

# Advanced Topics in Parallel Molecular Dynamics

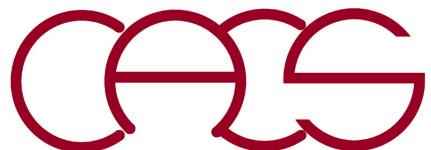
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Aiichiro Nakano

*Collaboratory for Advanced Computing & Simulations  
Department of Computer Science  
Department of Physics & Astronomy  
Department of Quantitative & Computational Biology  
University of Southern California*

Email: [anakano@usc.edu](mailto:anakano@usc.edu)



# Load Balancing

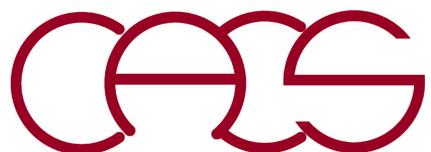
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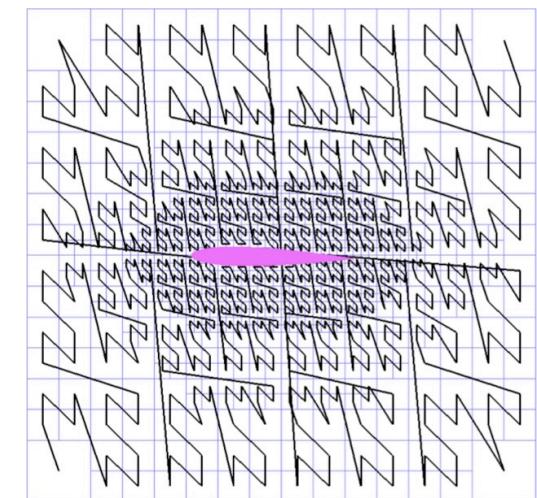
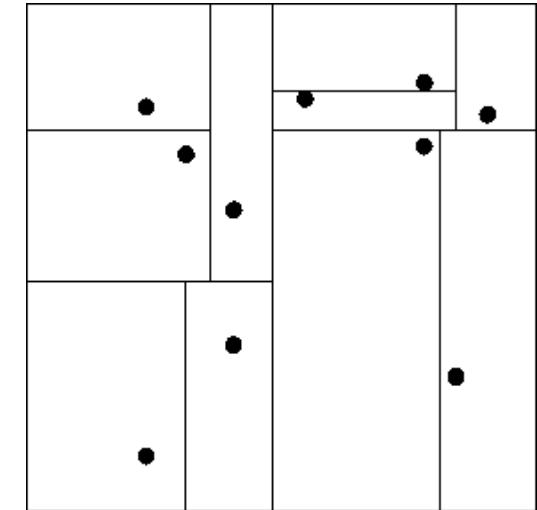
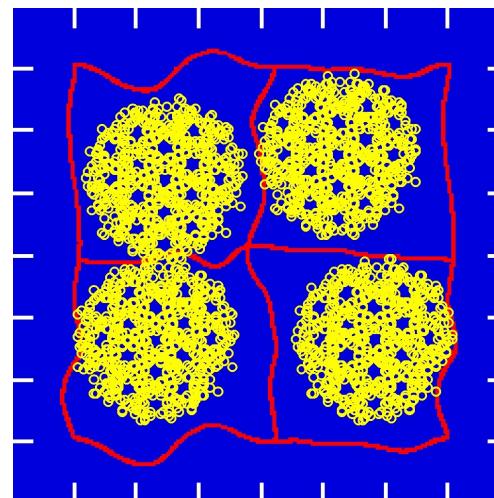
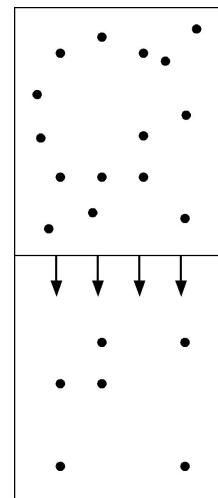
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Email: [anakano@usc.edu](mailto:anakano@usc.edu)



