Optimizing Molecular Dynamics

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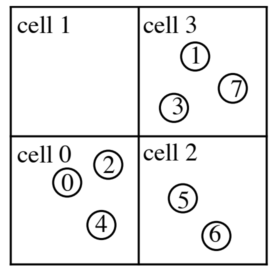
- **Intranode optimization: CPU & memory access**
- **Internode optimization: Communication**

Data/computation locality!

Intranode: Memory Access

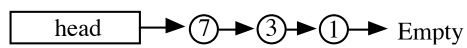
Data re-ordering

- **Linked-list cells—irregular memory access pattern**



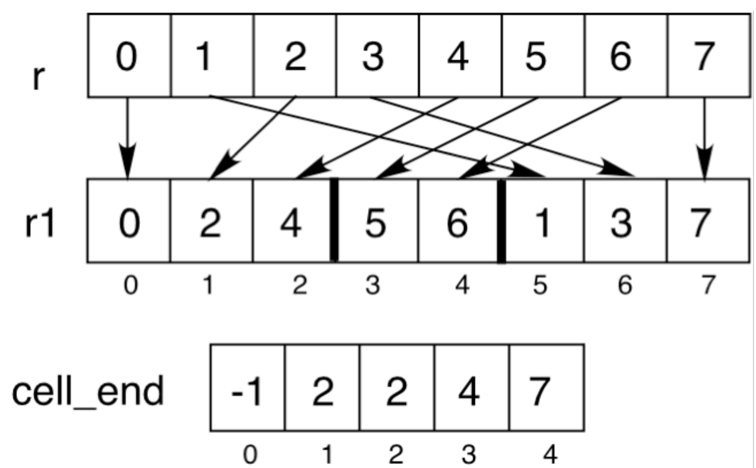
	0	1	2	3
head	4	E	6	7

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



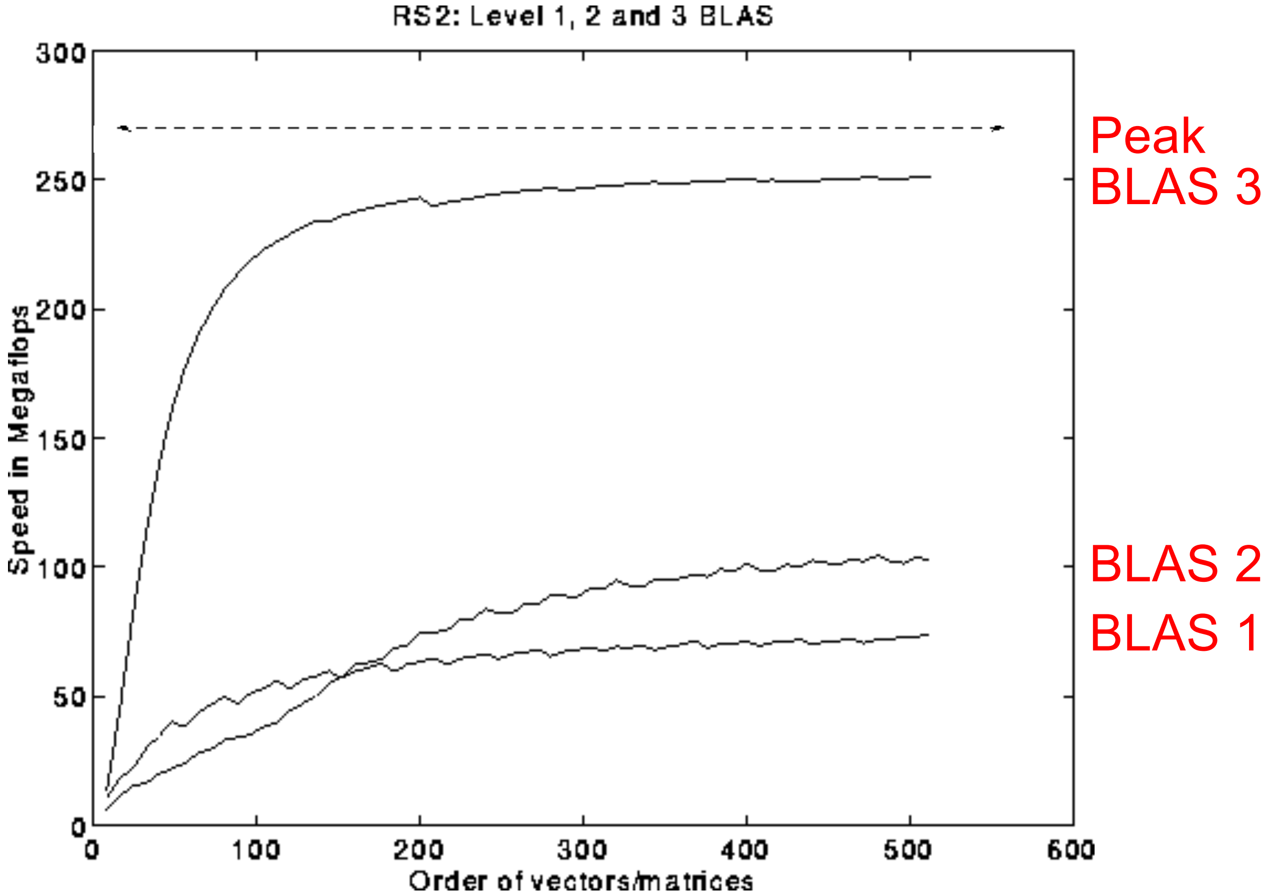
- **Data locality: Regular data layout**

```
for i = cell_end[c]+1 to cell_end[c+1]
  access r1[i]
endfor
```



BLAS3-Performance Molecular Dynamics?

- **BLAS3: q = 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 (AVX)?**

Floating Point Performance

- **BLAS-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)

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

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

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

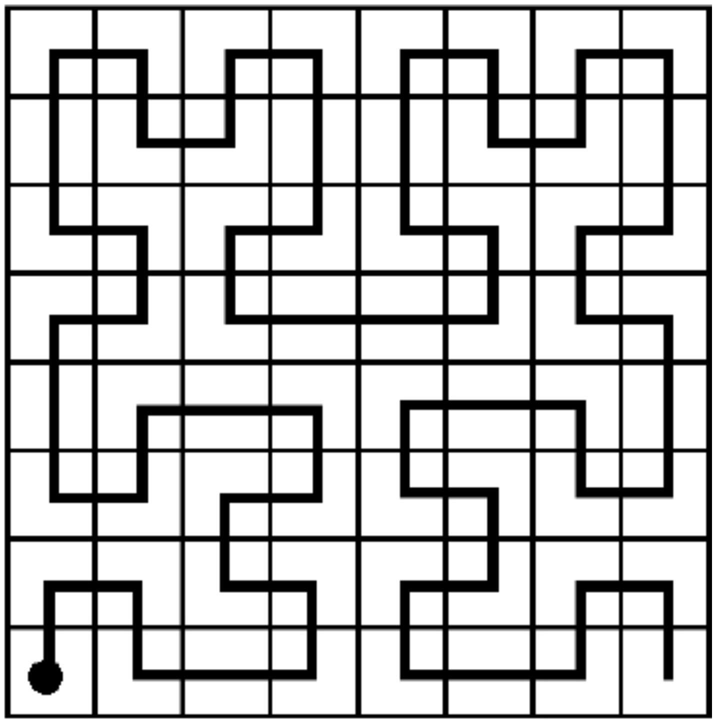
- **50.5% of the theoretical peak FLOP/s performance on 786,432 Blue Gene/Q cores (entire Mira at the Argonne Leadership Computing Facility)**
- **55% of the theoretical peak FLOP/s on Intel Xeon E5-2665**

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

Computation Locality

Data to computation re-ordering: How to traverse 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**



J. Mellor-Crummey *et al*., *Int'l J. Parallel Prog*. **29**, 217 ('01)

Hilbert-Peano Curve

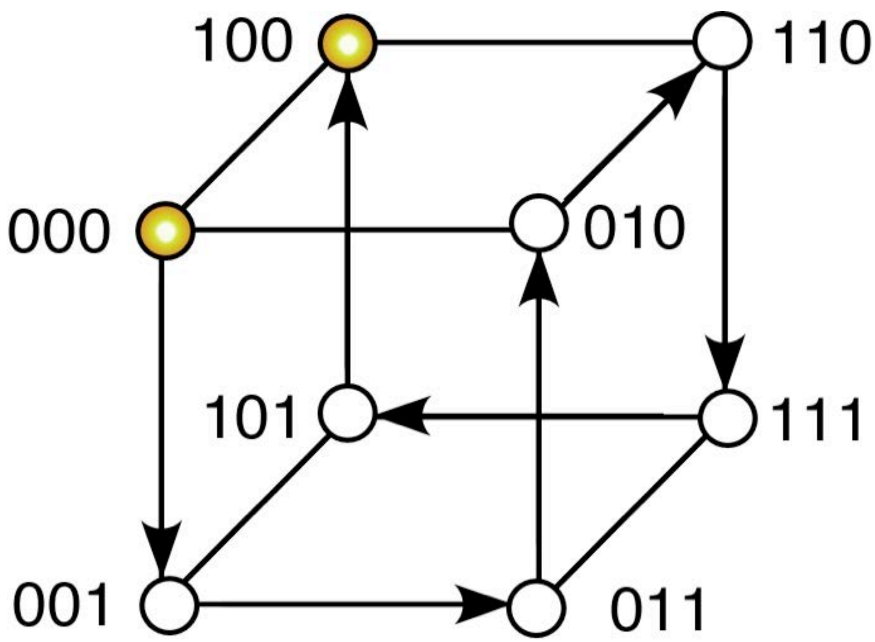
- **Gray code: a sequence of numbers such that successive numbers have Hamming distance 1**

