

# Optimizing Molecular Dynamics

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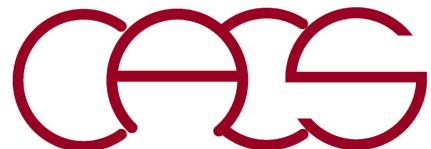
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*University of Southern California*

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- Intranode optimization: CPU & memory access
- Internode optimization: Communication

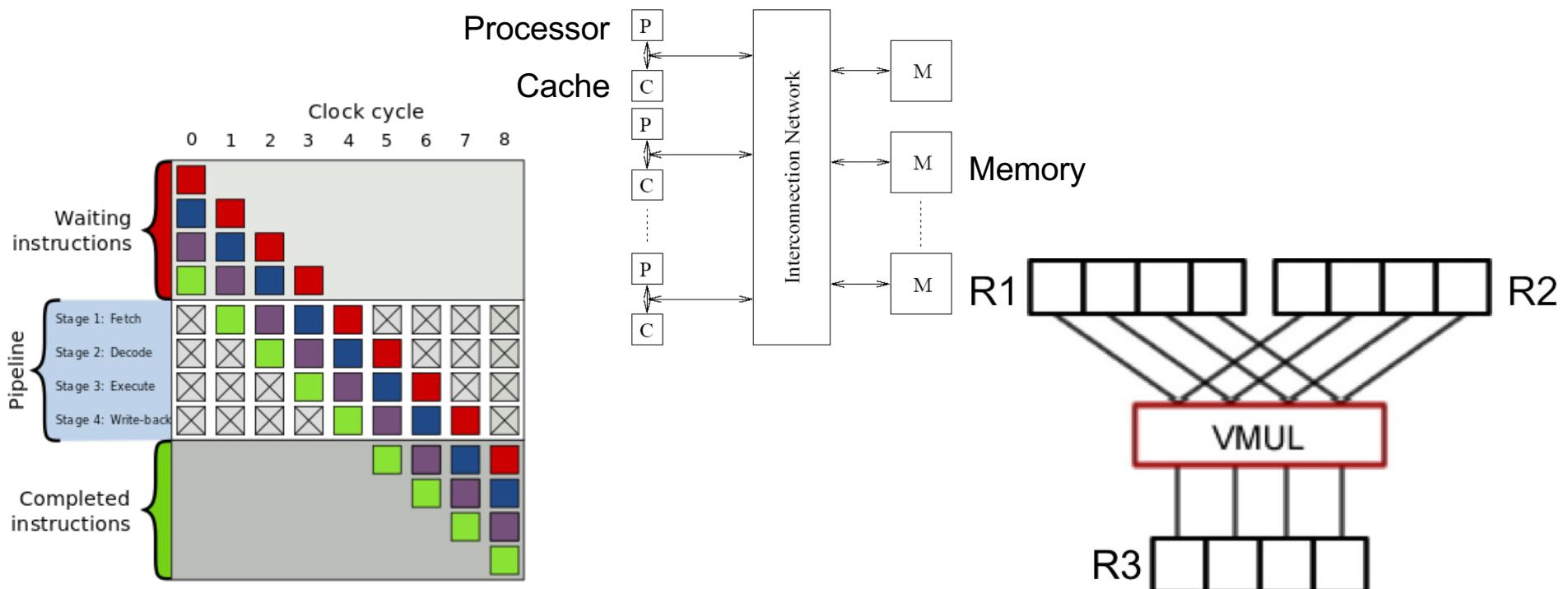


Data/computation locality!



# Key Hardware Features

- **Pipelining:** Multiple stages of computation are executed concurrently for multiple data elements
- **Cache:** Fast memory that holds a subset of main memory
- **Vectorization:** Single-instruction multiple-data (SIMD) parallelism on vector registers each holding multiple data elements simultaneously hold



# Roofline Model of Performance

- Off-chip memory bandwidth (from DRAM) is critical for performance (to feed enough data to be operated)
- *Operational intensity*: Operations per byte of DRAM traffic
- *Roofline model*: Predicts the floating-point (fp) performance from operation intensity, theoretical peak fp performance & peak memory bandwidth

$$\text{Attainable fp performance } \left[ \frac{\text{Gflop}}{\text{sec}} \right] = \min \left( \frac{\text{Peak fp performance}}{\left[ \frac{\text{Gflop}}{\text{sec}} \right]}, \frac{\text{Peak memory bandwidth}}{\left[ \frac{\text{GByte}}{\text{sec}} \right]} \times \text{Operational intensity} \left[ \frac{\text{flop}}{\text{Byte}} \right] \right)$$

$$\text{Peak fp } \left[ \frac{\text{Gflop}}{\text{sec}} \right] = \hat{f} \times \overbrace{n_{\text{core}}}^{\text{clock [GHz]}} \times \overbrace{n_{\text{vector}}}^{\text{\# of cores}} \times \overbrace{n_{\text{FMA}}}^{\text{\# of operands/vector}} \times 2 \overbrace{n_{\text{FMA}}}^{\text{\# of FMA}}$$

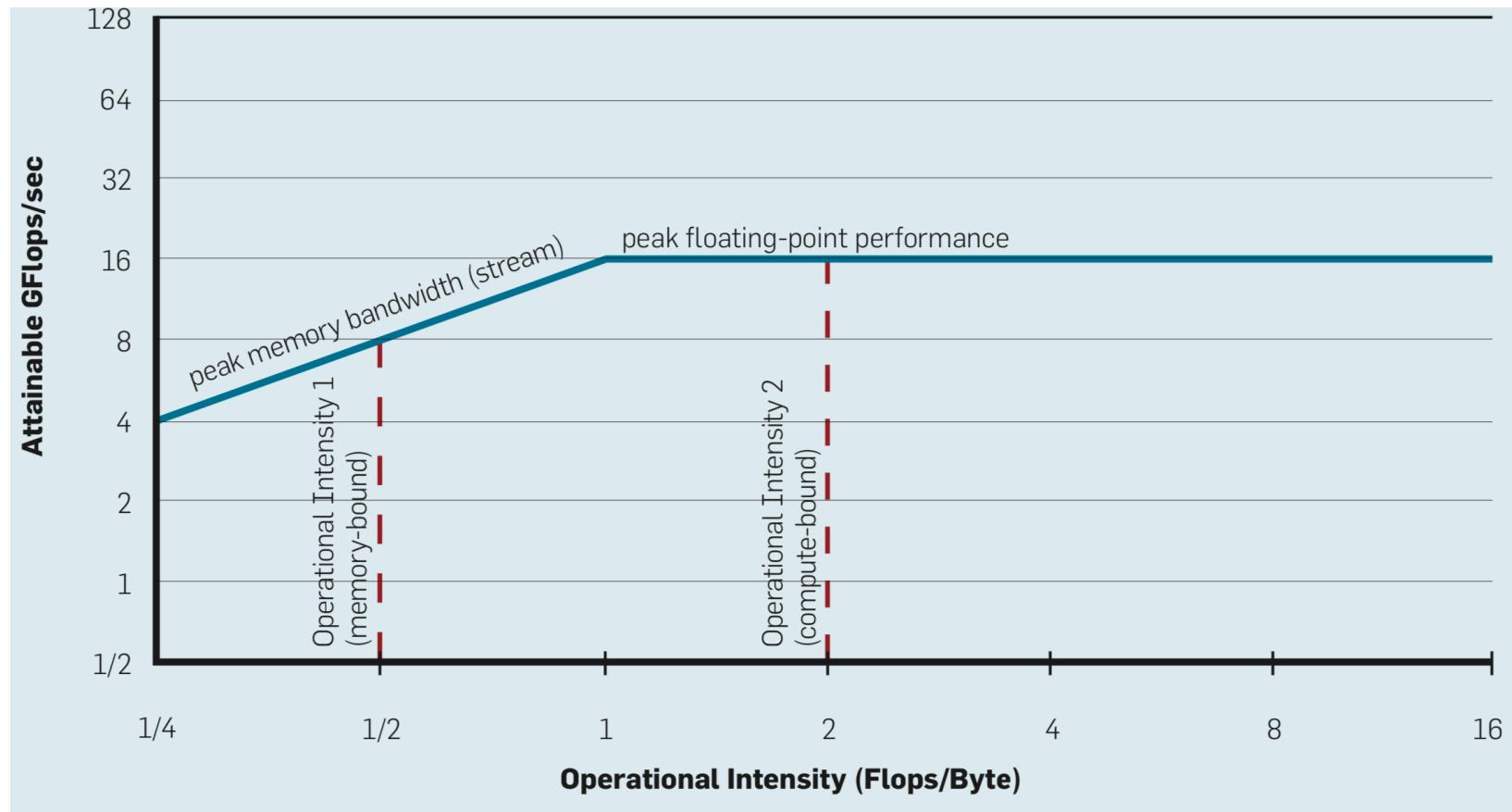
FMA: fused multiply-add unit

S. Williams et al., *Commun. ACM* 52(4), 65 ('09)

V. Elango et al., *ACM. T. Arch. Code Opt.* 11, 67 ('15)

# Roofline Model of Performance

$$\text{Attainable fp} \left[ \frac{\text{Gflop}}{\text{sec}} \right] = \min \left( \text{Peak fp} \left[ \frac{\text{Gflop}}{\text{sec}} \right], \text{Memory bandwidth} \left[ \frac{\text{GByte}}{\text{sec}} \right] \times \text{Operational intensity} \left[ \frac{\text{flop}}{\text{Byte}} \right] \right)$$



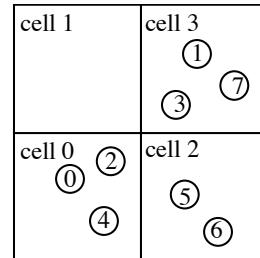
**Key: Data/computation locality:**

see Berkeley [CS267 lecture](#) on “memory hierarchies & matrix multiplication”

# Intranode: Memory Access

## Data re-ordering

- Linked-list cells—irregular memory access pattern



head	0	1	2	3			
	4	E	6	7			
lscl	0	1	2	3	4	5	6    7

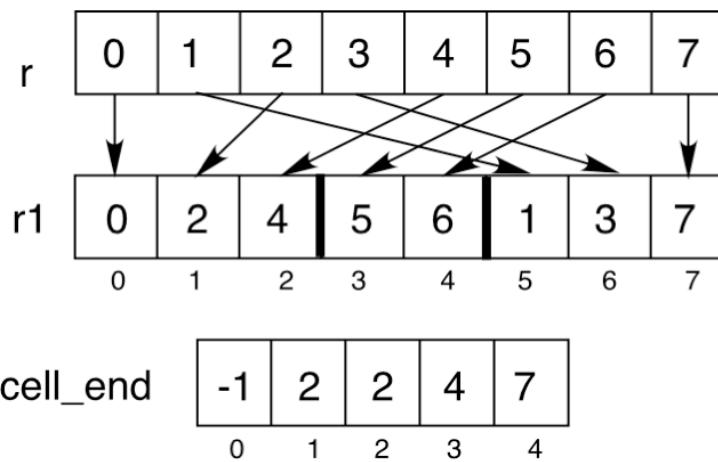
head → 7 → 3 → 1 → Empty

- Data locality: Regular data layout

for i = cell\_end[c]+1 to cell\_end[c+1]

