Parallel Quantum Molecular Dynamics

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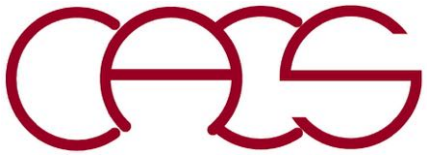
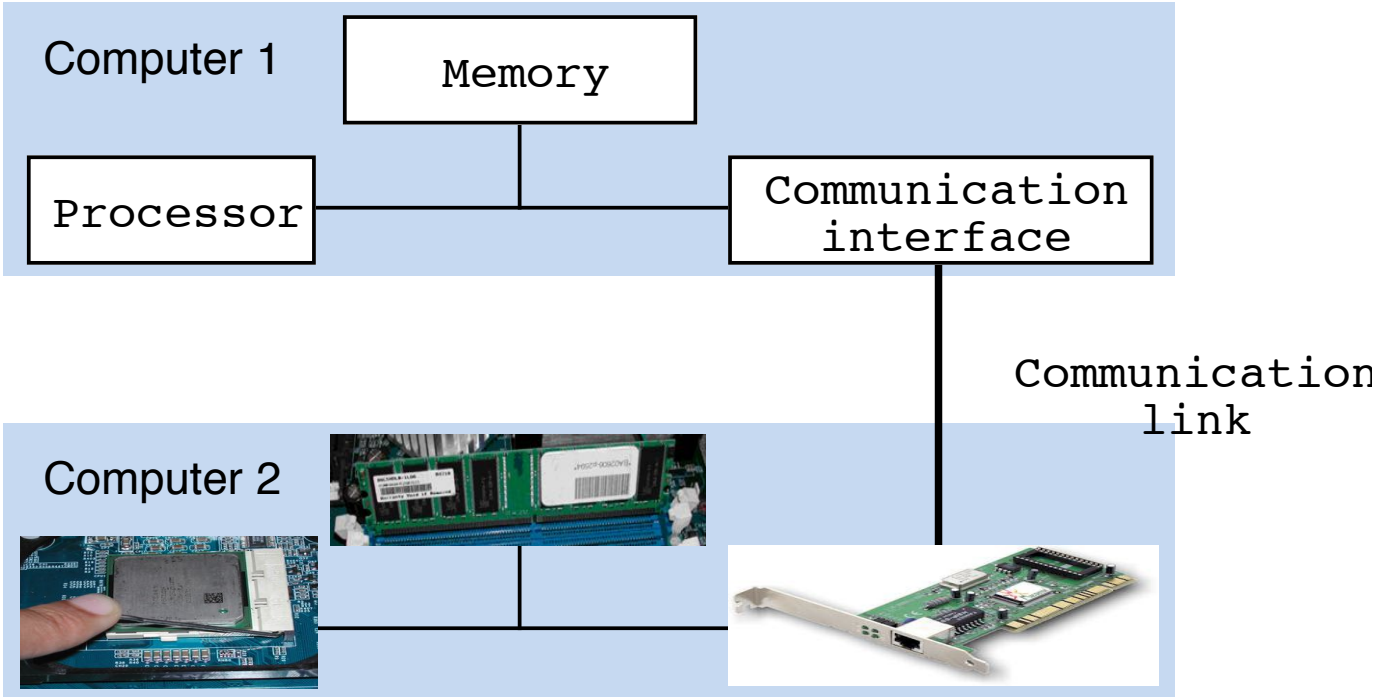


Parallel Computing Hardware

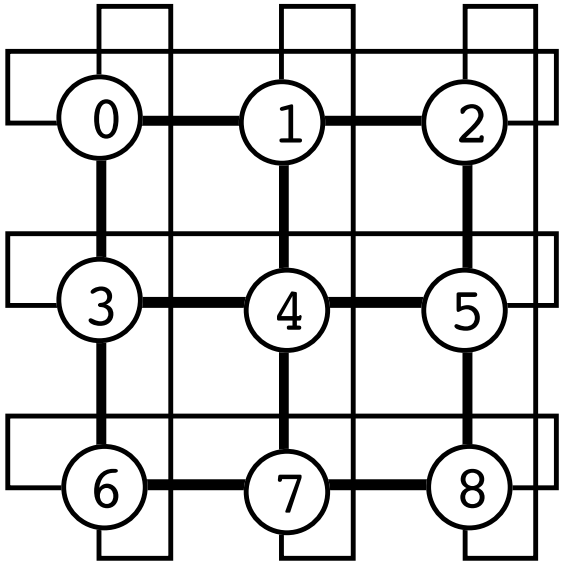


- **Processor: Executes arithmetic & logic operations**
- **Memory: Stores program & data (stored program computer)**
- **Communication interface: Performs signal conversion & synchronization between communication link & a computer**
- **Communication link: A wire capable of carrying a sequence of bits as electrical (or optical) signals**

See http://cacs.usc.edu/education/cs596.html

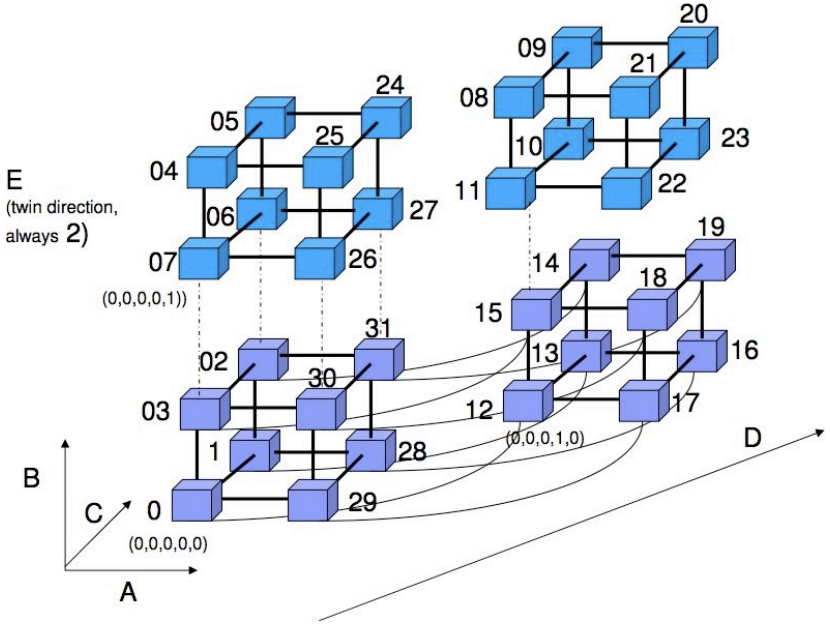
Communication Network

Mesh (torus)

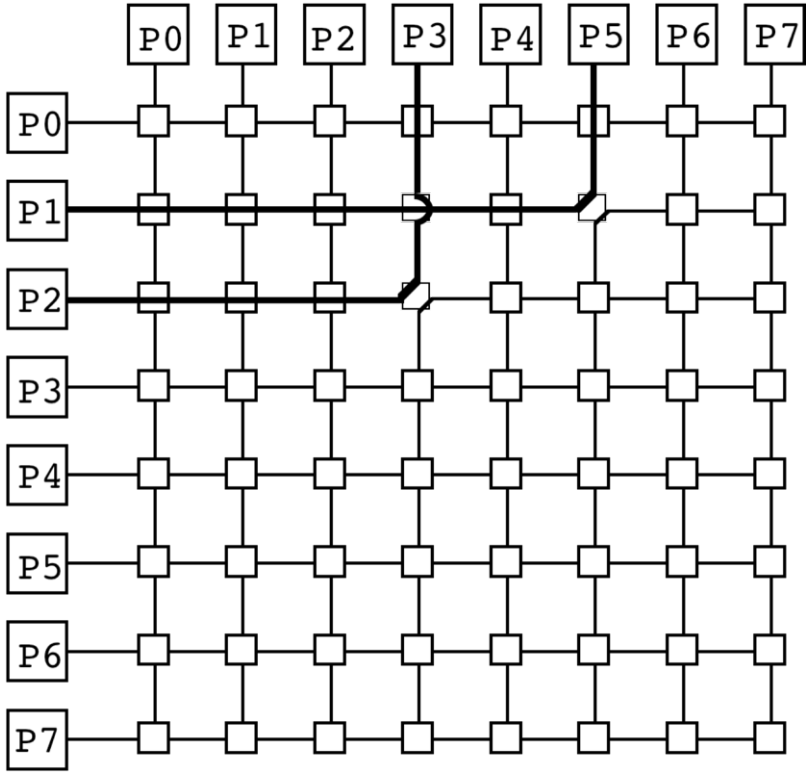


NEC Earth Simulator (640x640 crossbar)

IBM Blue Gene/Q (5D torus)



Crossbar switch



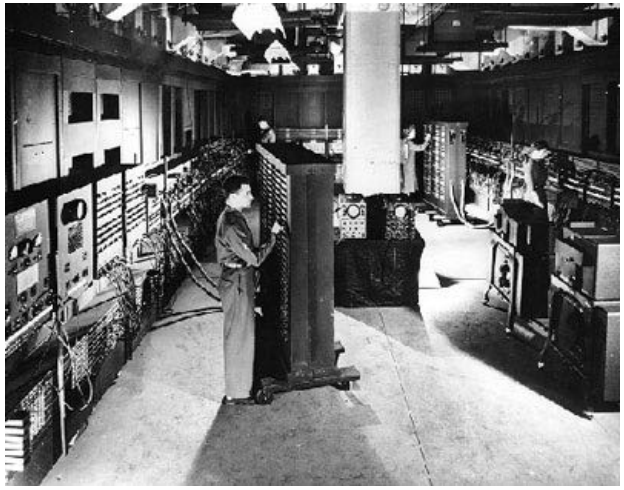
History of Supercomputers

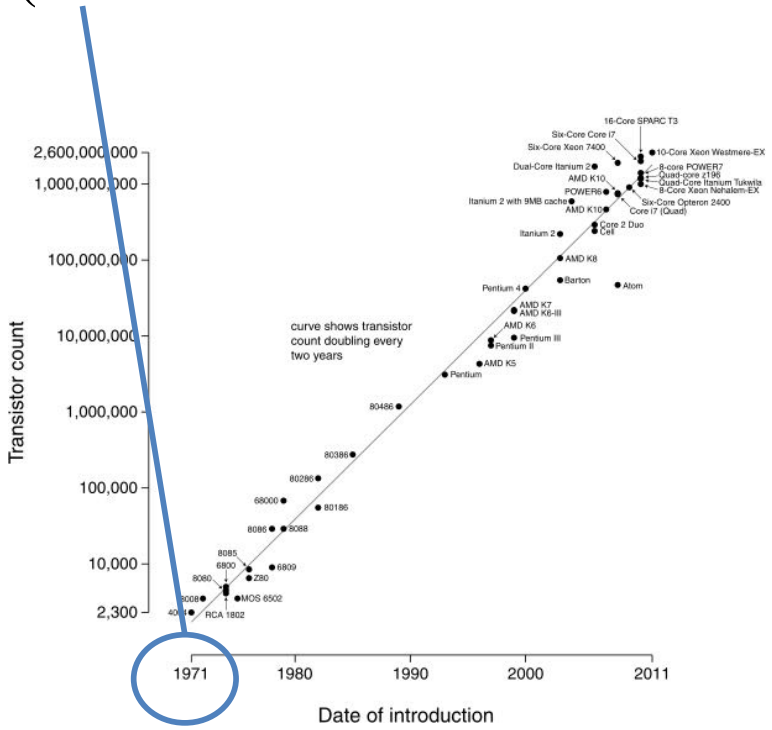
Early ’40s: ENIAC by Presper Eckert & John Mauchly at Univ. of Pennsylvania—First general-purpose electronic computer

’76: Cray 1 by Seymour Cray—beginning of vector supercomputer era

Late 80’s: massively parallel computers such as the Thinking Machines CM-2

(’71: Intel 4004—invention of microprocessor)





See lecture on “MD machines”

Merge of PC & Supercomputers

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China 太湖之光	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China 天河	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 Cray Inc.	361,760	19,590.0	25,326.3	2,272
4	Japan Agency for Marine-Earth Science and Technology Japan 暁光	**Gyoukou** - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz ExaScaler	19,860,000	19,135.8	28,192.0	1,350
5	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209

Theoretical performance

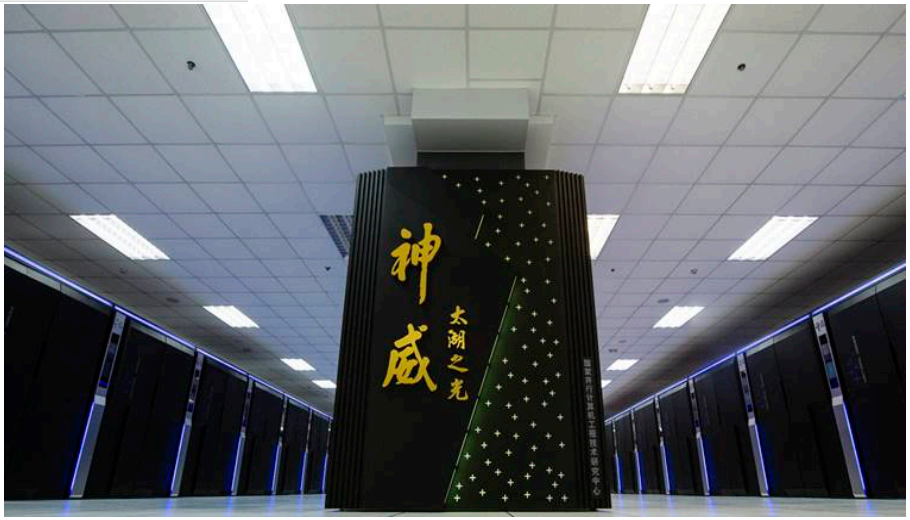
Measured performance (in Tflop/s)

Flop/s = floating-point operations/second

M (mega) = 10^6
G (giga) = 10^9
T (Tera) = 10^{12}
P (Peta) = 10^{15}
X (Exa) = 10^{18}

http://www.top500.org (November '17)

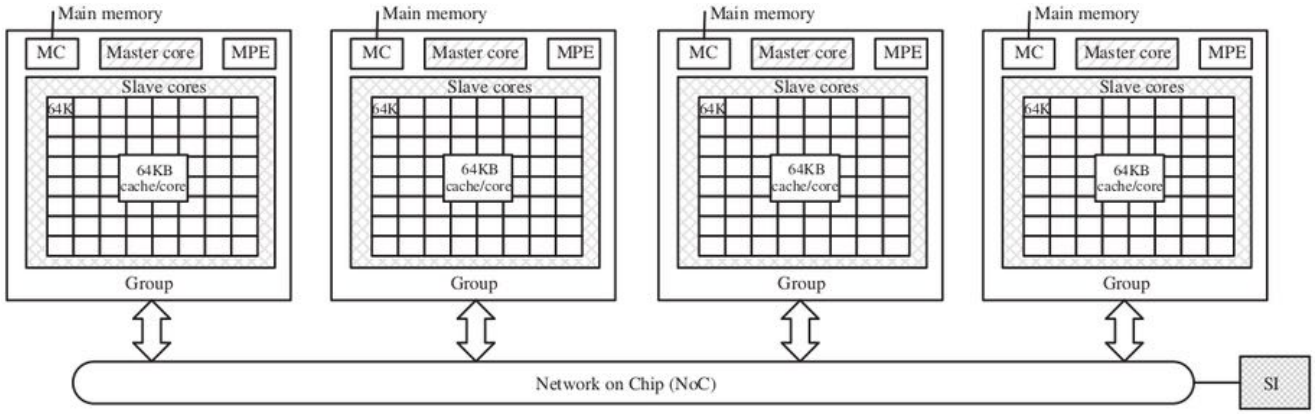
- **USC-HPC: 13,440 cores, 0.62 Pflop/s**
- **CACS: 4,096 cores**
- **CACS-INCITE: 200M core-hours/year on 786,432-core 8.6 Pflop/s Blue Gene/Q at Argonne Nat'l Lab**

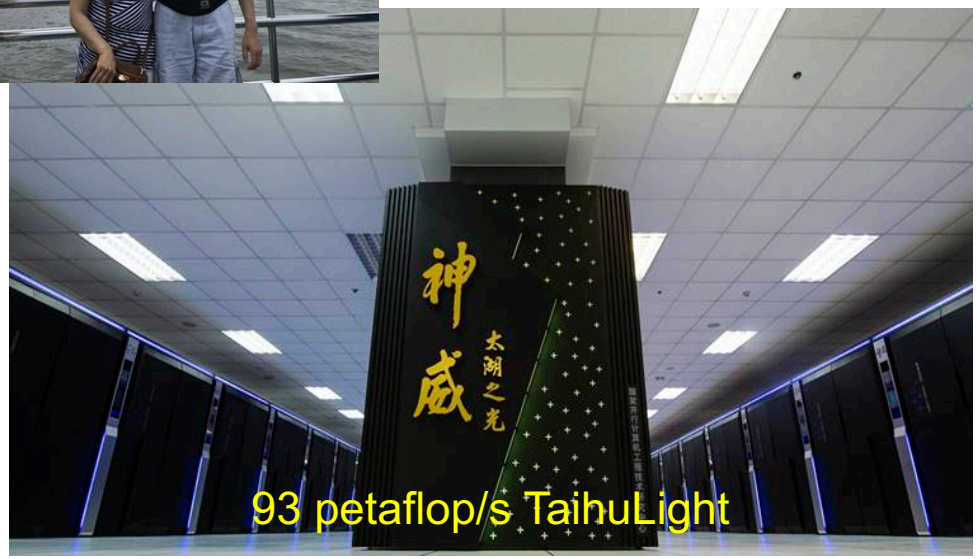


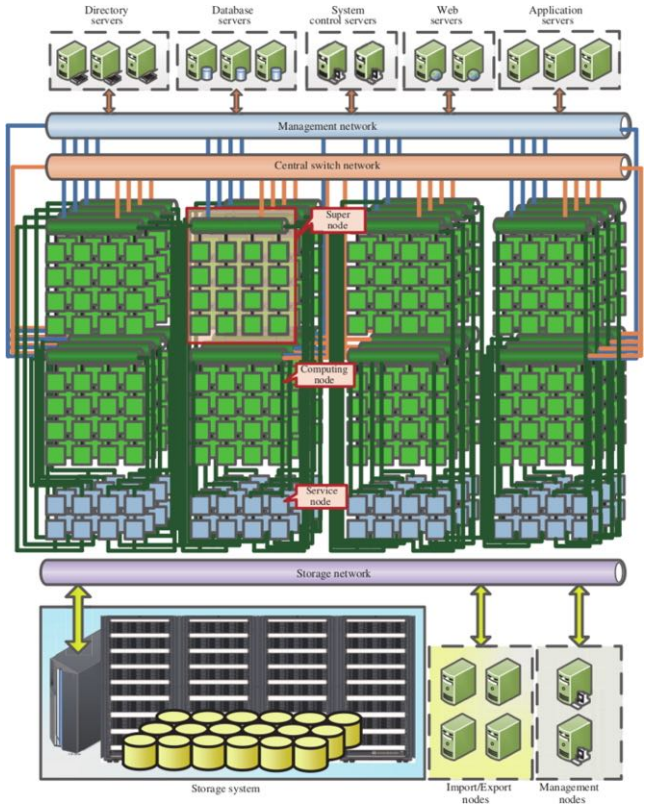
See lecture on "Beowulf clusters"

TaihuLight

256 cores/Sunway SW26010 processor × 40,960 = 10,485,760 cores

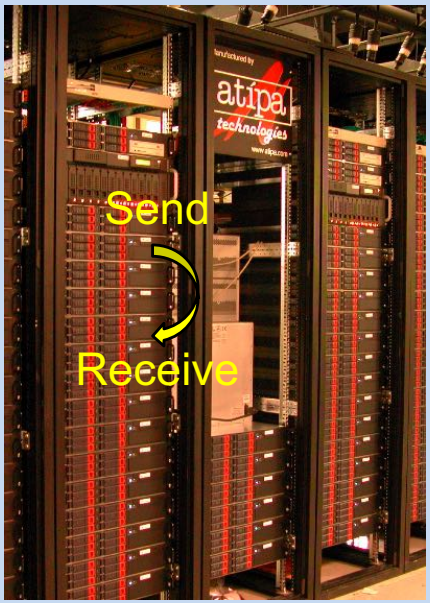






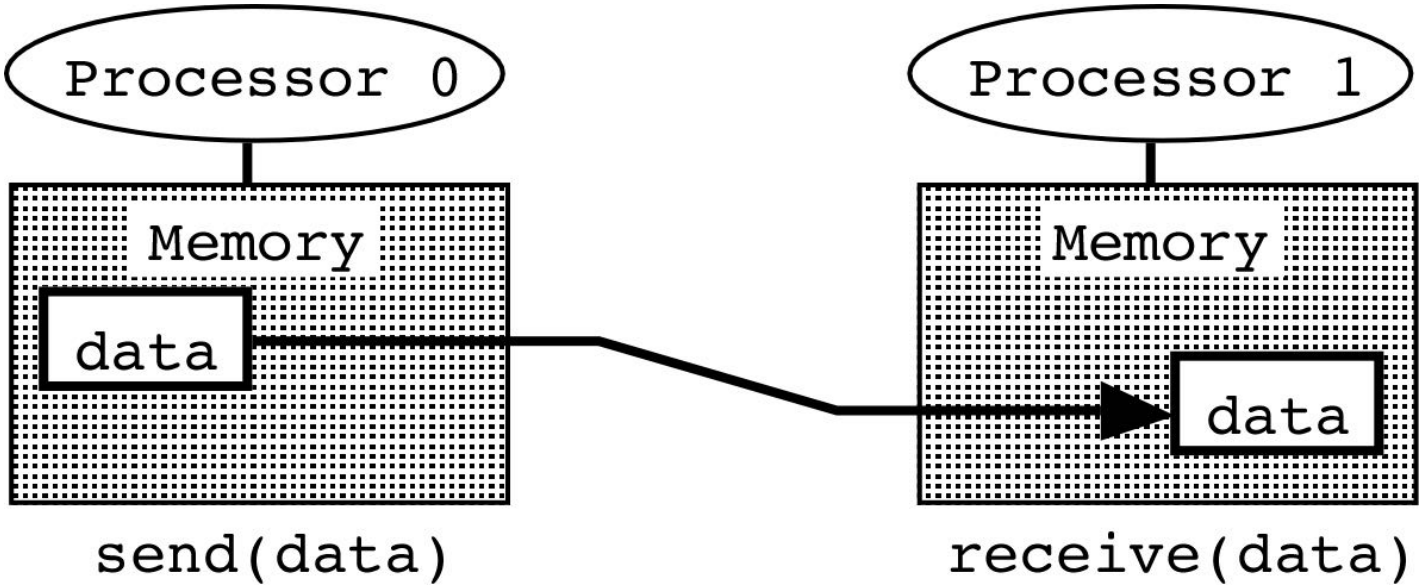
MPI Programming

```
#include "mpi.h"
#include <stdio.h>
main(int argc, char *argv[]) {
  MPI_Status status;
  int myid;
  int n;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myid);
  if (myid == 0) {
    n = 777;
    MPI_Send(&n, 1, MPI_INT, 1, 10, MPI_COMM_WORLD);
  }
  else {
    MPI_Recv(&n, 1, MPI_INT, 0, 10, MPI_COMM_WORLD, &status);
    printf("n = %d\n", n);
  }
  MPI_Finalize();
}
```



http://www.mcs.anl.gov/mpi

Single Program Multiple Data (SPMD)



Process 0

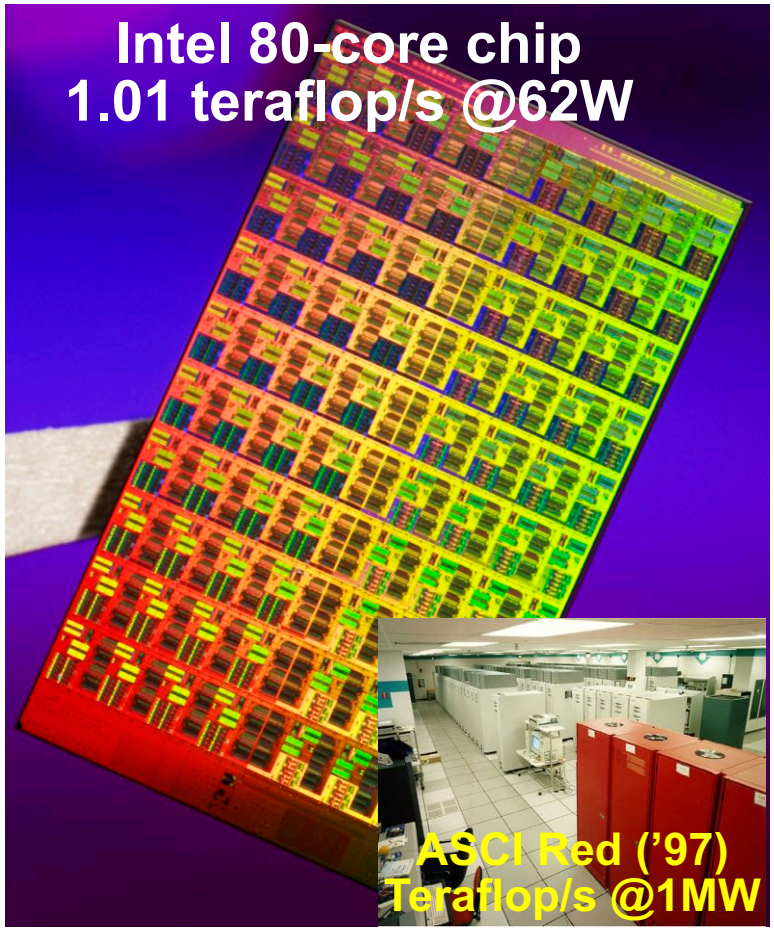
```
if (myid == 0) {
  n = 777;
  MPI_Send(&n,...);
}
else {
  MPI_Recv(&n,...);
  printf(...);
}
```