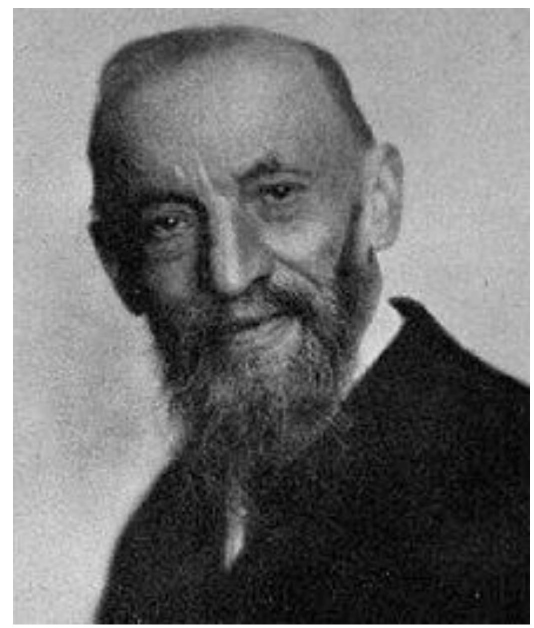
# of bits where two binary numbers differ

```
Algorithm: Recursive generation of k-bit Gray code G(k)
(1)G(1) is a sequence: 0 1.
(2)G(k+1) is constructed from G(k) as follows:
   a. Construct a new sequence by appending a 0 to the left of all members
      of G(k).
   b. Construct a new sequence by reversing G(k) & then appending a 1 to
      the left of all members of the sequence.
   c. 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)

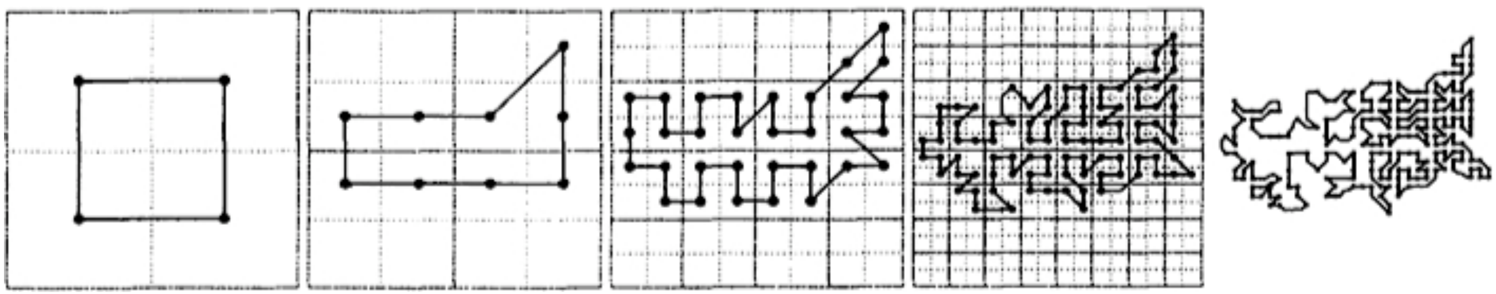




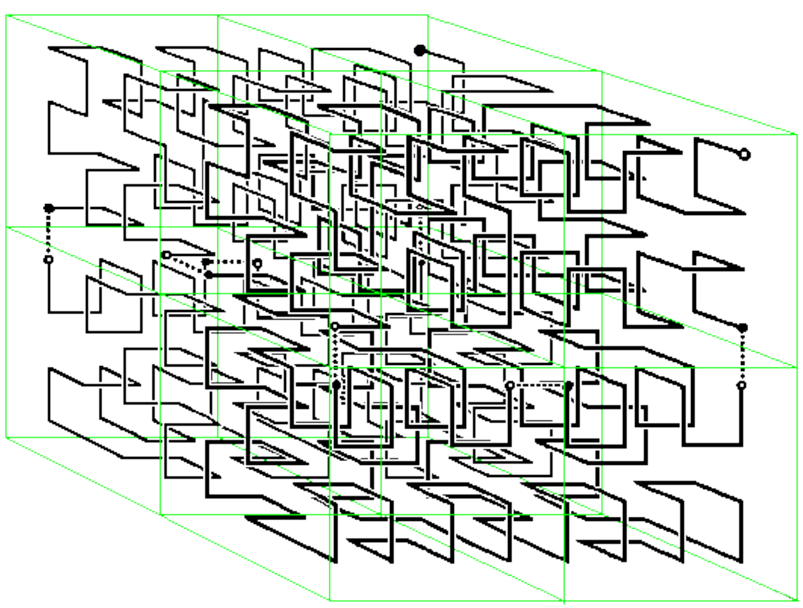
Giuseppe Peano (1858–1932)

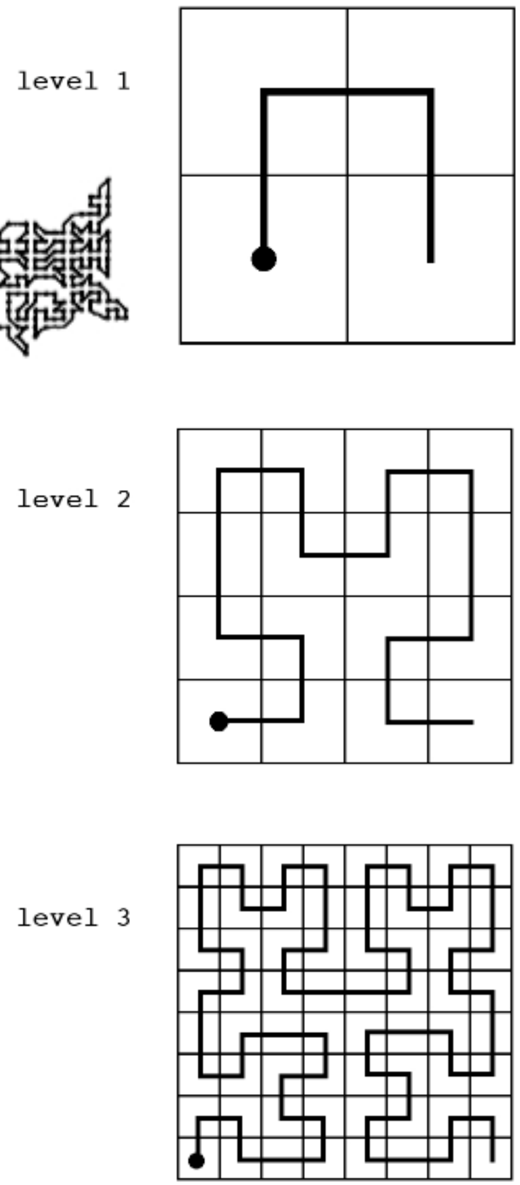
Hilbert-Peano Curve

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



- 3-dimensional Hilbert curve



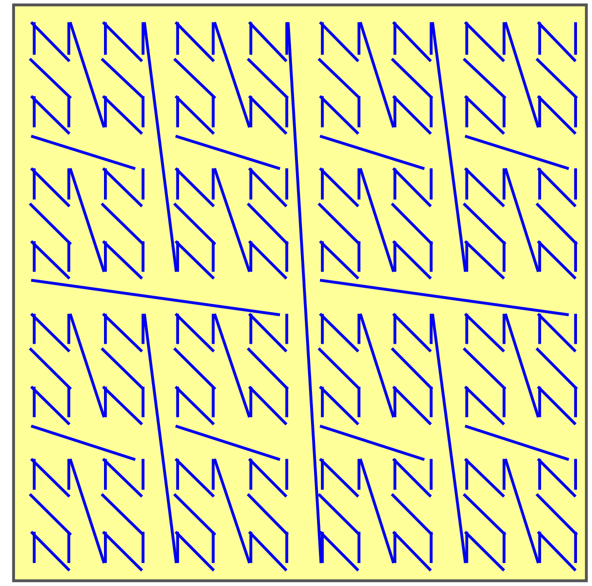


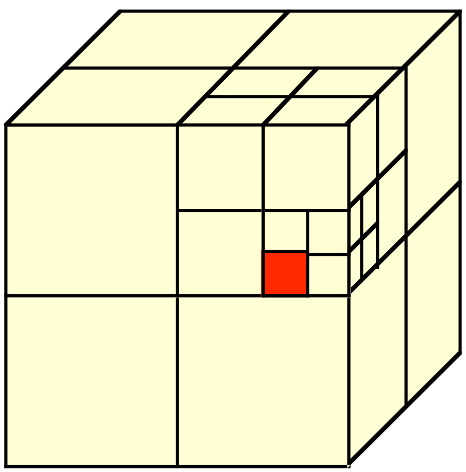
Morton (Z) Curve

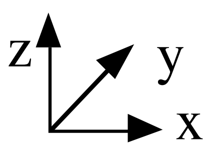
- Spacefilling curve based on octree index

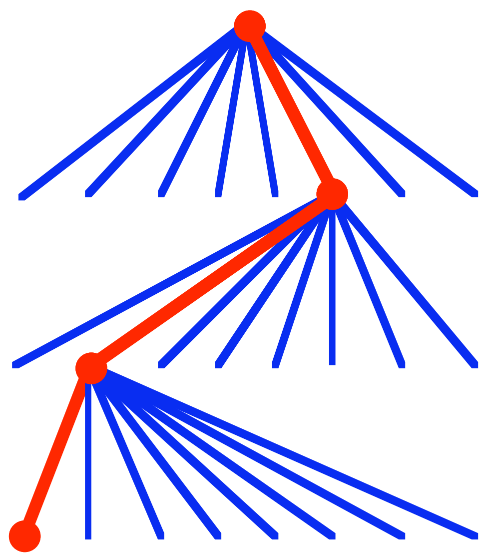
```
x =    1   1   0
y =   0   0   0
z = 1   0   0
R = 101 001 000
```

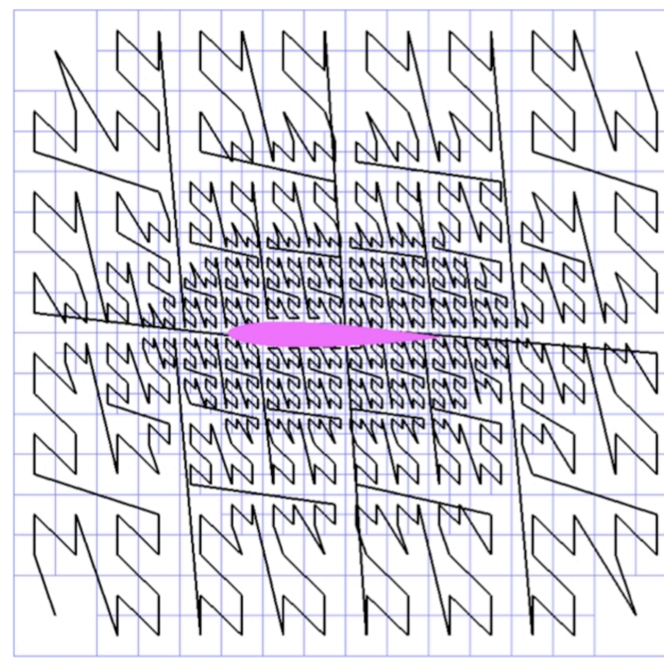
- 3D → list map preserves spatial proximity
- Multiresolution analysis made easy











A. Omeltchenko *et al.*, *Comput. Phys. Commun.* **131**, 78 ('00)