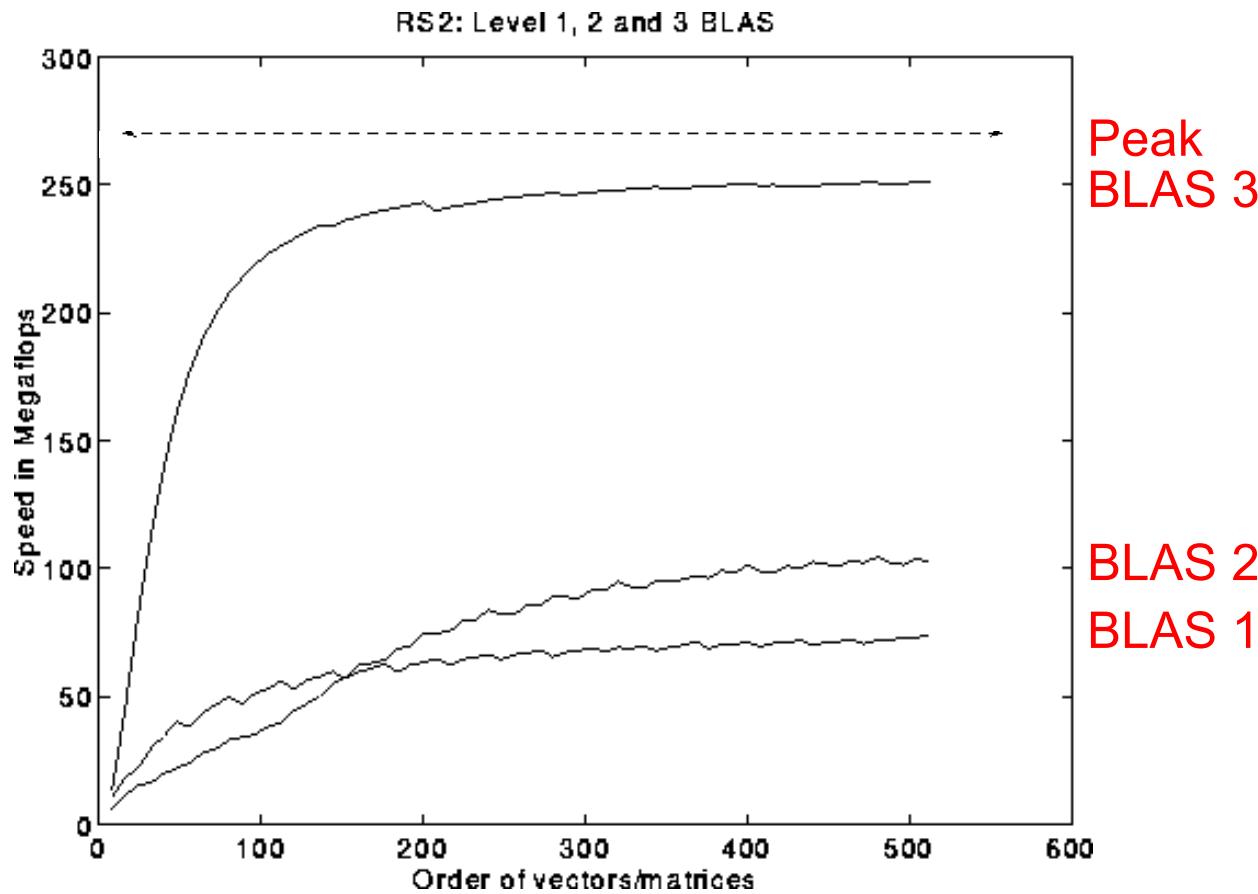
access r1[i]

endfor



# BLAS3-Performance Molecular Dynamics?

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



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

# Floating Point Performance

- **GEMM-ification:** Transform from band-by-band to all-band computations to utilize a matrix-matrix subroutine (DGEMM) in the BLAS3 library for the quantum molecular dynamics application
- Algebraic transformation of computations

## Example: Nonlocal pseudopotential operation

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

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



$$\Psi = [|\psi_1^\alpha\rangle, \dots, |\psi_{N_{\text{band}}}^\alpha\rangle] \quad \tilde{\mathbf{B}}(i) = [|\beta_{i,1}\rangle, \dots, |\beta_{i,N_{\text{atom}}}\rangle] \quad [\tilde{\mathbf{D}}(i,j)]_{I,J} = D_{ij,I} \delta_{IJ}$$

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

- **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**

# More GEMMification

- **GEMMification:** Switch of representation from finite-difference to Kohn-Sham (KS) orbital bases makes nonlocal correction into dense complex-matrix multiplications

$$\underbrace{\Psi(t)}_{\text{FP32}} = \delta \underbrace{\Psi(0)}_{\text{BF16}} \underbrace{\Psi^\dagger(0)}_{\text{BF16}} \underbrace{\Psi(t)}_{\text{BF16}}$$

$N_{\text{grid}} \times N_{\text{orb}}$        $N_{\text{grid}} \times N_{\text{orb}}$        $N_{\text{orb}} \times N_{\text{grid}}$        $N_{\text{grid}} \times N_{\text{orb}}$

- **Mixed-precision:** FP32 to accumulate perturbatively small BF16 matrix multiplications with sufficient precision

N. Piroozan et al., SCW24, DOI: 10.1109/SCW63240.2024.00187

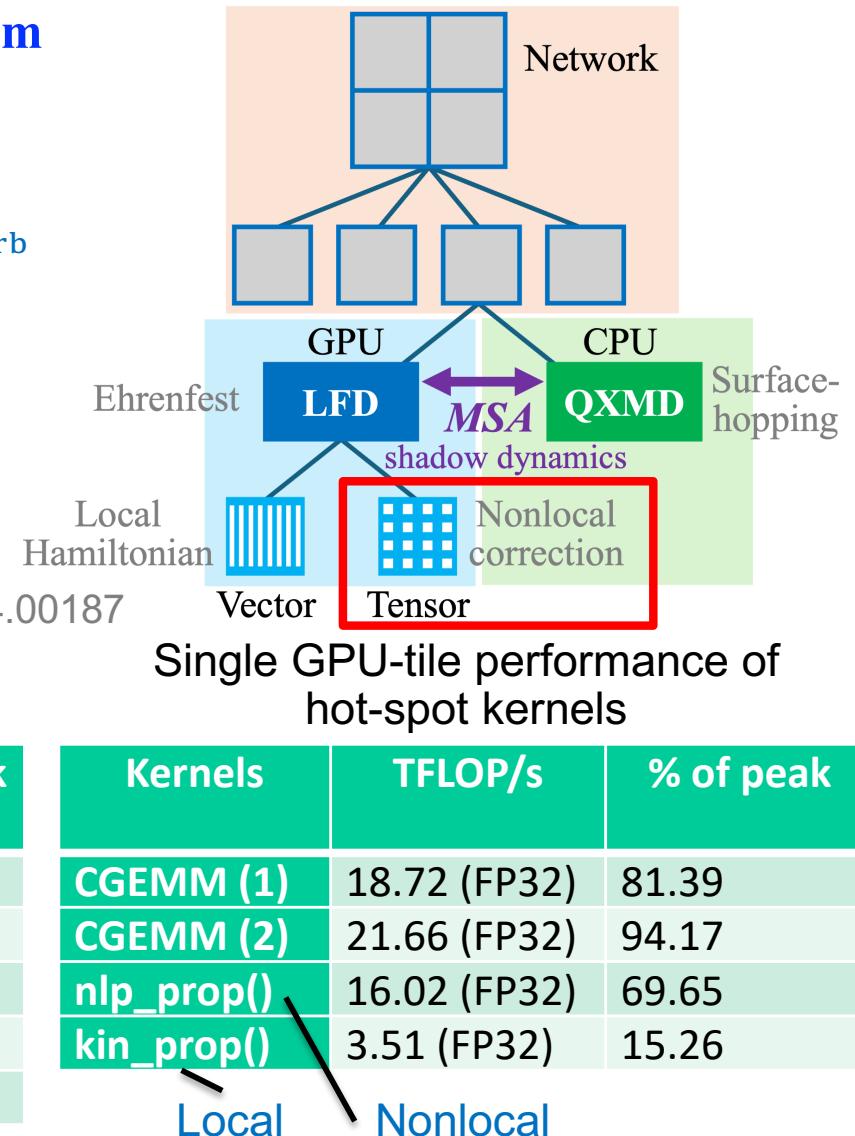
Single GPU-tile performance of DC-MESH for several problem sizes\*

Number of KS orbitals	TFLOP/s	% of FP64 peak (23 TFLOP/s)
256	5.22 (FP32)	22.69
864	9.74 (FP32)	42.35
1024	14.98 (FP32)	65.16
1024	<b>17.95 (FP32/BF16)</b>	<b>78.03</b>
1024	7.69 (FP64)	33.43

\*Intel Data Center GPU Max 1550 GPU (PVC)

- **Breaking the Exaflop/s barrier:** 1.87 Exaflop/s on 60,000 GPUs of Aurora (94% of FP64 peak)

T. M. Razakh et al., IEEE/ACM SC ('25); arXiv:2509.00966

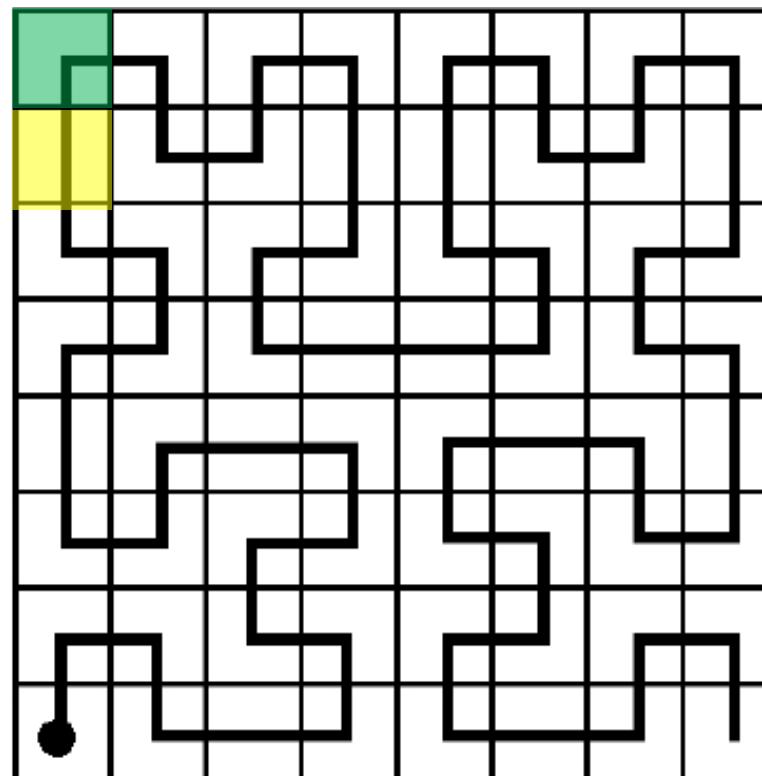


# Computation Locality

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**Data-to-computaion locality:** How to traverse the linked-list cells?

- **Pair-interaction computation:** Preserve nearest-neighbor cells' proximity in memory
- **Spacefilling curve:** Mapping from the  $d$ -dimensional space to one-dimensional list to preserve spatial proximity of consecutive list elements



# Hilbert-Peano Curve

- Gray code: a sequence of numbers such that successive numbers have Hamming distance 1

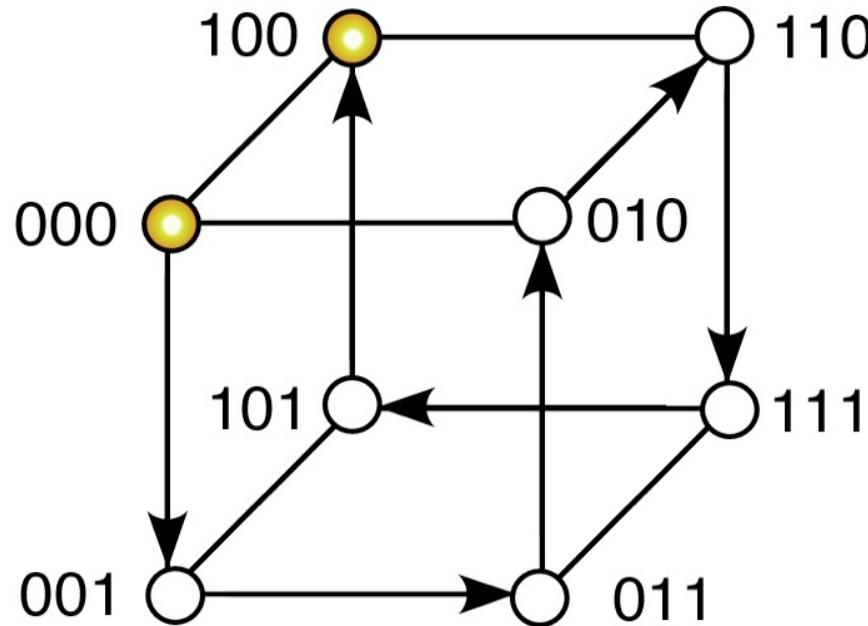
Algorithm: Recursive generation of k-bit Gray code  $G(k)$   
(1)  $G(1)$  is a sequence: 0 1.

