640 cores, 27.1125 PFlop/s, DOE/SC/Oak Ridge National Laboratory Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom, Titan - Cray XK7 , Opteron 6274 16C 2.200GHz, -
 - 1 572 864 cores, DOE/NNSA/LLNL \sim
- K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect, 705 024 cores \mathfrak{C}
 - 786 432 cores, DOE/SC/Argonne National Laboratory JUQUEEN BlueGene/Q, Power BQC 16C 1.600GHz, Custom BlueGene/Q, Power BQC 16C 1.60GHz, Custom, Mira -4
- Interconnect, 393 216 cores വ
- . . .
- Triolith Cluster Platform SL230s Gen8, Xeon E5-2660 8C 2.200GHz, Infiniband FDR, 19136 cores, National Supercomputer Centre, Sweden. 83

Titan – the first major supercomputing system to utilize a hybrid architecture: utilizes both conventional 16-core AMD Opteron CPUs and NVIDIA Tesla K20 GPU Accelerators. ୧୨୧୯ μų

Top 500, November 2012

BlueGene-Q:

- ▶ IBM PowerPC A2 1.6 GHz, 16 cores per node
 - Networks
- 5D Torus 40 GBps; 2.5 μsec latency (worst case)
 Collective network part of the 5D Torus; collective logic
 - operations supported
- 1 GB Control Network System Boot, Debug, Monitoring Global Barrier/Interrupt – part of 5D Torus
- L2 cache multi-versioned, supporting transactional memory and speculative execution; has hardware support for atomic operations.

- Tianhe-2 (MilkyWay-2) TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.2 GHz, TH Express-2, Intel Xeon Phi 31S1P, 3,120,000 cores, 54902.4 TFLOP Titan Cray XK7, Opteron 6274 16C 2.2 GHz, Cray Gemini inter-connect, NVIDIA K20x Cray Inc., 560 640 cores, 27112.5 TFLOP -
- \sim
- ... Beskow Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries inter-connect Cray Inc., 53,632 cores, 1,397 TFLOP ... 52

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Top 500, November 2012

Tianhe-2 (MilkyWay-2) :

- 16000 nodes, 32000 Intel Xeon CPUs, 48000 Intel Xeon Phis, 4096 FT CPUs
 - Memory 1PB in total, 88 GB per node
- Interconnect: fat-tree topology, opto-interconnection, bidirectional bandwidth at 160 Gbps

 ୧୦୧୯ jiiji ▲理・▲理・▲喧・▲□・ Models and metrics for the 'small-sized'

New performance models and metrics:

Examples:

Estimating Parallel Performance, A Skeleton-Based Approach Oleg Lobachev and Rita Loogen, Proceeding HLPP'10 Proceedings of the 4th international workshop on High-level parallel programming and applications, ACM New York, NY, USA, 2010, 25-34.

Roofline: An Insightful Visual Performance Model for Floating-Point Programs and Multicore Architectures Samuel Webb Williams, Andrew Waterman and David A. Patterson, Communications of the ACM, 52 (2009), 65-76.

The 'Skeleton' approach:

No of PEs - 'p', problem size - 'n', W(n), T(n) = W(n), T(n, p) - execution time on p PEs; assume W(n, p) = pT(n, p). In a parallel execution, the sequential work is distributed over the processors. This causes an overhead, A(n, p) (a penalty), which is also distributed over the p elements, thus, $A(n, p) = p\widetilde{A}(n, p)$. 2 Then

$$T(n,p) = T(n)/p + \widetilde{A}(n,p)$$

and

$$W(n, p) = T(n) + p\widetilde{A}(n, p) = T(n) + A(n, p)$$

Then we can predict T(n, p). Use 'skeletons' as abstract descriptions of the parallelization paradigm ('divide and conquer', Task: try to estimate accurately T(n) and A(n, p). 'iteration').

The 'Roofline' approach:



- Parallel performance
- Parallel performance metrics
 - time – speedup
- efficiency
- scalability
- Computational and communication complexity of algorithms •
- Examples: nonoptimal optimal algorithms
 - Energy efficiency models and metrics
 - Summary. Tendencies

A scalar product of two vectors of order n on p PE's (tree)



and we see that the theoretical speedup is degraded by the factor $(1+\alpha)^{-1}$ due to data transport. $S = \frac{T_1}{T_p} = \frac{2n-1}{(\log_2 n+1)} \cdot \frac{1}{1+\alpha}$

A scalar product of two vectors of order n on 3D hypercube



Matrix-vector product, distributed memory

Question: How is the matrix distributed over the processing units?