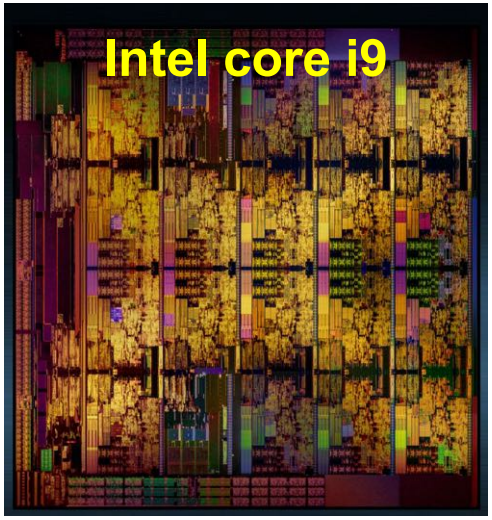
Process 1

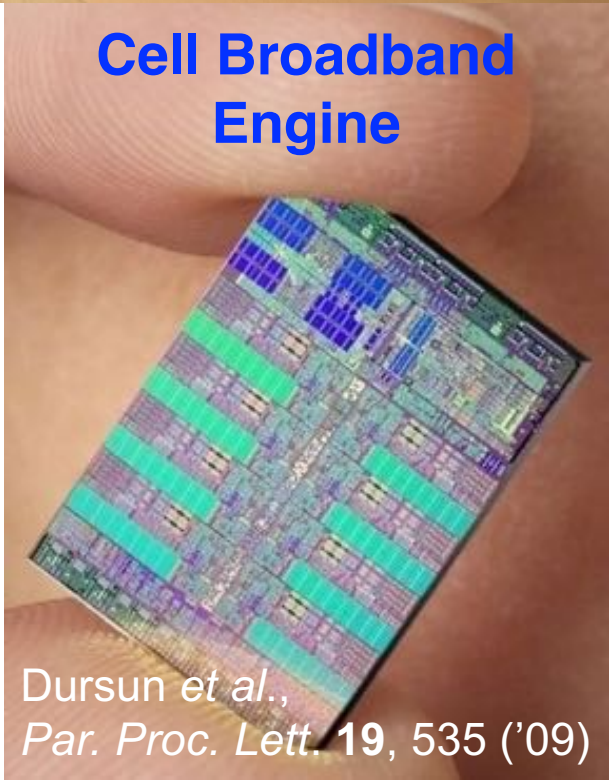
```
if (myid == 0) {
  n = 777;
  MPI_Send(&n,...);
}
else {
  MPI_Recv(&n,...);
  printf(...);
}
```

Parallel computing: Specifies "Who does what"

Multicore Processors







- **Multiple simple processors (or cores) sharing common memory**

Godson-T Many-core Architecture

J. Parallel Distrib. Comput. 73 (2013) 1469–1482

Contents lists available at ScienceDirect

J. Parallel Distrib. Comput.

journal homepage: www.elsevier.com/locate/jpdc

Scalability study of molecular dynamics simulation on *Godson-T* many-core architecture

狗剩

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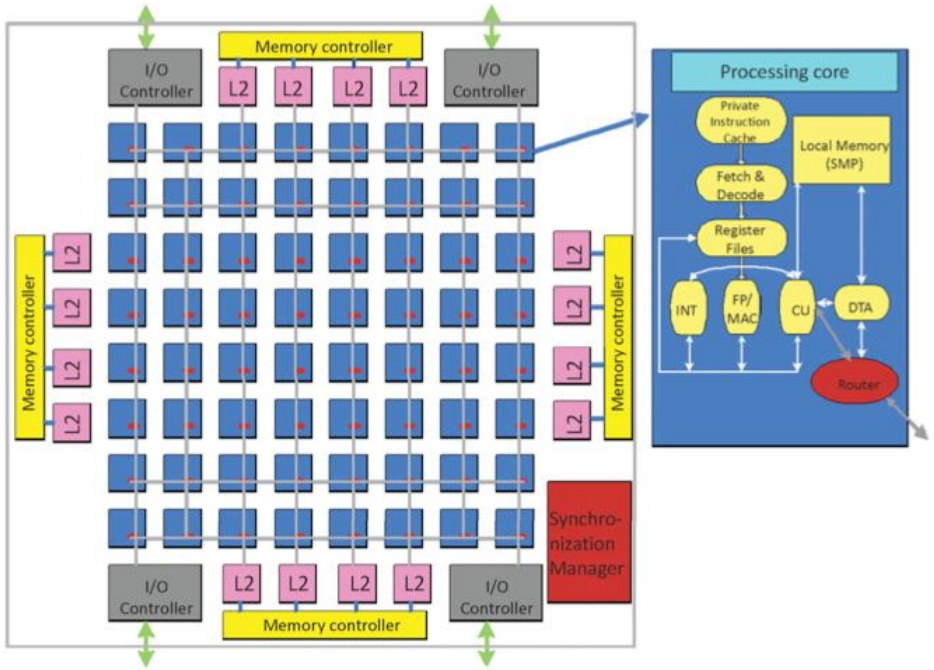
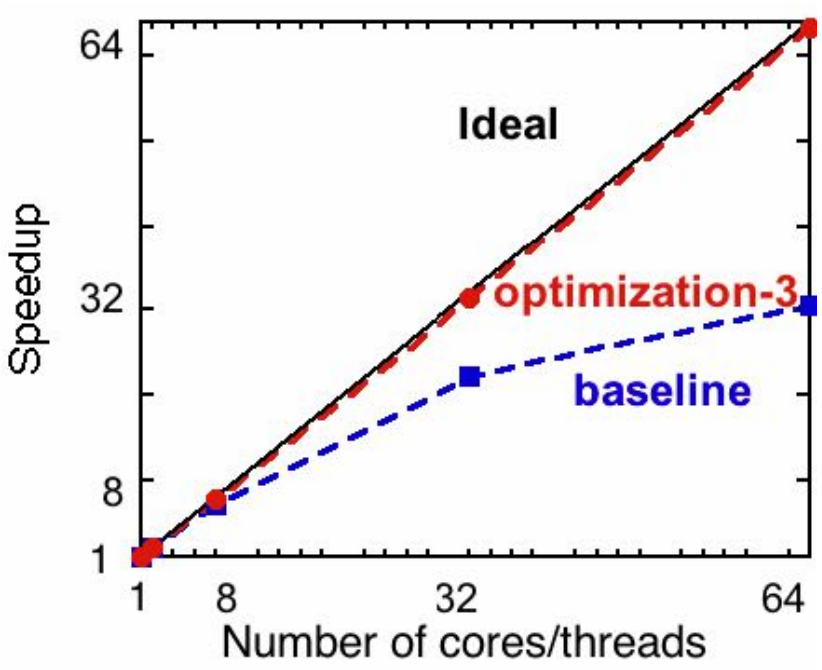
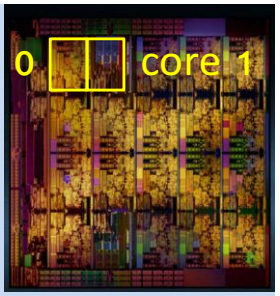




OpenMP Programming




```
#include <stdio.h>
#include <omp.h>
void main () {
  int nthreads,tid;
  nthreads = omp_get_num_threads();
  printf("Sequential section: # of threads = %d\n",nthreads);
  /* Fork multi-threads with own copies of variable */
  #pragma omp parallel private(tid)
  {
    /* Obtain & print thread id */
    tid = omp_get_thread_num();
    printf("Parallel section: Hello world from thread %d\n",tid);
    /* Only master thread does this */
    if (tid == 0) {
      nthreads = omp_get_num_threads();
      printf("Parallel section: # of threads = %d\n",nthreads);}
  } /* All created threads terminate */
}
```

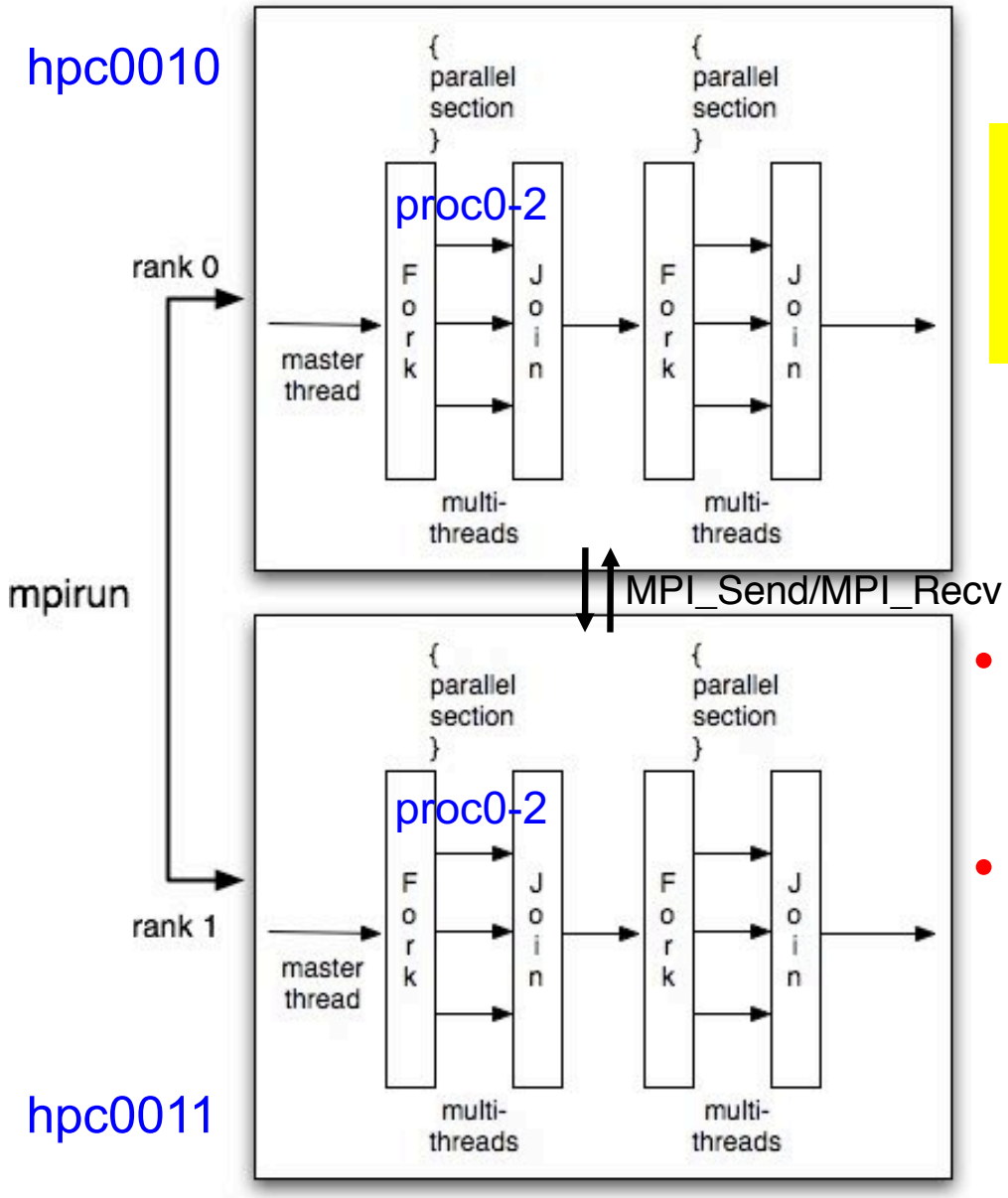
parallel section

- **Obtain the number of threads & my thread ID**
- **By default, all variables are shared unless selectively changing storage attributes using private clauses**

http://www.openmp.org

Hybrid MPI+OpenMP Programming

Each MPI process spawns multiple OpenMP threads




```
In a PBS script:
  mpirun –np 2
In the code:
  omp_set_num_threads(3);
```

- **MPI processes communicate by sending/receiving messages**
- **OpenMP threads communicate by writing to/reading from shared variables**

SIMD Vectorization: MD

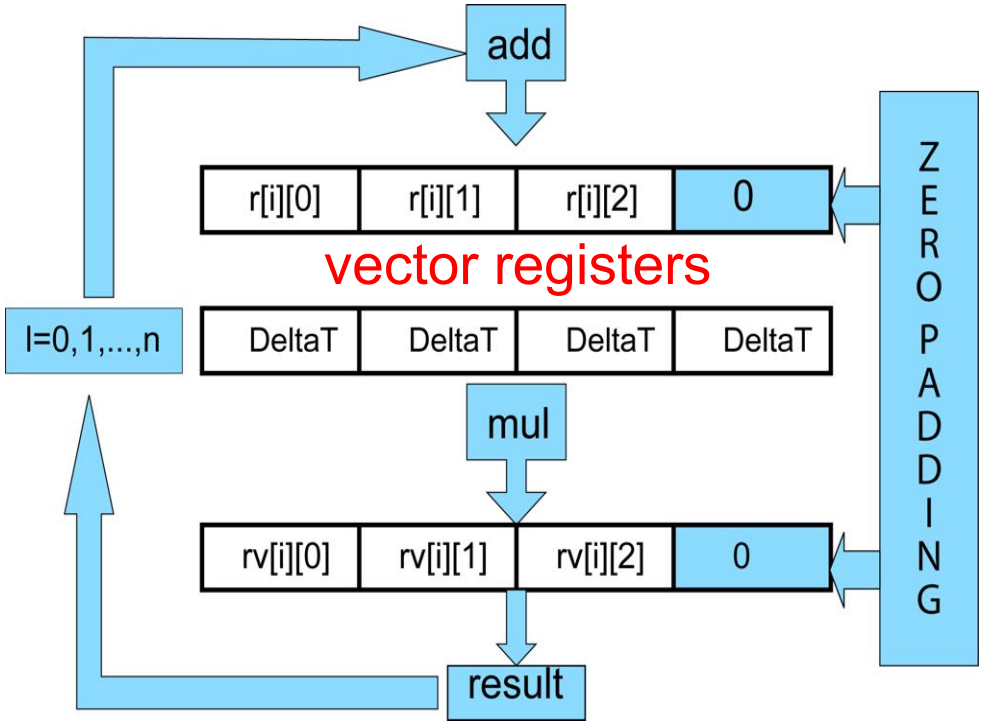
- **Single-instruction multiple-data (SIMD) parallelism using vector registers**

(Example) Zero padding to align complex data in molecular dynamics

Original solution

```
for (i=0; i<N; i++)
  for (a=0; a<3; a++)
    r[i][a] =
    r[i][a] +
    DeltaT*rv[i][a];
```

SIMD solution

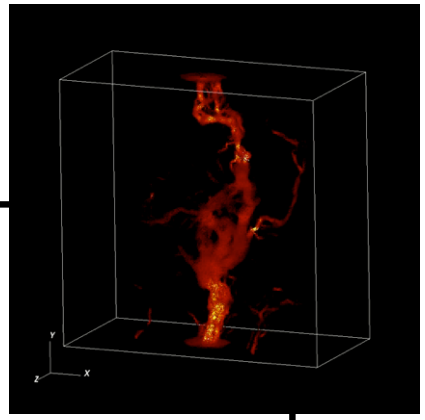


Peng *et al.*, *PDPTA 2009*; *UCHPC 2010; J. Supercomputing* **57**, 20 ('11)

SIMD Vectorization: LBM

- **Translocated statement fusion in lattice-Boltzmann flow simulation**

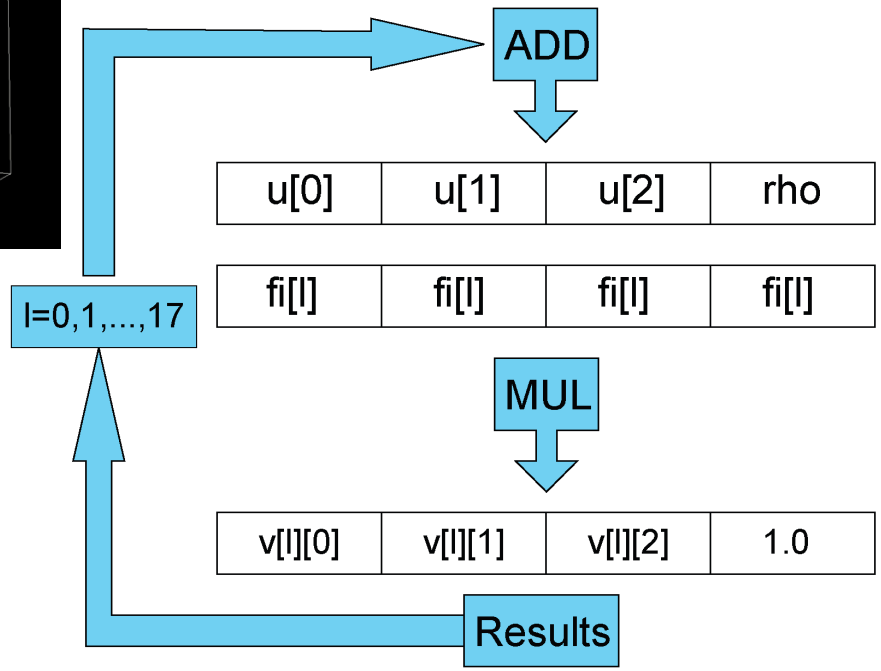
Original solution



```
for(i=0;i<3;i++){
  u[i]=0.0; rho=0.0;
  for(l=0;l<18;l++){
    fi[l] = f[18*cnz+1];
    u[i] += fi[l]*v[l][i];
    rho += fi[l];
  }
}
```

3×18×5 = 270 computation

SIMD solution



18×4 = 72 computation

Ideal Speedup 3.5

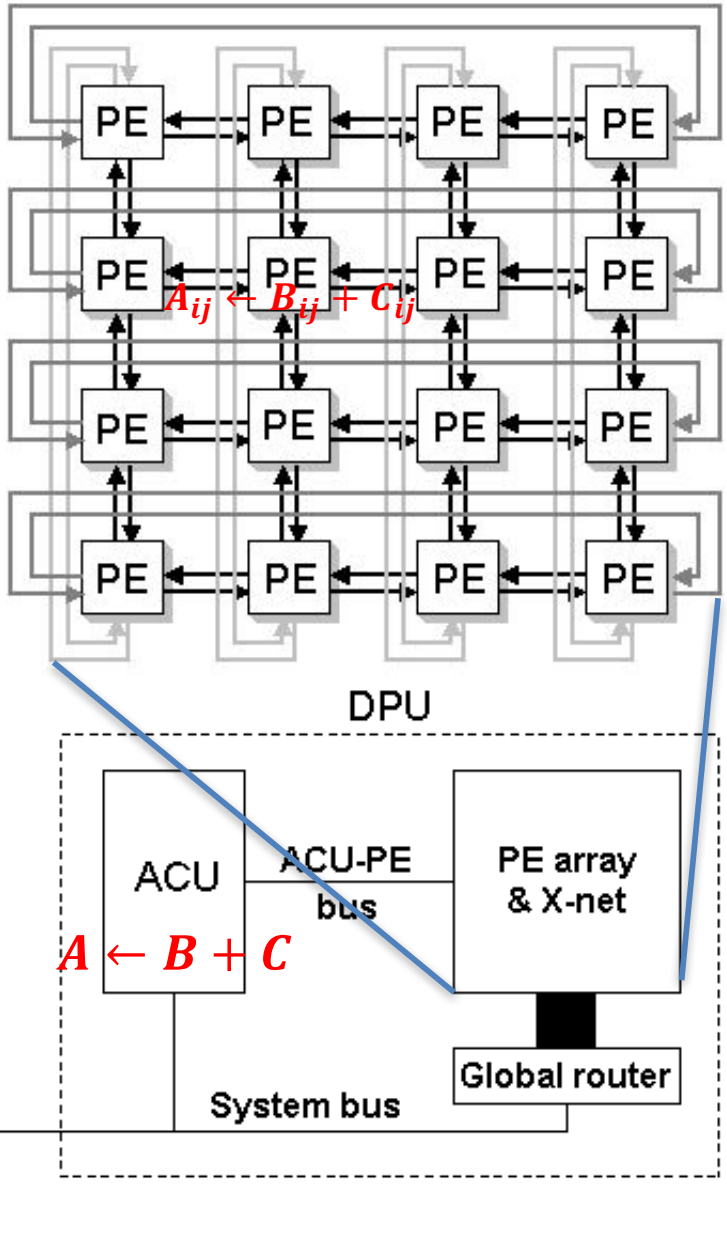
SIMDizable mathematical formulations:
Special relativity, quaternion, *etc.*

$$J^{\alpha} = (c\rho, j^1, j^2, j^3)$$

$$A^{\alpha} = (\phi/c, A^1, A^2, A^3)$$

$$\boxdot A^{\alpha} = \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) A^{\alpha} = \frac{4\pi}{c} J^{\alpha}$$

Massive SIMD Data Parallelism



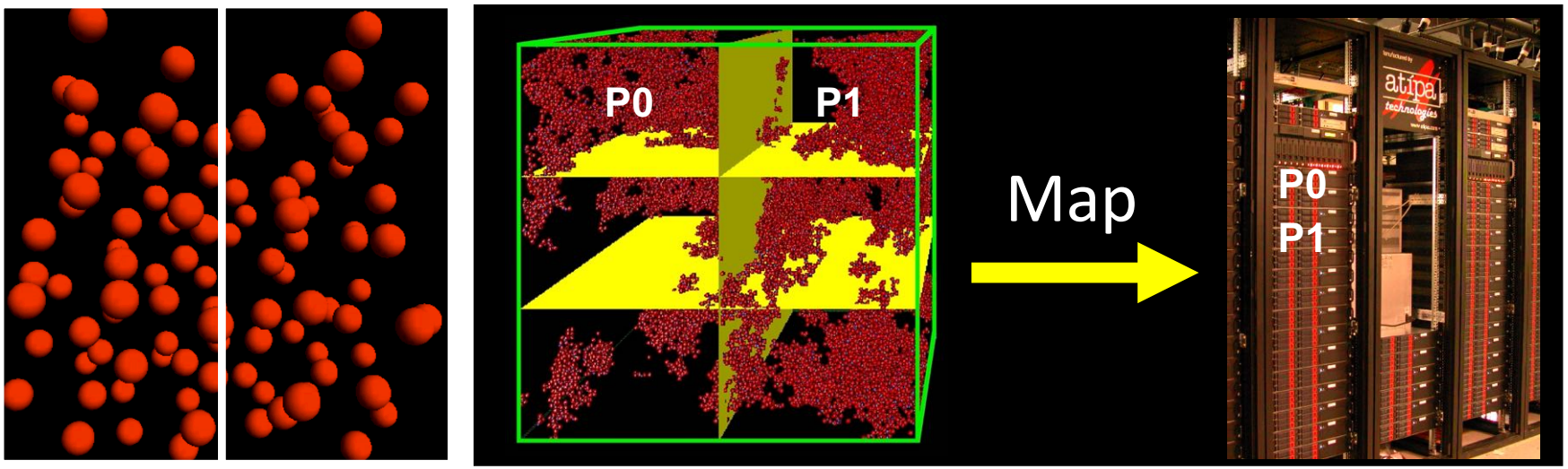
Quantum dynamics on 8,192-processor (128 × 64) MasPar 1208B

Nakano,
Comput. Phys. Commun.
83, 181 ('94)

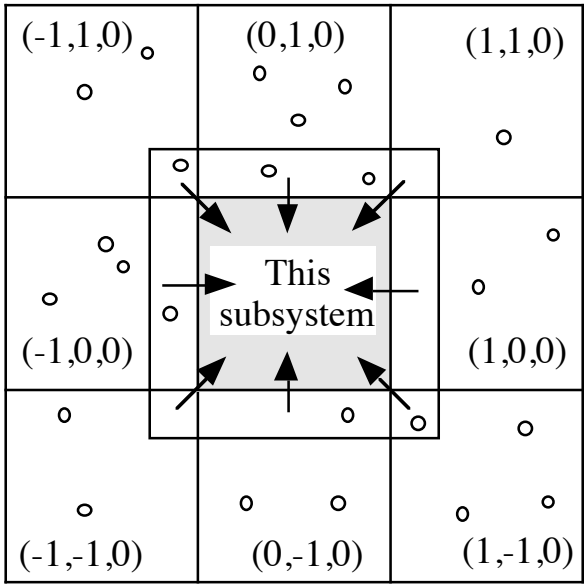
See lecture on "pre-Beowulf parallel computing"

Parallel Molecular Dynamics

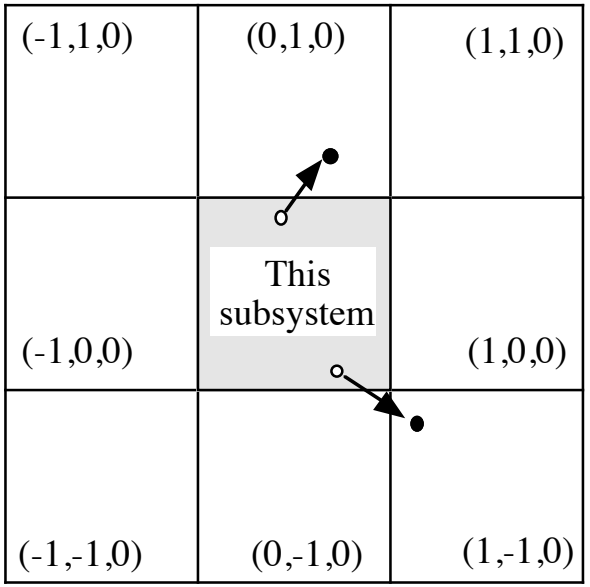
Spatial decomposition (short ranged): $O(N/P)$ computation