# of bits where two binary numbers differ

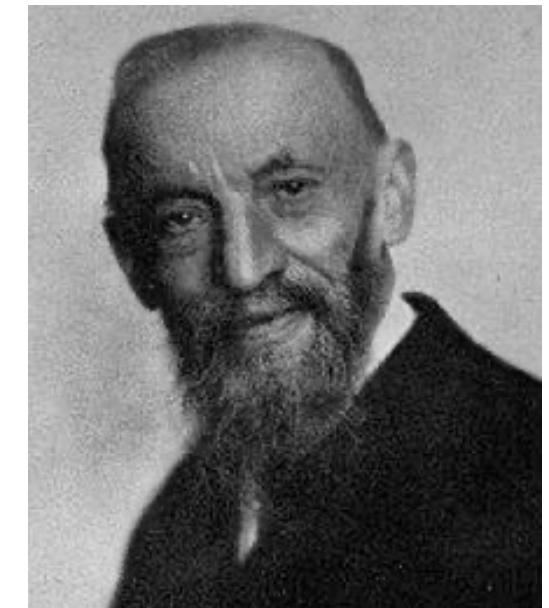
(2)  $G(k+1)$  is constructed from  $G(k)$  as follows:

- Construct a new sequence by appending a 0 to the left of all members of  $G(k)$ .
- Construct a new sequence by reversing  $G(k)$  & then appending a 1 to the left of all members of the sequence.
- $G(k+1)$  is the concatenation of the sequences defined in steps a & b.

- $G(3): 000 \ 001 \ 011 \ 010 \ 110 \ 111 \ 101 \ 100$



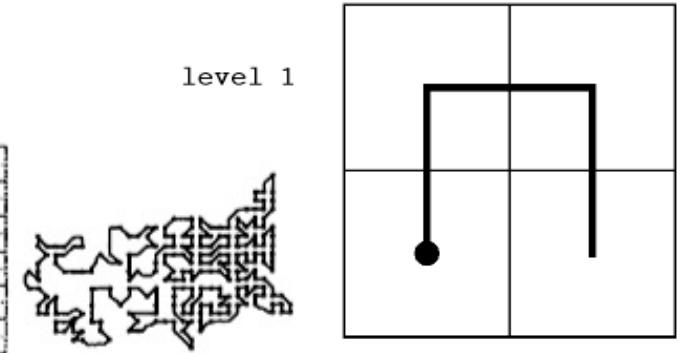
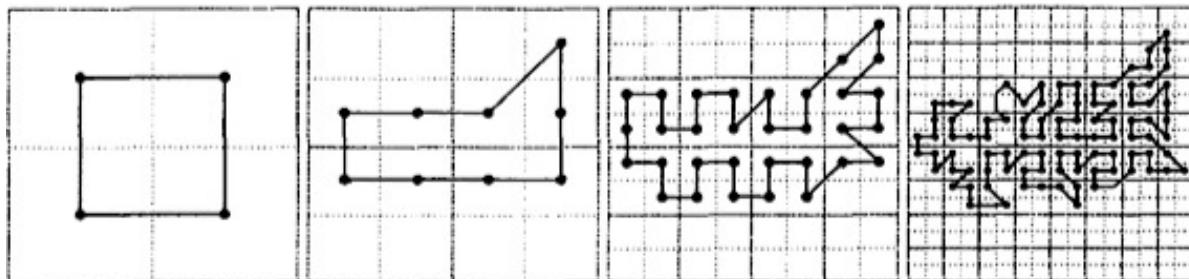
David Hilbert (1862–1943)



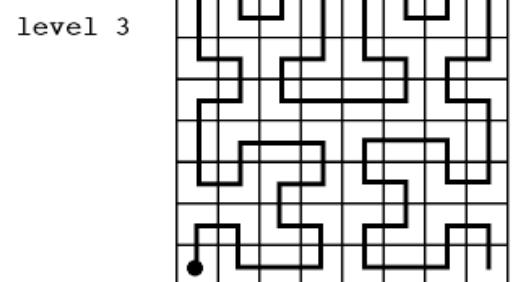
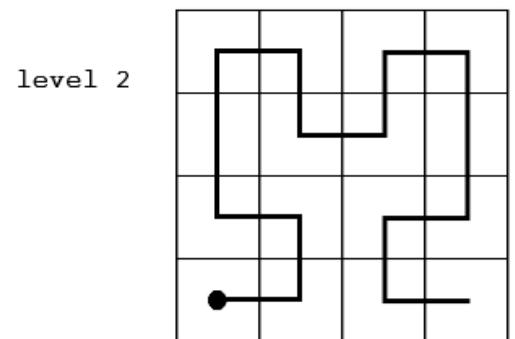
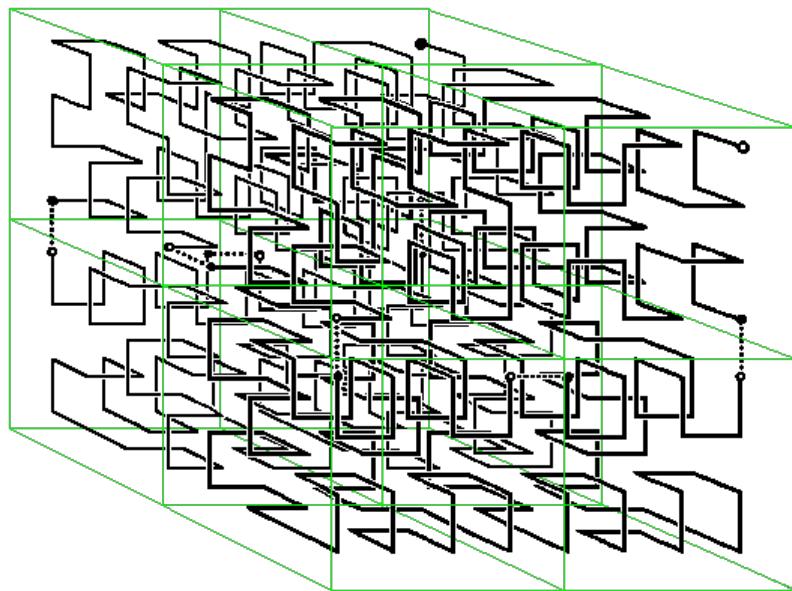
Giuseppe Peano (1858–1932)

# Hilbert-Peano Curve

- Hilbert curve: recursive application of the  $d$ -dimensional Gray codes
- 2-dimensional Hilbert curve



- 3-dimensional Hilbert curve

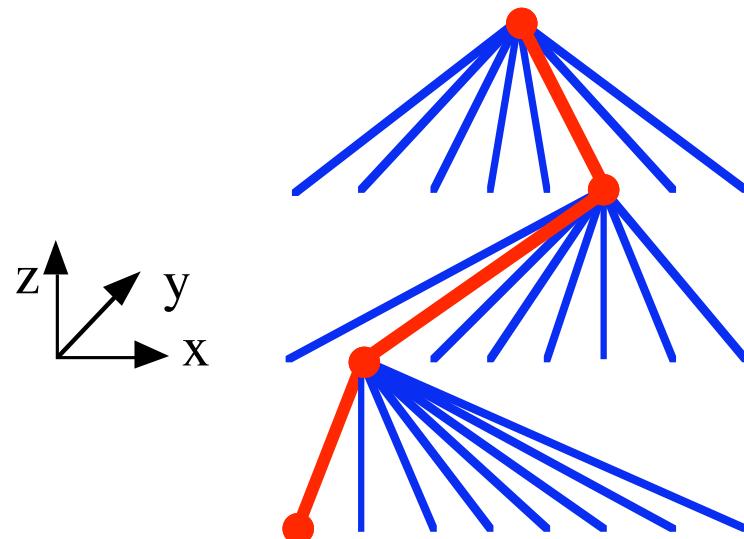
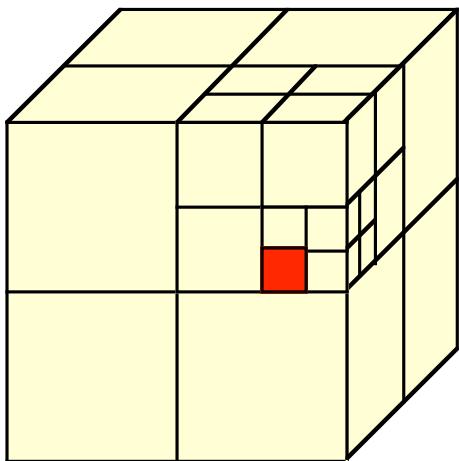


# Morton (Z) Curve

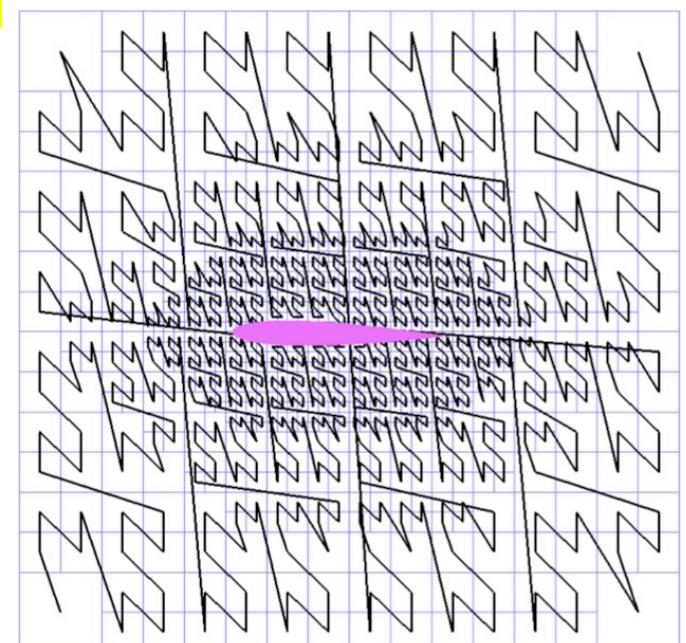
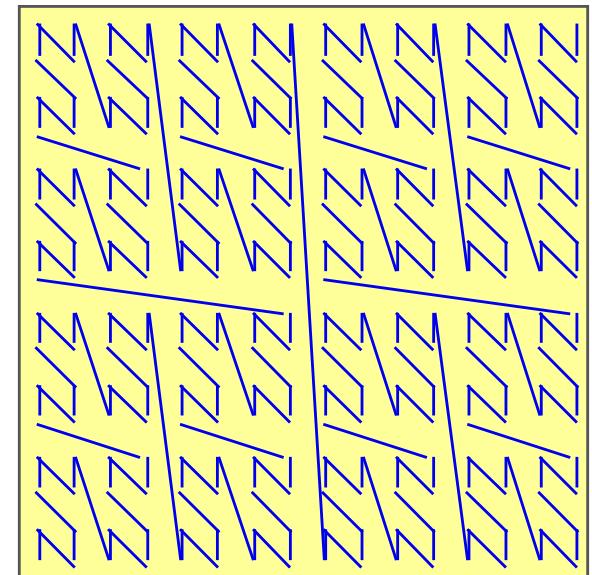
- Spacefilling curve based on octree index

$$\begin{array}{r} \mathbf{x} = \quad 1 \quad 1 \quad 0 \\ \mathbf{y} = \quad 0 \quad 0 \quad 0 \\ \mathbf{z} = 1 \quad 0 \quad 0 \\ \hline \mathbf{R} = 101 \ 001 \ 000 \end{array}$$

- 3D  $\rightarrow$  list map preserves spatial proximity
- Multiresolution analysis made easy



A. Omeltchenko et al., [Comput. Phys. Commun. 131, 78 \('00\)](#)



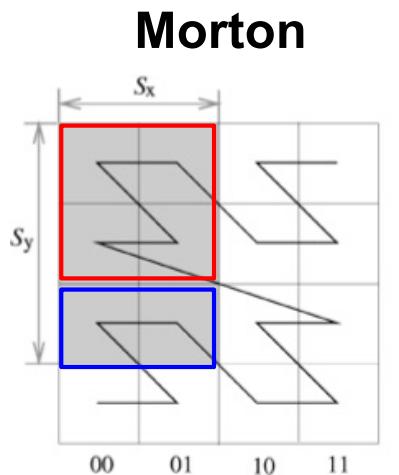
# Analysis of Data Locality

124

IEEE TRANSACTIONS ON KNOWLEDGE AND DATA ENGINEERING, VOL. 13, NO. 1, JANUARY/FEBRUARY 2001

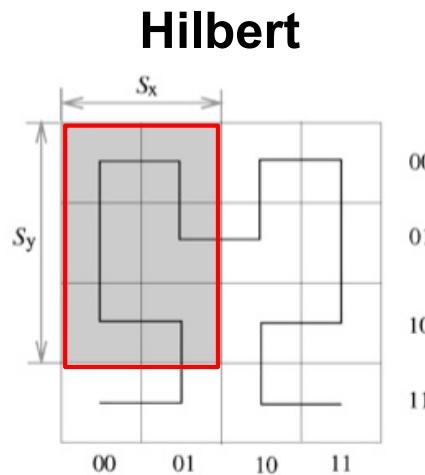
## Analysis of the Clustering Properties of the Hilbert Space-Filling Curve