	broc 1			1	Droc 3	200	proc 4	
	ģ	b_2	\mathbf{p}_3	b_4	b_{S}	b_6	b₁	å
				I	I			
	X ₁	\mathbf{X}_{2}	\mathbf{X}_3	X ₄	Х ₅	х ₆	\mathbf{X}_{7}	X ₈
1					•			
Uption 1: PEISc-style	a ₁₁ a ₁₂	a ₂₁ a ₂₃ a ₂₃	a32a33a34	a43a44a45	a ₅₄ a ₅₅ a ₅₆	a ₆₅ a ₆₆ a ₆₇	a ₇₆ a ₇₇ a ₇₈	a ₈₇ a ₈₈

Matrix-vector product, distributed memory

Question: How is the matrix distributed over the processing units? Option 2: METIS-style



An algorithm which should scale very well ...



... but does not scale ...

ed Conjugate	
n code stencil-bas	:pc
shelf Fortraı	ent metho
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	ime/lt	.0061	.0297		Time/It	0.0233	0.0816
2	Time T	7.77 0	72.72 0	ω	Time	56.96	386.58
	土	1273	2447		느	2447	4737
	Time/It	0.0051	0.0228		Time/It	0.0134	0.0477
	Time	3.86	33.66	4	Time	19.69	137.03
	ㅗ	756	1474		<u>+</u>	1474	2873
Local	problem size	500^{2}	1000^{2}	Problem size		500^{2}	1000^{2}

Numerical efficiency – parallel efficiency – time

FEM-DD-PCG-SPAI

Assume A, B and b are distributed and the initial guess $\mathbf{x}^{(0)}$ is replicated.

	$\mathbf{g}^{(0)} = replicate(\mathbf{g}^{(0)})$	$\mathbf{h} = replicate(\mathbf{h})$	nce		$\mathbf{g}^{(k+1)} = replicate(\mathbf{g}^{(k+1)})$	$\mathbf{h} = replicate(\mathbf{h})$	$\delta_0 = \delta_1$
CG-FEM-METIS style	$g^{(0)} = Ax^{(0)} - b,$ $h - Ba^{(0)}$	$ \begin{array}{rcl} \delta_0 &= & \mathbf{g}_{(0)}, \mathbf{h} \\ \mathbf{d}^{(0)} &= & -\mathbf{h} \\ \end{array} $	For $k = 0, 1, \cdots$ until converge (1) $\mathbf{h} = A\mathbf{d}^{(k)}$	(2) $\tau = \delta_0/(\mathbf{h}, \mathbf{d}^{(k)})$ (3) $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \tau \mathbf{d}^{(k)}$	(4) $g^{(k+1)} = g^{(k)} + \tau h$, (5) $h = B \sigma^{(k+1)}$	(6) $\delta_1 = (\mathbf{g}^{(k+1)}, \mathbf{h})$	(7) $\beta = \delta_1/\delta_0,$ (8) $\mathbf{d}^{(k+1)} = -\mathbf{h} + \beta \mathbf{d}^{(k)}$

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Poisson's equation

F		11	11	10	10	10	6
Comm.	Time	0	0.2217	0.2209	0.3424	0.3648	0.3962
Total	Time	3.8375	3.8994	3.5908	4.2601	4.3697	4.1379
E(n, P)	$(n = 2^{10})$	1.0	0.9841	1.0687	0.9008	0.8782	0.9274
Probl.	size	1048576	4194304	16777216	67108864	268435456	1073741824
h_l		$1/2^{10}$	$1/2^{11}$	$1/2^{12}$	$1/2^{13}$	$1/2^{14}$	$1/2^{15}$
ط		1	4	16	64	256	1024

Borrowed from a presentation by Ridgway Scott, Valpariaso, Jan 2011.

Parallel performance of U-cycle multigrid on IBM Blue Gene/L

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		D11 /			
	197129	0.005	0.28	7.01	
16	49408	0.180	0.07	0.29	
54	12416	0.098	0.02	0.03	
		Problem si	ize: 78745	9	
		Solution me	ethod: PC	ĴĈ	
				(

Relative stopping criterium: $< 10^{-6}$

FEM-SPAI: Scalability figures: Constant problem size

# iter	2	£	Ð
t _{solution} [s]	7.01	0.29	0.03
t _{repl} [s]	0.28	0.07	0.02
$t_{{\mathcal B}_{11}^{-1}}/t_{\mathcal A}$	0.005	0.180	0.098
nfine	197129	49408	12416
# proc	4	16	64