# Load Balancing

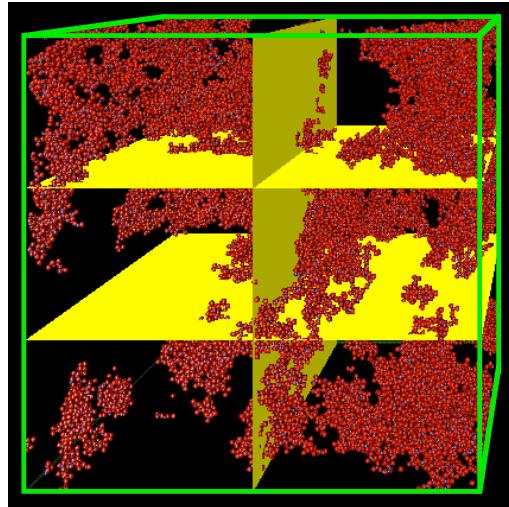
- Goal: Keep all processors equally busy while minimizing inter-processor communication for irregular parallel computations
- Issues:
  - Spatial data vs. generic graph
  - Static vs. adaptive
  - Incremental vs. non-incremental
- Load-balancing schemes:
  - Recursive bisection
  - Spectral method
  - Spacefilling curve
  - Curved space
  - Load diffusion



# Data Locality in Parallelization

Challenge: Load balancing for irregular data structures

Irregular  
data-structures/  
processor-speed



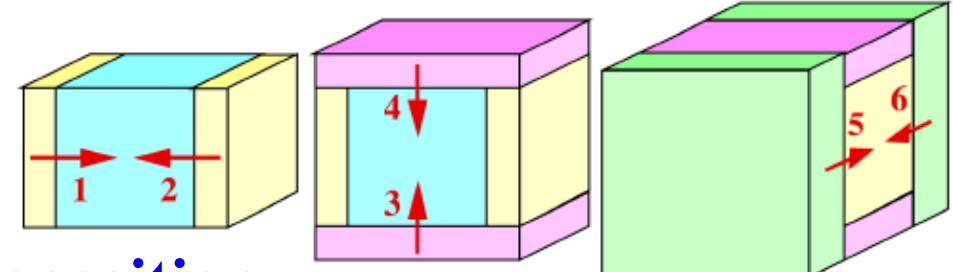
Map  
→



Parallel  
computer

Optimization problem:

- Minimize the load-imbalance cost
- Minimize the communication cost
- Topology-preserving spatial decomposition  
→ structured 6-step message passing minimizes latency



$$E = t_{\text{comp}} \left( \max_p |\{i \mid \mathbf{r}_i \in p\}| \right) + t_{\text{comm}} \left( \max_p |\{i \mid \|\mathbf{r}_i - \partial p\| < r_c\}| \right) \\ + t_{\text{latency}} \left( \max_p [N_{\text{message}}(p)] \right)$$