Atom caching: $O((N/P)^{2/3})$



Atom migration



See also "parallel quantum dynamics" lecture

History of Particle Simulations

'44 **John von Neumann memo on a stored-program computer:** ***"Our present analytical methods seem unsuitable for the solution of the important problems arising in connection with nonlinear partial differential equations. The really efficient high-speed computing devices may provide us with those heuristic hints which are needed in all parts of mathematics for genuine progress"***

'53 **First Monte Carlo simulation of liquid by Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller on MANIAC at Los Alamos Nat'l Lab**

'55 **Enrico Fermi, John Pasta, and Stanislaw Ulam studied the dynamics of an one-dimensional array of particles coupled by anharmonic springs on MANIAC**

'56 **Dynamics of hard spheres (billiards) studied by Alder and Wainwright at the Lawrence Livermore Nat'l Lab.**

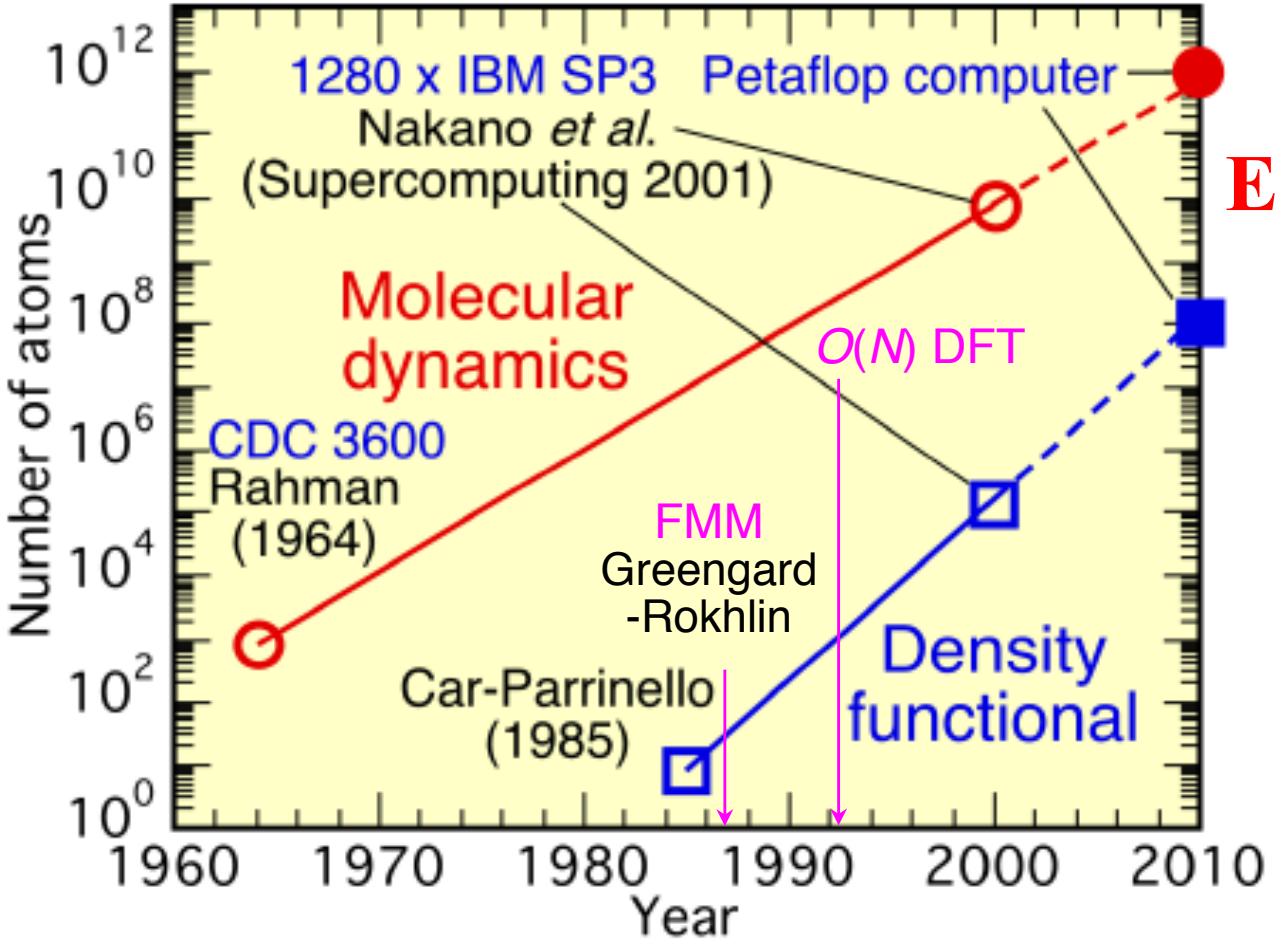
'60 **Radiation damage in crystalline Cu studied with short-range repulsion and uniform attraction toward the center by George Vineyard's group at Brookhaven Nat'l Lab**

'64 **First MD simulation of liquid (864 argon atoms) using interatomic potentials by Aneesur Rahman at the Argonne Nat'l Lab on a CDC 3600**

Moore's Law in Scientific Computing

Number of particles in MD simulations has doubled:

- **Every 19 months in the past 50 years for classical MD**
- **Every 22 months in the past 30 years for DFT-MD**



Exaflop/s?

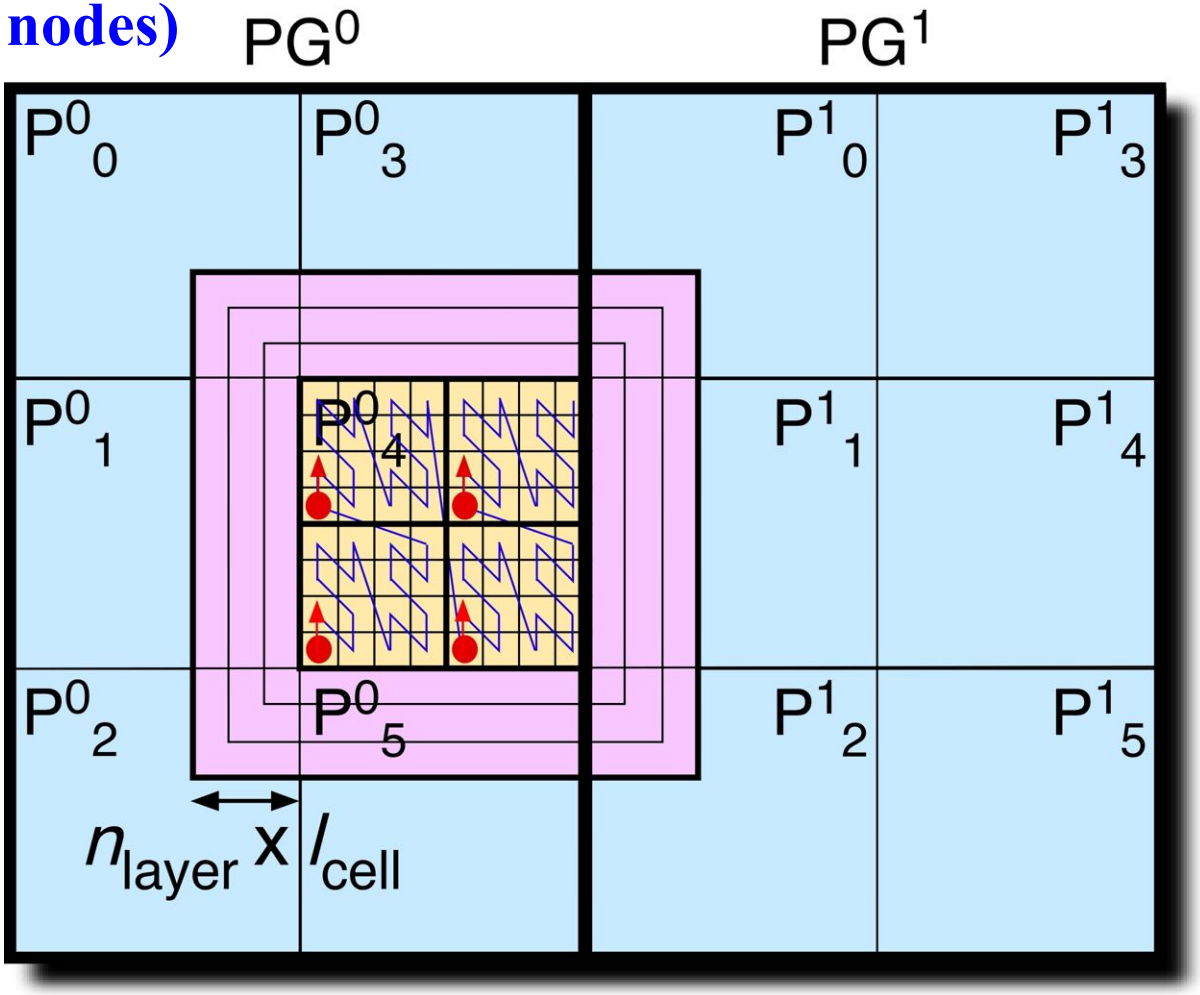
2014: 10^{12}-atom MD & 10^{8}-electron DFT on a 10 petaflop/s Blue Gene/Q with advances in algorithmic & parallel-computing techniques

Tunable Hierarchical Cellular Decomposition

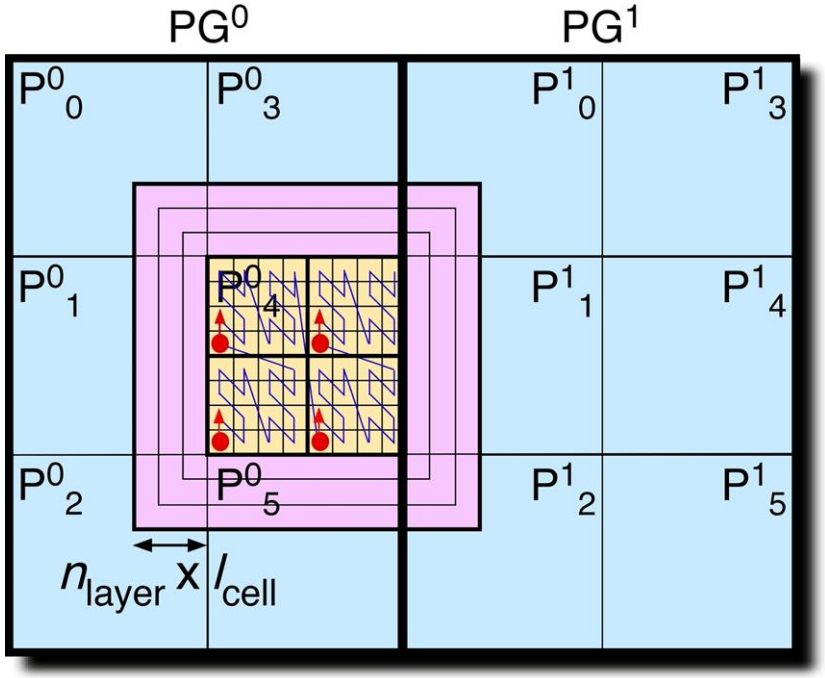
Mapping $O(N)$ divide-&-conquer algorithms onto memory hierarchies

- Spatial decomposition with data "caching" & "migration"
- Computational cells (*e.g.* linked-list cells in MD) < cell blocks (threads) < processes ($P^{\gamma}{}_{\pi}$, spatial decomposition subsystems) < process groups (P^{γ}, Grid nodes)
- Multilayer cellular decomposition (MCD) for n-tuples (n = 2–6)
- Tunable cell data & computation structures: Data/computation re-ordering & granularity parameterized at each decomposition level
- Tunable hybrid MPI + OpenMP + SIMD implementation

Nomura *et al.*, *IPDPS 2009*

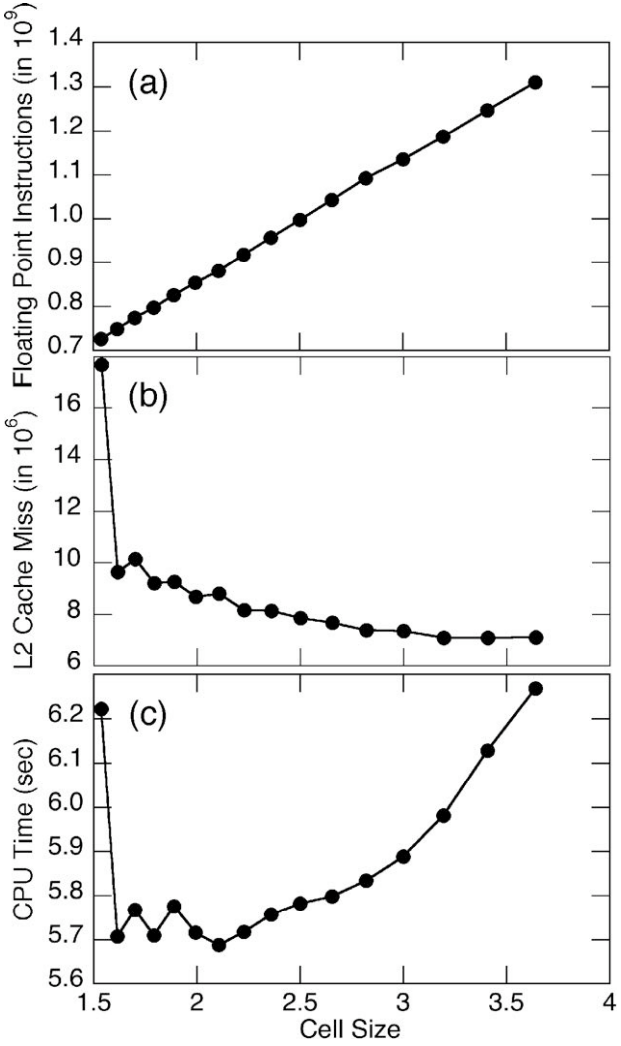


Performance Tunability



Floating-point operation/L2 cache miss trade-off:

331,776-atom silica MRMD on 1.4GHz Pentium III



MPI/OpenMP parallelism trade-off:

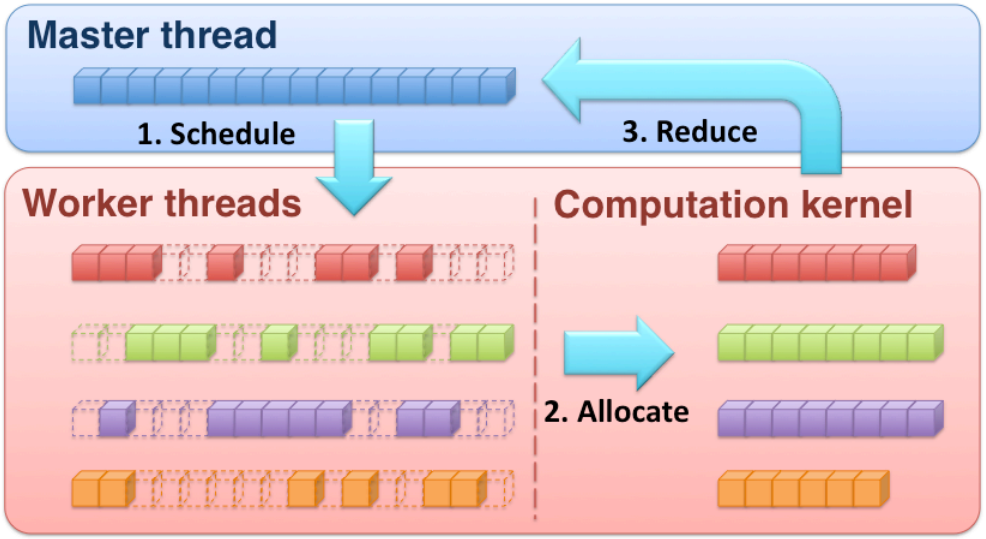
8,232,000-atom silica MRMD & 290,304-atom RDX F-ReaxFF on 8-way 1.5 GHz Power4

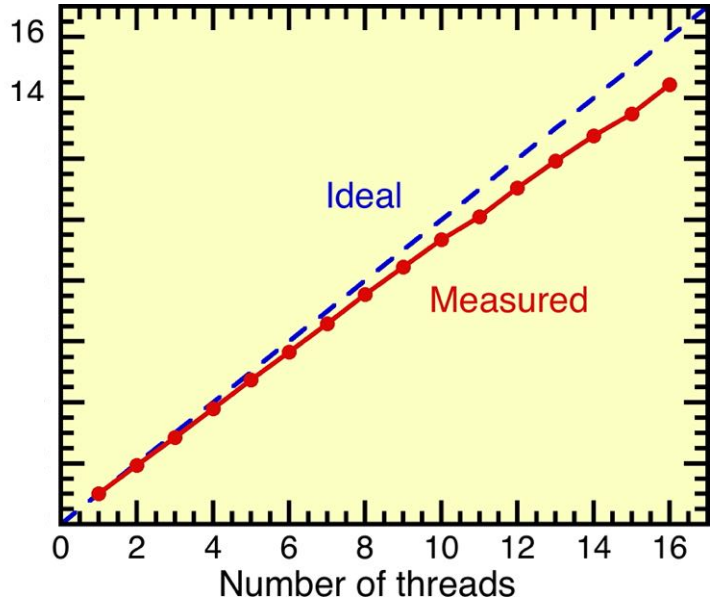
Number of OpenMP threads, n_{td}	Number of MPI processes, n_p	Execution time/MD time step (sec)	
		MRMD	P-ReaxFF
1	8	4.19	62.5
2	4	5.75	58.9
4	2	8.60	54.9
8	1	12.5	120

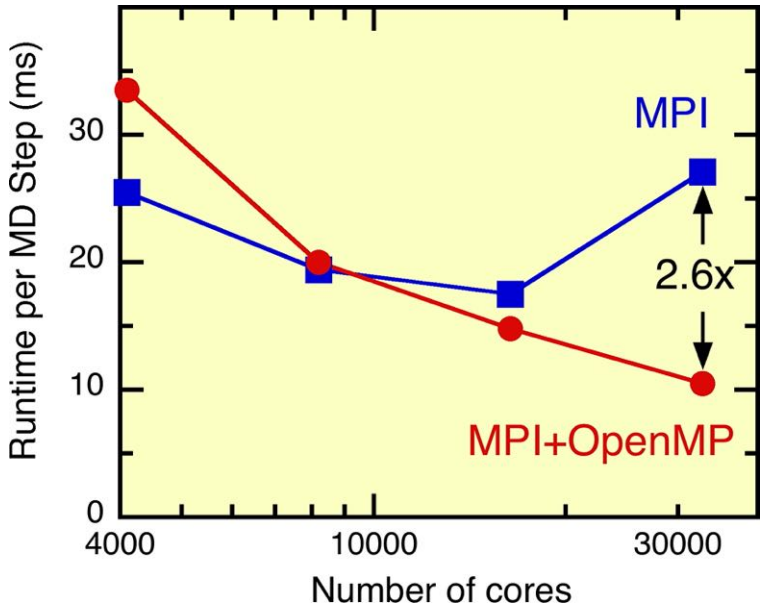
Spatially Compact Thread Scheduling

Concurrency-control mechanism: Data privatization

- **Reduced memory:** # of atoms / # of threads
  $\Theta(nq) \rightarrow \Theta(n+n^{2/3}q^{1/3})$
- **Strong scaling parallel efficiency 0.9 on quad quad-core AMD Opteron**
- **2.6× speedup over MPI by hybrid MPI+OpenMP on 32,768 IBM Blue Gene/P cores**







M. Kunaseth *et al.*, *PDPTA'11*; *J. Supercomput.* ('13)

Concurrency-Control Mechanisms

A number of concurrency-control mechanisms (CCMs) are provided by OpenMP to coordinate multiple threads:

- **Critical section: Serialization**
- **Atomic update: Expensive hardware instruction**
- **Data privatization: Requires large memory $\Theta(nq)$**
- **Hardware transactional memory: Rollbacks (on IBM Blue Gene/Q)**

# of atoms per node

# of threads

CCM performance varies:

- **Depending on computational characteristics of each program**
- **In many cases, CCM degrades performance significantly**

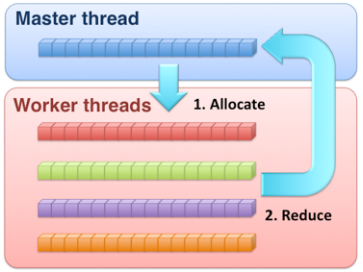
HTM/critical section

```
#pragma omp <critical|tm_atomic>
{
  ra[i][0] += fa*dr[0];
  ra[i][1] += fa*dr[1];
  ra[i][2] += fa*dr[2];
}
```

Atomic update

```
#pragma omp atomic
ra[i][0] += fa*dr[0];
#pragma omp atomic
ra[i][1] += fa*dr[1];
#pragma omp atomic
ra[i][2] += fa*dr[2];
```

Data privatization



Goal: Provide a guideline to choose the "right" CCM

Hardware Transactional Memory

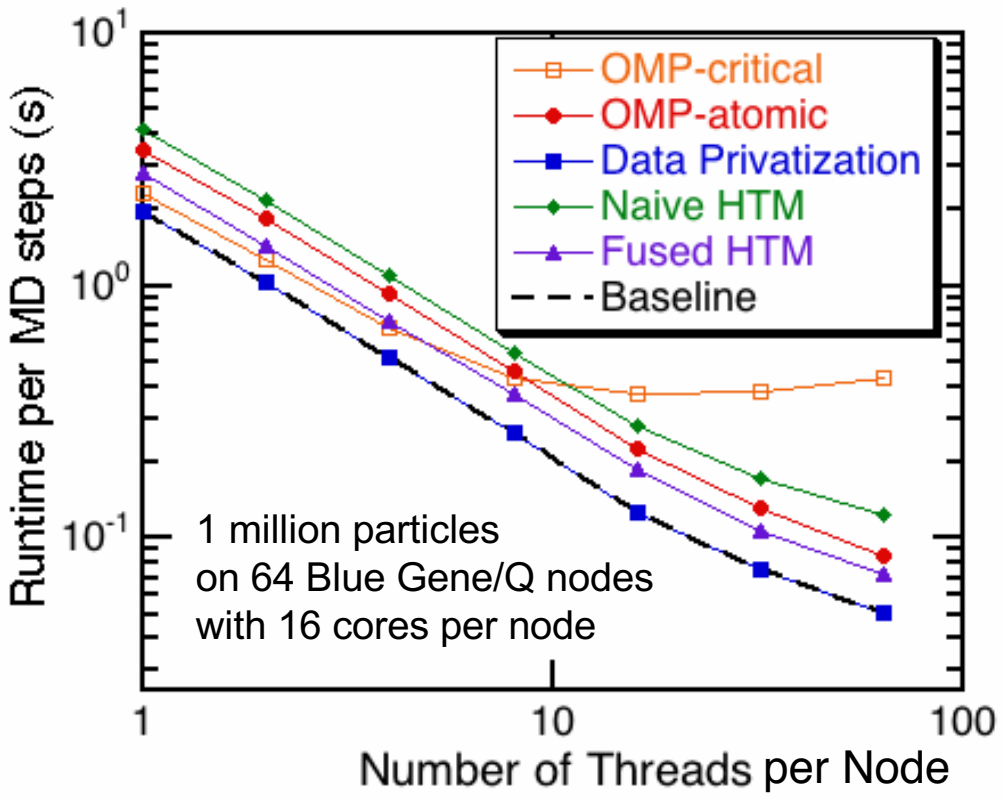
Transactional memory (TM): An opportunistic CCM

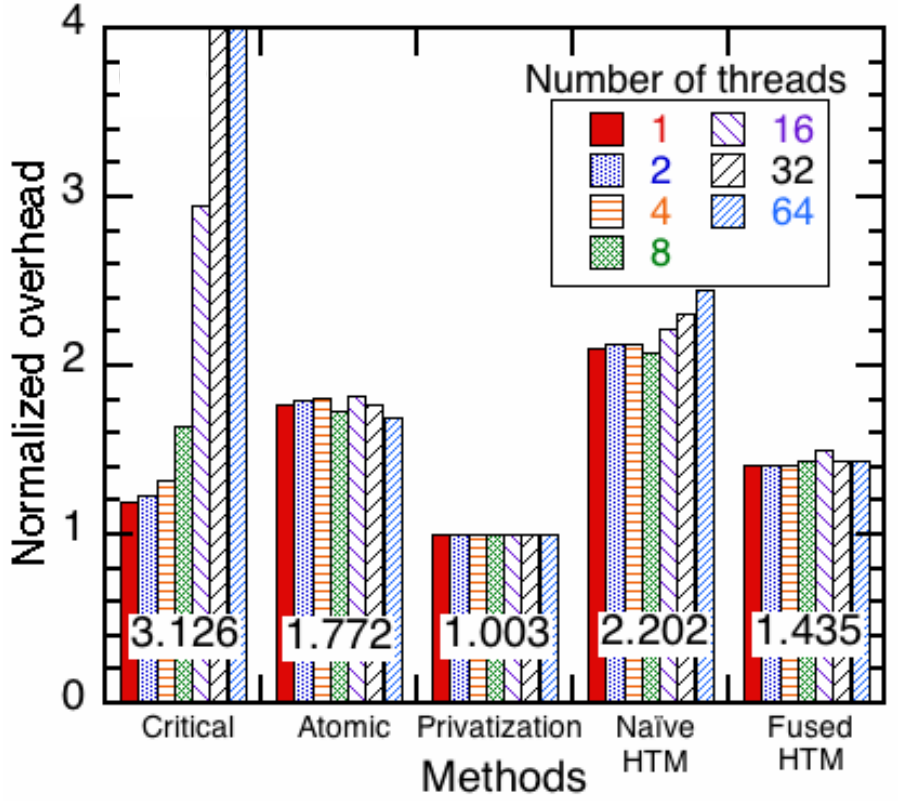
- **Avoids memory conflicts by monitoring a set of speculative operations (*i.e.* transaction)**
- **If two or more transactions write to the same memory address, transaction(s) will be restarted—a process called rollback**
- **If no conflict detected in the end of a transaction, operations within the transaction becomes permanent (*i.e.* committed)**
- **Software TM usually suffers from large overhead**