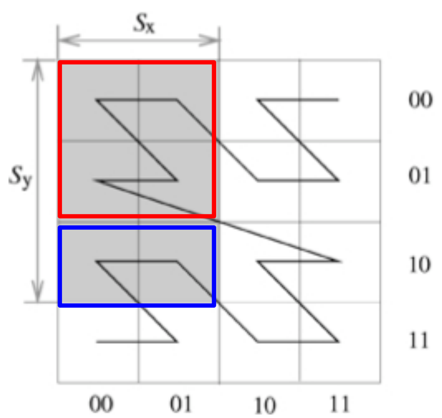
Analysis of Data Locaility

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

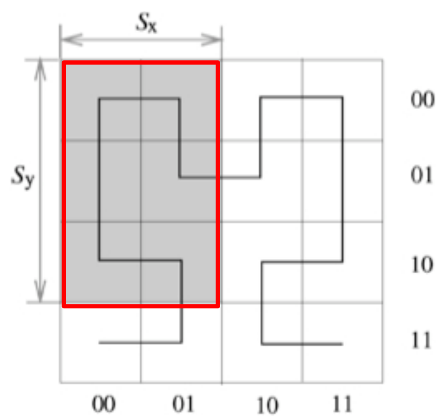
Analysis of the Clustering Properties of the Hilbert Space-Filling Curve

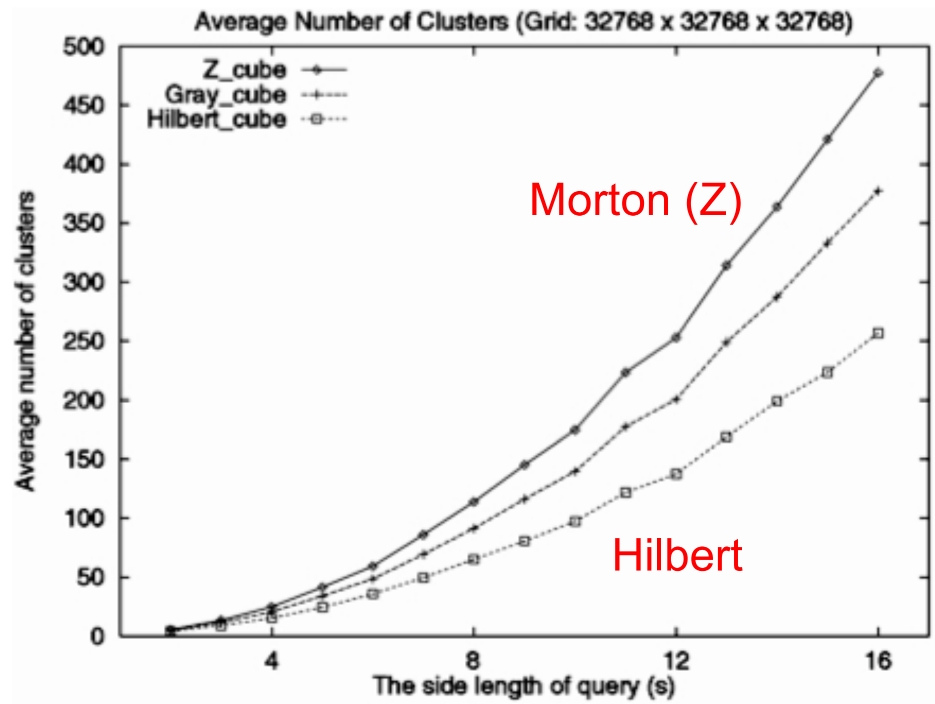
Bongki Moon, H.V. Jagadish, Christos Faloutsos, *Member, IEEE*, and Joel H. Saltz, *Member, IEEE*

Morton



Hilbert





2 clusters **1 cluster**

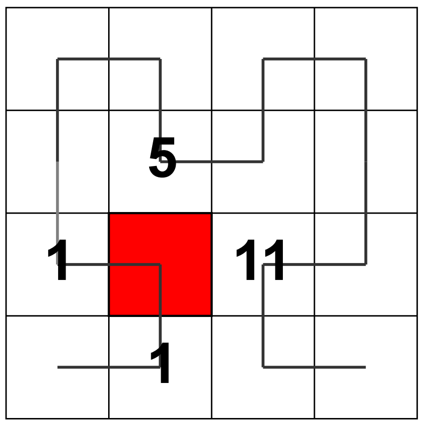
Cluster ~ cache line ~ latency cost

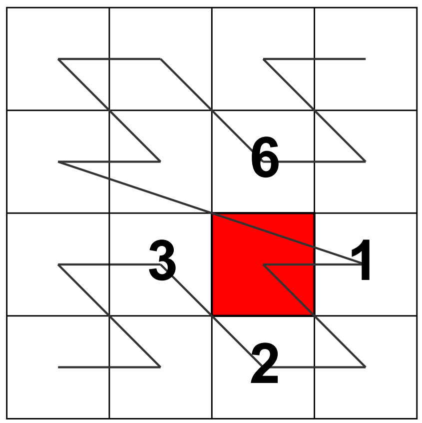
Hilbert curve is better than Morton curve for spatial range query

Alternative Locality Measure for MD

Which curve is better for spatial "pair" query?

- **Evaluate curves based on curve distances to neighbors**
- **Compare number below & 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 $2 < k_c < 13$

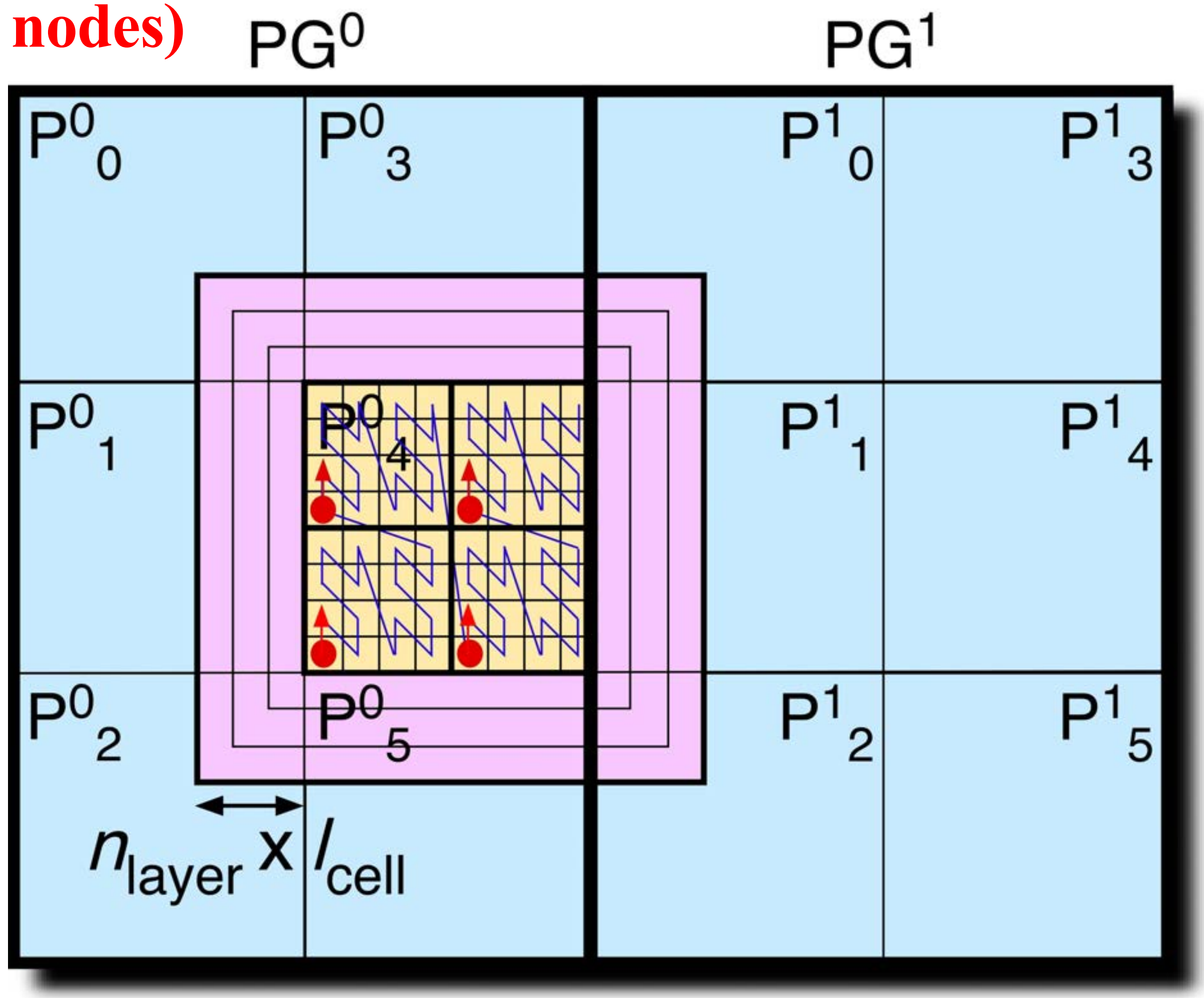
Scott Calaghan (CSCI 596 final project)

Tunable Hierarchical Cellular Decomposition

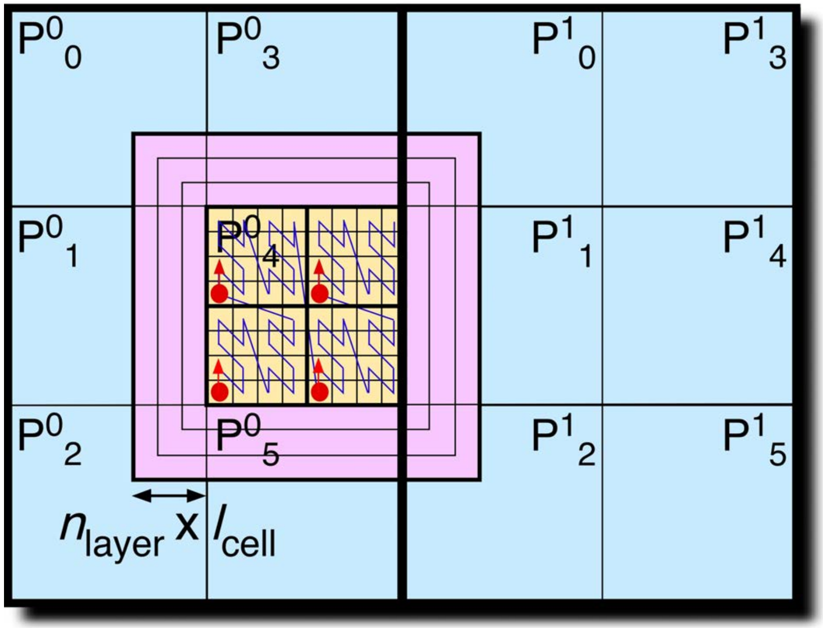
Mapping $O(N)$ divide-&-conquer algorithms onto memory hierarchies

- **Spatial decomposition with data "caching" & "migration"**