# Computational-Space Decomposition

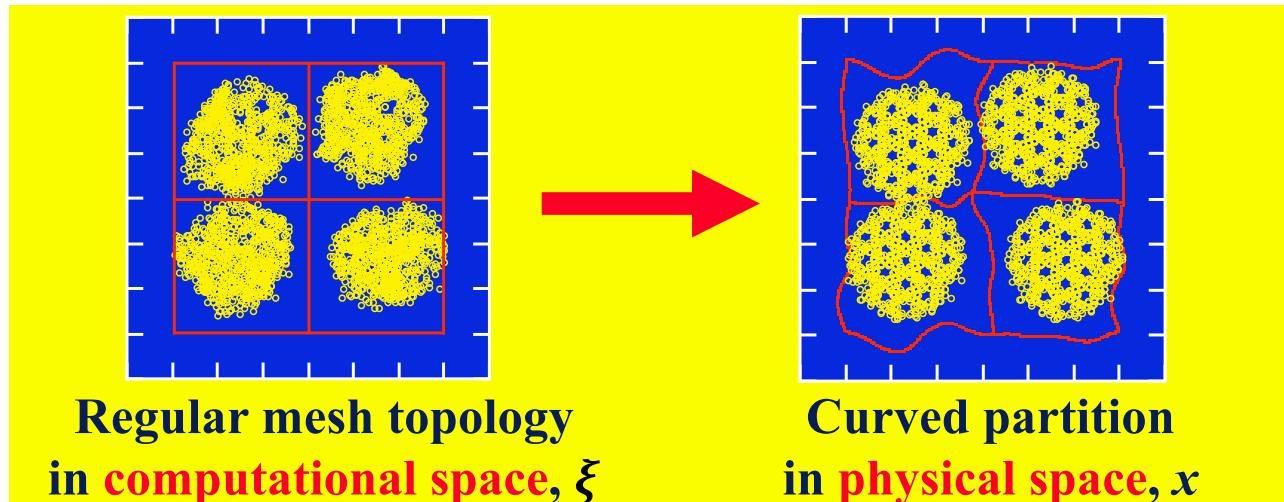
Topology-preserving “computational-space” decomposition in curved space (*cf.* general relativity)

Curvilinear coordinate transformation

$$\xi = \mathbf{x} + \mathbf{u}(\mathbf{x})$$

Particle-processor mapping: regular 3D mesh topology

$$\begin{cases} p(\xi_i) = p_x(\xi_{ix})P_yP_z + p_y(\xi_{iy})P_z + p_z(\xi_{iz}) \\ p_\alpha(\xi_{i\alpha}) = \lfloor \xi_{i\alpha} P_\alpha / L_\alpha \rfloor \quad (\alpha = x, y, z) \end{cases}$$