Hardware TM on IBM Blue Gene/Q:

- **The first commercial platform implementing TM support at hardware level *via* multiversioned L2-cache**
- **Hardware support is expected to reduce TM overhead**
- **Performance of HTM on molecular dynamics has not been quantified**

Strong-Scaling Benchmark for MD





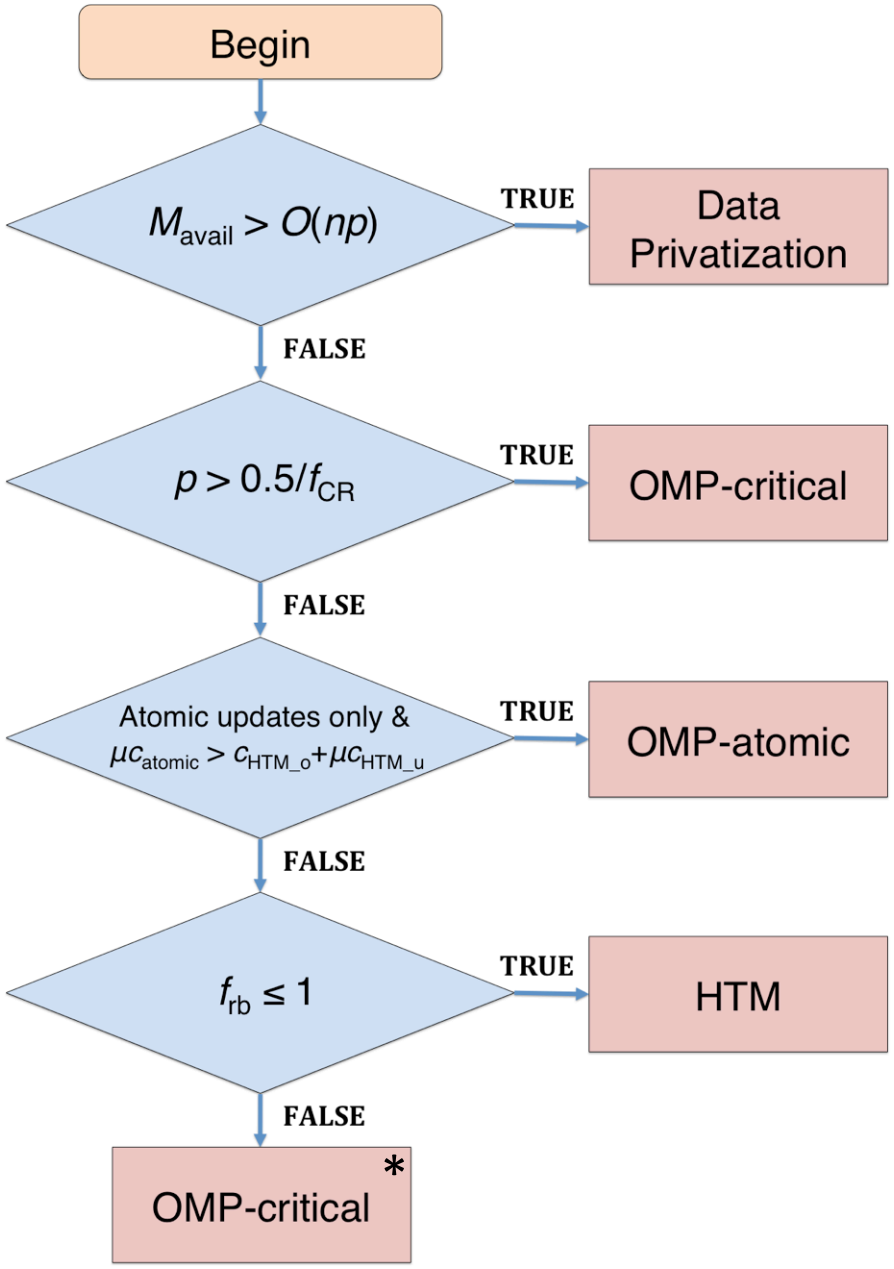
*Baseline: No CCM; the result is wrong

Developed a fundamental understanding of CCMs:

- **OMP-critical has limited scalability on larger number of threads ($q > 8$)**
- **Data privatization is the fastest, but it requires $\Theta(nq)$ memory**
- **Fused HTM performs the best among constant-memory CCMs**

M. Kunaseth *et al.*, *PDSEC'13*

Threading Guideline for Scientific Programs



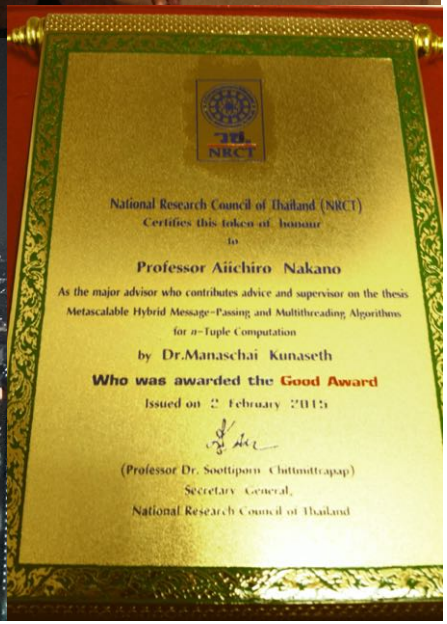
M. Kunaseth *et al.*, *PDSEC'13*

Focus on minimizing runtime (best performance):

- **Have enough memory → data privatization**
- **Conflict region is small → OMP-critical**
- **Small amount of updates → OMP-atomic**
- **Conflict rate is low → HTM**
- **Other → OMP-critical* (poor performance)**

Concurrency control mechanism	Parallel efficiency
OMP-critical	$e = \min(\frac{1}{pf_{CR}}, 1)$
OMP-atomic	$e = \frac{t_{total}}{t_{total} + m\mu c_{atomic}}$
Data privatization	$e = \frac{t_{total}}{t_{total} + c_{reduction} n \log p}$
HTM	$e = \frac{t_{total}}{t_{total} + m(c_{HTM\_overhead} + \mu c_{HTM\_update})}$

IEEE PDSEC Best Paper & Beyond



GPU Programming: CUDA

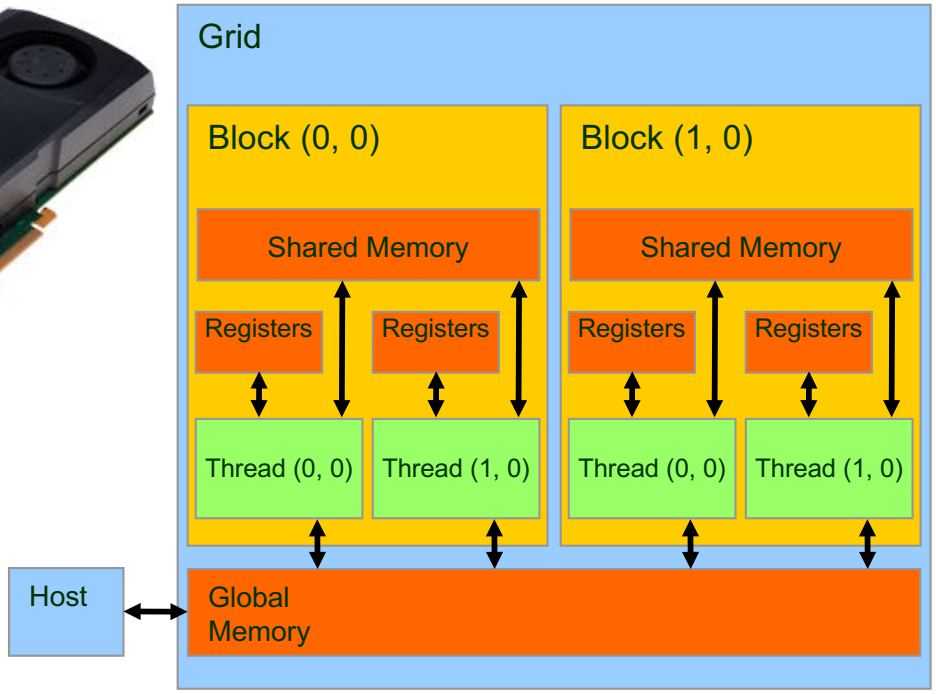
- **Compute Unified Device Architecture**
- **Integrated host (CPU) + device (GPU) application programming interface based on C language developed at NVIDIA**
- **CUDA homepage**

  `http://www.nvidia.com/object/cuda_home_new.html`
- **Compilation**

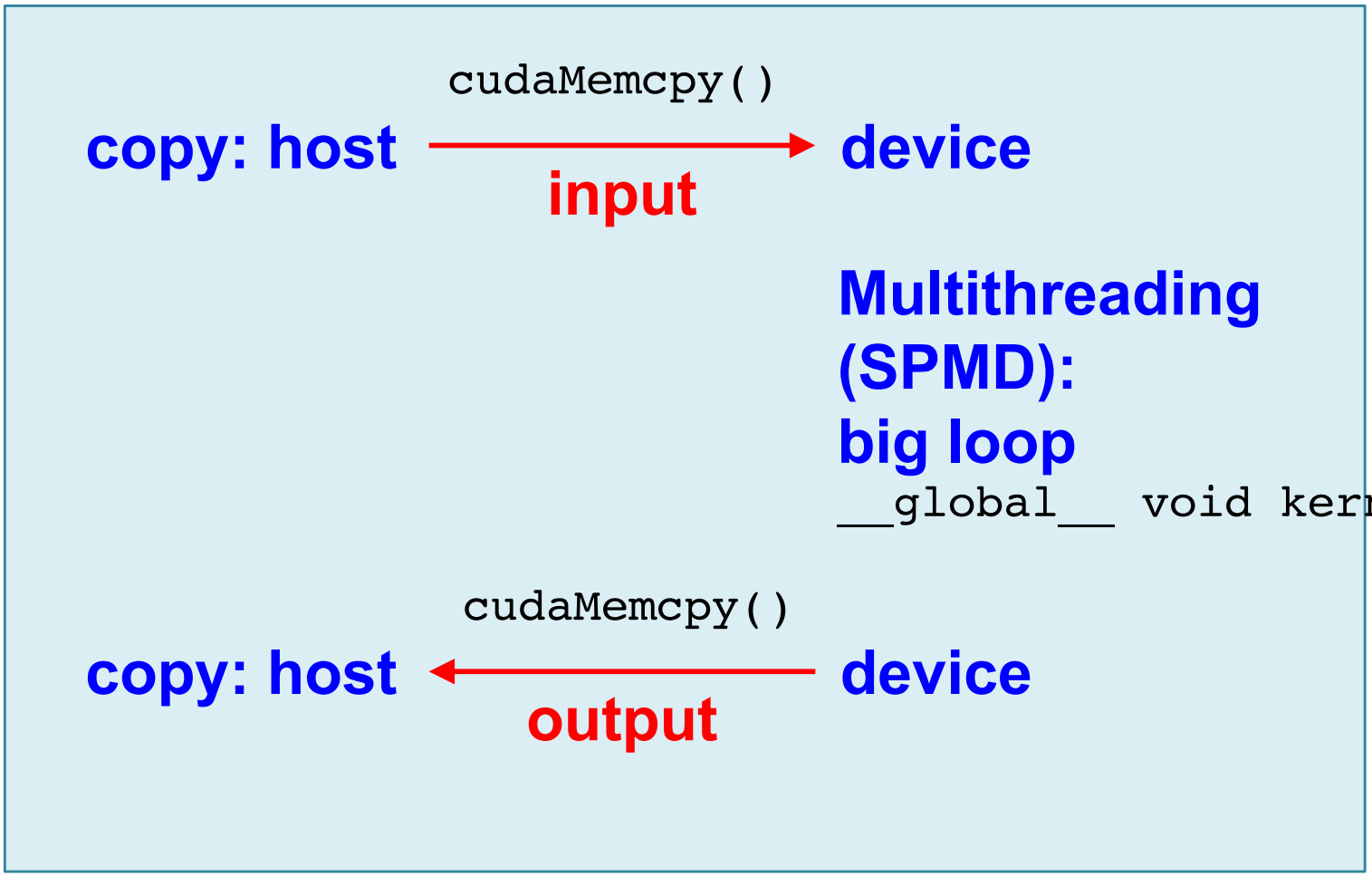
  `$ nvcc pi.cu`
- **Execution**

  `$ a.out`

  `PI = 3.141593`



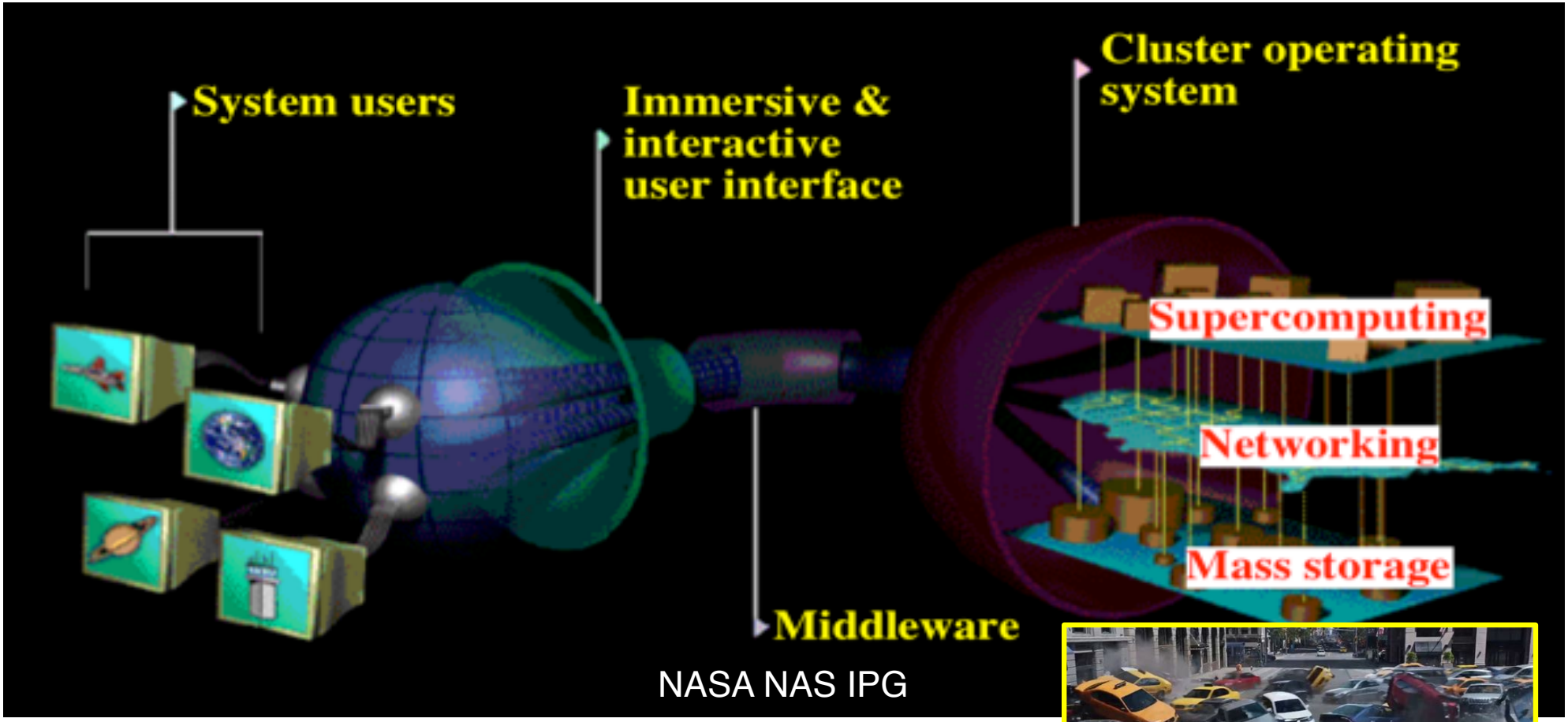
Summary: CUDA Computing



See http://cacs.usc.edu/education/cs596.html

Grid Computing

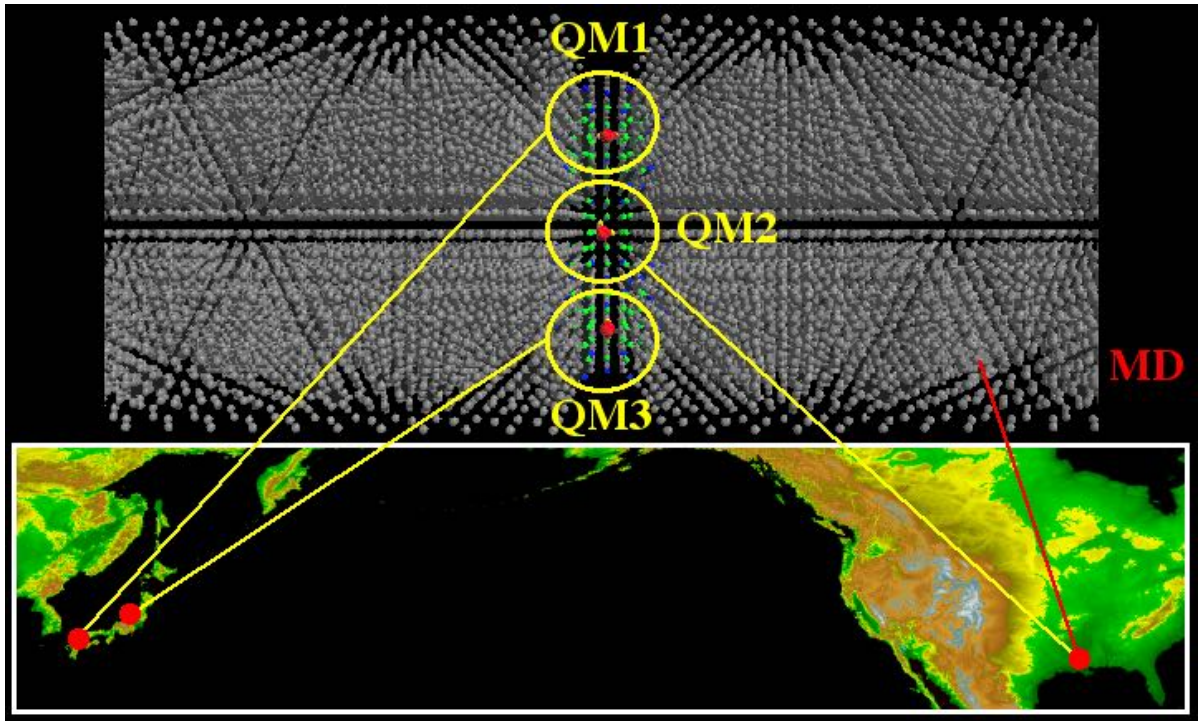
- **World Wide Web:** Universal interface to digital library on the Internet
- **Information Grid:** Pervasive (from any place in the world at any time) access to everything (computing, mass storage, experimental equipments, distributed sensors, *etc*., on high-speed networks)

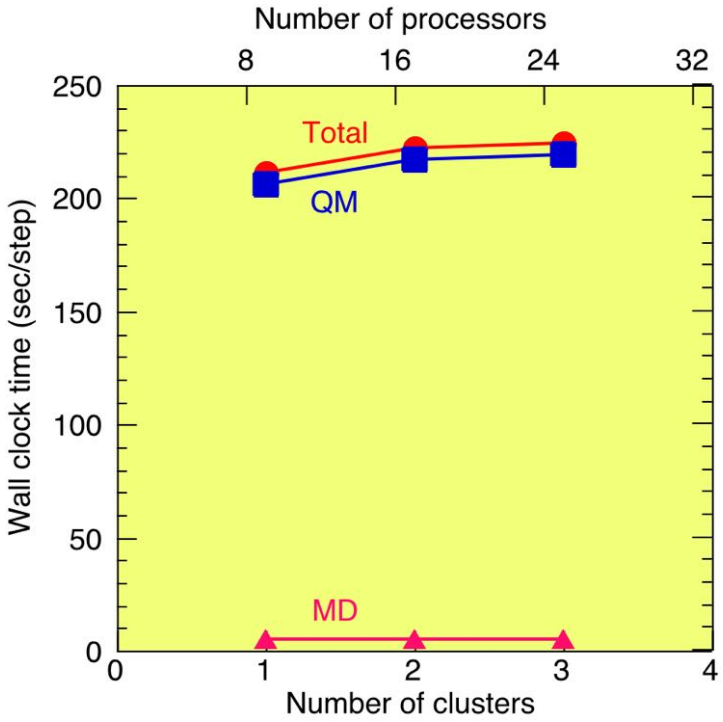


Global Collaborative Simulation

Multiscale MD/QM simulation on a Grid of distributed PC clusters in the US & Japan

- Task decomposition (MPI Communicator) + spatial decomposition
- MPICH-G2/Globus





Japan: Yamaguchi—65 P4 2.0GHz
Hiroshima, Okayama, Niigata—3×24 P4 1.8GHz
US: Louisiana—17 Athlon XP 1900+

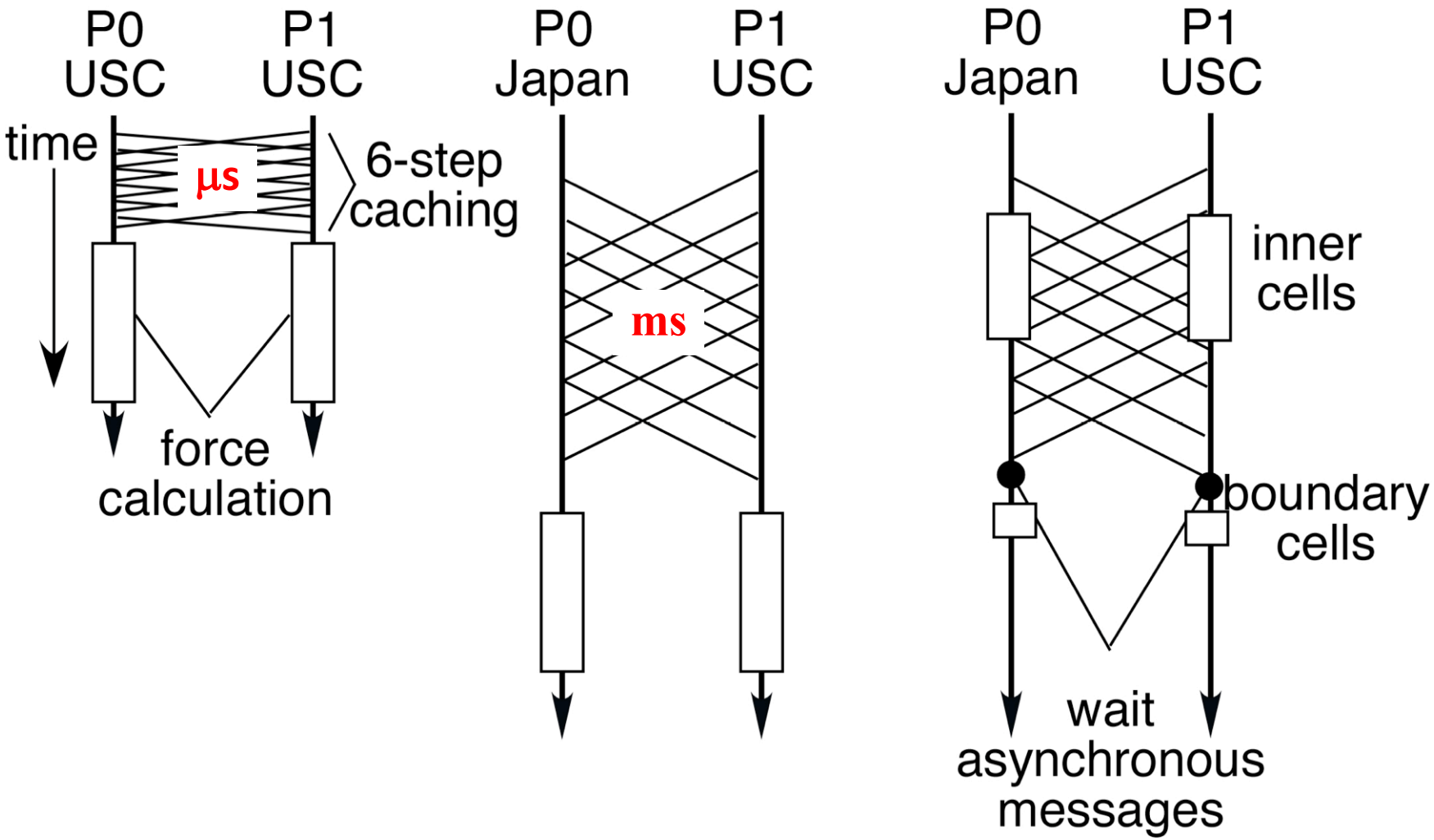
MD — 91,256 atoms
QM (DFT) — 76*n* atoms on *n* clusters

- Scaled speedup, $P = 1$ (for MD) + $8n$ (for QM)
- Efficiency = 94.0% on 25 processors over 3 PC clusters