- **Computational cells (*e.g*. linked-list cells in MD) < cell blocks (threads) < processes (P^{γ}_{π}, 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*

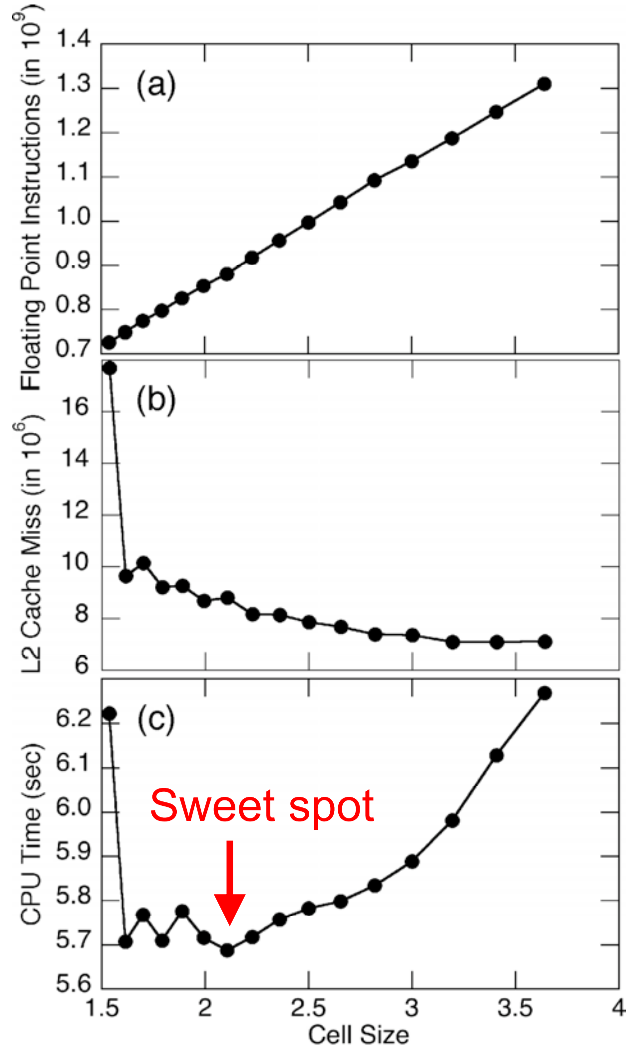


Performance Tunability



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

SIMD Vectorization

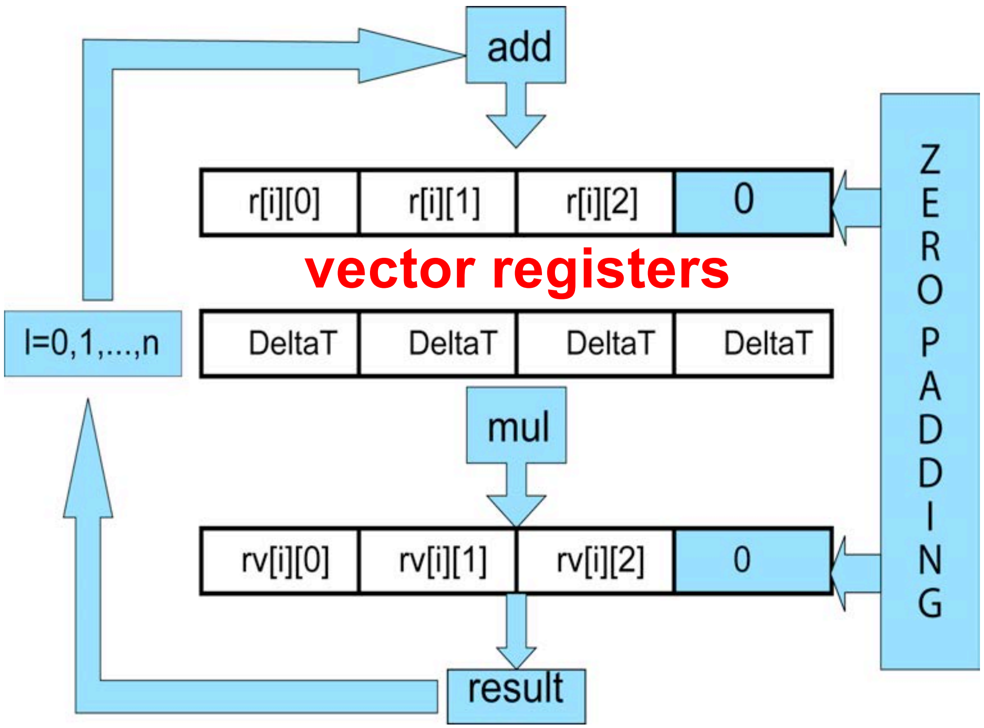
- **Single-instruction multiple-data (SIMD) parallelism**

(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

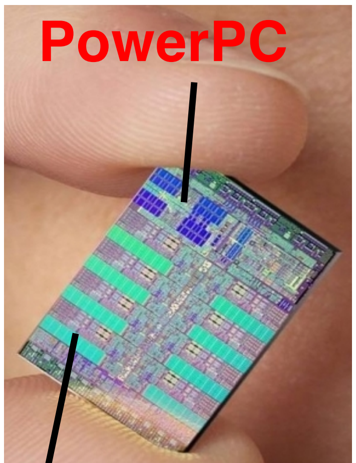


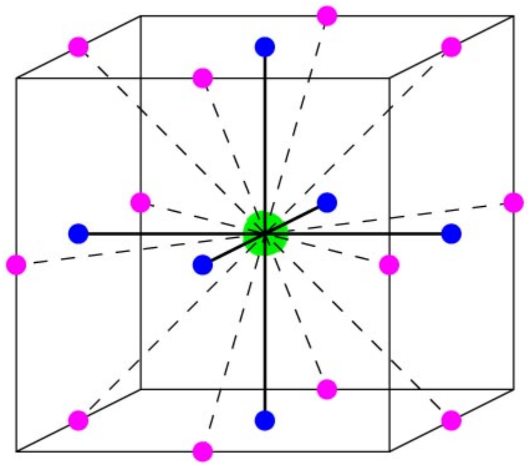
***cf.* False-sharing avoidance**

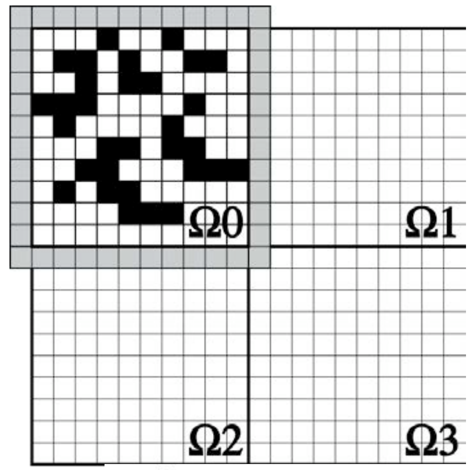
Peng *et al.*, *PDPTA 2009*; *UCHPC 2010; J. Supercomputing* **57**, 20 ('11)

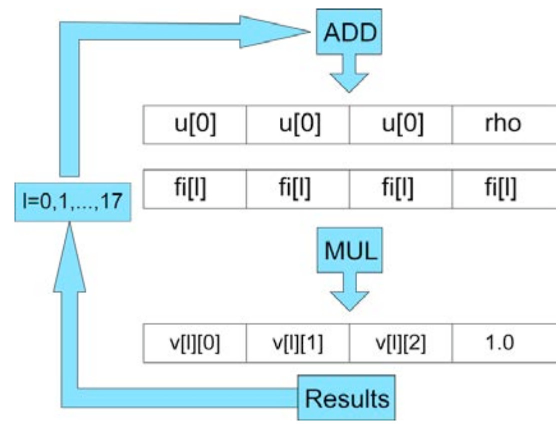
Hierarchical Parallelization

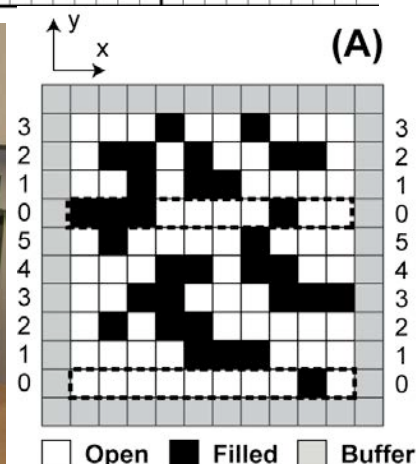
- **Developed a hierarchical parallel lattice Boltzmann method (pLBM) for flow simulation on a cluster of Cell Broadband Engine-based Playstation3 consoles & IBM BlueGenes**
  1. **Spatial decomposition *via* message passing**
  2. **Multithreading through critical section-free, dual representation**
  3. **Single-instruction multiple data (SIMD) parallelism *via* new vector transforms**

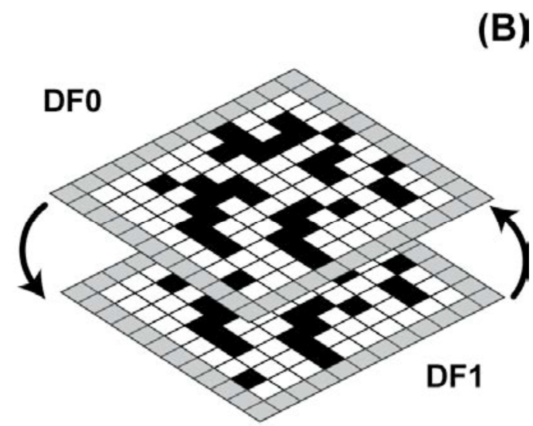












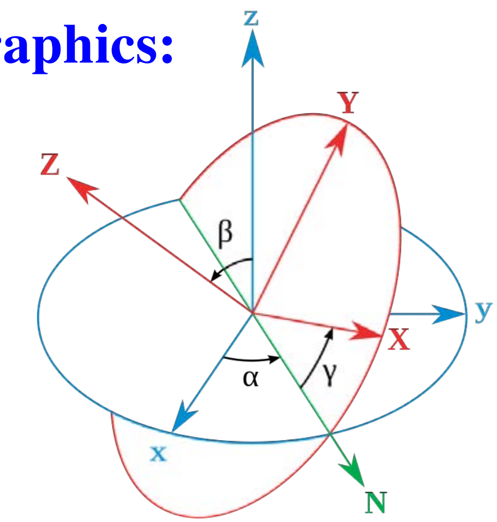