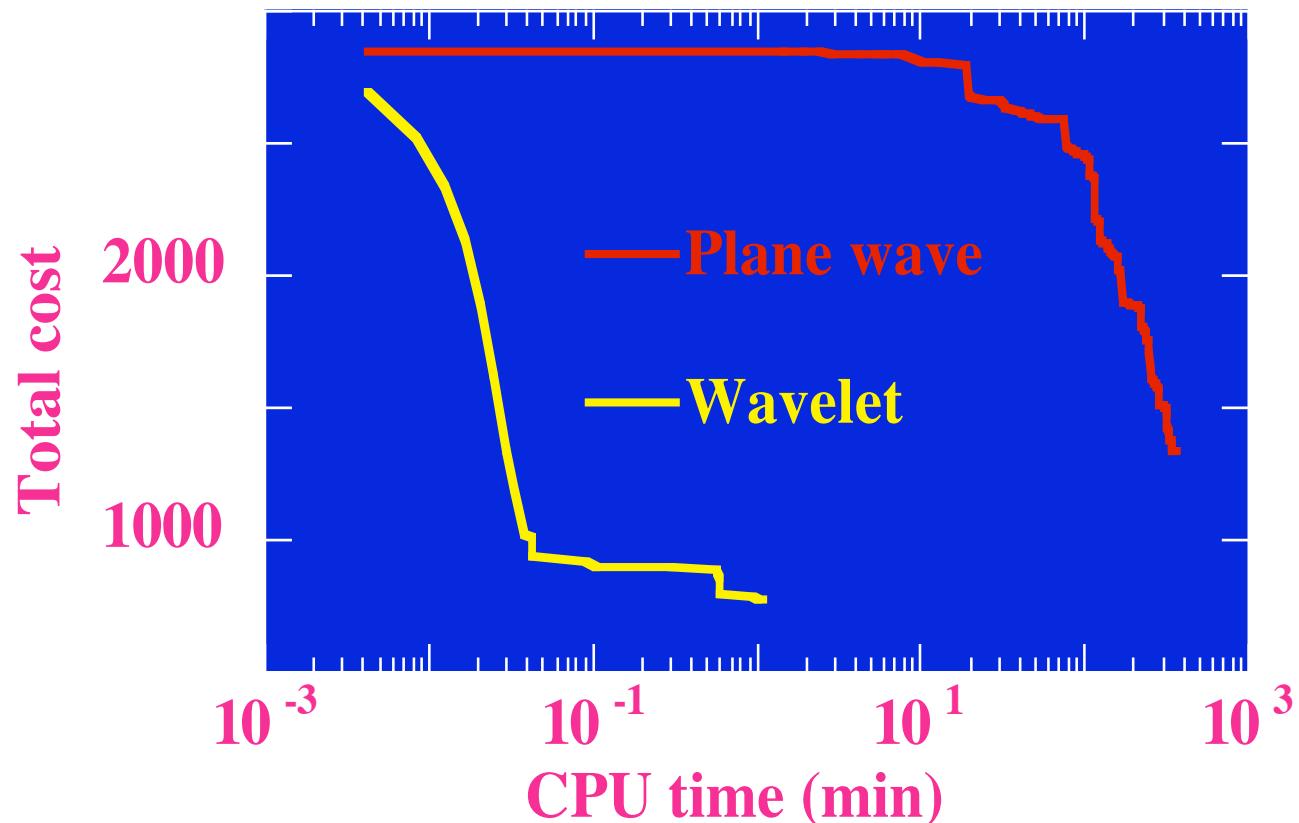


A. Nakano & T. J. Campbell, *Parallel Comput.* 23, 1461 ('97)

# Wavelet-based Adaptive Load Balancing

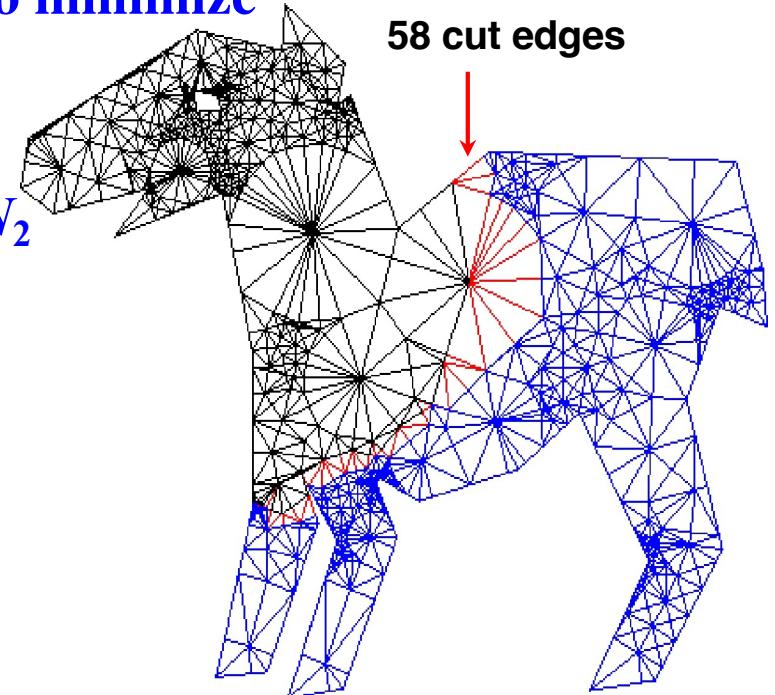
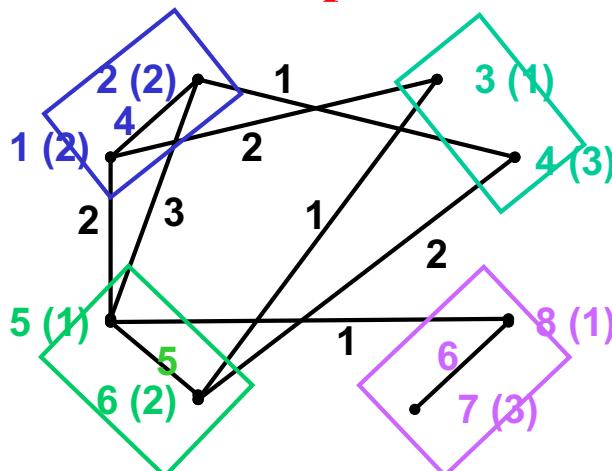
- Simulated annealing to minimize the load-imbalance & communication costs,  $E[\xi(x)]$
- Wavelet representation speeds up the optimization