Kikuchi *et al.*
IEEE/ACM SC02

Internode Optimization

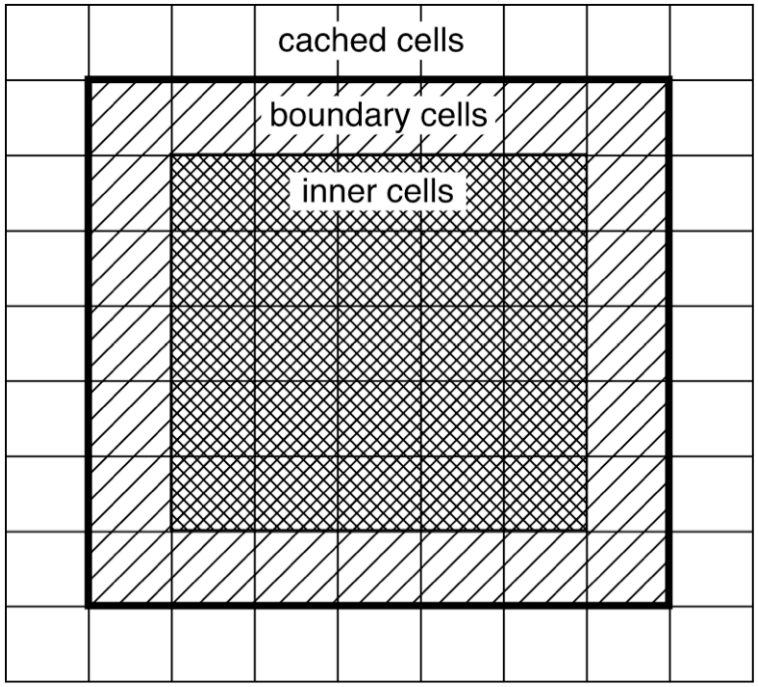
- **Communication bottleneck in metacomputing on a Grid**



Grid-Enabled MD Algorithm

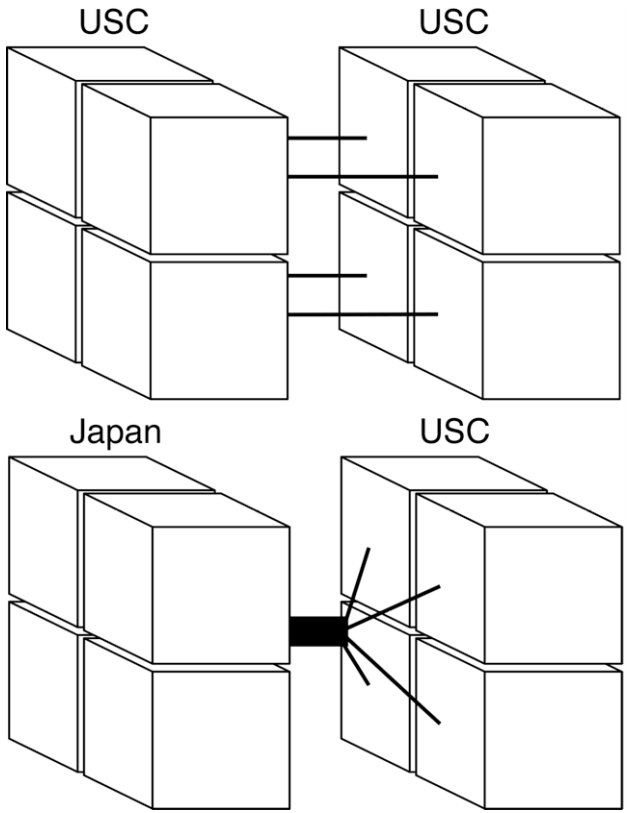
Grid MD algorithm:

1. asynchronous receive of cells to be cached **MPI_Irecv()**
2. send atomic coordinates in the boundary cells
3. compute forces for atoms in the inner cells
4. wait for the completion of the asynchronous receive **MPI_Wait()**
5. compute forces for atoms in the boundary cells



Renormalized Messages:

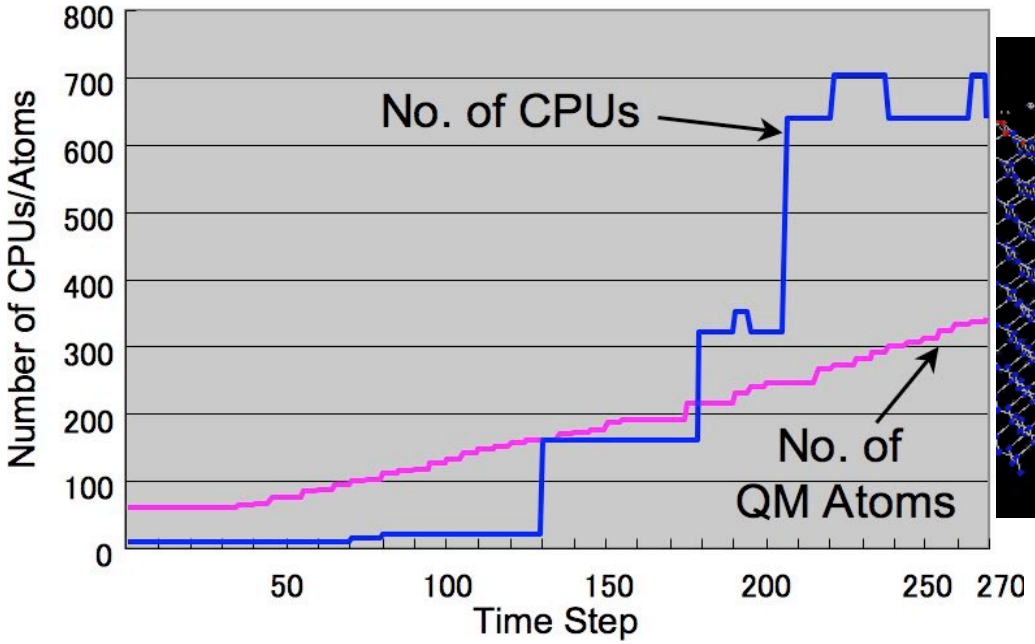
Latency can be reduced by composing a large cross-site message instead of sending all processor-to-processor messages

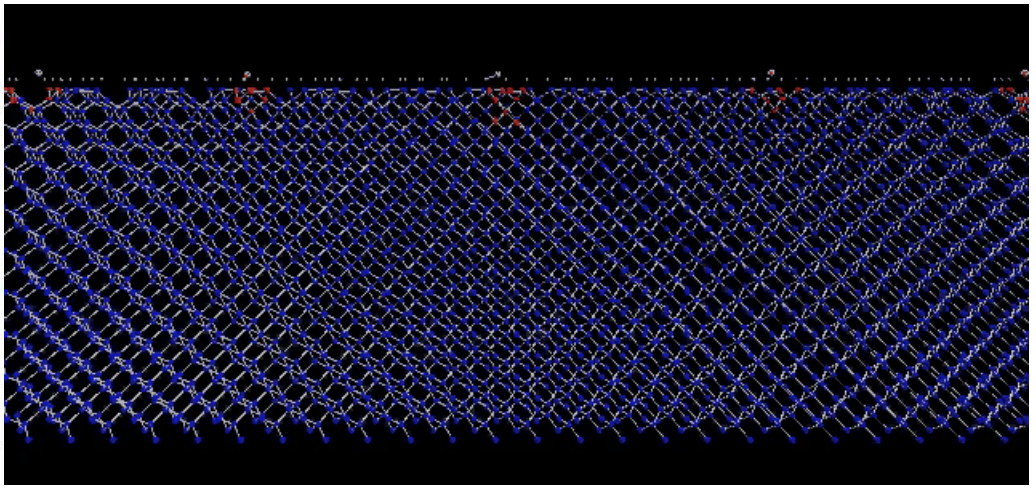


Sustainable Grid Supercomputing

- **Sustained (> months) supercomputing (> 10^3 CPUs) on a Grid of geographically distributed supercomputers**
- **Hybrid Grid remote procedure call (GridRPC) + message passing (MPI) programming**
- **Dynamic allocation of computing resources on demand & automated migration due to reservation schedule & faults**

Ninf-G GridRPC: ninf.apgrid.org; MPICH: www.mcs.anl.gov/mpi





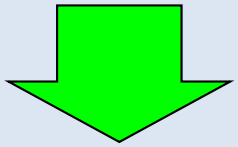
Takemiya *et al.*, *IEEE/ACM SC06*
Song *et al.*, *IJCS* ('09)

Multiscale QM/MD simulation of high-energy beam oxidation of Si

Grid Remote Procedure Call (RPC)

- **Simple RPC API (application program interface)**
- **Existing libraries & applications into Grid applications**
- **IDL (interface definition language) embodying call information, with minimal client-side management**

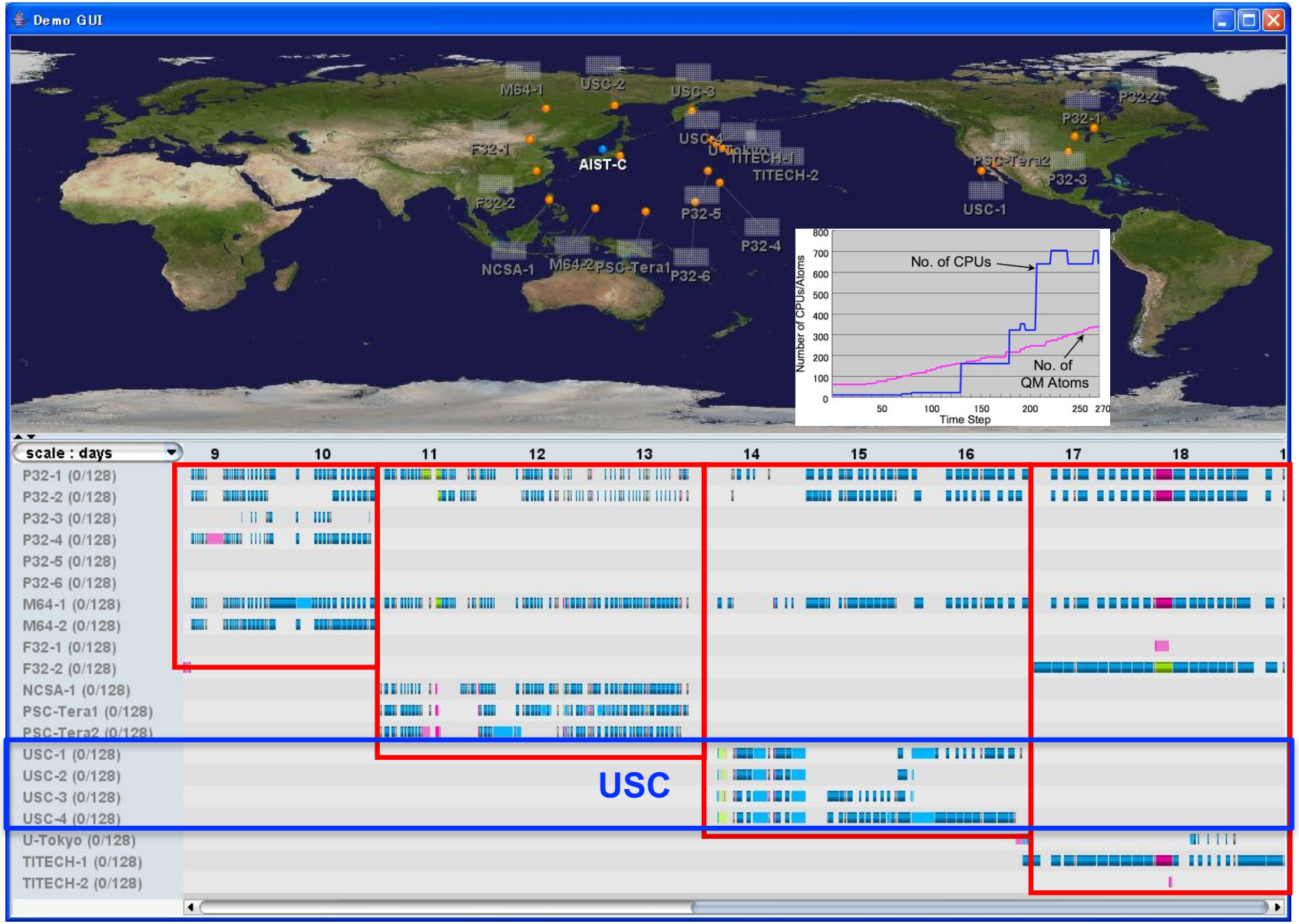
```
double A[n][n],B[n][n],C[n][n];      /* Data Declaration */
dmmul(n,A,B,C);                      /* Call local function */
```



```
grpc_function_handle_default(&hdl, "dmmul");
grpc_call(hdl,n,A,B,C);   /* Call server side routine */
```

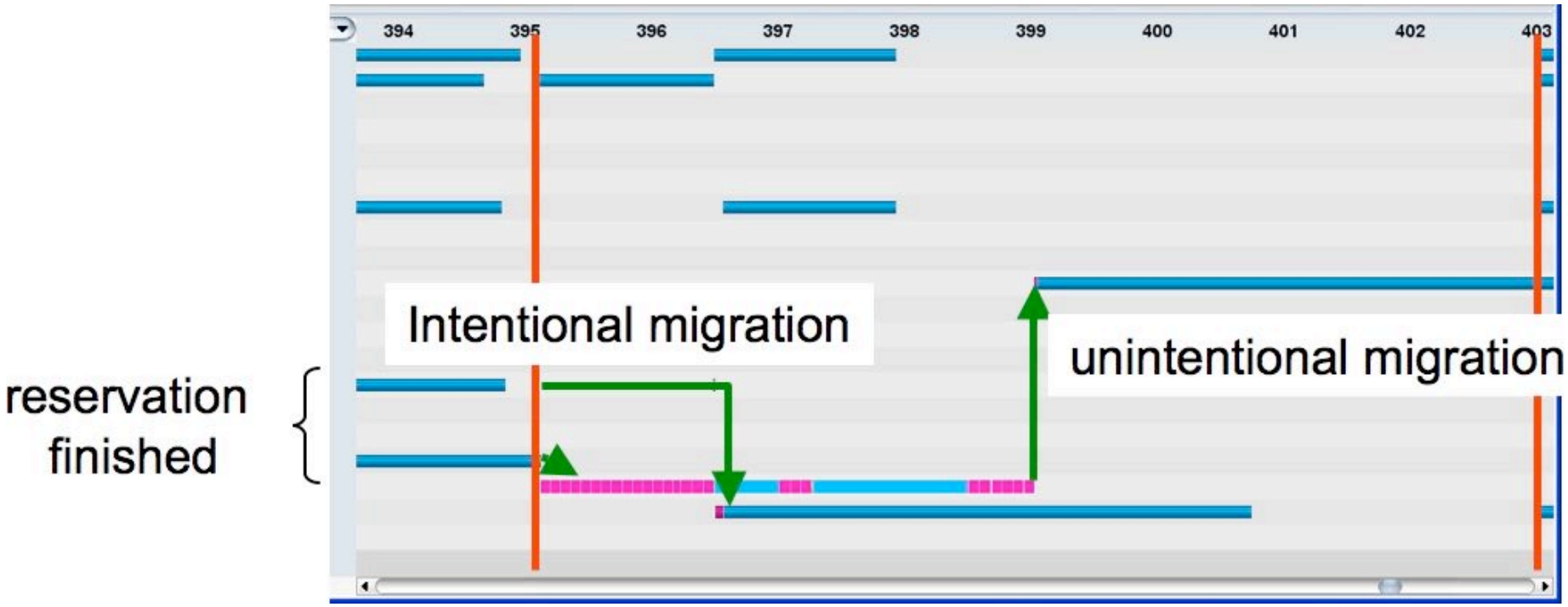
- **Ninf–G Grid RPC system**
  http://ninf.apgrid.org

US-Japan Grid Testbed



Fault Tolerance

- **Automated migration in response to unexpected faults**



Current & Future Computing Platforms

- **Won two DOE supercomputing awards to develop & deploy metascalable ("design once, scale on future platforms") simulation algorithms (2017-2020)**

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

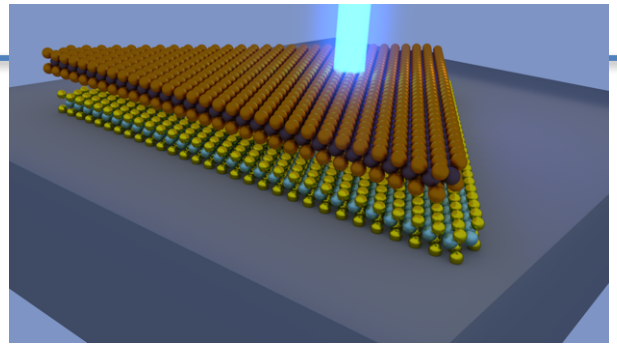
- **NAQMD & RMD simulations on full 800K cores**

Innovative & Novel Computational Impact on Theory & Experiment

Title: "Petascale Simulations for Layered Materials Genome"

Principal Investigator: Aiichiro Nakano, University of Southern California
Co-Investigator: Priya Vashishta, University of Southern California

786,432-core IBM Blue Gene/Q

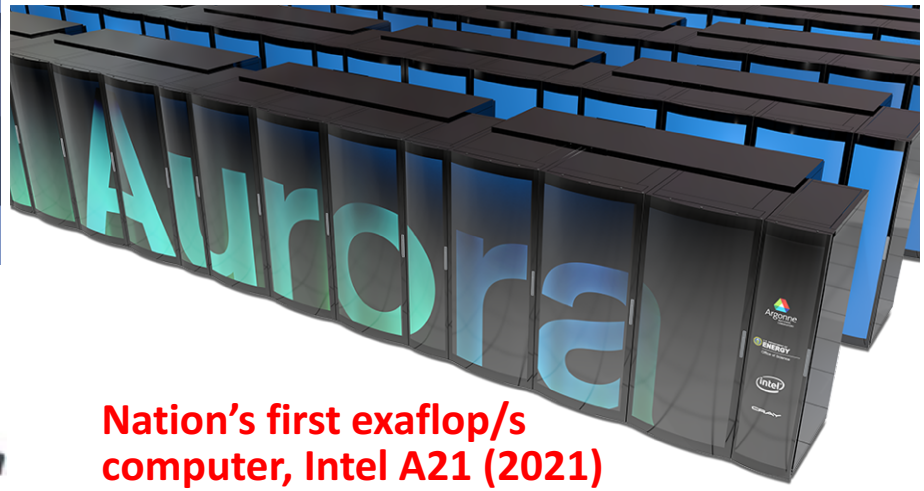


AURORA | EARLY SCIENCE PROGRAM

Early Science Projects for Aurora Supercomputer Announced

Metascalable layered materials genome

Investigator: Aiichiro Nakano, University of Southern California



Nation's first exaflop/s computer, Intel A21 (2021)

- **One of 10 exclusive users of the next-generation DOE supercomputer**

USC@A21 in the Global Exascale Race

R. F. Service, *Science* **359**, 617 ('18)

SUPERCOMPUTING

Design for U.S. exascale computer takes shape

Competition with China accelerates plans for next great leap in supercomputing power

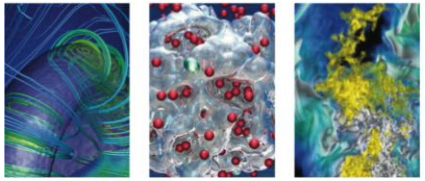
By **Robert F. Service**

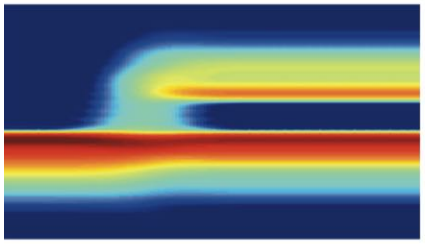
In 1957, the launch of the Sputnik satellite vaulted the Soviet Union to the lead in the space race and galvanized the United States. U.S. supercomputer researchers are today facing their own

Lemont, Illinois. That's 2 years earlier than planned. "It's a pretty exciting time," says Aiichiro Nakano, a physicist at the University of Southern California in Los Angeles who uses supercomputers to model materials made by layering stacks of atomic sheets like graphene.

pace reflects a change of strategy by DOE officials last fall. Initially, the agency set up a "two lanes" approach to overcoming the challenges of an exascale machine, in particular a potentially ravenous appetite for electricity that could require the output of a small nuclear plant.

BES





BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

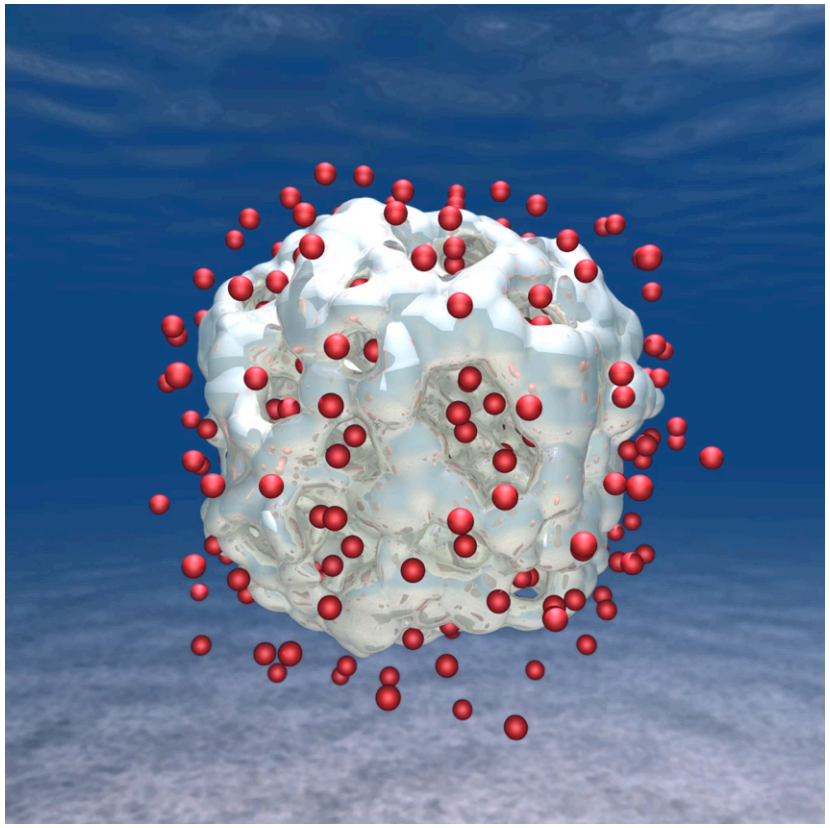
An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND

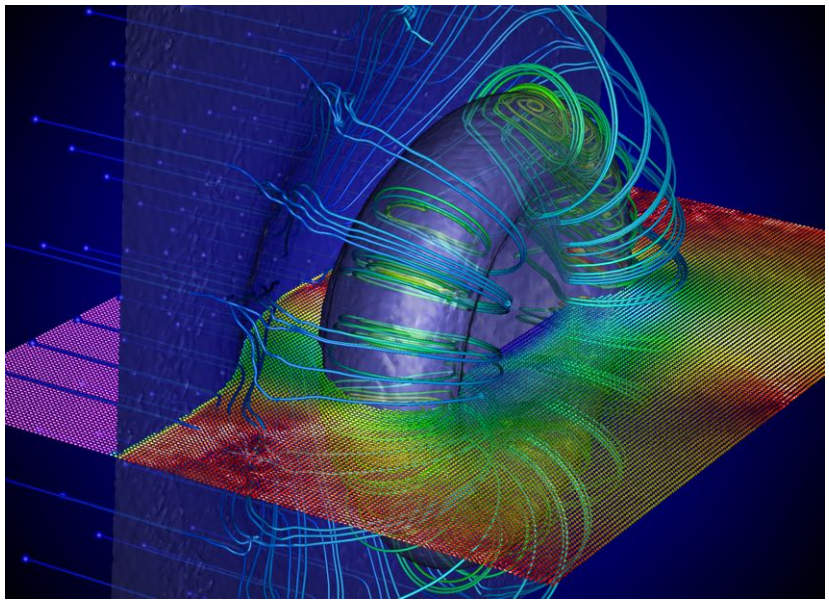
16,611-atom quantum molecular dynamics

Shimamura *et al*.,
Nano Lett.
14, 4090 ('14)



Billion-atom reactive molecular dynamics

Shekhar *et al*.,
Phys. Rev. Lett.
111, 184503 ('13)



U.S. DEPARTMENT OF ENERGY

But...

TOP 500 The List.