Peng *et al*., *IJCS 08*; *Euro-Par 08*; *IPDPS 09*; *cf.* https://en.wikipedia.org/wiki/Four-vector

More Four-Vectors for SIMD

Use SIMD-efficient four-vectors abundant in mathematical physics!

- **Special relativity in physics: space (x, y, z)-time (t) four-vector**
  $X^\mu = (ct, x, y, z)$; c: light speed
- **Quaternion representation of rotation in computer graphics:**

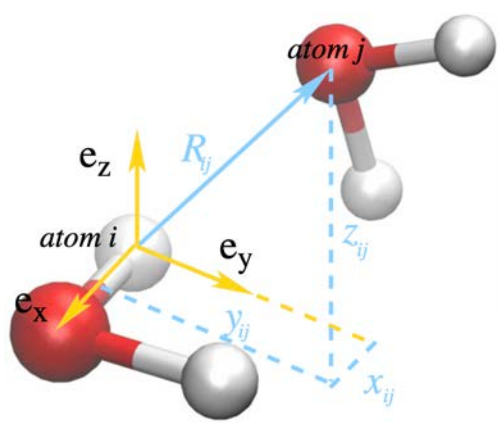
$$\begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} \cos\frac{\theta}{2}\cos\frac{\phi+\psi}{2} \\ \sin\frac{\theta}{2}\cos\frac{\phi-\psi}{2} \\ \sin\frac{\theta}{2}\sin\frac{\phi-\psi}{2} \\ \cos\frac{\theta}{2}\sin\frac{\phi+\psi}{2} \end{bmatrix}; \ (\theta, \phi, \psi)\text{: Euler angles}$$



- **Feature vector in deep-learning molecular dynamics:**

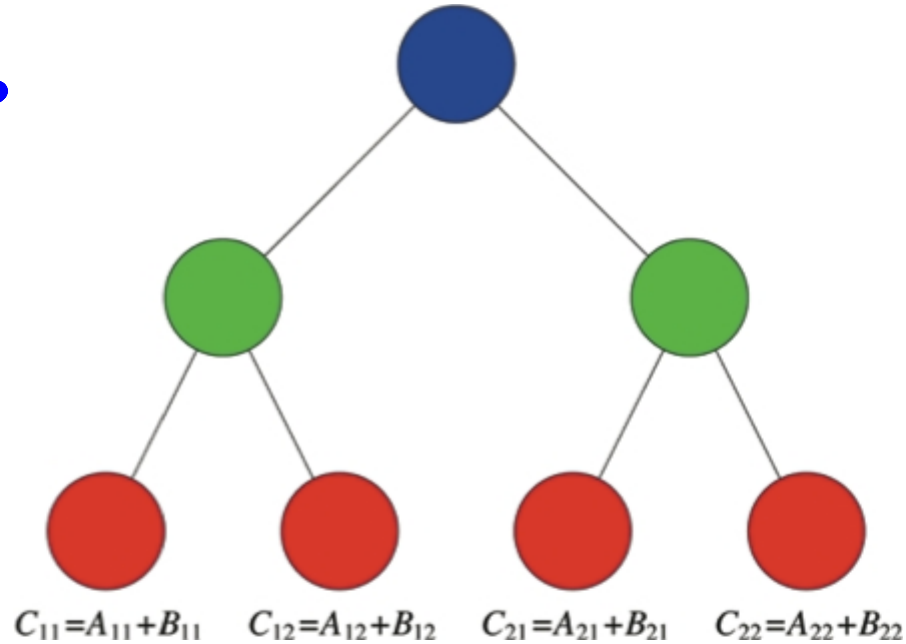
$$D_{ij} = \left(1/R_{ij}, x_{ij}/R_{ij}, y_{ij}/R_{ij}, z_{ij}/R_{ij}\right)$$

L. Zhang *et al.*, *Phys. Rev. Lett.* **120**, 143001 ('18)



Cache-Oblivious Linked-List Cell MD?

- **Recursive blocking for cells?**



Cache-Oblivious Algorithms

EXTENDED ABSTRACT SUBMITTED FOR PUBLICATION. In *Proc. FOCS99*

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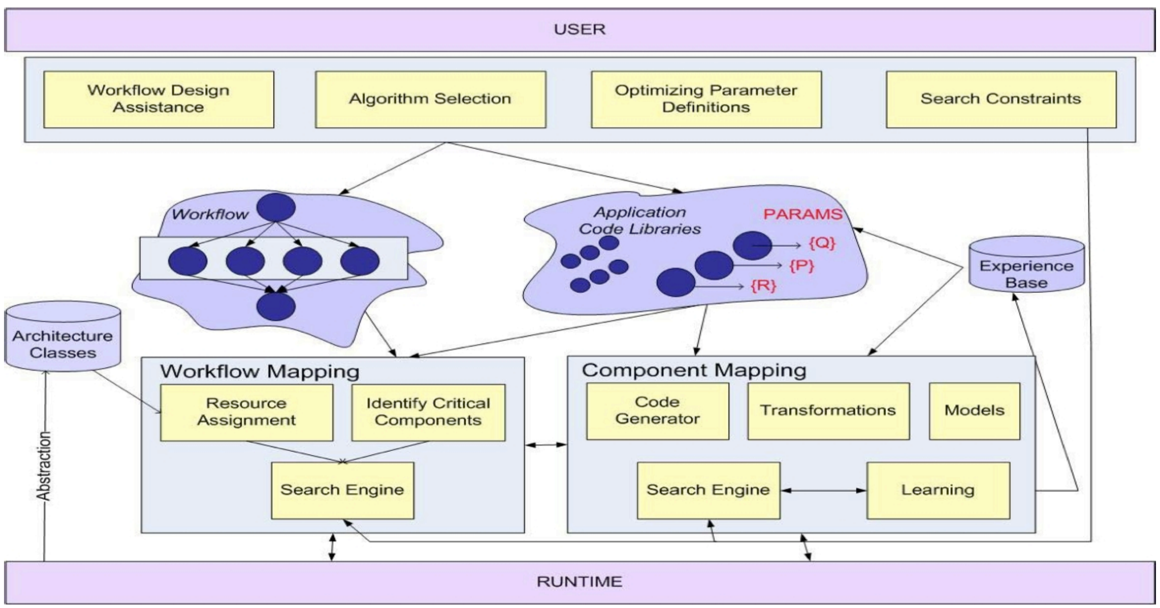
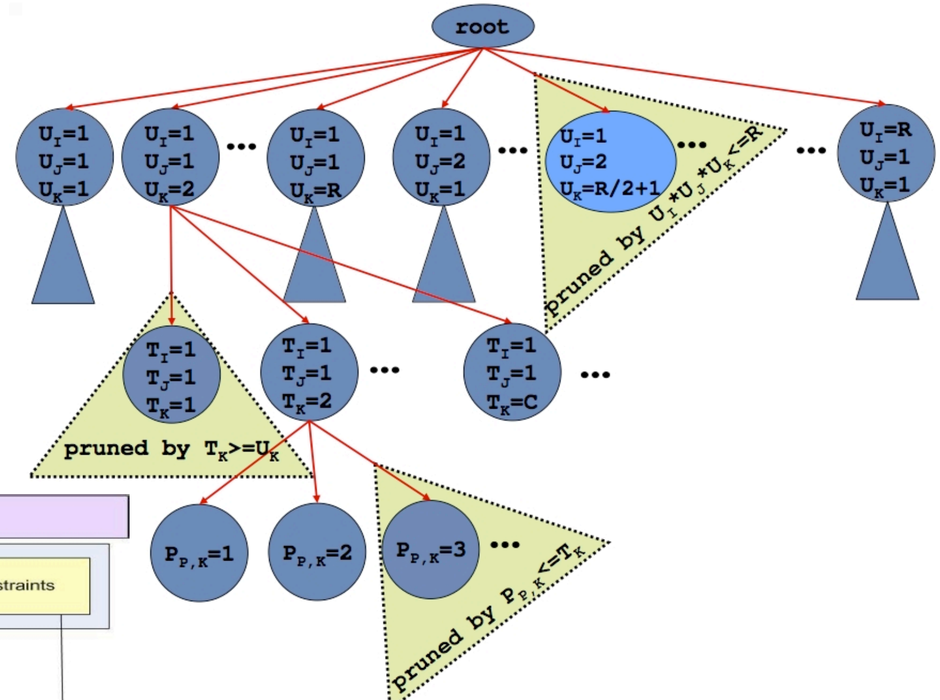