$$\xi(x) = x + \sum_{l,m} d_{lm} \psi_{lm}(x)$$



# Load Balancing as Graph Partitioning

- Need: Decompose tasks without spatial indices
- **Graph partitioning:** Given a graph  $G = (N, E, W_N, W_E)$ 
  - $N$ : node set =  $\{j \mid \text{tasks}\}$
  - $W_N$ : node weights =  $\{w_N(j) : \text{task costs}\}$
  - $E$ : edge set =  $\{(j,k) \mid \text{messages from } j \text{ to } k\}$
  - $W_E$ : edge weights =  $\{w_E(j,k) : \text{message sizes}\}$
- choose a partition  $N = N_1 \cup N_2 \cup \dots \cup N_p$  to minimize
  - $\max_p \{\sum_{j \in N_p} w_N(j)\}$
  - $\max_{(p,q)} \{\sum_{j \in N_p, k \in N_q} w_E(j,k)\}$
- **Graph bisection:** Special case of  $N = N_1 \cup N_2$
- Choosing optimal partitioning is known to be NP-complete → need heuristics



Prof. James Demmel (UC Berkeley)

# Spectral Bisection: Motivation

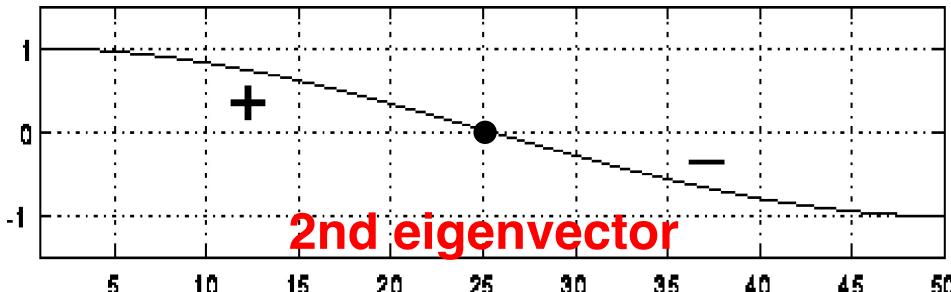
1. Graph as point masses connected via harmonic springs
2. The node of the eigenvector of the Hessian matrix,  $\partial^2 / \partial x^2$ , corresponding to the 2nd smallest eigenvalue separates the graph into 2