Bongki Moon, H.V. Jagadish, Christos Faloutsos, *Member, IEEE*, and  
Joel H. Saltz, *Member, IEEE*

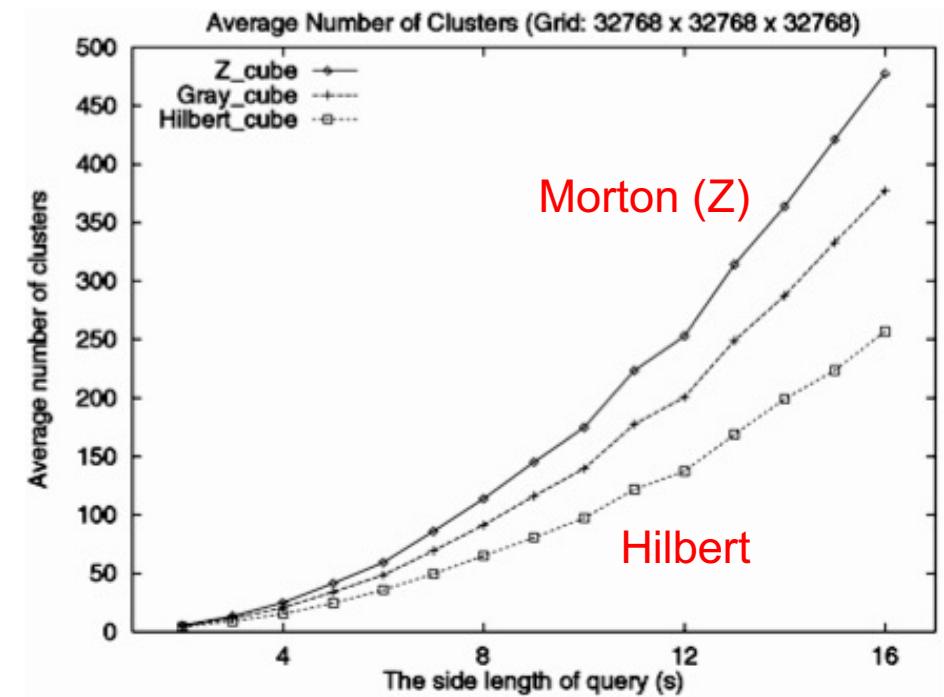


**2 clusters**

**Cluster ~ cache line ~ latency cost**



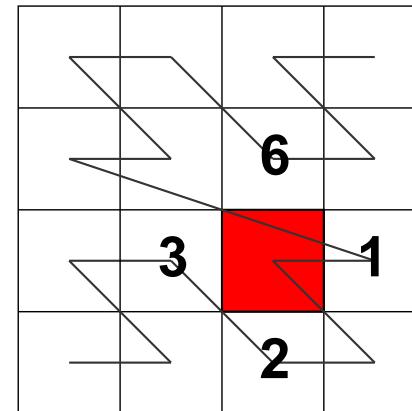
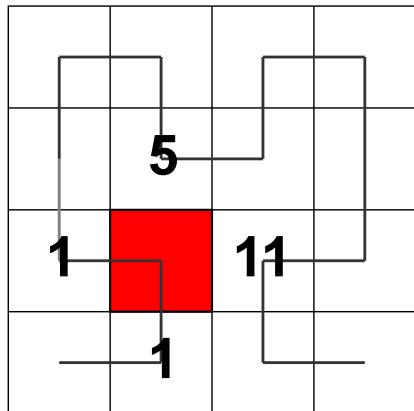
**1 cluster**



Hilbert curve is better than Morton curve for spatial range query

# Alternative Locality Measure for MD

- Doubly nested loops of cell access
- Evaluate curves based on along-curve distances to neighbors
- Compare number below and above threshold cutoff  $k_c$  (like cache)



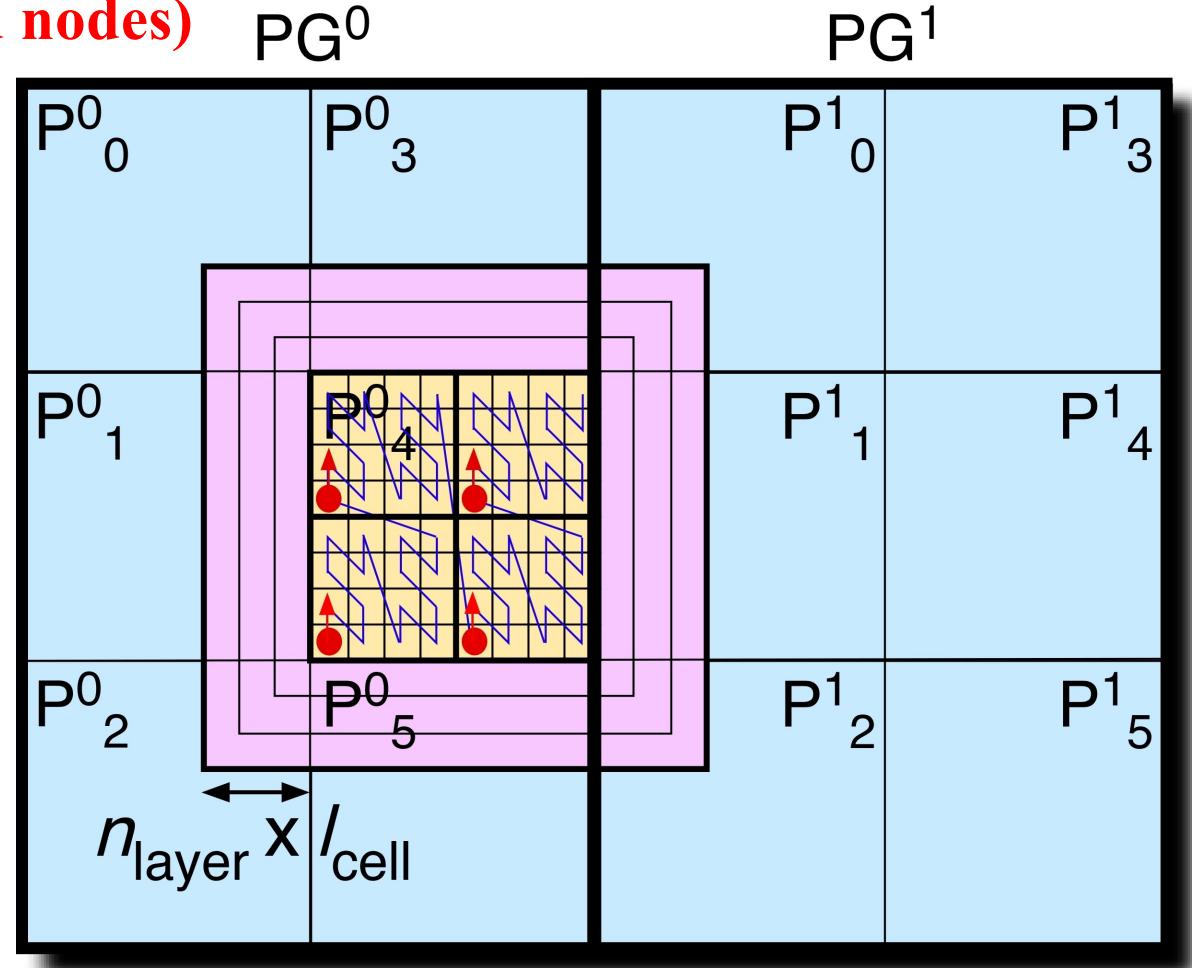
- 4x4 Hilbert:
  - 30 1s
  - 10 3s
  - 4 5s
  - 2 11s
  - 2 13s
- Lower median, higher variance
- Better for  $k_c=1$

- 4x4 Z-curve:
  - 16 1s
  - 16 2s
  - 8 3s
  - 8 6s
- Higher median, lower variance
- Better for  $2 < k_c < 13$

# Tunable Hierarchical Cellular Decomposition

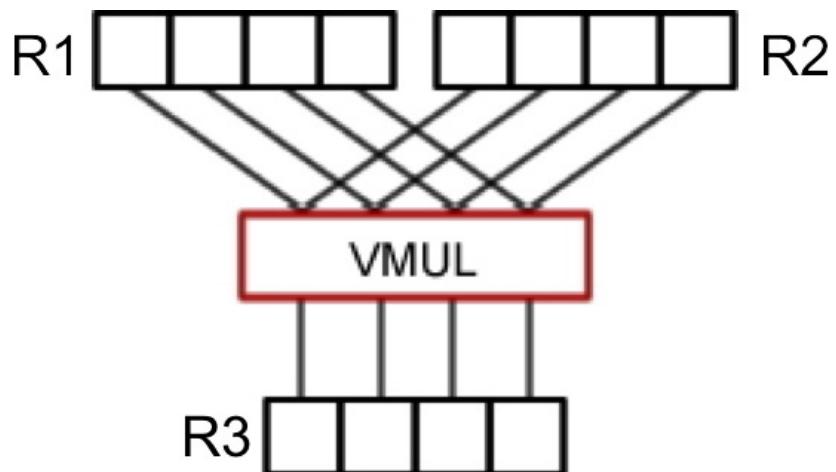
Mapping  $O(N)$  divide-&-conquer algorithms onto memory hierarchies

- 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 ( $P^{\gamma}$ , Grid nodes)
- Multilayer cellular decomposition (MCD) for  $n$ -tuples ( $n = 2\text{--}6$ )
- Tunable cell data & computation structures: Data/computation re-ordering & granularity parameterized at each decomposition level
- Tunable hybrid MPI + OpenMP + SIMD implementation



# SIMD/Vector Operation

- Single-instruction multiple-data (SIMD) parallelism: An arithmetic operation is operated on multiple operand-pairs stored in vector registers, each of which can hold multiple double-precision numbers.

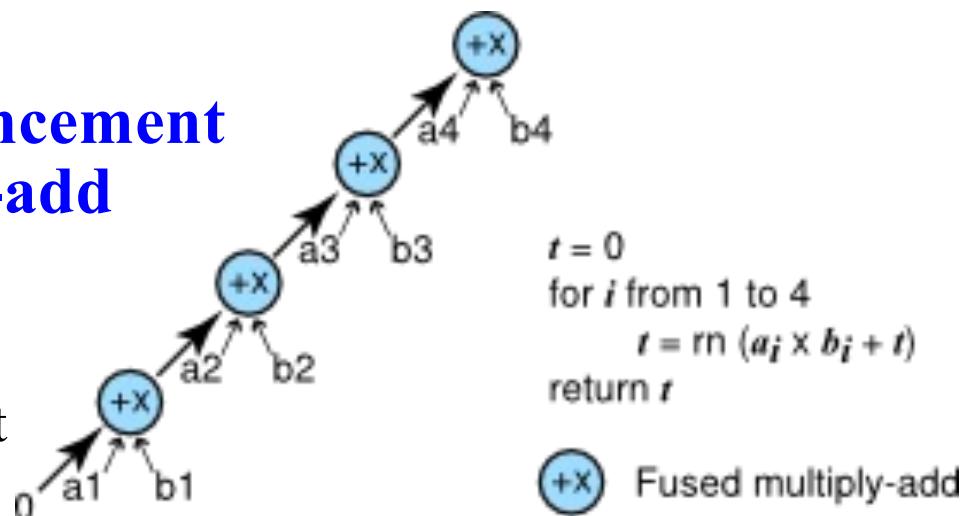


**Example:** Vector multiplier (VMUL) loads data from two vector registers, R1 and R2, each holding 4 double-precision numbers, concurrently performs 4 multiplications, and stores the results on vector register R3.