We introduce an "ideal-cache" model to analyze our algorithms, and we prove that an optimal cache-oblivious algorithm designed for two levels of memory is also optimal for multiple levels.

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**

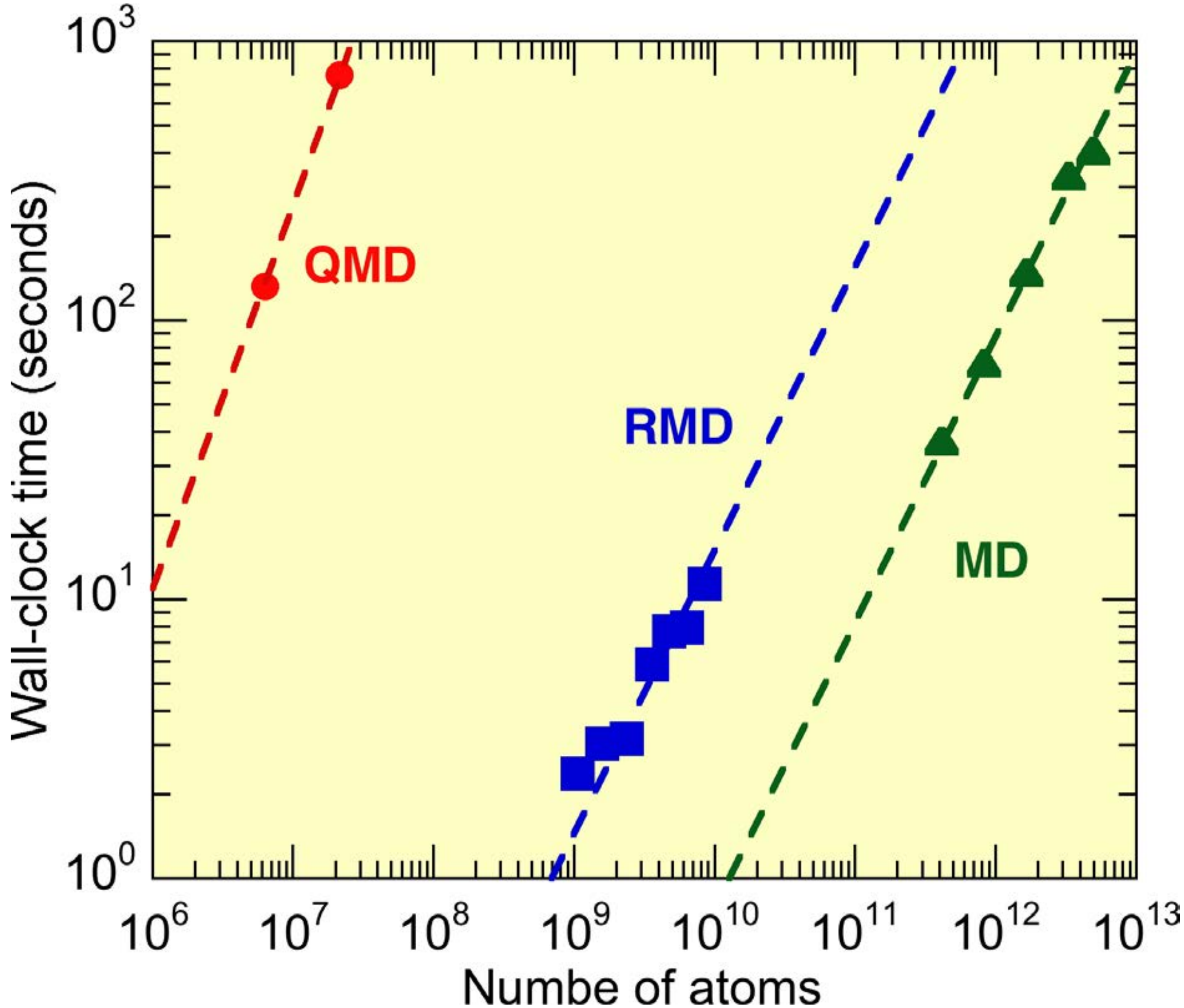


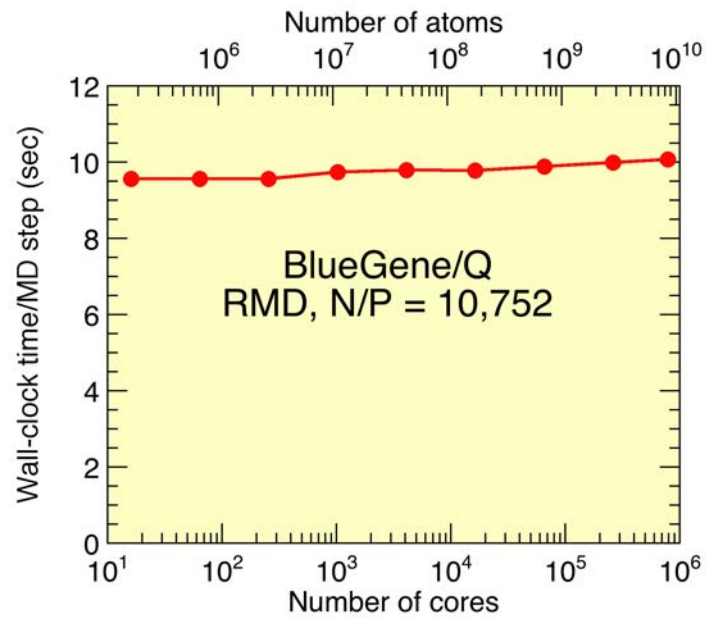


Pruned decision tree
C. Chen, *Ph.D. Thesis* (Computer Science, USC, '07)

"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)*

Scalable Simulation Algorithm Suite





QMD (quantum molecular dynamics): DC-DFT

RMD (reactive molecular dynamics): F-ReaxFF

MD (molecular dynamics): MRMD

Nomura *et al.*, *IEEE/ACM SC14*

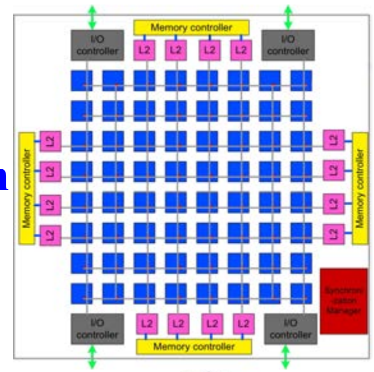
- **4.9 trillion-atom space-time multiresolution MD (MRMD) of SiO_2**
- **8.5 billion-atom fast reactive force-field (F-ReaxFF) RMD of RDX**
- **39.8 trillion grid points (50.3 million-atom) DC-DFT QMD of SiC**

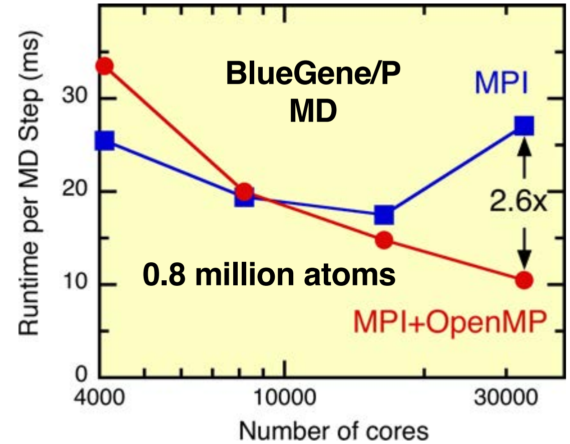
parallel efficiency 0.984 on 786,432 Blue Gene/Q cores

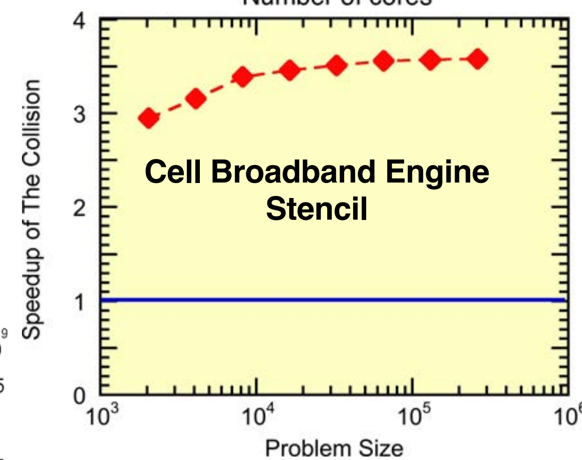
Scalability on Multicore Clusters

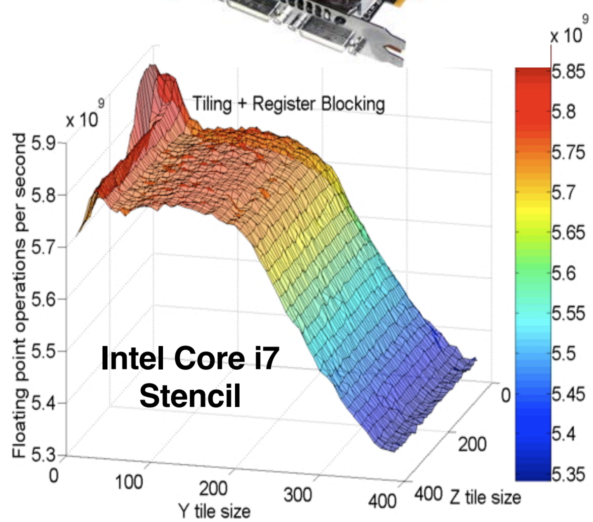
Hybrid message-passing (MPI) + multithreading (OpenMP) + single-instruction multiple-data (SIMD) programming