1D example

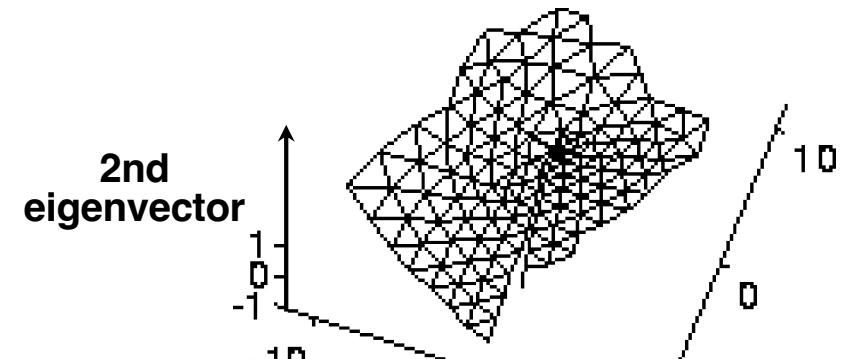


1st eigenvector

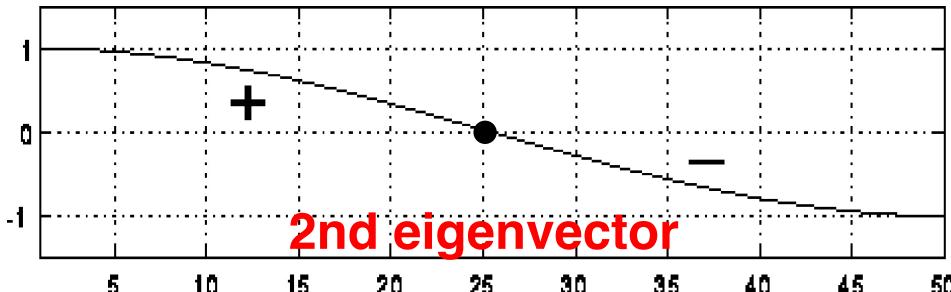
2nd eigenvector



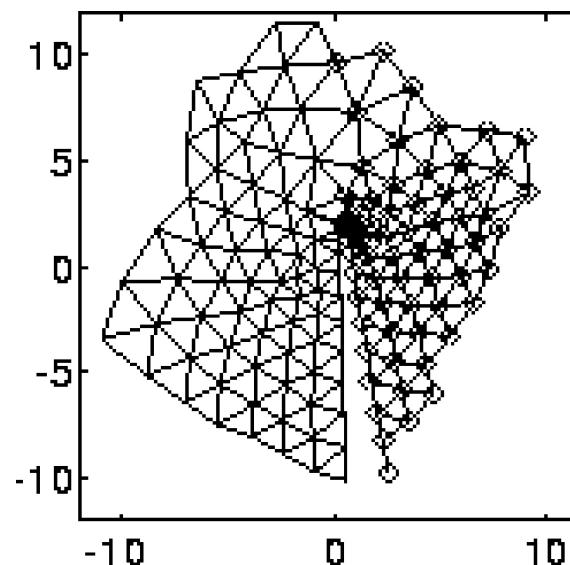
2D example



2nd eigenvector



3rd eigenvector



Partitioned half circled

# Spectral Bisection

Laplacian matrix:

$\mathbf{L}(G)$  of a graph  $G(N,E)$  is an  $|N|$  by  $|N|$  symmetric matrix:

- $\mathbf{L}(G)(i,i) = \text{degree of node } i$  (number of incident edges)
- $\mathbf{L}(G)(i,j) = -1$  if  $i \neq j$  and there is an edge  $(i,j)$
- $\mathbf{L}(G)(i,j) = 0$  otherwise

Theorems:

1. The eigenvalues of  $\mathbf{L}(G)$  are nonnegative:

$$\lambda_1 = 0 \leq \lambda_2 \leq \dots \leq \lambda_N$$

2.  $\lambda_2(\mathbf{L}(G)) \neq 0$  if and only if  $G$  is connected

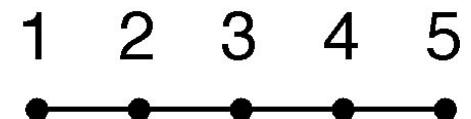
Spectral bisection algorithm:

1. Compute eigenvector  $\mathbf{v}_2$  corresponding to  $\lambda_2(\mathbf{L}(G))$

2. For each node  $i$  of  $G$

- if  $\mathbf{v}_2(i) < 0$ , put node  $i$  in partition  $N_-$
- else put node  $i$  in partition  $N_+$

Example



$$\begin{matrix} & 1 & 2 & 3 & 4 & 5 \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \left[ \begin{matrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{matrix} \right] \end{matrix}$$

# $O(N)$ $\lambda_2$ Computation

Lanczos algorithm:

- Given an  $N \times N$  symmetric matrix  $A$  (e.g.,  $L(G)$ ), compute a  $K \times K$  “approximation”  $T$  by performing  $K$  matrix-vector products, where  $K \ll N$
- Approximate  $A$ ’s eigenvalues & eigenvectors using  $T$ ’s