- Peak performance enhancement on top of fused multiply-add (FMA) unit.

$$a \leftarrow a + b \times c$$

with 1-cycle throughput



# Vector Processing at CARC

## Node information

CPU model	Microarchitecture	Partitions	SSE	SSE2	SSE3	SSE4	AVX	AVX2	AVX-512
xeon-2650v2	ivybridge	oneweek, debug	✓	✓	✓	✓	✓		
xeon-2640v3	haswell	main, oneweek, debug	✓	✓	✓	✓	✓	✓	
xeon-2640v4	broadwell	main, gpu, debug	✓	✓	✓	✓	✓	✓	
xeon-4116	skylake_avx512	main	✓	✓	✓	✓	✓	✓	✓
xeon-6130	skylake_avx512	gpu	✓	✓	✓	✓	✓	✓	✓
epyc-7542	zen2	epyc-64	✓	✓	✓	✓	✓	✓	
epyc-7513	zen3	epyc-64, gpu, largemem	✓	✓	✓	✓	✓	✓	✓
epyc-7282	zen2	gpu	✓	✓	✓	✓	✓	✓	

## Intel & AMD advanced vector extension (AVX):

- AVX2 operates on 4 double-precision floating-point numbers
- AVX512

# SIMD Vectorization: MD

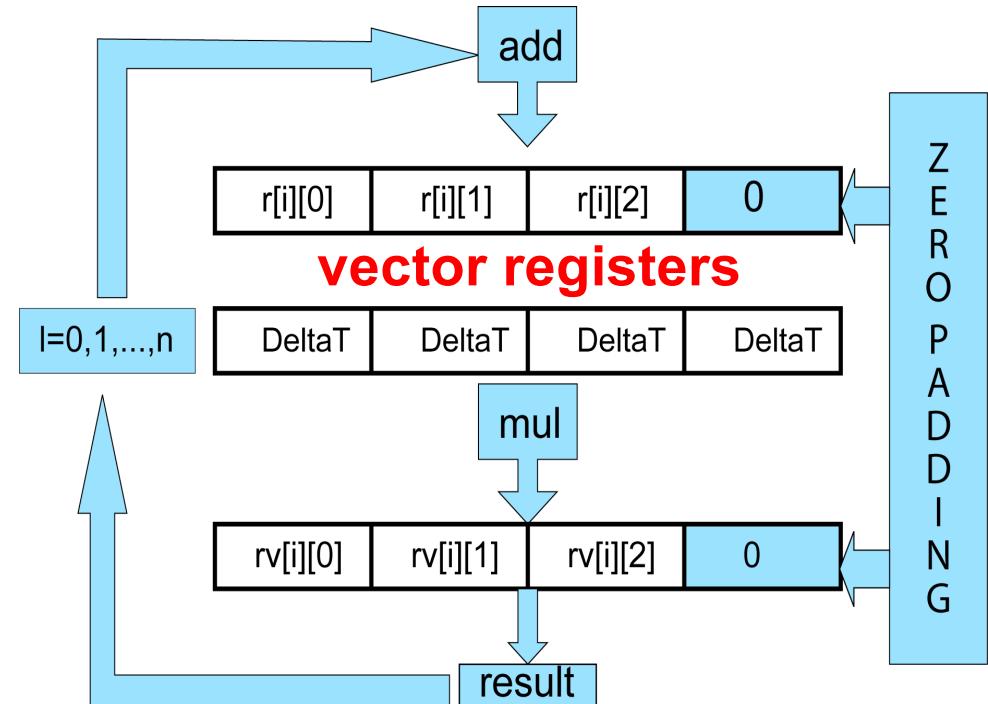
- Single-instruction multiple-data (SIMD) parallelism

(Example) Zero padding to align complex data

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



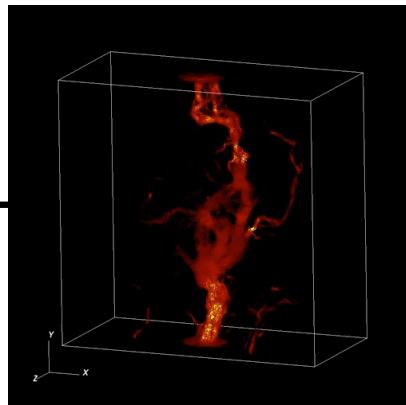
cf. False-sharing avoidance

# SIMD Vectorization: LBM

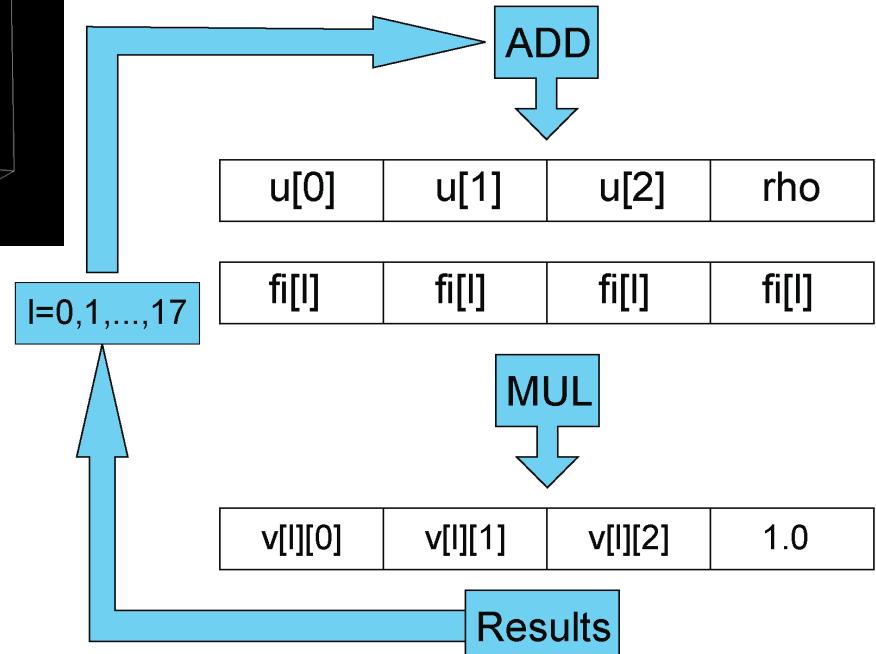
- Translocated statement fusion in lattice-Boltzmann flow simulation