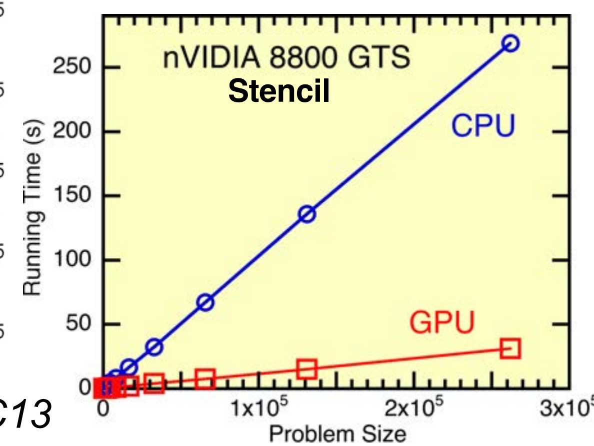
- **2.6× speedup over MPI by hybrid MPI+OpenMP on 32,768 IBM BlueGene/P cores**
- **Multithreading parallel efficiency 0.99 for MD on 64-core Godson-T processor**
- **SIMD efficiency 0.93 on PlayStation3**
- **8.8× speedup on an NVIDIA GeForce 8800 GTS graphics processing unit (GPU) over an AMD Sempron CPU**
- **55% of theoretical peak performance on 2.67 GHz Intel Core i7 920**







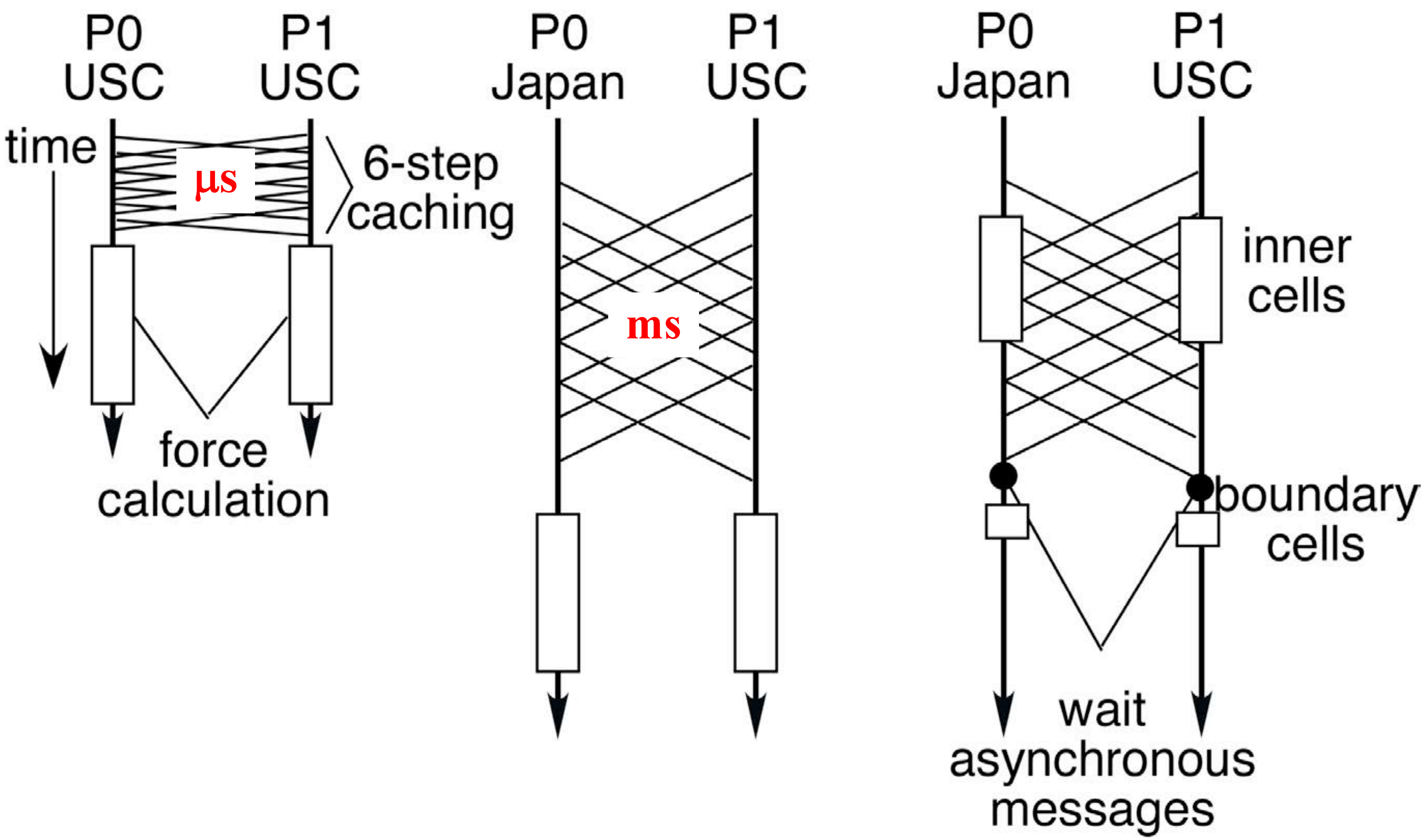




IJCS08; IPDPS09; PPL09; ICS10; CF11; Euro-Par12; JSC12; JPDC13; SC13

Internode Optimization

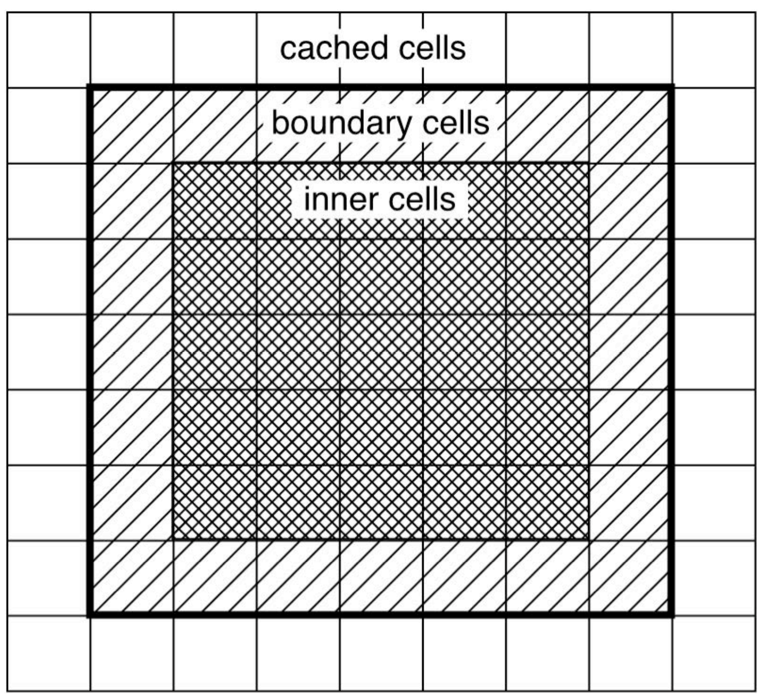
- **Communication bottleneck in metacomputing on a Grid**



Grid-Enabled MD Algorithm

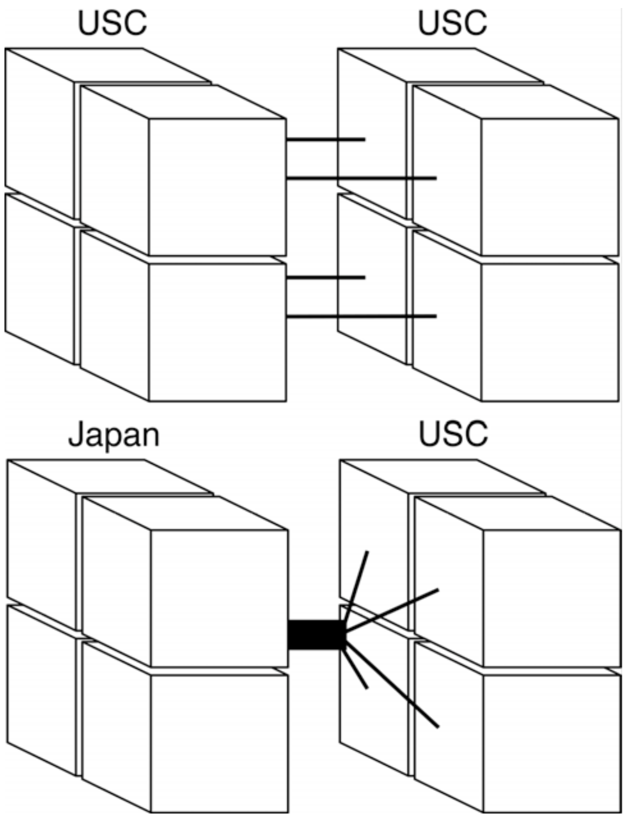
Grid MD algorithm:

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



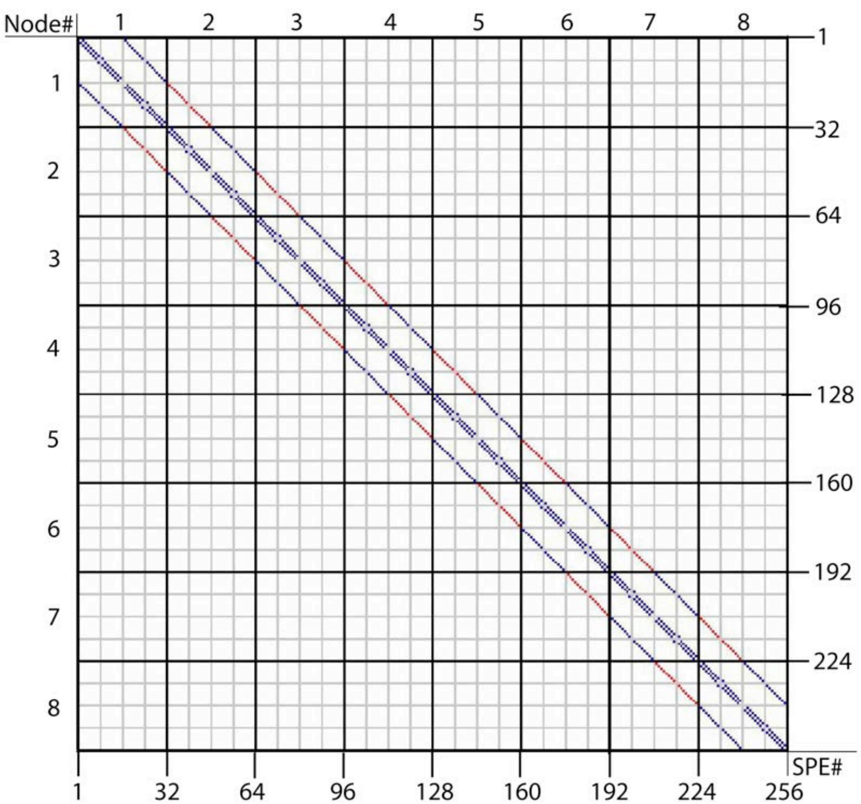
Renormalized Messages:

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

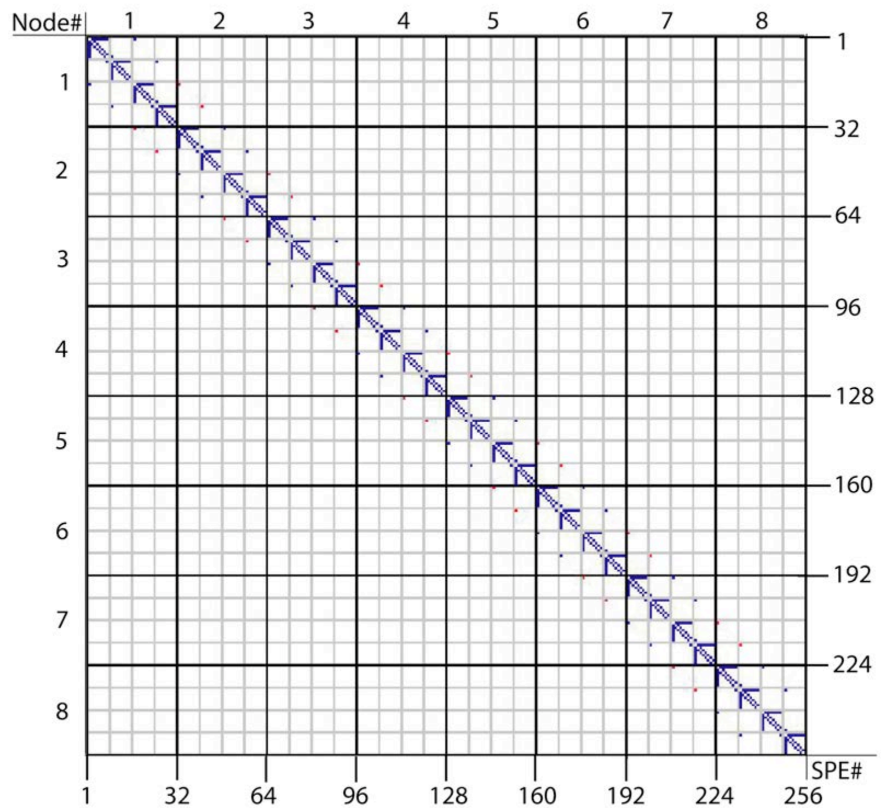


Renormalized Messages

Communication pattern of a 3D particle transport simulation code on a cluster of quad-Cell (32 cores) nodes



Original



Renormalized

H. Dursun *et al.*, *Parallel Processing Letters* **19**, 535 ('09)

Where to Go from Here