Choose an arbitrary starting vector  $r$

$b(0) = ||r||$

$j=0$

repeat

$j=j+1$

$q(j) = r/b(j-1)$

$r = A * q(j)$

$r = r - b(j-1) * v(j-1)$

$a(j) = v(j)^T * r$

$r = r - a(j) * v(j)$

$b(j) = ||r||$

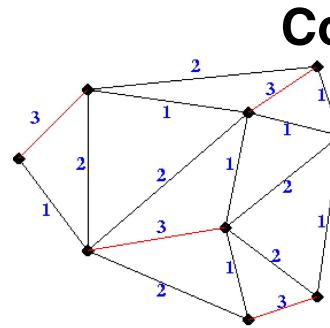
until convergence

$$T = \begin{bmatrix} a_1 & b_1 & & & \\ b_1 & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{K-2} & a_{K-1} & b_{K-1} \\ & & & b_{K-1} & a_K \end{bmatrix}$$

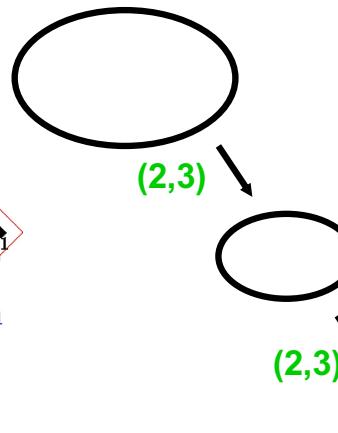
# Multilevel Partitioning

Recursively apply:

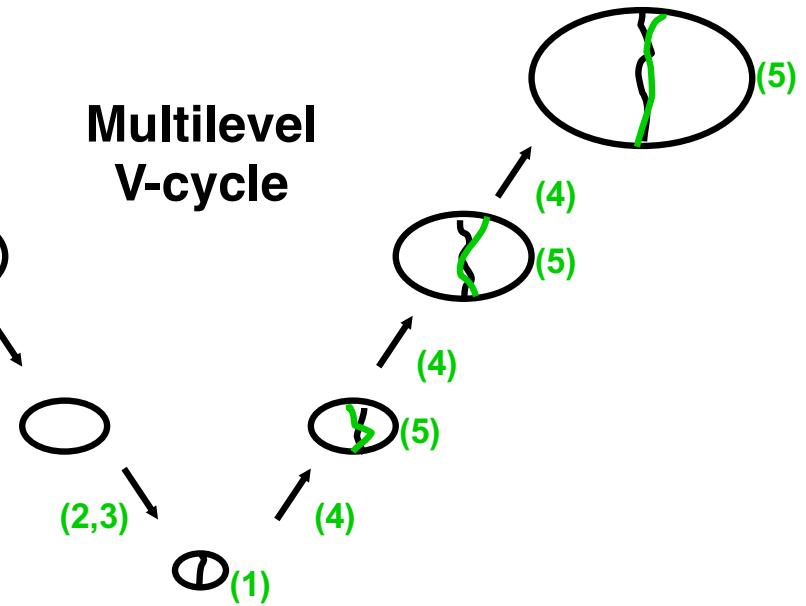
1. Replace  $G(N,E)$  by a coarse approximation  $G_c(N_c,E_c)$ , & partition  $G_c$
2. Use partition of  $G_c$  to obtain a rough partitioning of  $G$ , then uncoarsen & iteratively improve it