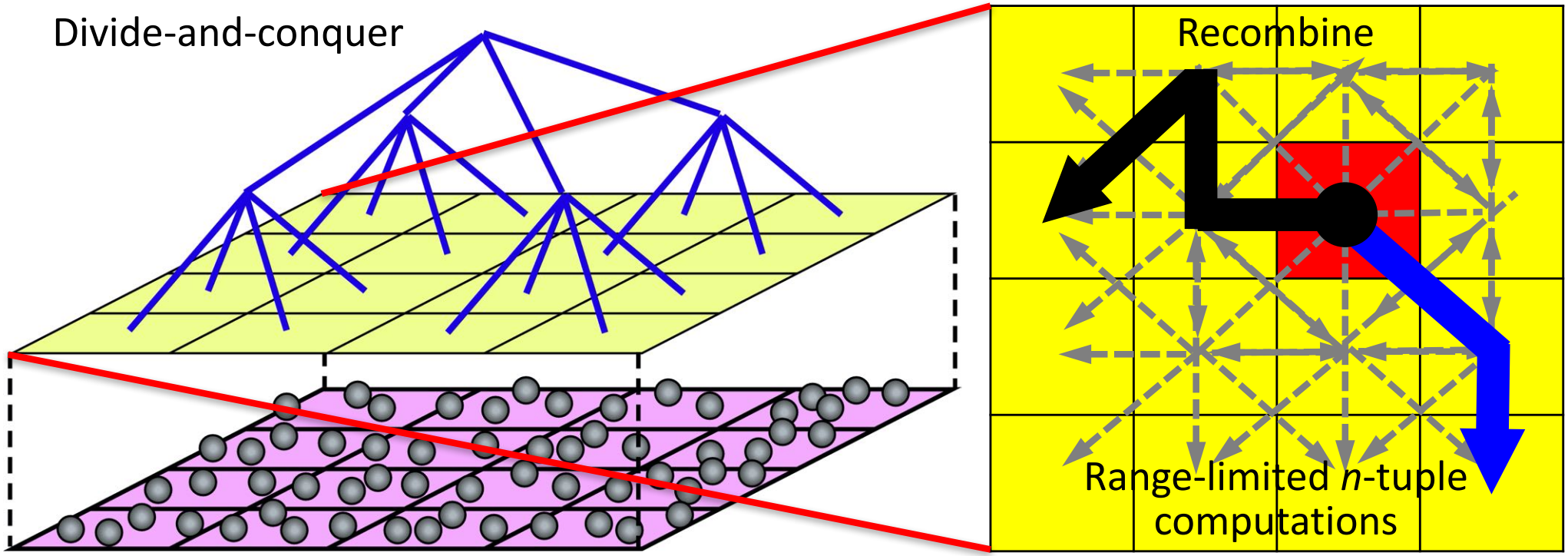
Intel Dumps Knights Hill, Future of Xeon Phi Product Line Uncertain

Michael Feldman | November 15, 2017 04:34 CET

https://www.top500.org/news/

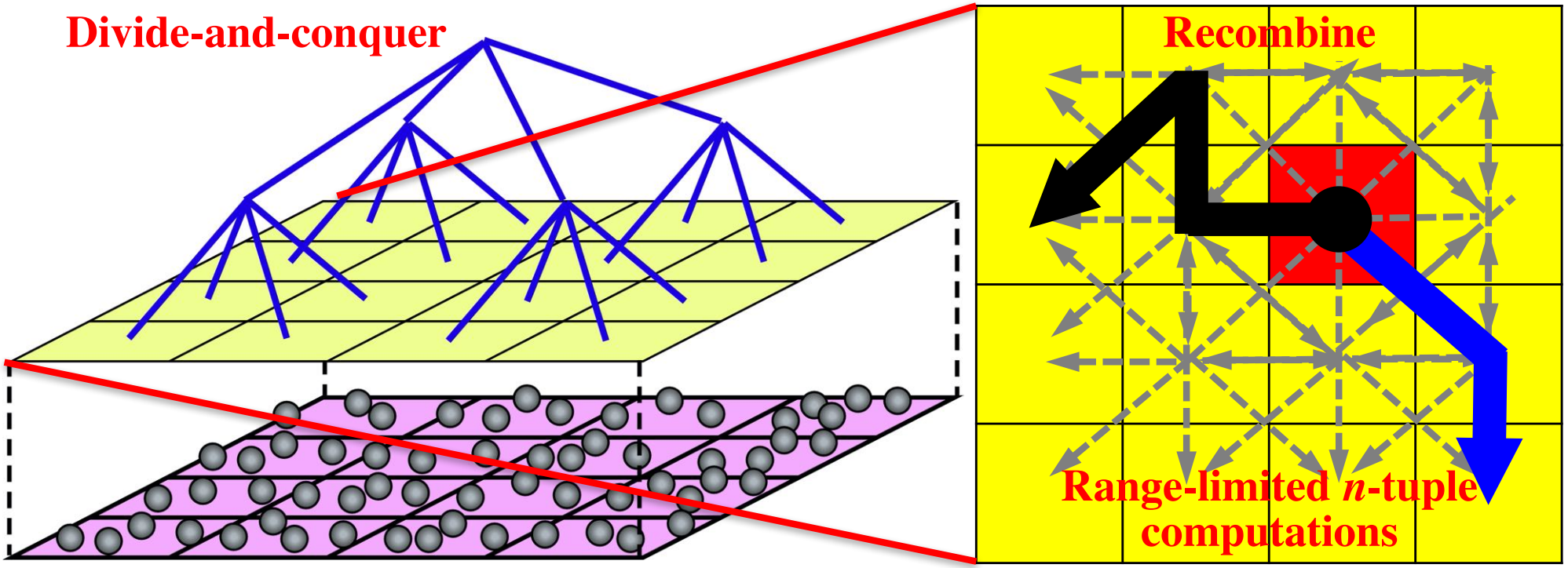
- **Need *metascalable* (or "design once, scale on new architectures") parallel applications**
- **Proposed *divide-conquer-recombine***

F. Shimojo *et al.*, *J. Chem. Phys.* **140**, 18A529 ('14);
K. Nomura *et al.*, *ACM/IEEE SC14* ('14)



M. Kunaseth *et al.*, *ACM/IEEE SC13* ('13)

Divide-Conquer-Recombine (DCR) Engines



M. Kunaseth *et al.*, *ACM/IEEE SC13*

See lecture on "shift-collapse" algorithm

- **Lean divide-&-conquer density functional theory (LDC-DFT) algorithm minimizes the prefactor of $O(N)$ computational cost**

  F. Shimojo *et al.*, *J. Chem. Phys.* **140**, 18A529 ('14); K. Nomura *et al.*, *IEEE/ACM SC14*

- **Extended-Lagrangian reactive molecular dynamics (XRMD) algorithm eliminates the speed-limiting charge iteration**

  K. Nomura *et al.*, *Comput. Phys. Commun.* **192**, 91 ('15)

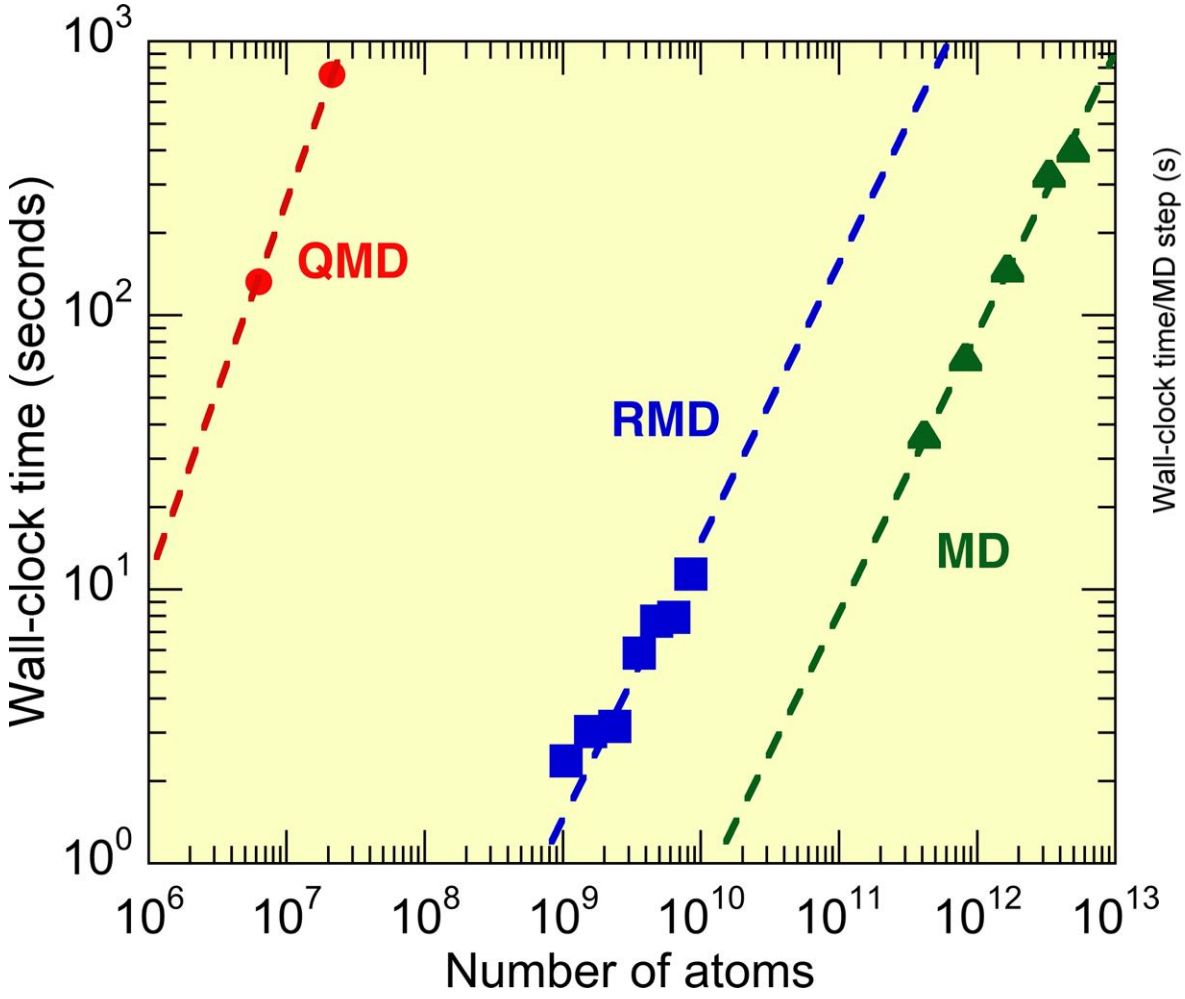
Divide-Conquer-(Re)combine

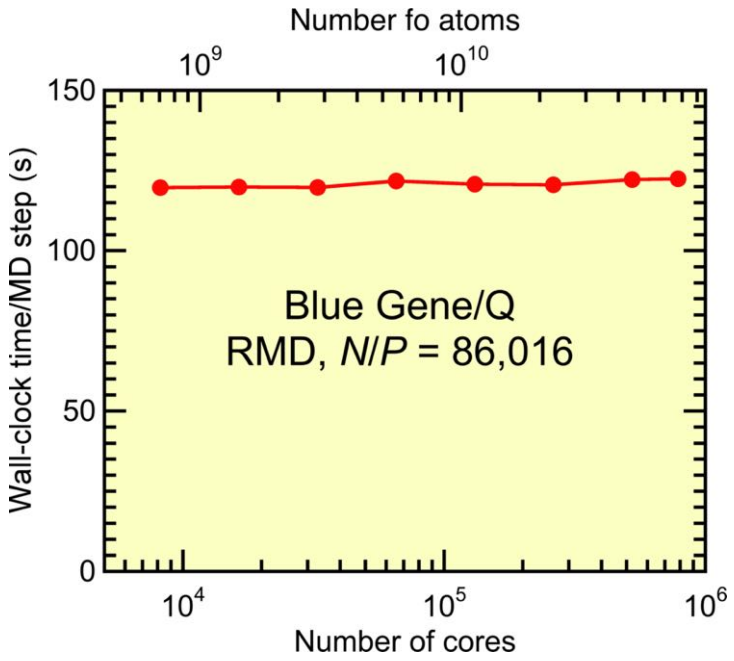
- **"The first was to never accept anything as true which I could not accept as obviously true. The second was to divide each of the problems in as many parts as I should to solve them. The third, beginning with the simplest and easiest to understand matters, little by little, to the most complex knowledge. And the last resolution was to make my enumerations so complete and my reviews so general that I could be assured that I had not omitted anything." (René Descartes, *Discourse on Method*, 1637)**
- **「モデルの分割ー再統合の方法の優れた点は、分割した要素的概念を、モデルの理解に役立つように再構成することができ、そこに創造の入り込む余地があるという点にある。」（福井謙一学問の創造、1987）**

room for creativity

Kenichi Fukui [*Nobel Chemistry Prize*, '98]

Scalable Simulation Algorithm Suite





QMD (quantum molecular dynamics): DC-DFT

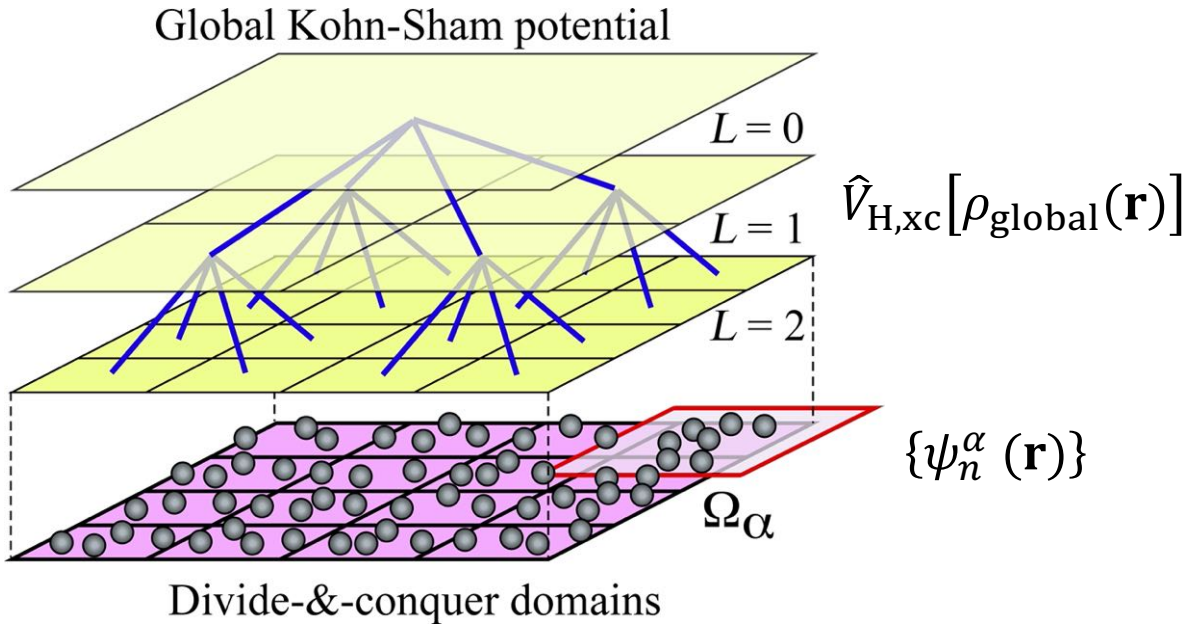
RMD (reactive molecular dynamics): F-ReaxFF

MD (molecular dynamics): MRMD

- **4.9 trillion-atom space-time multiresolution MD (MRMD) of SiO_2**
- **67.6 billion-atom fast reactive force-field (F-ReaxFF) RMD of RDX**
- **39.8 trillion grid points (50.3 million-atom) DC-DFT QMD of SiC**

parallel efficiency 0.984 on 786,432 Blue Gene/Q cores

Divide-&-Conquer Density Functional Theory



- **Overlapping spatial domains:** $\Omega = \cup_\alpha \Omega_\alpha$
- **Domain Kohn-Sham equations**

Global-local self-consistent field (SCF) iteration

$$\left(-\frac{1}{2}\nabla^2 + \hat{V}_{\mathrm{ion}} + \hat{V}_{\mathrm{H,xc}}[\rho_{\mathrm{global}}(\mathbf{r})]\right)\psi_n^\alpha(\mathbf{r}) = \epsilon_n^\alpha \psi_n^\alpha(\mathbf{r})$$

- **Global & domain electron densities**

$$\rho_{\mathrm{global}}(\mathbf{r}) = \Sigma_\alpha\, p_\alpha(\mathbf{r})\rho_\alpha(\mathbf{r}) \leftarrow \rho_\alpha(\mathbf{r}) = \Sigma_n |\psi_n^\alpha|^2\, \Theta(\mu - \epsilon_n^\alpha)$$

Domain support function

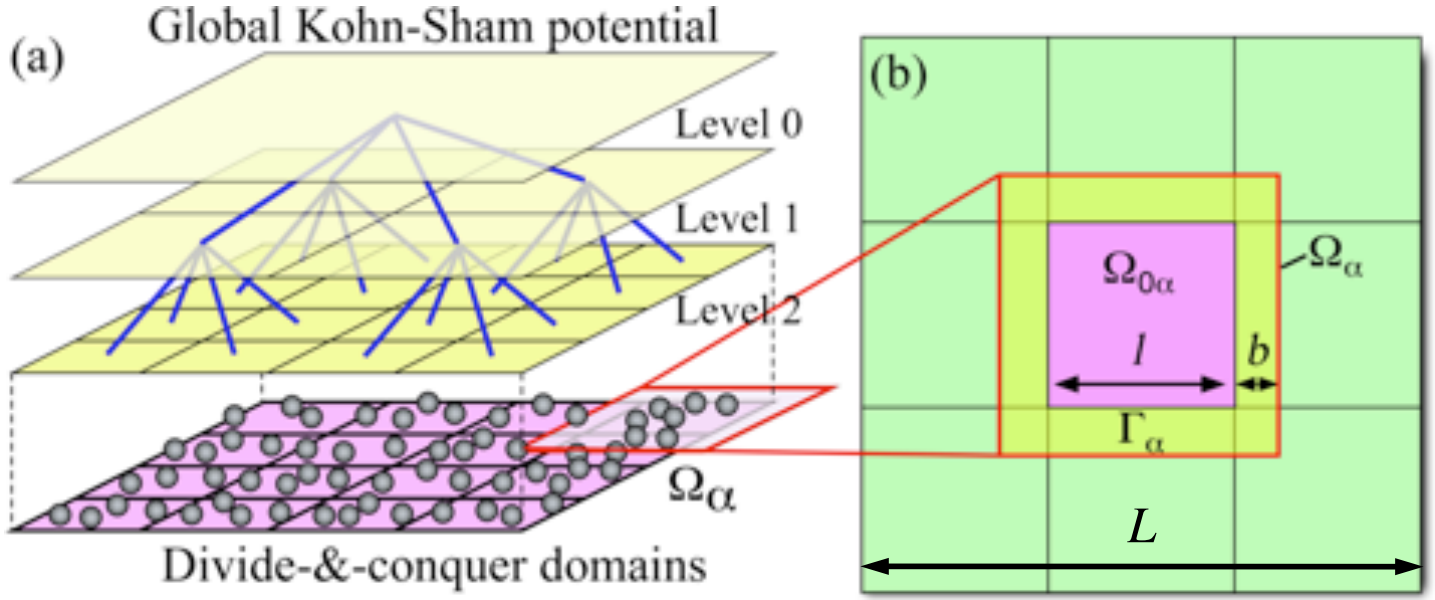
$$\Sigma_\alpha\, p_\alpha(\mathbf{r}) = 1$$

Global chemical potential

$$N = \int d\mathbf{r}\, \rho_{\mathrm{global}}(\mathbf{r})$$

Optimization of Divide-&-Conquer DFT

- **Computational parameters of DC-DFT = domain size (l) + buffer thickness (b)**



- **Complexity analysis to optimize the domain size l**

$$l_* = \mathrm{argmin}\left(T_{\mathrm{comp}}(l)\right) = \mathrm{argmin}\left(\left(\frac{L}{l}\right)^3 (l+2b)^{3\nu}\right) = \frac{2b}{\nu-1}$$

Per-domain computational complexity of DFT = $O(n^\nu)$: $\nu = 2$ or 3 ($n <$ or $> 10^3$)

- **Error analysis: Buffer thickness b is dictated by the accuracy requirement**

$$b = \lambda \ln\left(\max\left\{|\Delta\rho_\alpha(\mathbf{r})| \,|\, \mathbf{r} \in \partial\Omega_\alpha\right\}\right)/\varepsilon\langle\rho_\alpha(\mathbf{r})\rangle$$

Decay length — $\rho_\alpha(\mathbf{r}) - \rho_{\mathrm{global}}(\mathbf{r})$ — Error tolerance

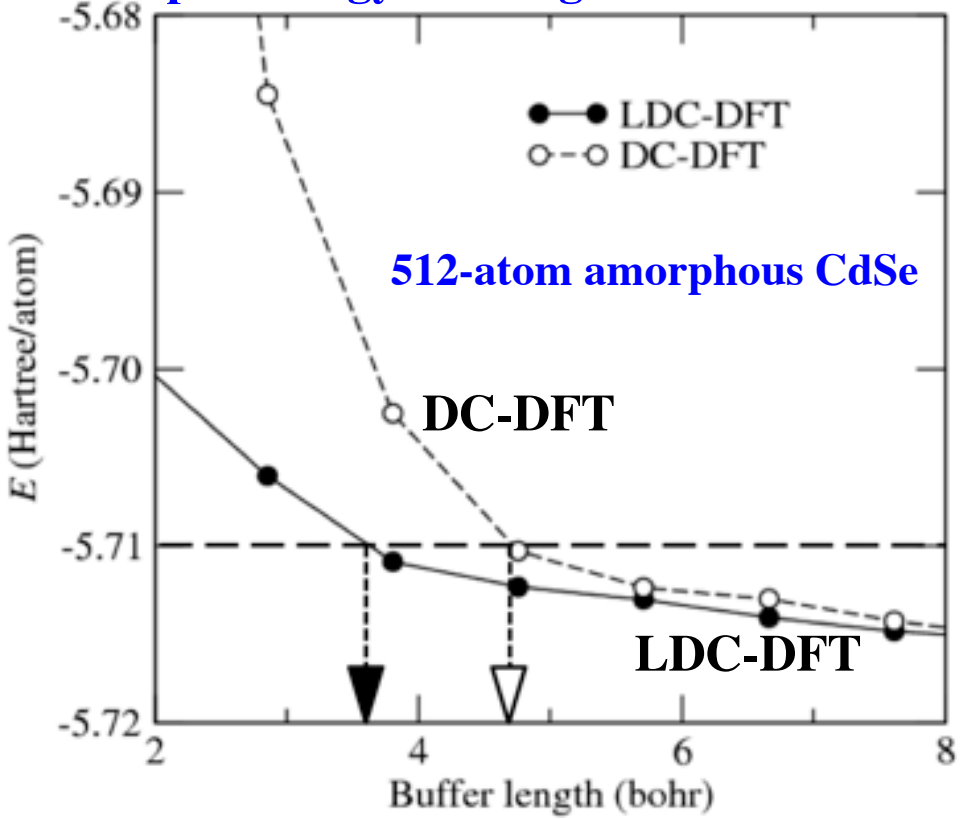
cf. quantum nearsightedness [Kohn, *Phys. Rev. Lett.* **76**, 3168 ('96)]

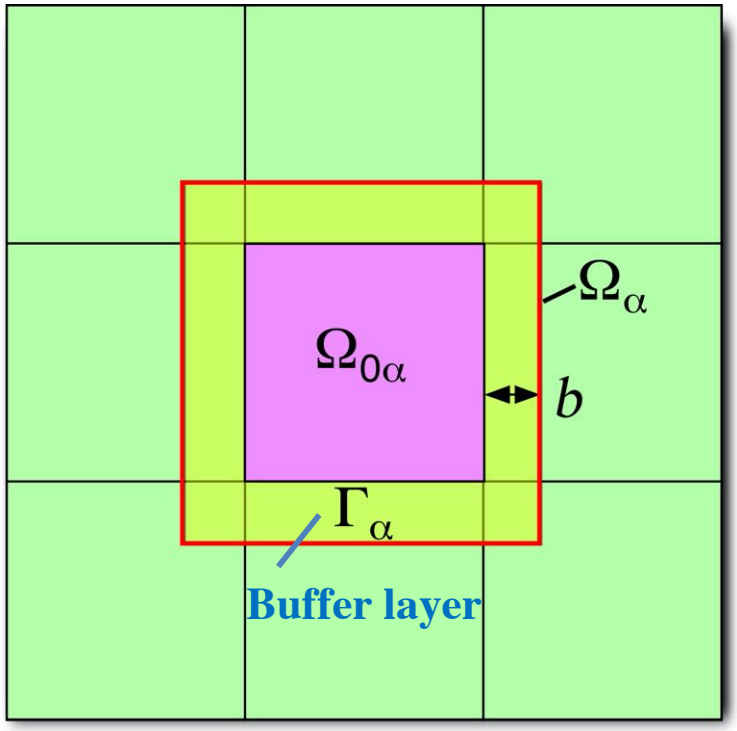
Lean Divide-&-Conquer (LDC) DFT

- **Density-adaptive boundary potential to reduce the *O*(*N*) prefactor**

$$v_\alpha^{\mathrm{bc}}(\mathbf{r}) = \int d\mathbf{r}' \frac{\partial v(\mathbf{r})}{\partial \rho(\mathbf{r}')}\Big(\rho_\alpha(\mathbf{r}) - \rho_{\mathrm{global}}(\mathbf{r})\Big) \cong \frac{\rho_\alpha(\mathbf{r}) - \rho_{\mathrm{global}}(\mathbf{r})}{\xi}$$