- **Performance profiling: First thing is to know how well/badly your program is performing in terms of flop/s performance, vectorization, cache miss, *etc*.**
- **Use professional tools like Intel VTune/Advisor if available on your computer:**
  https://software.intel.com/content/www/us/en/develop/tools/vtune-profiler.html
  https://www.intel.com/content/www/us/en/developer/tools/oneapi/advisor.html
  https://www.youtube.com/watch?reload=9&v=ymy139CuAx8

Advisor can show you the "roofline" of your application

- **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**

$$Attainable\,fp\;performance\left[\frac{\mathrm{Gflop}}{\mathrm{sec}}\right] =$$

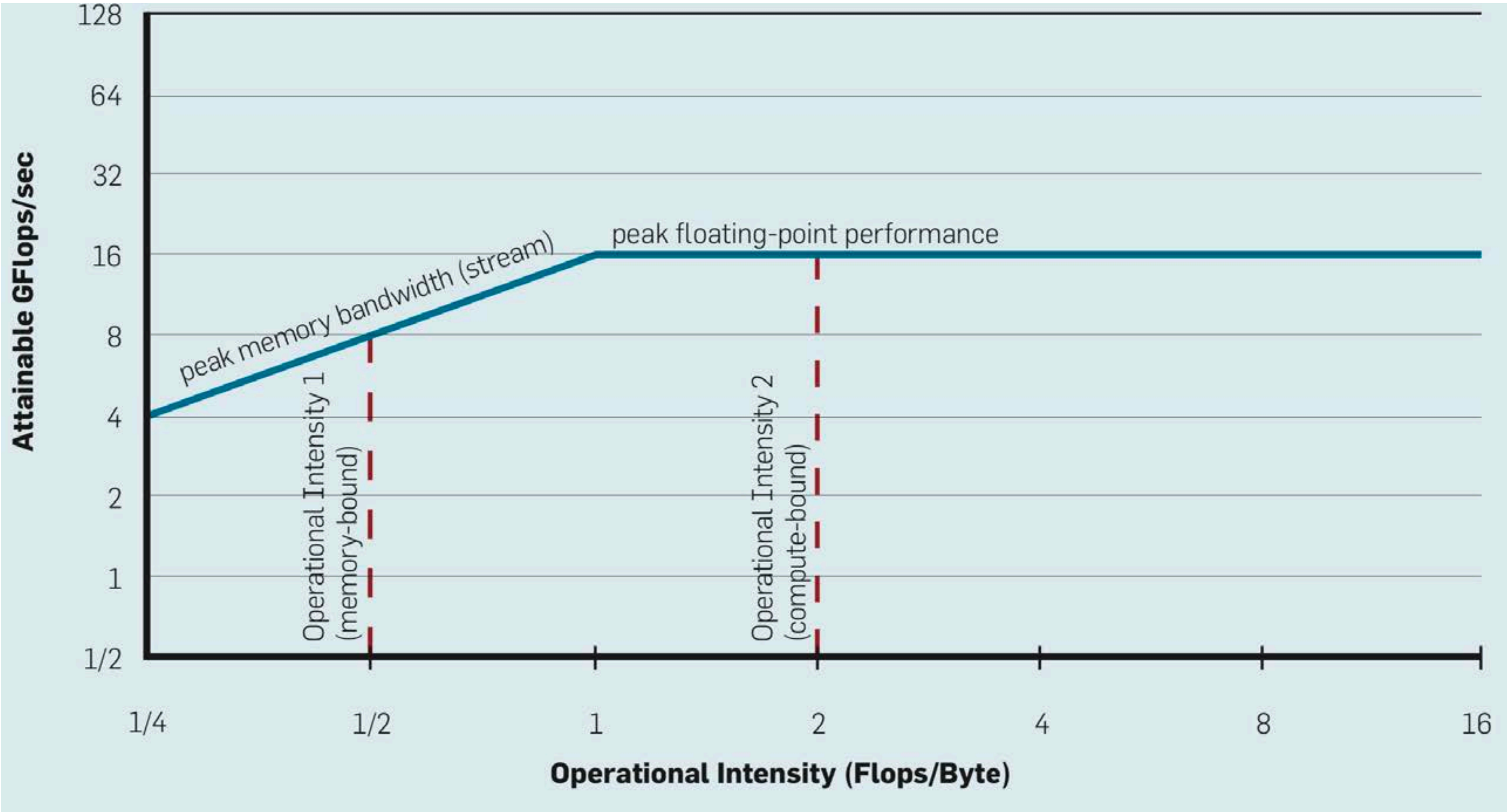
$$\min\left(\begin{array}{c} Peak\;fp\;performance\left[\frac{\mathrm{Gflop}}{\mathrm{sec}}\right], \\ Peak\;memory\;bandwidth\left[\frac{\mathrm{GByte}}{\mathrm{sec}}\right]\times Operational\;intensity\left[\frac{\mathrm{flop}}{\mathrm{Byte}}\right] \end{array}\right)$$

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

$$Attainable\ fp \left[\frac{\text{Gflop}}{\text{sec}}\right] =$$

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



Key: Data/computation locality

see Berkeley CS267 lecture on “memory hierarchies & matrix multiplication”