 ୧୦୧୦ μų ▲□▼ ▲□▼ ▲□▼ FEM-SPAI: Scalability figures: Constant load per processor

# iter	5	5	5	Ð
t _{solution} [s]	0.17	7.01	4.55	12.43
t_{repl} [s]	ı	0.28	0.24	0.23
$t_{B_{11}^{-1}}/t_{\mathcal{A}}$	0.0050	0.0032	0.0035	0.0040
#proc		4	16	64

Local number of degrees of freedom: 197129 Solution method: PCGRelative stopping criterium: $< 10^{-6}$

Linear elasticity:

Solve
$$\begin{bmatrix} F & B^T \\ B & -M \end{bmatrix}$$
, preconditioned by $\begin{bmatrix} F & 0 \\ B & -S \end{bmatrix}$.

Linear elasticity, MPI

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5 907 203 5 907 203 23 610 883	$\begin{array}{c} \frac{1}{100} \left(8,1 \right) \\ 10(8,1) \\ 10(8,1) \\ 10(8,1) \\ 10(8,1) \\ 10(8,1) \\ 10(8,1) \\ 10(8,1) \\ 10(9,1) \\ 10(9,1) \\ 10(9,1) \\ 10(9,1) \\ 10(11,1) \\ 10(11,1) \\ 10(11,1) \\ 10(11,1) \\ 10(11,1) \\ 10(11,1) \\ 10(12,1) \\ 10(1$	Setup 25.3 7.11 3.6.1 3.6.1 1.26 1.26 1.26 1.26 1.26 1.4.6 8.68 1.4.66 1.4.6 5.42 5.22 5.22 5.22 5.22 5.22 5.66 1.4.6 8.66 1.65 1.65 1.65 1.65 1.65 1.65 1.1.1 1.26 1.1.26 1.1.26 1.26 1.26 1.26	Solve 86.9 86.9 86.9 9.51 9.51 9.51 9.51 99.2 21.1 21.1 21.1 21.1 205 257 253 60.8 33.3 257 507 503 507 507 507 507 507 507 507 507 507 507
128 256	94 407 683	10(12, 1) 10(11, 1)	21.5 14	272 98.9
512		10(11, 1)	9.79	72.9

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Does this algorithm scale or not?

A version of $\ensuremath{\mathsf{wave}}$: Solve 2D advection equation with forcing term numerically with the Leap-frog scheme

16		1	I	I		0.33	2.49	19.69	
ω)	0.73	5.93	52.62		0.42	3.17	29.25
4		0.72	5.83	47.25		0.77	6.78	48.17	
2	Dec, 2010	1.37	11.23	88.75	ec, 2011	1.49	11.45	105.32	
1		2.71	21.79	172.35		3.26	25.99	208.04	
Problem size		256^{2}	512^{2}	1024^{2}		256^{2}	512^{2}	1024^{2}	

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The Speedup of the wave solver



An algorithm that scales ...

	Coarsest		N	umber of F	РEs		
Grid	level No						Time
size	(total no.	4	ω	16	32	64	(sec)
	of levels)						
256^{2}	10(16)	403.49	189.06	93.86	49.18	28.71	outer
		5.31	5.93	5.58	4.62	3.89	comm.
				632.60	304.24	154.65	total
512^{2}	12(18)			629.44	302.71	153.81	outer
				14.28	12.14	10.14	comm.
					1662.73	829.71	total
1024^{2}	12(20)				1655.73	826.22	outer
					29.89	22.26	comm.

Stokes problem: Performance results on the Cray T3E-600 computer

Another algorithm that scales ..

Ultrascalable implicit finite element analyses in solid mechanics

with over a half a billion degrees of freedom

M.. Adams, H.. Bayraktar, T.. Keaveny, P. Papadopoulos ACM/IEEE Proceedings of SC2004: High Performance Networking and Computing, 2004

Bone mechanics, AMG, 4088 processors, the ACSI White machine (TRNL):

multigrid method (smoothed aggregation) is computationally effective for large deformation finite element analysis of solid mechanics problems "We have demonstrated that a mathematically optimal algebraic with up to 537 million degrees of freedom.

We have achieved a sustained flop rate of almost one half a Teraflop/sec on 4088 IBM Power3 processors (ASCI White)

problems with complex geometry that we are aware of, with an average These are the largest published analyses of unstructured elasticity

time per linear solve of about 1 and a half minutes.

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ACM/IEEE Proceedings of SC2004: High Performance Networking Ultrascalable implicit finite element analyses in solid mechanics M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos with over a half a billion degrees of freedom and Computing, 2004

... Additionally, this work is significant in that no special purpose algorithms or implementations were required to achieve a highly scalable performance on a common parallel computer.