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];  
    }  
}
```



SIMD solution



$3 \times 18 \times 5 = 270$  computation

SIMDizable mathematical formulations:

Special relativity, quaternion, etc.

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

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

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

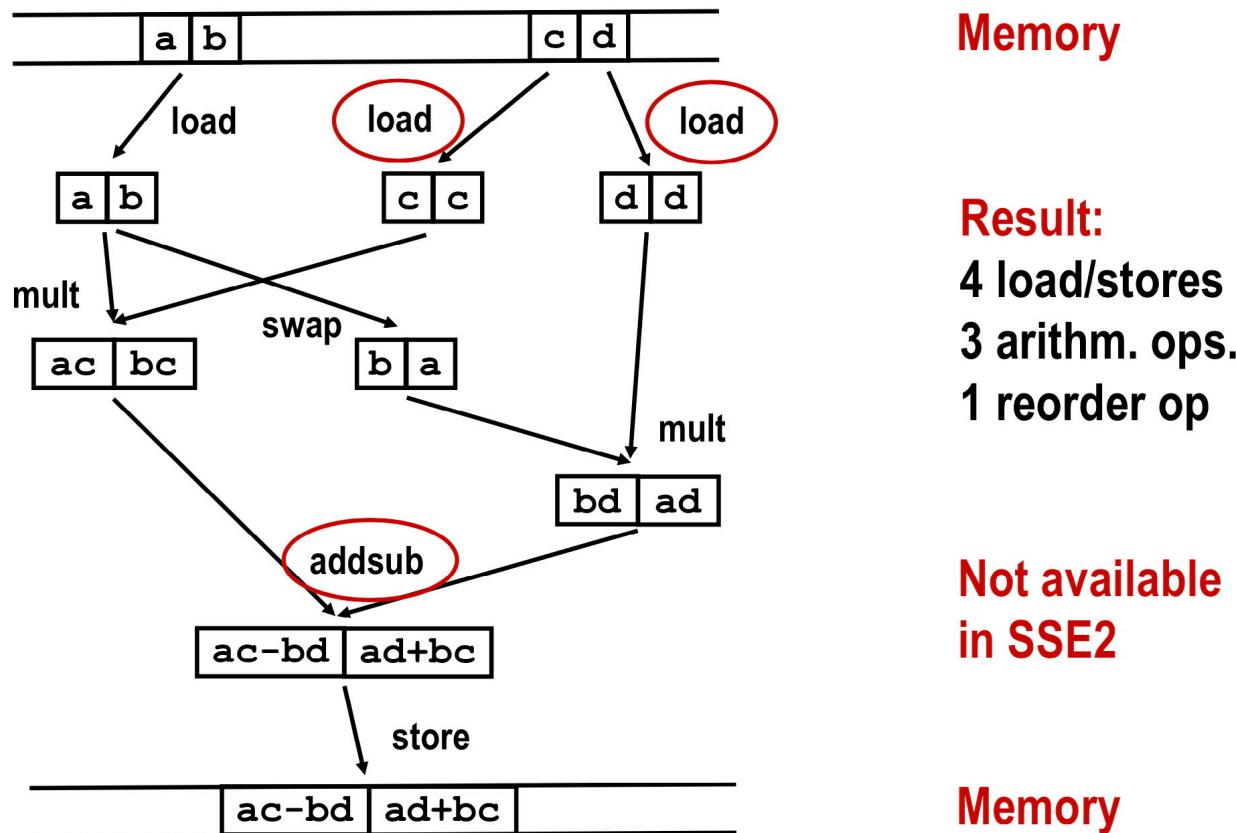
$18 \times 4 = 72$  computation

Ideal Speedup 3.5

# SIMDized Complex Multiplication

- SSE (streaming SIMD extension) instruction set  
Pre-AVX instruction set
- For quantum dynamics?

$$(a + ib)(c + id) = (ac - bd) + i(ad + bc)$$

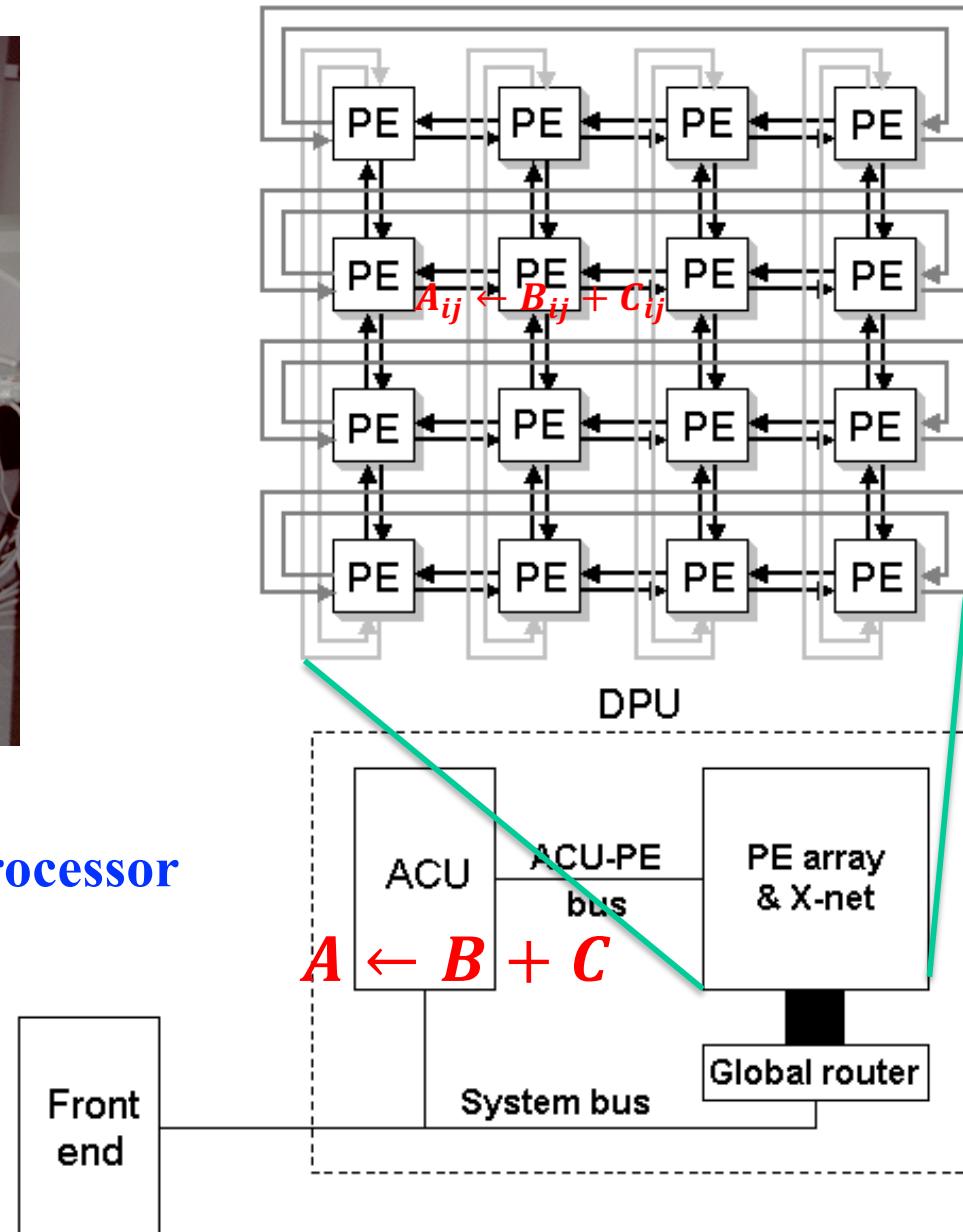


# Massive SIMD Data Parallelism



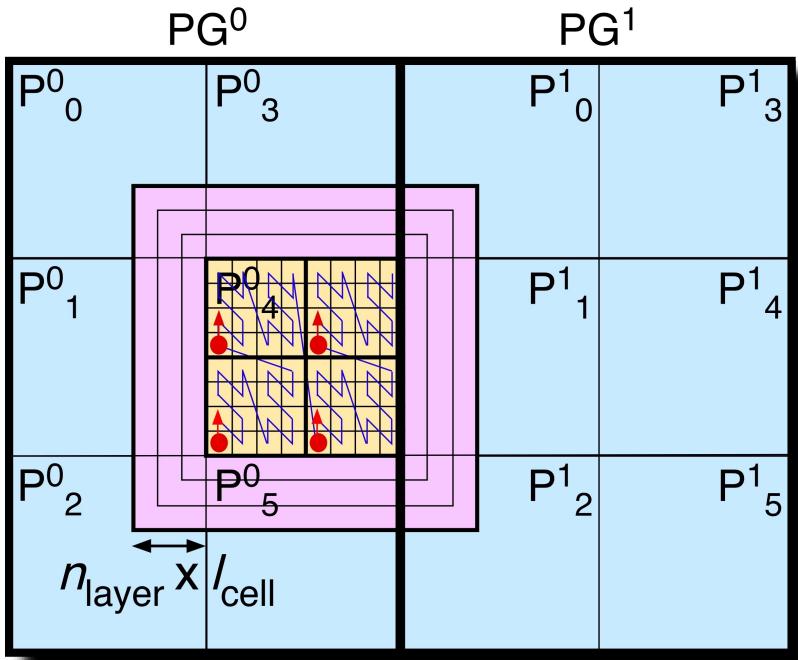
Quantum dynamics on 8,192-processor  
( $128 \times 64$ ) MasPar 1208B

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



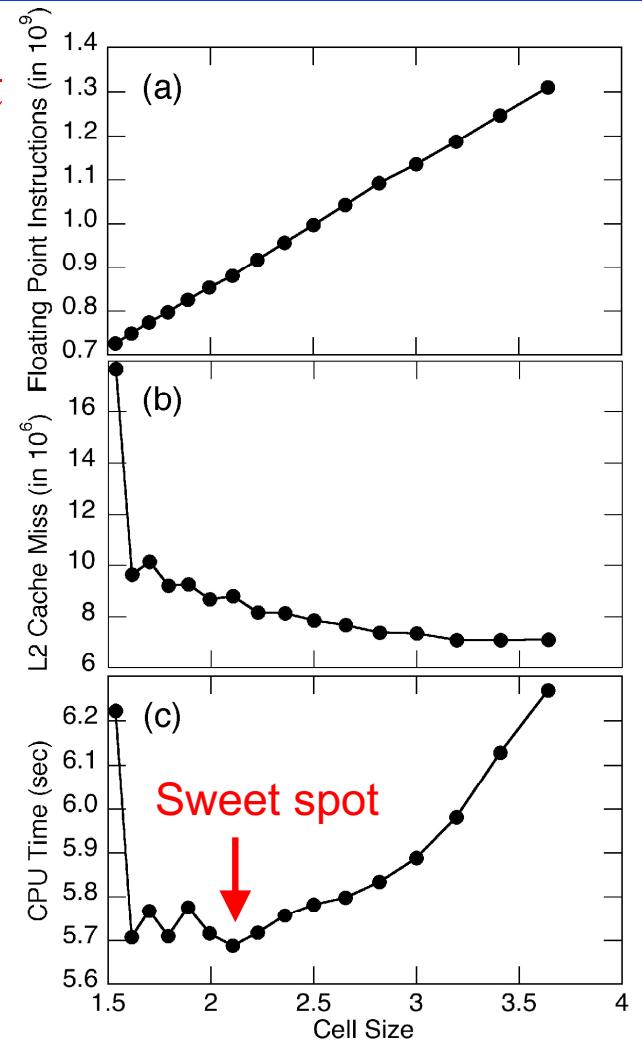
See lecture on pre-Beowulf parallel computing

# Performance Tunability



**MPI/OpenMP parallelism trade-off:**  
**8,232,000-atom silica MRMD & 290,304-atom RDX F-ReaxFF on 8-way 1.5 GHz Power4**

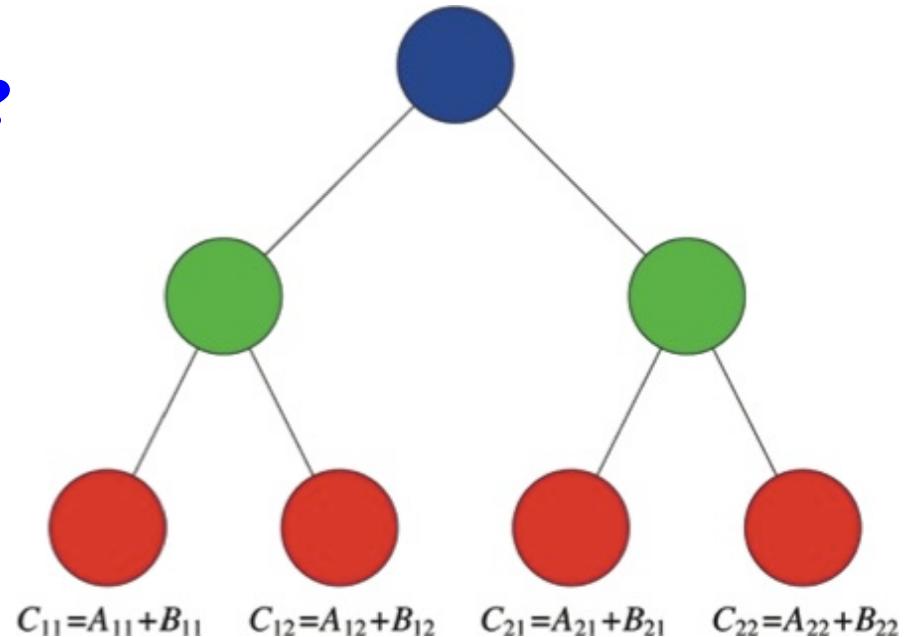
**Floating-point operation/L2 cache miss trade-off:  
 331,776-atom silica MRMD on 1.4GHz Pentium III**



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

# Cache-Oblivious Linked-List Cell MD?

- Recursive blocking for cells?



## Cache-Oblivious Algorithms

EXTENDED ABSTRACT SUBMITTED FOR PUBLICATION. In Proc. FOCS99

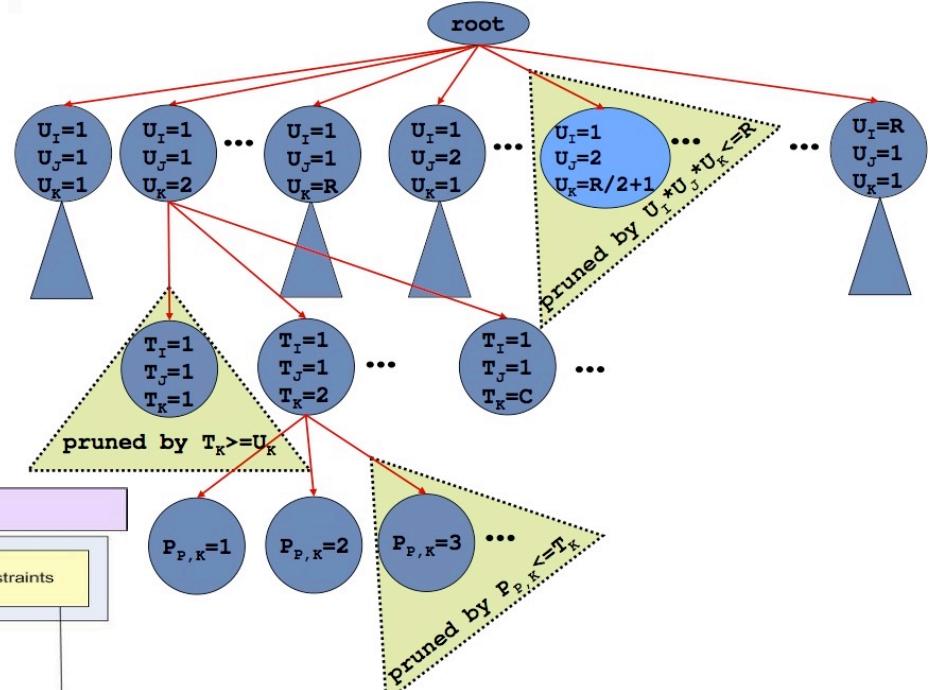
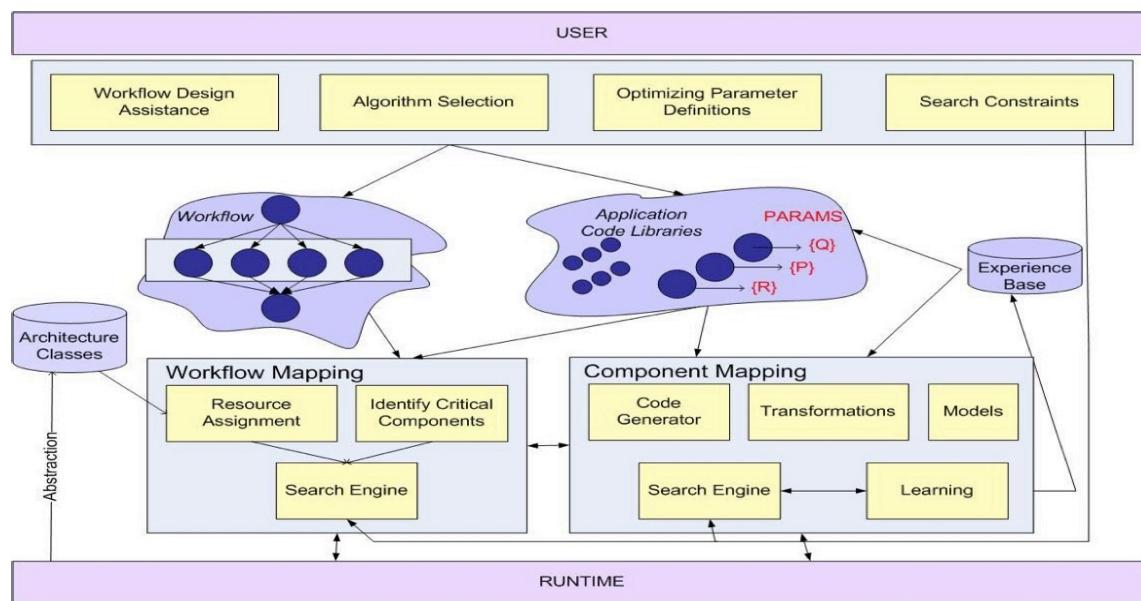
Matteo Frigo      Charles E. Leiserson      Harald Prokop      Sridhar Ramachandran  
MIT Laboratory for Computer Science, 545 Technology Square, Cambridge, MA 02139  
`{athena, cel, prokop, sridhar}@supertech.lcs.mit.edu`

We introduce an “ideal-cache” model to analyze our algorithms, and we prove that an optimal cache-oblivious algorithm designed for two levels of memory is also optimal for multiple levels.

# Intelligent Performance Optimization

- Knowledge representation to express concurrency/data locality & machine learning to optimally map them to hardware

cf. Tunable hierarchical cellular decomposition exposes maximal data locality



Pruned decision tree  
C. Chen, Ph.D.  
Thesis (Computer  
Science, USC, '07)