- **More rapid energy convergence of LDC-DFT compared with nonadaptive DC-DFT**



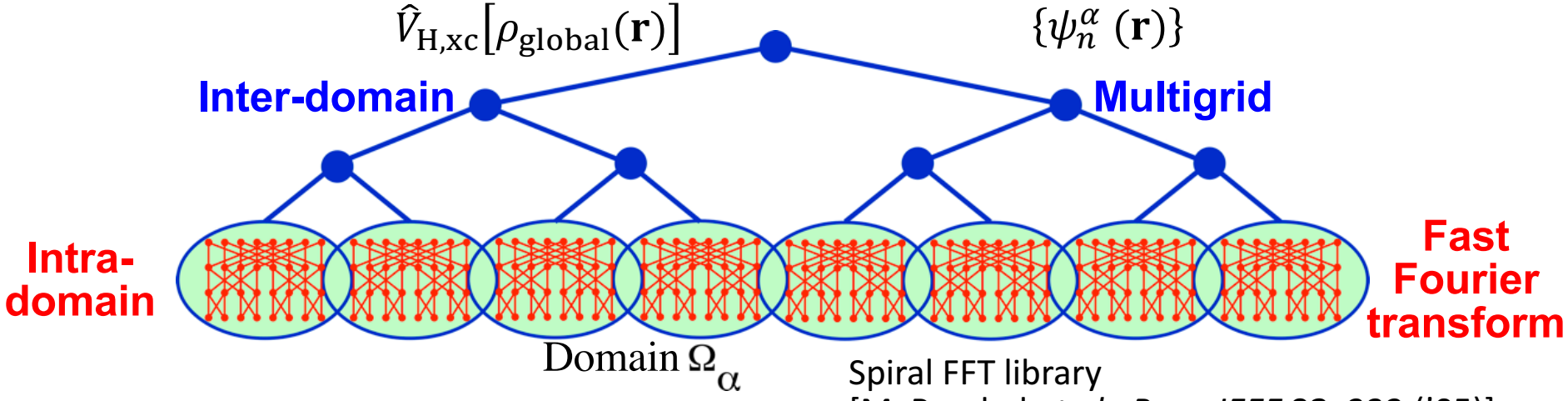


- **Factor 2.03 (for ν = 2) ~ 2.89 (for ν = 3) reduction of the computational cost with an error tolerance of 5×10^{-3} a.u. (per-domain complexity: n^ν)**

F. Shimojo *et al.*, *J. Chem. Phys.* **140**, 18A529 ('14);
Phys. Rev. B **77**, 085103 ('08); *Comput. Phys. Commun.* **167**, 151 ('05)

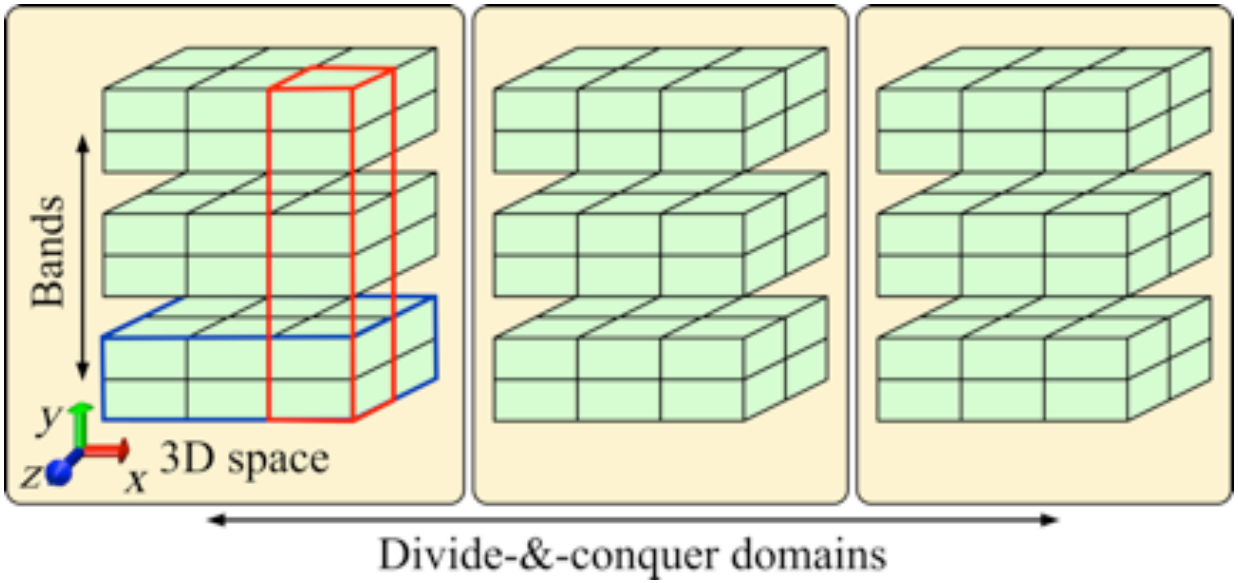
Hierarchical Computing

- **Globally scalable (real-space multigrid) + locally fast (plane wave) electronic solver**



Spiral FFT library
[M. Puschel *et al.*, *Proc. IEEE* **93**, 232 ('05)]

- **Hierarchical band (*i.e.* Kohn-Sham orbital) + space + domain (BSD) decomposition**



F. Shimojo *et al.*, *J. Chem. Phys.* **140**, 18A529 ('14)

Parallel Efficiency

Parallel computing = solving a big problem (W) in a short time (T) using many processors (P)

- **Execution time: $T(W,P)$**

  W: Workload

  P: Number of processors

- **Speed:** $$S(W,P) = \frac{W}{T(W,P)}$$

- **Speedup:** $$S_P = \frac{S(W_P,P)}{S(W_1,1)} = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)}$$

- **Efficiency:** $$E_P = \frac{S_P}{P} = \frac{W_P T(W_1,1)}{P W_1 T(W_P,P)}$$

How to scale W_P with P?

See http://cacs.usc.edu/education/cs596-lecture.html

Fixed Problem-Size (Strong) Scaling

Solve the same problem faster

$W_P = W$—constant (strong scaling)

- **Speedup:** $$S_P = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)} = \frac{T(W,1)}{T(W,P)}$$
- **Efficiency:** $$E_P = \frac{T(W,1)}{PT(W,P)}$$
- **Amdahl's law:** f (= sequential fraction of the workload) limits the asymptotic speedup

$$T(W,P) = fT(W,1) + \frac{(1-f)T(W,1)}{P}$$

$$\therefore S_P = \frac{T(W,1)}{T(W,P)} = \frac{1}{f + (1-f)/P}$$

$$\therefore S_P \to \frac{1}{f} \quad (P \to \infty)$$

Isogranular (Weak) Scaling

Solve a larger problem within the same time duration

$W_P = Pw$ **(weak scaling)**
w **= constant workload per processor (granularity)**

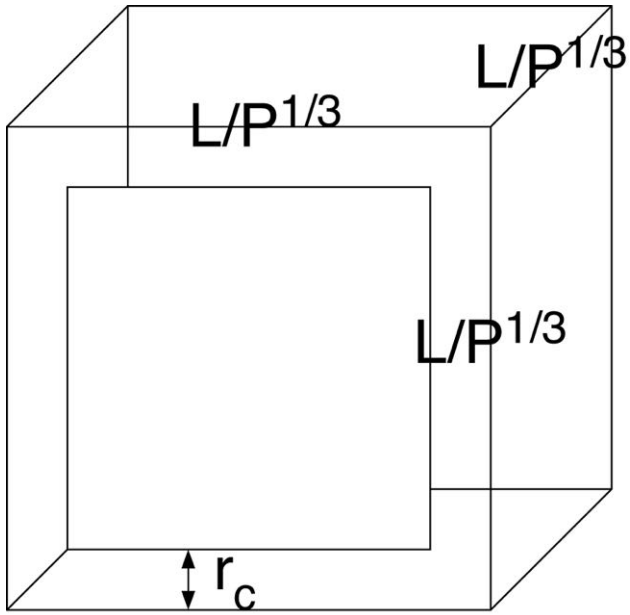
- **Speedup:** $$S_P = \frac{S(P \bullet w, P)}{S(w,1)} = \frac{P \bullet w / T(P \bullet w, P)}{w / T(w,1)} = \frac{P \bullet T(w,1)}{T(P \bullet w, P)}$$

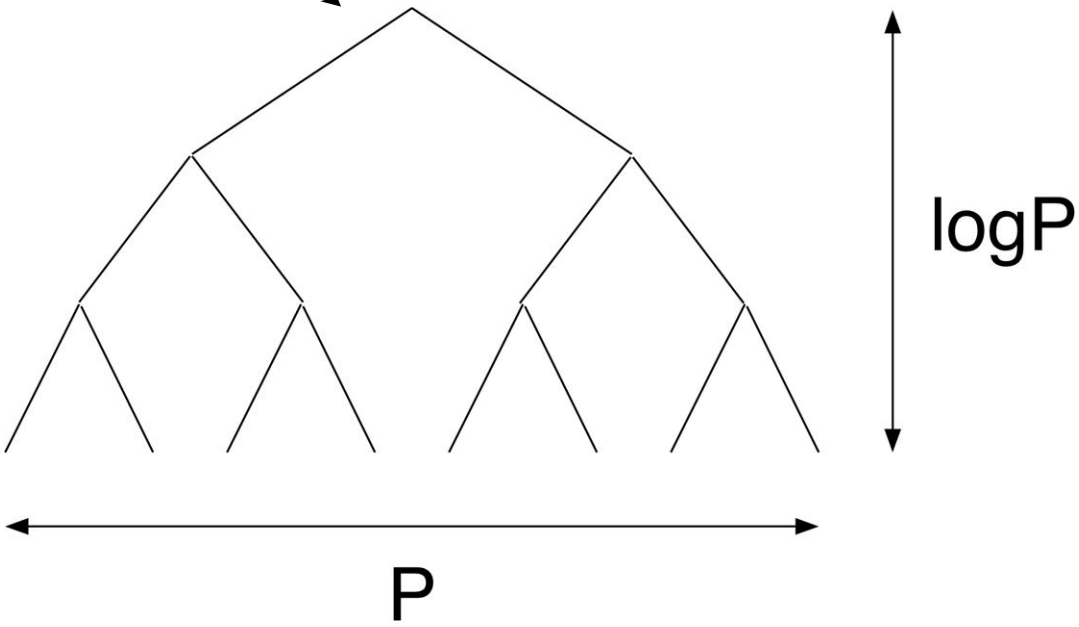
- **Efficiency:** $$E_P = \frac{S_P}{P} = \frac{T(w,1)}{T(P \bullet w, P)}$$

Analysis of Parallel MD

- **Parallel execution time:**
  Workload ∝ Number of atoms, *N* (linked-list cell algorithm)

$$T(N,P) = T_{\text{comp}}(N,P) + T_{\text{comm}}(N,P) + T_{\text{global}}(P)$$
$$= a\frac{N}{P} + b\left(\frac{N}{P}\right)^{2/3} + c\log P$$





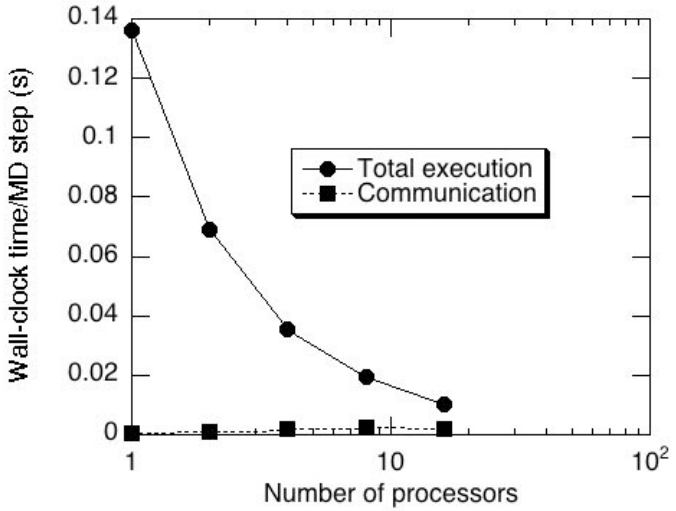
Fixed Problem-Size Scaling

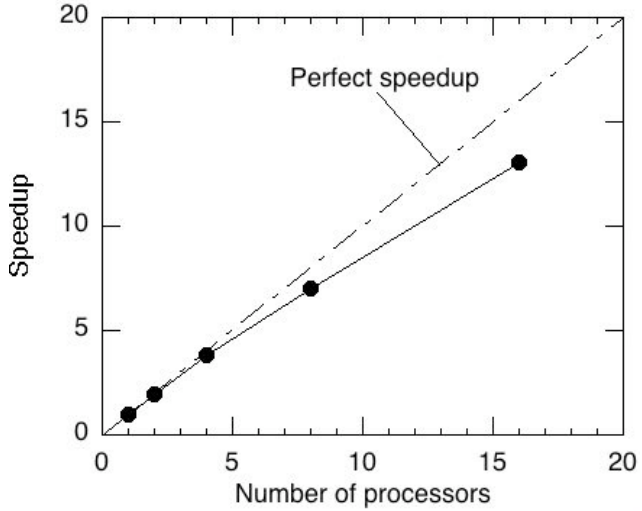
- **Speedup:**

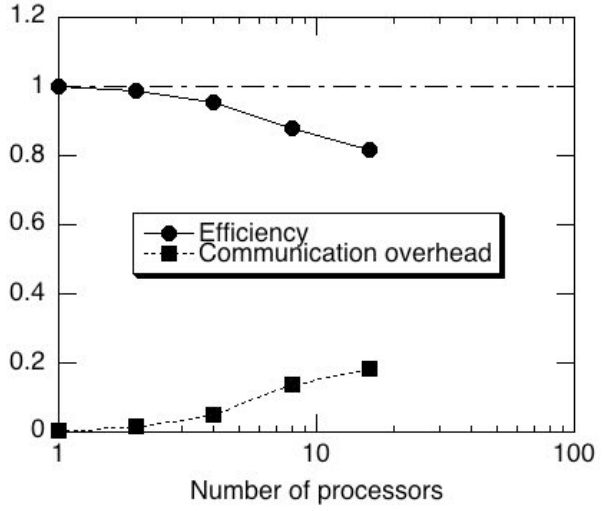
$$S_P = \frac{T(N,1)}{T(N,P)} = \frac{aN}{\frac{aN/P + b(N/P)^{2/3} + c\log P}{P}} = \frac{}{1 + \frac{b}{a}\left(\frac{P}{N}\right)^{1/3} + \frac{c}{a}\frac{P\log P}{N}}$$

- **Efficiency:**

$$E_P = \frac{S_P}{P} = \frac{1}{1 + \frac{b}{a}\left(\frac{P}{N}\right)^{1/3} + \frac{c}{a}\frac{P\log P}{N}}$$





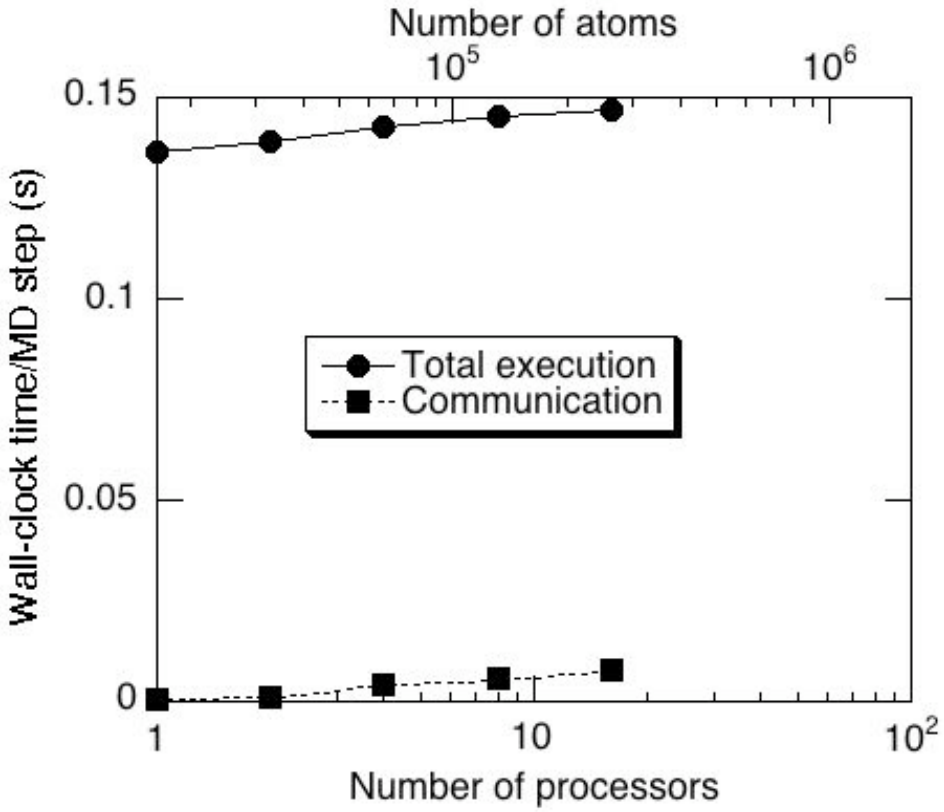


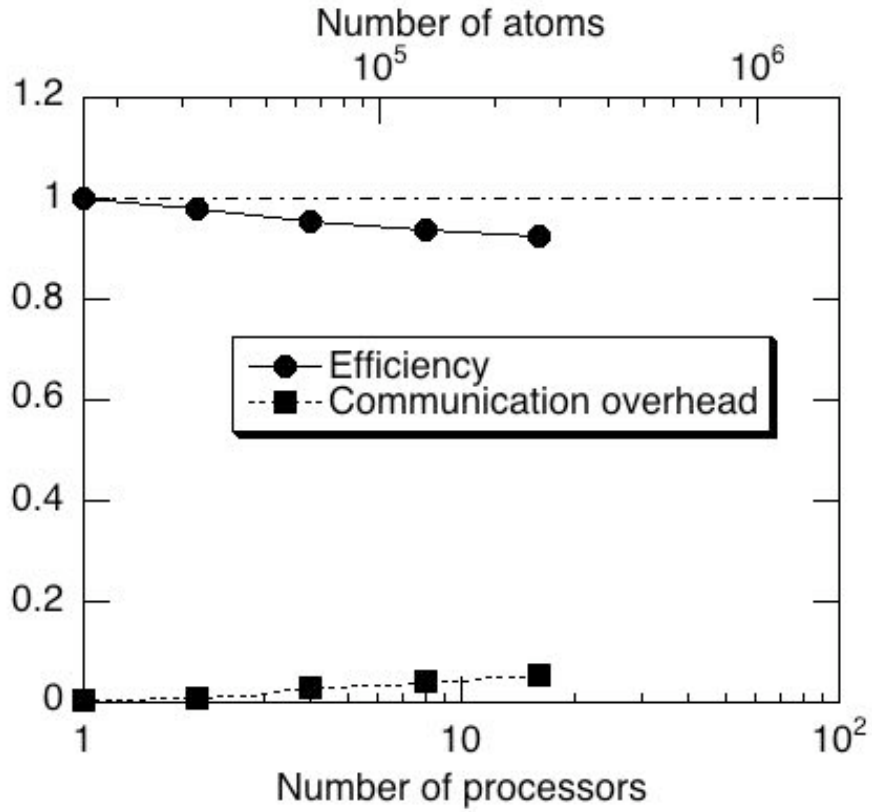
pmd.c: N = 16,384, on HPC

Isogranular Scaling of Parallel MD

- $n = N/P$ = constant
- **Efficiency:**

$$E_P = \frac{T(n,1)}{T(nP,P)} = \frac{an}{an + bn^{2/3} + c\log P} = \frac{1}{1 + \frac{b}{a}n^{-1/3} + \frac{c}{an}\log P}$$

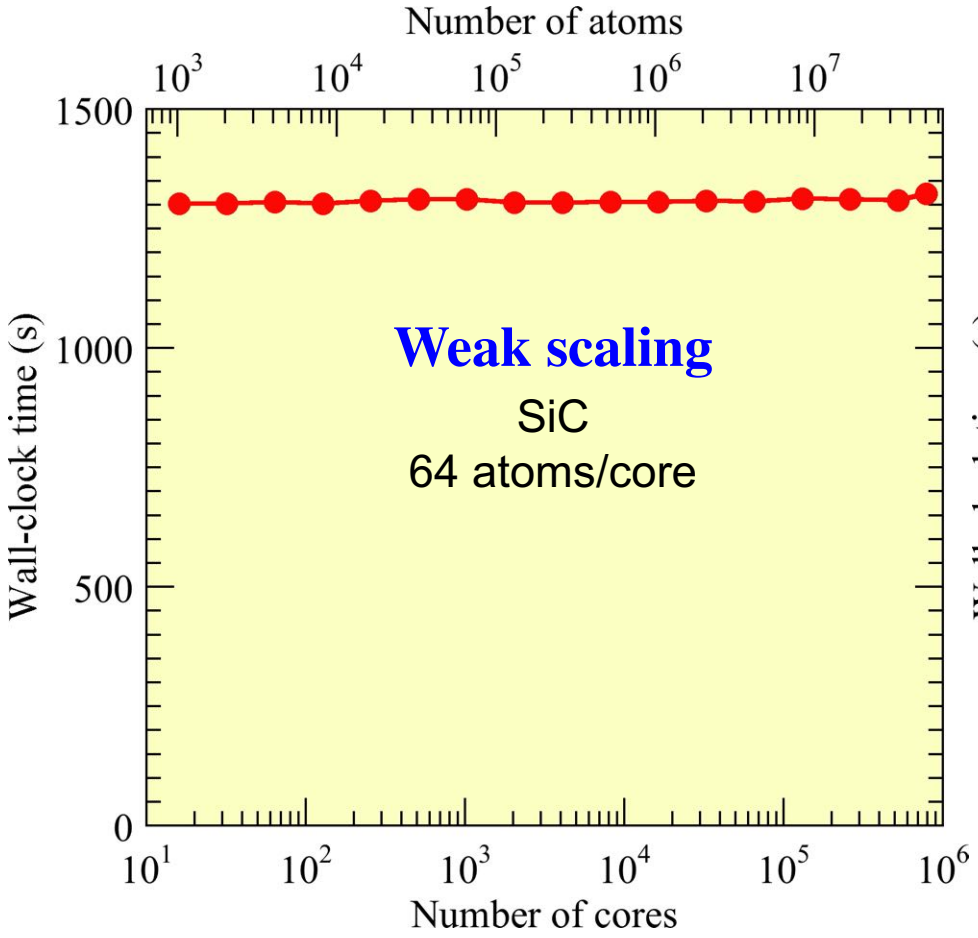


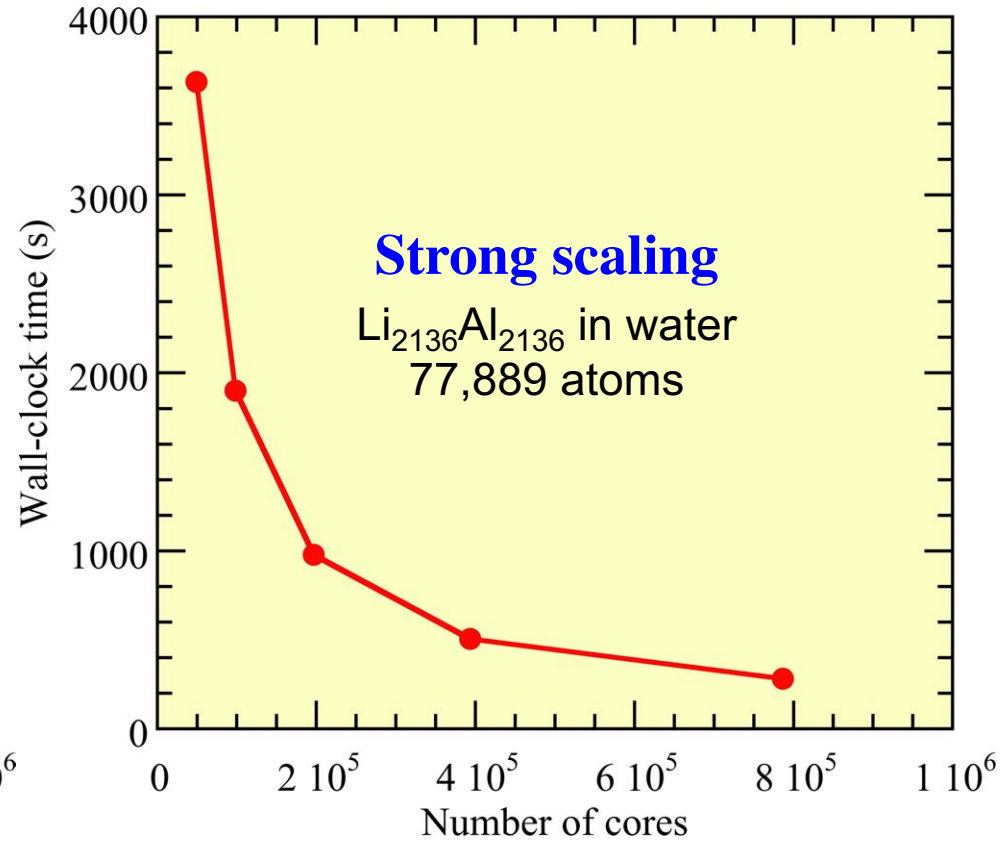


pmd.c: N/P = 16,384, on HPC

Parallel Performance of QXMD

- **Weak-scaling parallel efficiency is 0.984 on 786,432 Blue Gene/Q cores for a 50,331,648-atom SiC system**
- **Strong-scale parallel efficiency is 0.803 on 786,432 Blue Gene/Q cores**





- **62-fold reduction of time-to-solution** [441 s/SCF-step for 50.3M atoms] **from the previous state-of-the-art** [55 s/SCF-step for 102K atoms, Osei-Kuffuor *et al.*, *PRL* '14]

K. Nomura *et al.*, *IEEE/ACM Supercomputing, SC14* ('14)

BLASification

- **Transform from band-by-band to all-band computations to utilize a matrix-matrix subroutine (DGEMM) in the level 3 basic linear algebra subprograms (BLAS3) library**
- **Algebraic transformation of computations**

Example: Nonlocal pseudopotential operation

D. Vanderbilt, *Phys. Rev. B* **41**, 7892 ('90)

$$\hat{v}_{\mathrm{nl}}|\psi_n^\alpha\rangle = \sum_I^{N_{\mathrm{atom}}} \sum_{ij}^{L_{\max}} |\beta_{i,I}\rangle D_{ij,I} \langle\beta_{j,I}|\psi_n^\alpha\rangle \quad (n = 1, \ldots, N_{\mathrm{band}})$$

$$\boldsymbol{\Psi} = \left[|\psi_1^\alpha\rangle, \ldots, |\psi_{N_{\mathrm{band}}}^\alpha\rangle\right] \widetilde{\mathbf{B}}(i) = \left[|\beta_{i,1}\rangle, \ldots, |\beta_{i,N_{\mathrm{atom}}}\rangle\right] \left[\widetilde{\mathbf{D}}(i,j)\right]_{I,J} = D_{ij,I}\delta_{IJ}$$