3D Multiphase flow simulations

4293378		2 / 10 / 5	287.40	7.79		18/5	236.97	7.09
549250	CG with AMG	2 / 11 / 5	36.86	7.64	CG with AMG	20/5	33.42	6.66
71874	(i1), F	2 / 12 / 5	4.82		(i2), F	26/4	5.02	
Size		$N_1/N_2/N_3$	T	R		N_1/N_3	T	Я

Average iteration counts N_1 , N_2 , and N_3 , average wall time T in seconds and factor R of increase of T for three consecutive mesh refinements, methods (i1) and (i2) on one processor.

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3D Multiphase flow simulations

1	1	1	I.					1				1
270011394	512		3 / 10 / 103	520.7	1.64	1.77		14 / 95	355.6	1.70	1.64	verage iteration
33949186	64		3 / 11 / 57	293.9	1.65	2.16		17 / 56	217.2	1.60	1.71	$M + \varepsilon \sqrt{R}K = \Delta$
4293378	œ	(i1)	3 / 10 / 38	136.4	1.32	3.49	(i2)	18 / 35	127.4	1.60	1.81	d for systems with
549250	1		3 / 12 / 24	39.1				20 / 22	70.2			ity test CG lise
Size	No. cores		$N_1/N_2/N_3$	T	R_{CG}	Я		N_1/N_3	T	R_{CG}	R	Weak scalahil

Weak scalability test, UG used for systems with $M + \varepsilon_V \beta K$. Average iteration counts M_1 , M_2 , and M_3 , average wall time T in seconds, factor R_{G} of increase of the inner CG iterations and factor R of increase of T after one mesh refinement

3D Multiphase flow simulations

270011394	512		3 / 9 / 6	275.20	1.89		14/6	140.59	1.03
33949186	64		3 / 6 / 6	145.66	1.60		17/6	136.56	2.02
4293378	ω	(i1)	3 / 10 / 6	91.02	2.57	(i2)	17/5	67.53	2.15
549250	1		3 / 11 / 5	35.36			20/5	31.45	
Size	No. cores		$N_1/N_2/N_3$	T	R		N_1/N_3	T	R

Weak scalability test, PCG with AMG preconditioner used for systems with $M + \varepsilon \sqrt{\beta}K$. Average iteration counts N_1 , N_2 , and N_3 , average wall time T in seconds and factor R of increase of T after one refinement of the mesh

Gauss Elimination

Dependences in Gaussian elimination System of equations and standard sequential algorithm for Gaussian elimination:

Sequential Gaussian elimination: multiple loops

Gauss Elimination



The iteration space for the standard sequential algorithm for Gaussian elimination forms a trapezoidal region with square cross-section in the i, j plane. Within each square (with k fixed) there are no dependencies.

Gauss Elimination

(1) The dominant part of the computation when solving a system with a direct solver is the factorization, in which L and U are determined.

loops (the *i* and *j* loops) because i, j > k. Therefore, these loops (2) There are no loop-carried dependences in the inner-most two can be decomposed in any desired fashion. (3) The algorithm for Gaussian elimination can be parallelized The triangular system solves require less computation.

using a message-passing paradigm. It is based on decomposing the middle loop (the j loop). A typical decomposition would be cyclic, matrix column-wise, and it corresponds to a decomposition of the since it provides a good load balance.

Gauss Elimination

```
a(i,j) - l(i,k) * a(k,j)
                                                                                                                for j=k+1,n ("modulo owning column j")
for i=k+1,n
                                             = a(i,k)/a(k,k)
                                                                                     else "receive" l(k+1 : n)
                                                                           . n)
              if("I own column k"
                                                                       "broadcast" 1(k+1
                                                                                                                                                   II
                                                                                                                                               a(i,j)
                              for i=k+1, n
                                         l(i,k) =
                                                                                                                                                              endfor(i)
                                                           endfor(i)
                                                                                                                                                                               endfor(j)
for k=1,n
                                                                                                                                                                                            endfor(k)
                                                                                                         endif
```

Standard column-storage parallelization Gaussian elimination.

Gauss Elimination

references) are executed, all of which can be done in parallel. Thus divisions are performed in computing the multipliers l(i, k), then these multipliers are broadcast to all other processors. Once these are received, $(n - k)^2$ multiply-add pairs (as well as some memory We can estimate the time of execution of the standard Gaussian elimination algorithm as follows. For each value of k, n - kthe time of execution for a particular value of k is

$$c1(n-k)+c2\frac{(n-k)^2}{P}$$

The constant $\ensuremath{c_{1}}$ can measure the time both to compute a quotient compute a 'multiply-add pair' a = a - b * c for a single processor. operations. Here, c_2 can be taken to be essentially the time to where the constants c_i model the time for the respective basic and to transmit a word of data.