"Intelligent optimization of parallel & distributed applications," B. Bansal, U. Catalyurek, J. Chame, C. Chen, E. Deelman, Y. Gil, M. Hall, V. Kumar, T. Kurc, K. Lerman, A. Nakano, Y. L. Nelson, J. Saltz, A. Sharma, and P. Vashishta, in *Proc. of Next Generation Software Workshop, Int'l Parallel & Distributed Processing Symp. (IPDPS 07)*

# Key Internode Feature

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## Simple communication cost model

$$t_{\text{comm}} = t_l + m/b$$

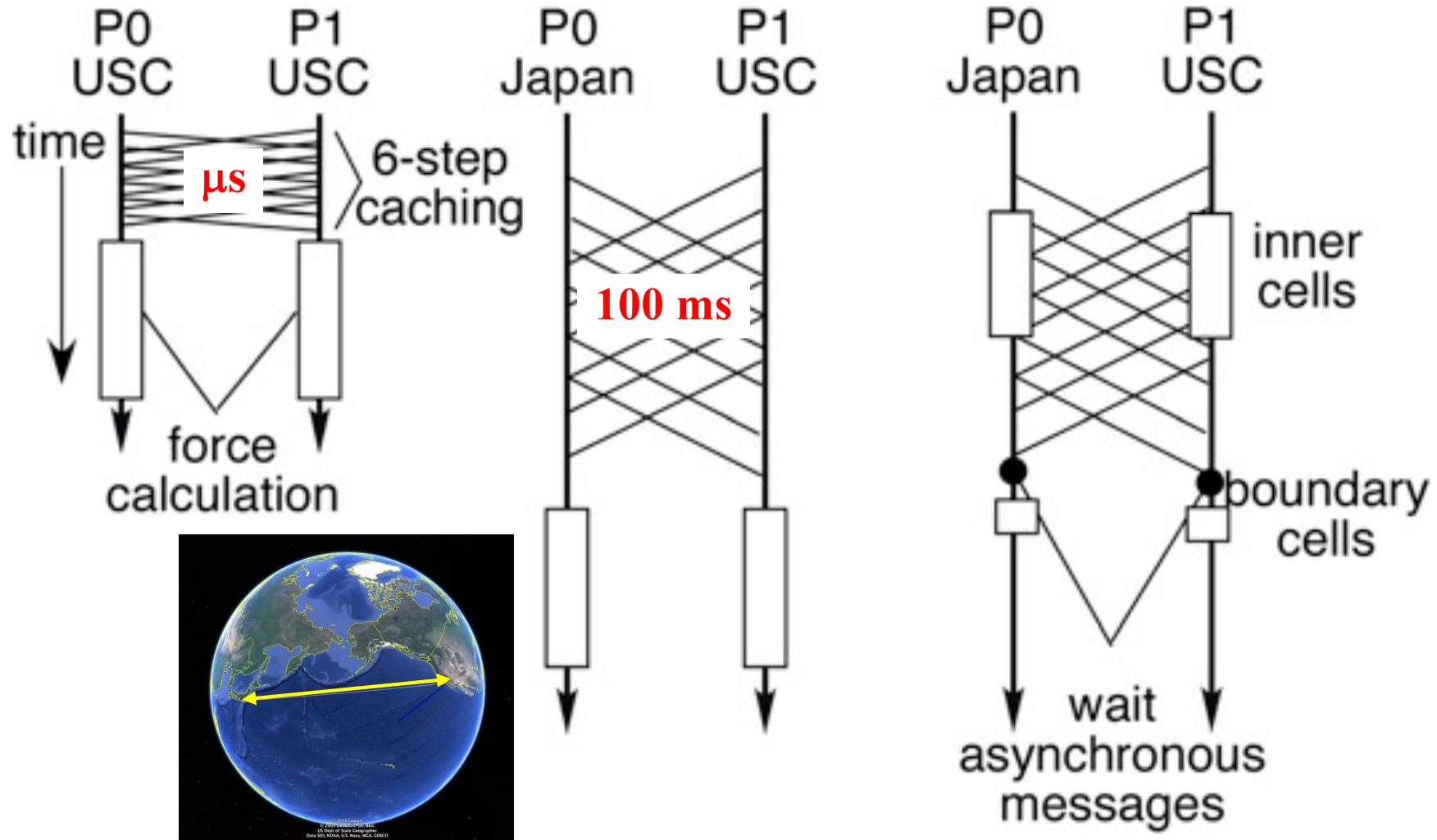
$t_{\text{comm}}$ : Total communication time for  $m$  Bytes

$t_l$ : Latency = time delay for the head of a message to travel between the source & destination nodes

$b$ : Bandwidth = number of Bytes per second that can be transmitted through the communication link

# Internode Optimization

- Communication bottleneck in metacomputing on a Grid

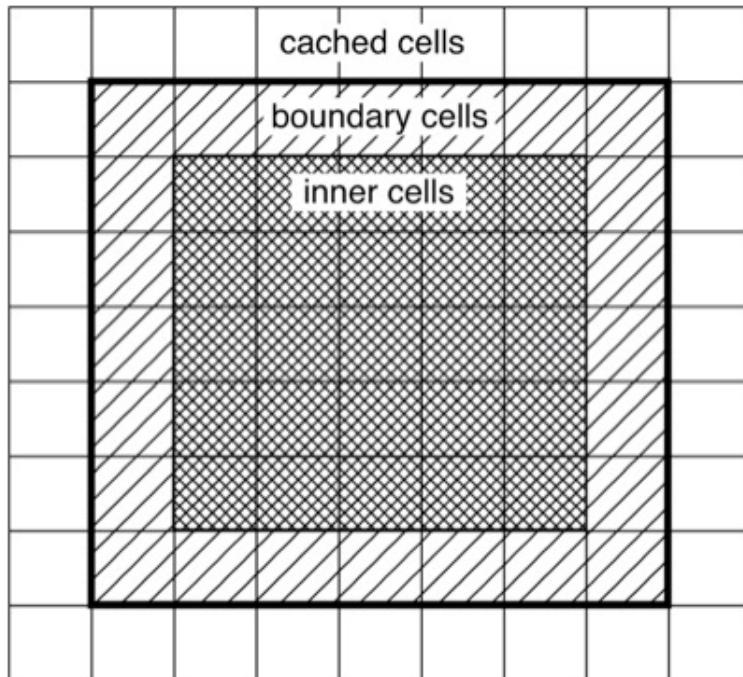


- Overlap computation & communication to hide the latency

# Grid-Enabled MD Algorithm

## Grid MD algorithm:

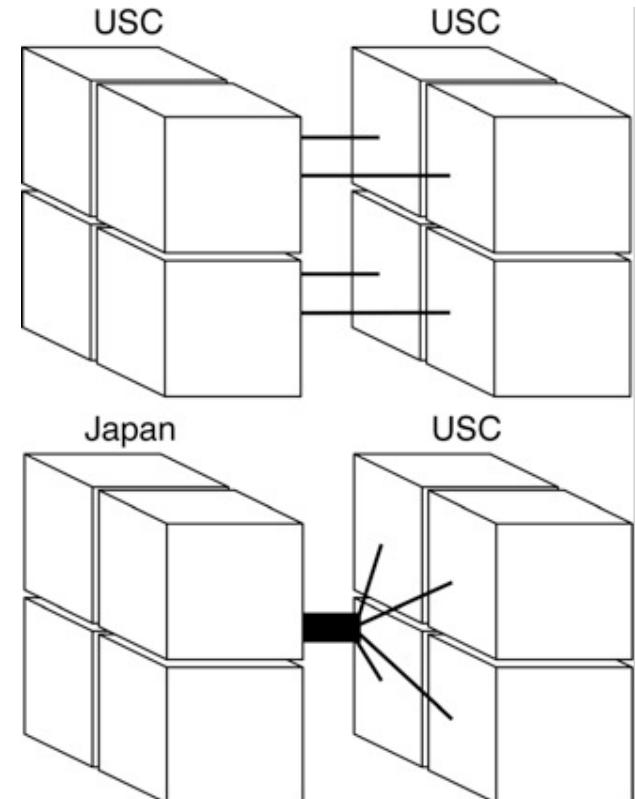
1. asynchronous receive of cells to be cached
2. send atomic coordinates in the boundary cells
3. compute forces for atoms in the inner cells
4. wait for the completion of the asynchronous receive
5. compute forces for atoms in the boundary cells



Kikuchi *et al.*, in Proc. SC02

## Renormalized Messages:

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

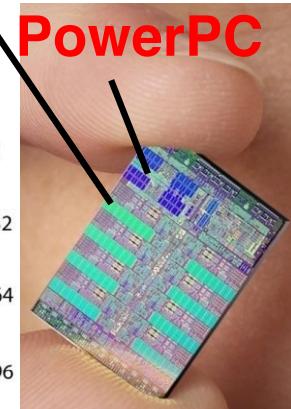
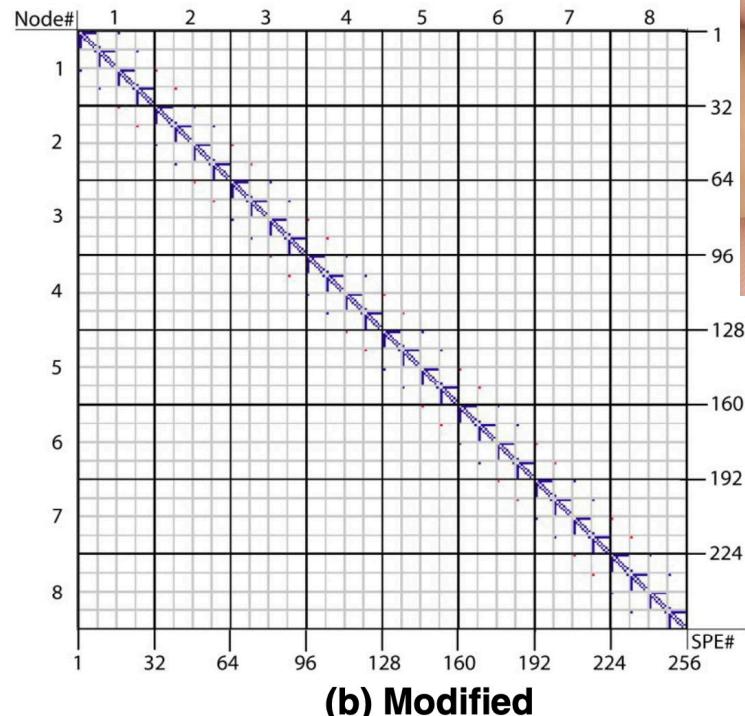
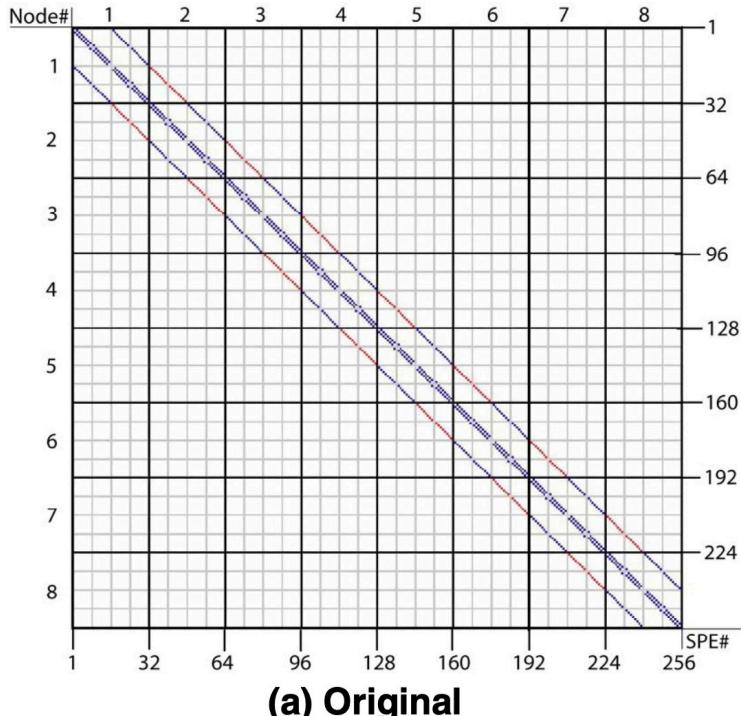


# Renormalized Message Passing

- Mapping a 3D-lattice problem onto 8 computing nodes each with 4 Cell processors (or 32 cores)
- Renormalized message passing reduce the number of internode communications

H. Dursun et al., *Par. Proc. Lett.* **19**, 535 ('09)

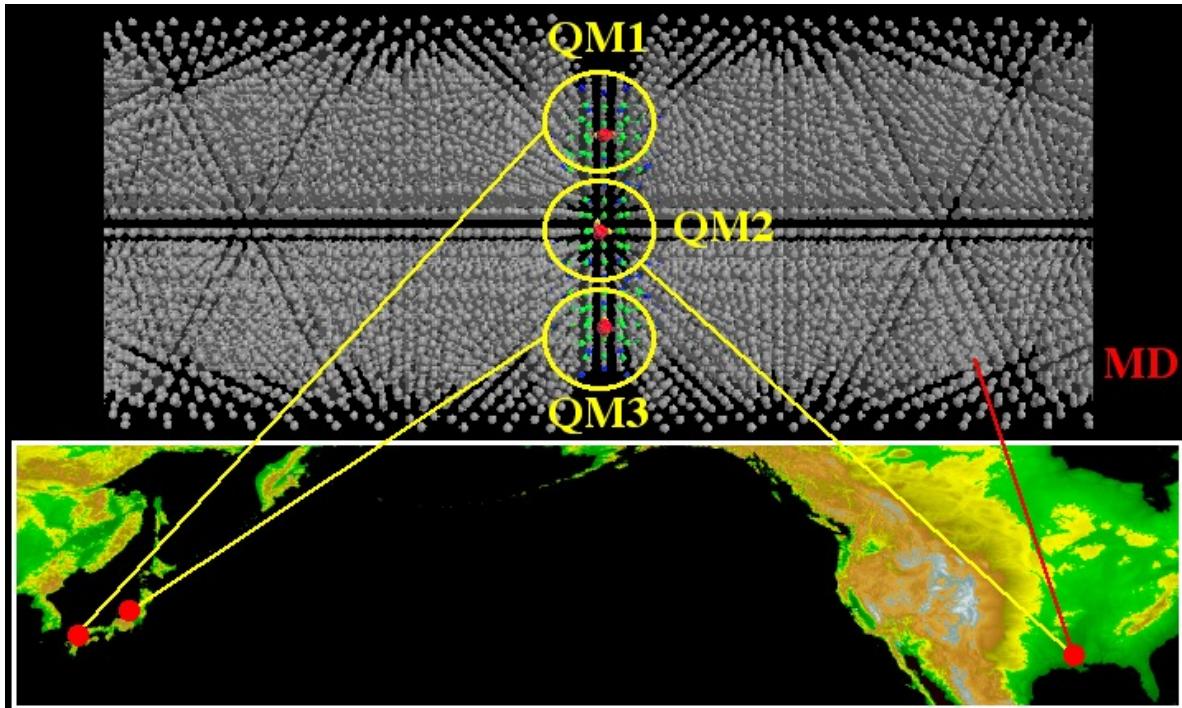
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband, IBM DOE/NNSA/LANL United States	122,400	1,026.00	1,375.78	2,345



# Global Collaborative Simulation

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

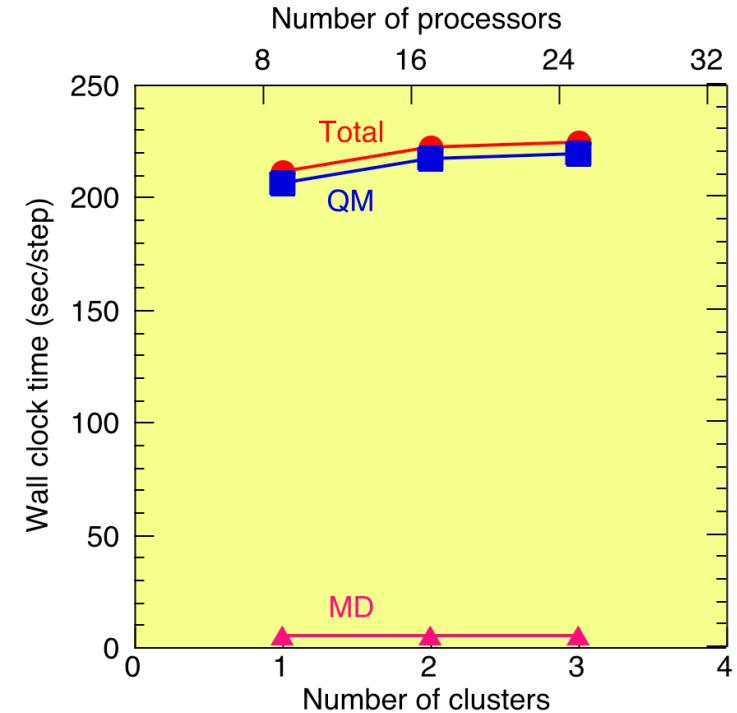
- Task decomposition (MPI Communicator) + spatial decomposition
- MPICH-G2 ([www.niu.edu/mpi](http://www.niu.edu/mpi))/Globus ([www.globus.org](http://www.globus.org))



Japan: Yamaguchi—65 P4 2.0GHz

Hiroshima, Okayama, Niigata—3×24 P4 1.8GHz

US: Louisiana—17 Athlon XP 1900+

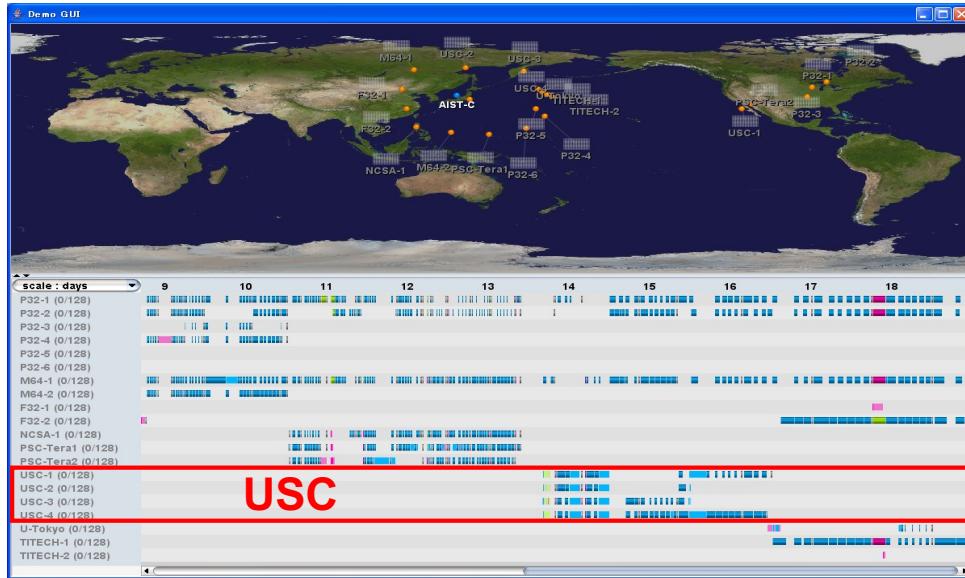


MD — 91,256 atoms