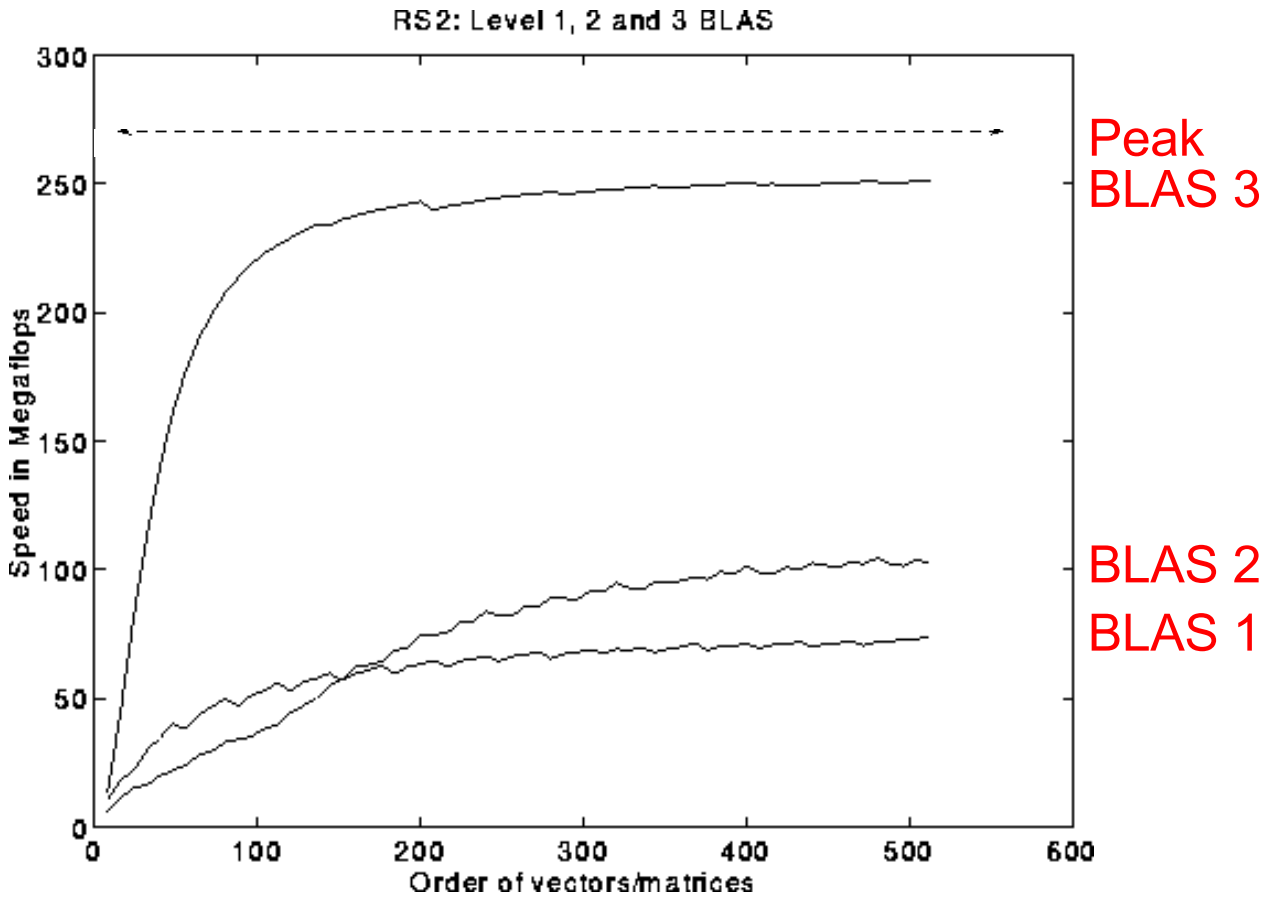
$$\hat{v}_{\mathrm{nl}}\boldsymbol{\Psi} = \sum_{i,j}^{L} \widetilde{\mathbf{B}}(i)\widetilde{\mathbf{D}}(i,j)\widetilde{\mathbf{B}}(j)^T$$

- **50.5% of the theoretical peak FLOP/s performance on 786,432 Blue Gene/Q cores (entire Mira at the Argonne Leadership Computing Facility)**
- **55% of the theoretical peak FLOP/s on Intel Xeon E5-2665**

K. Nomura *et al.*, *IEEE/ACM Supercomputing, SC14* ('14)

BLAS3-Performance Molecular Dynamics?

- **BLAS3: q = flop/memory access = (block size)$^{1/2}$**



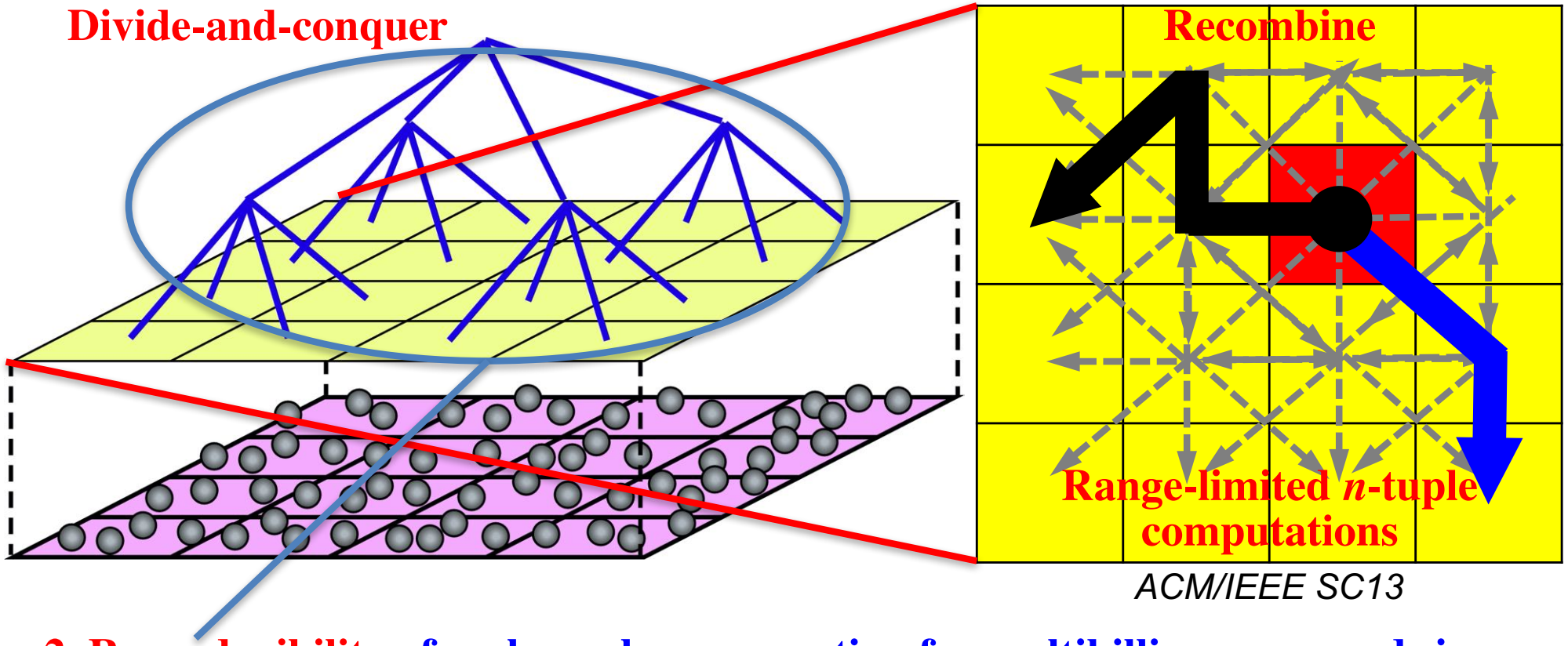
- **Molecular dynamics: $q = O(n^2)/O(n) = O(n$: block size)**
  > Use of SIMD (single instruction multiple data) instructions on Cell, multicore (SSE)?

Exascale Computing Challenge

1. Scalability for billion-way parallelism

J. Chem. Phys. **140**, 18A529 ('14)
IEEE/ACM SC14
IEEE Computer **48(11)**, 33 ('15)

Divide-conquer-recombine (DCR) algorithmic framework
Metascalable ("design once, scale on future architectures")

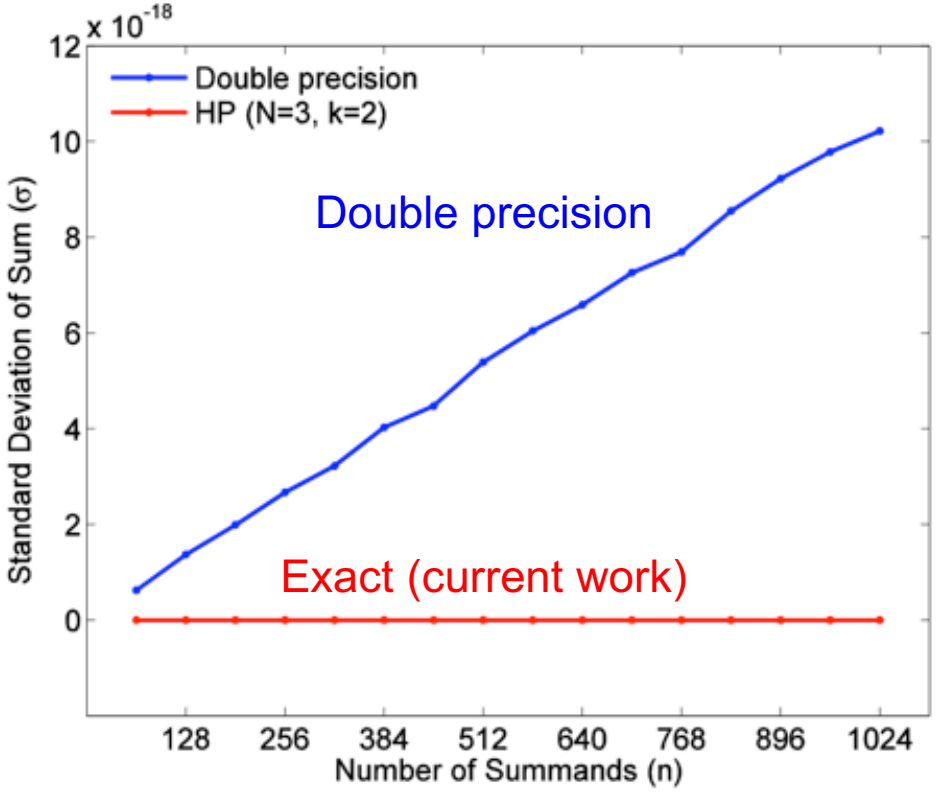


ACM/IEEE SC13

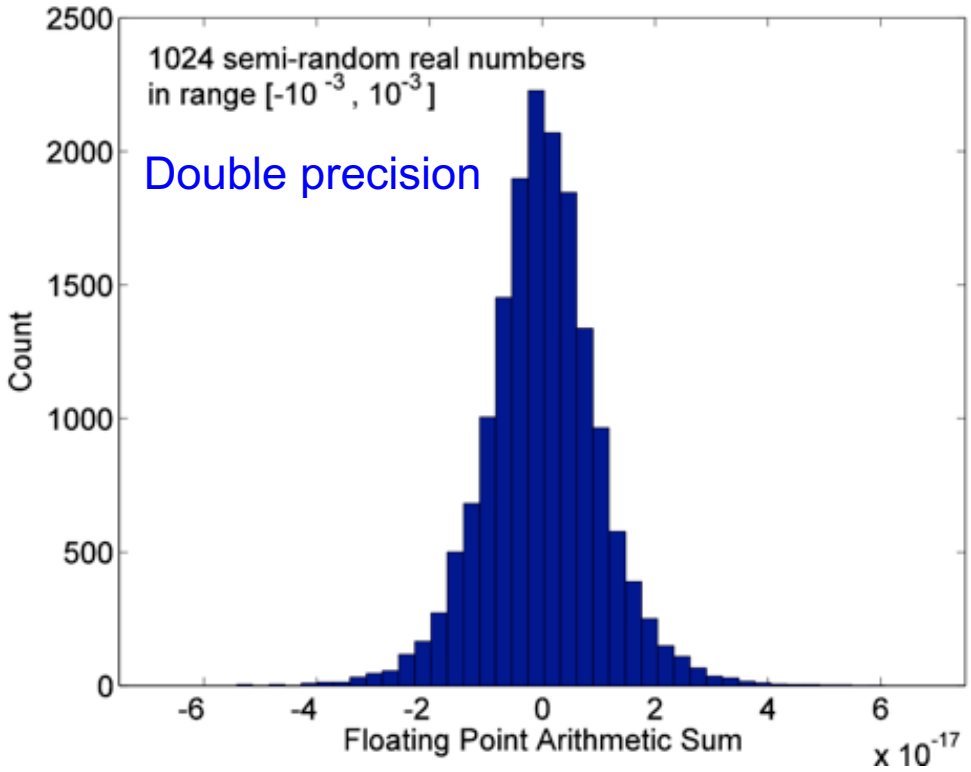
2. Reproducibility of real-number summation for multibillion summands in the global sum; double-precision arithmetic began to produce different results on different high-end architectures

Reproducibility Challenge

- **Rounding (truncation) error makes floating-point addition non-associative**



Standard deviation of sum with random summation orders



Distribution of sum with random summation orders

- **Sum becomes a random walk across the space of possible rounding error**

High-Precision (HP) Method

- **Propose an extension of the order-invariant, higher-precision intermediate-sum method by Hallberg & Adcroft** [*Par. Comput.* **40**, 140 ('14)]
- **The proposed variation represents a real number *r* using a set of *N* 64-bit unsigned integers, a_i ($i = 0, N\text{-}1$)**

$$r = \sum_{i=0}^{N-1} a_i 2^{64(N-k-i-1)}$$

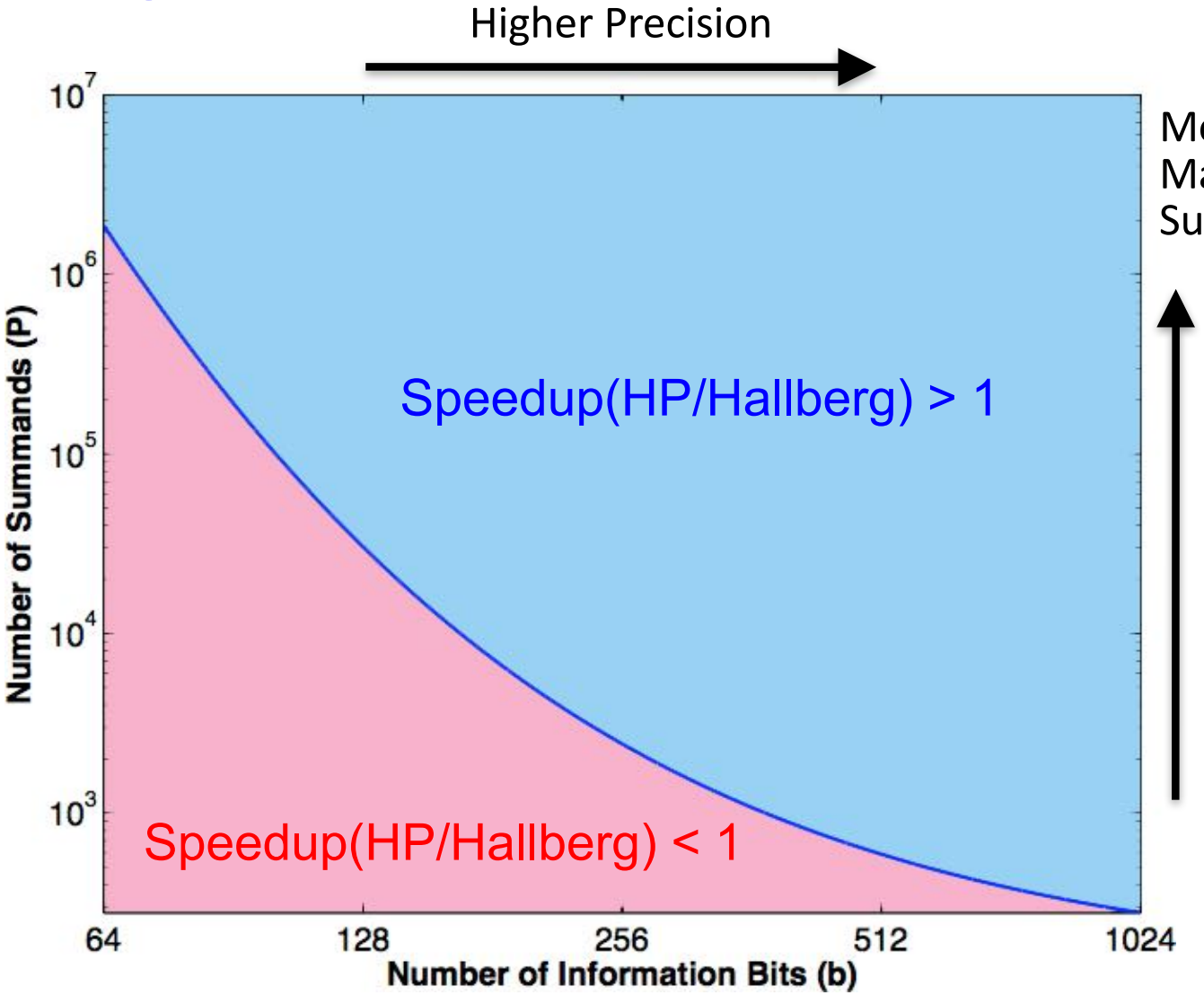
$$= \underbrace{a_0 2^{64(N-k-1)} + \cdots + a_{N-k-1}}_{N-k} + \cdots + \underbrace{a_{N-k} 2^{-64} + \cdots + a_{N-1} 2^{-64k}}_{k}$$

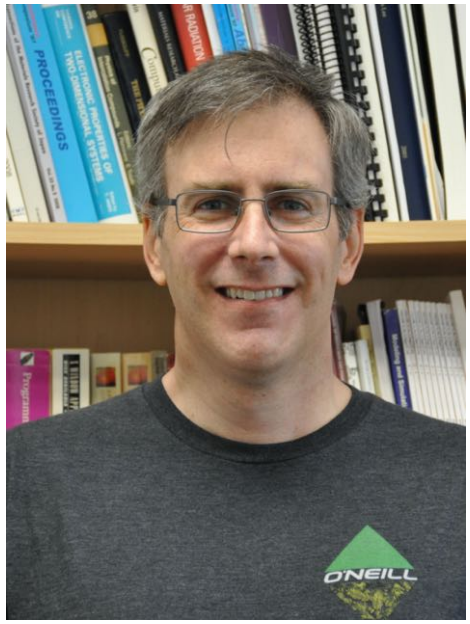
- ***k* is the number of 64-bit unsigned integers assigned to represent the fractional portion of *r* ($0 \le k \le N$), whereas *N*-*k* integers represent the whole-number component**
- **Negative number is represented by two's complement in integer representation, using only 1 bit**

P. E. Small *et al.*, *IEEE IPDPS 2016*

Performance Projection

- **HP sum is faster than Hallberg sum for higher precision & larger numbers of summands**



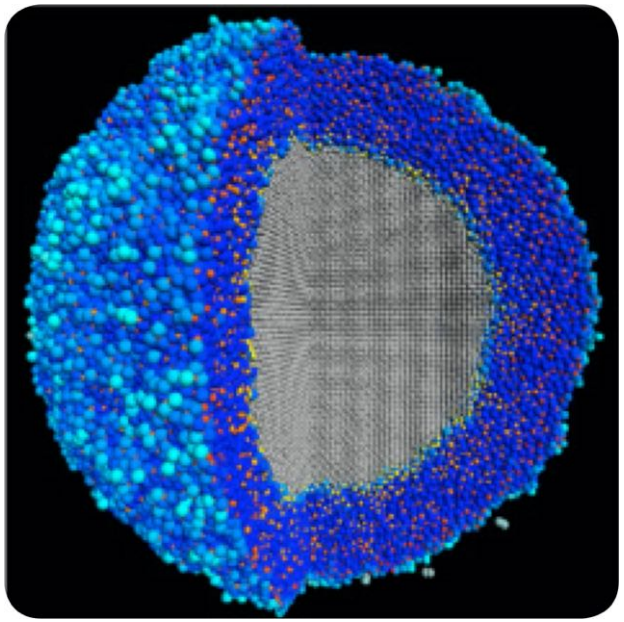


P. E. Small *et al.*, *IEEE IPDPS 2016*

U.S. National Initiatives

Materials Genome Initiative for Global Competitiveness

June 2011

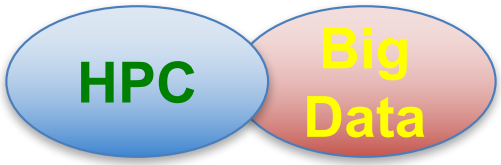


- **MGI will accelerate materials developments using data sciences**

EXECUTIVE ORDER

BARACK OBAMA

CREATING A NATIONAL STRATEGIC COMPUTING INITIATIVE

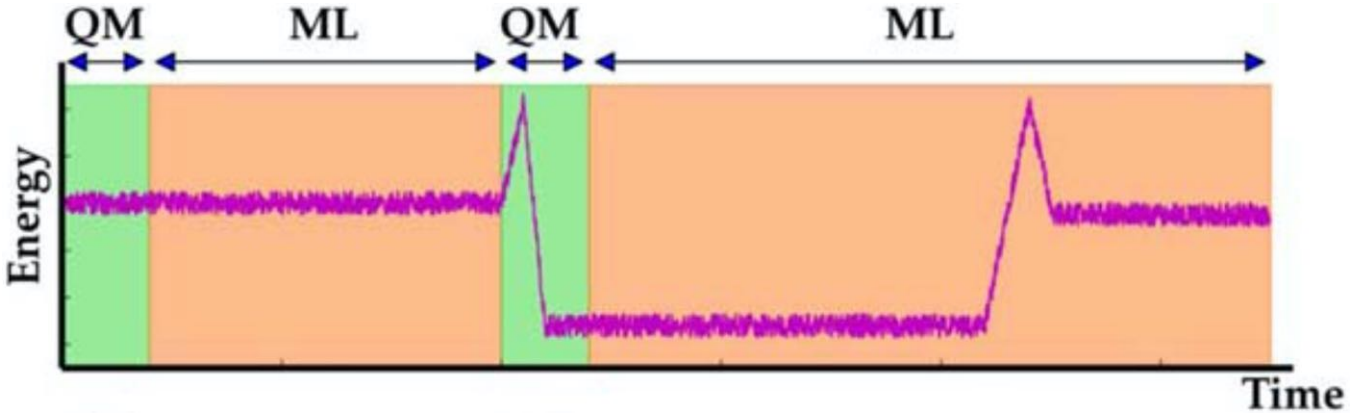


- **NSCI will merge exaflop/s (10^{18} floating-point operations per second) high performance computing (HPC) & exabyte (10^{18} bytes) "big data" to advance the frontier of sciences, economic growth & national security**

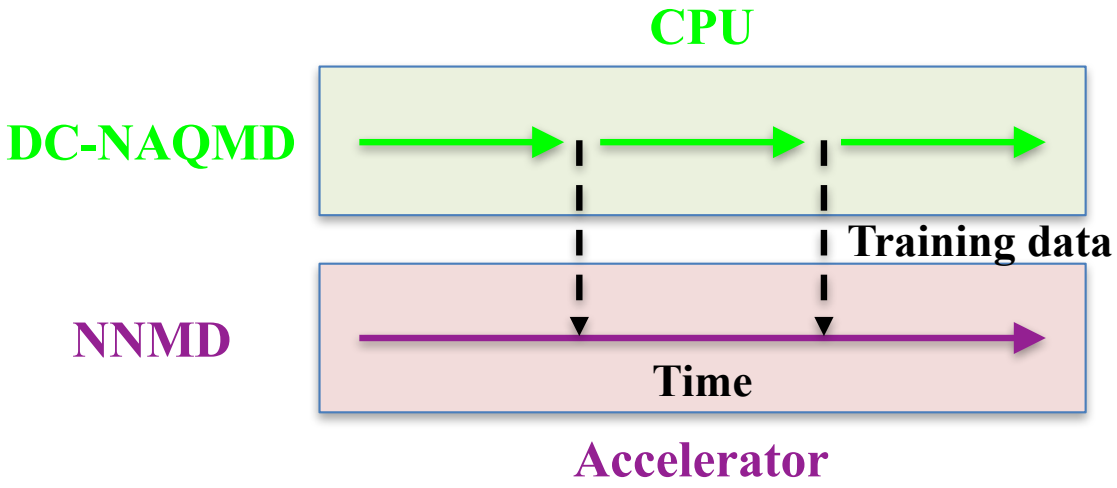
QM/NN(TN) on A21?

- **Sequential QM-machine learning (ML) molecular dynamics**

  [Botu & Ramprasad, *Int. J. Quant. Chem*. **115**, 1074 ('15)]



- **Concurrent nonadiabatic quantum-neural-network (NN) molecular dynamics with accelerators?**



- **NAQMD augmented w/ tensor network (TN)?** [Orus, *Ann. Phys*. **349**, 117 ('14)]