Gauss Elimination - speedup, efficiency and scalability

Summing over k, the total time of execution is

$$\sum_{k=1}^{n-1} \left(c_1(n-k) + c_2 \frac{(n-k)^2}{P} \right) \approx \frac{1}{2} c_1 n^2 2 + \frac{1}{3} c_2 \frac{n^3}{P}$$

Time to execute this algorithm sequentially is $\frac{1}{3}c_2n^3$. Speed-up for standard column-storage parallelization of Gaussian elimination is

$$S_{P,n} = \left(\frac{2}{3}\frac{\gamma}{n} + \frac{1}{P}\right)^{-1} = P\left(\frac{2}{3}\frac{\gamma}{n}P + 1\right)^{-1}$$

where $\gamma=c_{\rm l}/c_{\rm 2}$ - ratio of communication to computation time. Efficiency

<u>.</u>

$$E_{P,n} = \left(rac{2}{3}rac{\gamma P}{n} + rac{1}{P}
ight)^{-1} pprox 1 - rac{2}{3}rac{\gamma P}{n}.$$

Thus the algorithm is scalable; we can take $P_n n = \epsilon n$ and have a fixed efficiency of

$$\left(rac{2}{3}\gamma\epsilon+1
ight)^{-1}.$$

The efficiency will be the same for values of P and n which have the same ratio P/n. jiiji

- Parallel performance •
- performance metrics Parallel
- time
- speedup
- efficiency L
- scalability
- Computational and communication complexity of algorithms •
- Examples: nonoptimal optimal algorithms •

 - Energy efficiency models and metrics ٠
 - Summary. Tendencies •

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Energy efficiency

The topic is very broad and has various aspects:

- Hardware design
- Scheduling policies
- Algorithmic aspects

Metrics: MIPS per Watt

Speedup per Watt Power per speedup Dynamic Voltage Frequency Scaling (DVFS) MIPS² per Watt FLOPS per Watt Energy per operation

Energy per target

Performance per Watt

MIPS³ per Watt

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Energy efficiency, hardware design

- (A. Martin, Mika Nyström, P. Pénzes) Observation: Et^2 is independent of the voltage Et^2 On the level of VLSI (CMOS)
 - Power-aware speedup
- As the system scales, maintain constant per-node performance Iso-energy efficiency: (Song, Su, Ge, Vishnu, Cameron) to power

Energy efficiency, scheduling policies

Speedup per Watt - how to use power to achieve high performance Metrics and task scheduling policies for energy saving in multicore performance unit (find out the best hardware configuration that uses min energy and still achieve the required performance. Power per speedup - how much power is needed for each Power efficiency is not equal to energy efficiency. Majr, Leung, Huang, 2010 Energy=Power×time computers

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Energy efficiency, algorithmic aspects

Costas Bekas and Alessandro Curioni, Computer Science, Volume A new energy aware performance metric 25, Nr. 3-4, 187-195, 2010

designed in harmony and simultaneously optimized such that both Computing systems and algorithms that run on them should be power consumption and time to solution are minimized. Consider the following target:

The proposed metric is

f(time to solution) energy (FTTSE) where $f(\cdot)$ is an application-dependent function of time. (Contrast to Flops per Watt, where the two ingredients are optimized separately.)

- Parallel performance ٠
- performance metrics Parallel
- speedup - time
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- Computational and communication complexity of algorithms ٠
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 - Summary. Tendencies

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Final words: High Performance Computing, where are we?

- Performance:
- Sustained performance has increased substantially during the last years.
 - parallel systems has become smaller than that of specialized On many applications, the price-performance ratio for the supercomputers. But ..
 - Still, some applications remain hard to parallelize well (adaptive methods).
- ♦ Languages and compilers:
- Message passing programming is tedious and hard to debug. Standardized, portable, high-level languages exist. But ...
 - OpenMP has its limitations. Combination good.
 - GPUs still rather specialized
- Programming difficulties remain still a major obstacle for mainstream scientists to parallelize existing codes. Revisit some 'old' algorithms, come up with new languages.
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Final words: High Performance Computing, where are we?

We are witnessing and we are given the chance to participate in the exiting process of parallel computing achieving its full potential power and solving the most challenging problems in Scientific Computing/Computational Mathematics/Bioinformatics/Data Mining etc. して、 正、 ● 三、 シスペ