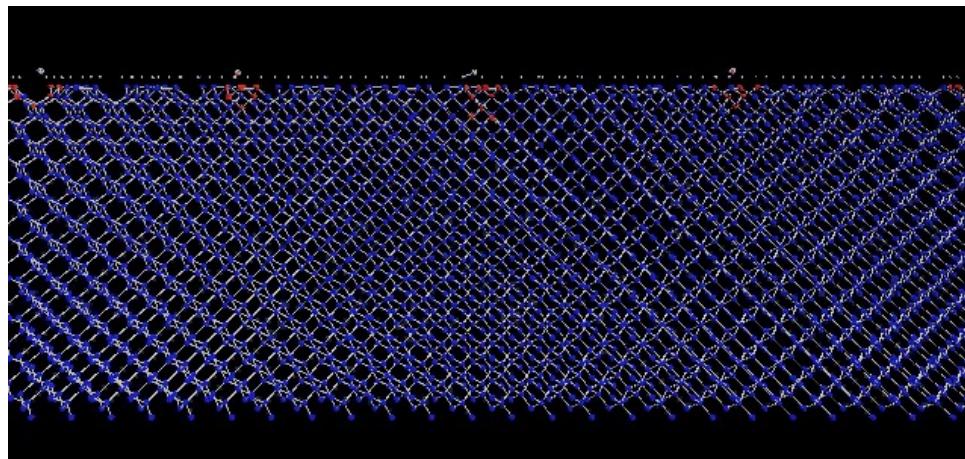
QM (DFT) — 76 $n$  atoms on  $n$  clusters

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

# Global Grid QM/MD

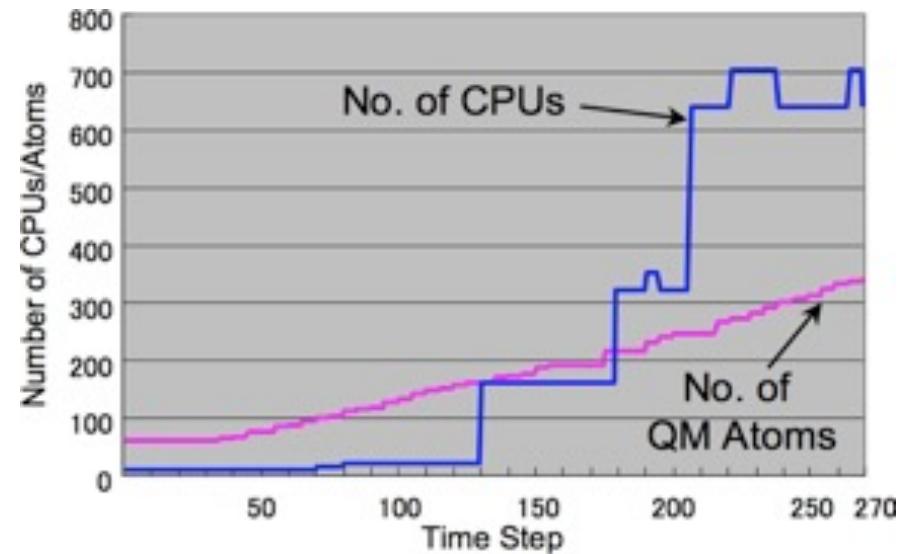


High-energy beam oxidation of Si



H. Takemiya et al., Proc. IEEE/ACM SC06

- Sustained (153,600 cpu-hrs) Grid supercomputing at 6 centers in the US (USC, NCSA, PSC) & Japan (AIST, U Tokyo, TITECH)
- Dynamic allocation of computing resources on demand & automated migration due to reservation schedule & faults
- Hybrid GridRPC ([ninf.apgrid.org](http://ninf.apgrid.org)) + MPI ([www.mcs.anl.gov/mpi](http://www.mcs.anl.gov/mpi)) Grid computing



# Fast TCP

## BBC NEWS WORLD EDITION

Last Updated: Thursday, 5 June, 2003, 10:48 GMT 11:48 UK

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### Promise of ultra-fast downloads

Soon you could be downloading an entire movie off the net far faster than you do now.

US researchers are working on ways to improve the way that net protocols decide how quickly data travels around the net.

Early tests of the new system show that it can triple data transmission speeds.

By linking lots of the faster systems together the researchers have produced data transfer speeds many times higher than is possible today.



Fast net tech could soon take off

### Packet tracking promises ultrafast internet

10:54 05 June 03

Exclusive from New Scientist Print Edition. [Subscribe](#) and get 4 free issues.

Imagine an internet connection so fast it will let you download a whole movie in just five seconds, or access TV-quality video servers in real time. That is the promise from a team at the California Institute of Technology in Pasadena, who have developed a system called Fast TCP.

#### HOW TO SPEED UP THE NET

##### Standard internet

Data packets sent across internet

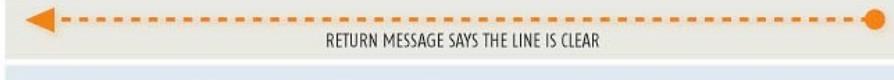


If a packet is lost, the transmission speed is halved



With Fast TCP higher speed connection paths can be ganged together to boost speed to more than 6000 times the capacity of today's broadband links

Data transmitted in same way as on standard internet



When return message says delays are low, packet transmission rate is boosted to highest rate connection can support



**Fast TCP: Achieved 8.6 Gb/s between Sunnyvale, CA & CERN, Switzerland**

**Steven Low (Caltech)**

<http://netlab.caltech.edu/FAST>