Coarsening



Multilevel  
V-cycle



```

( $N^+, N^-$ ) = Multilevel_Partition( $N, E$ )
// returns  $N^+$  and  $N^-$  where  $N = N^+ \cup N^-$ 
if  $|N|$  is small
1 Partition  $G = (N, E)$  directly to get  $N = N^+ \cup N^-$ 
    Return  $(N^+, N^-)$ 
else
2 Coarsen  $G$  to get an approximation  $G_c = (N_c, E_c)$ 
3  $(N_c^+, N_c^-) = \text{Multilevel\_Partition}(N_c, E_c)$ 
4 Expand  $(N_c^+, N_c^-)$  to a partition  $(N^+, N^-)$  of  $N$ 
5 Improve the partition  $(N^+, N^-)$ 
    Return  $(N^+, N^-)$ 
endif

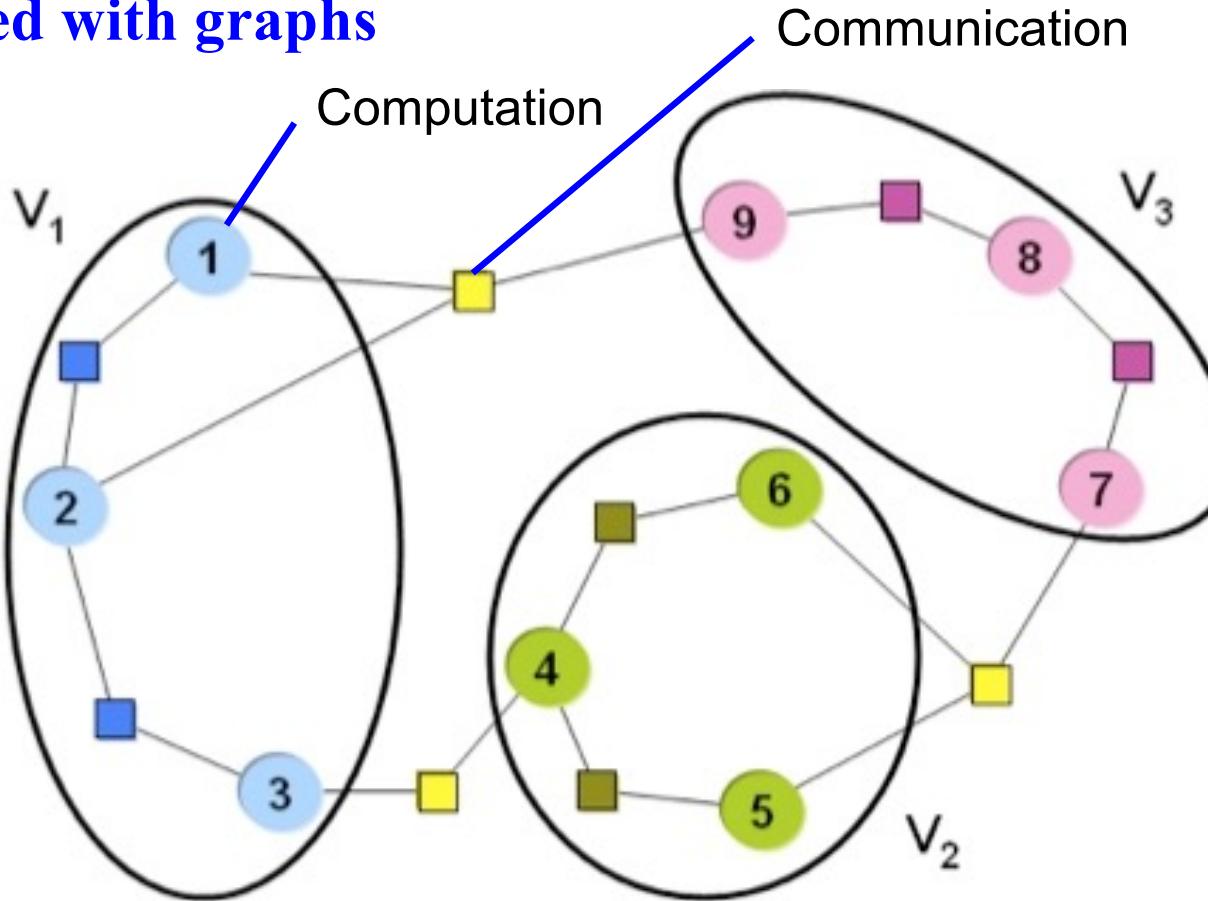
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*cf. Multigrid method*

*cf. Shang-Hua Teng, <https://dl.acm.org/doi/10.1145/3627708>*

# Hypergraph-based Load Balancing

1. Hypergraph = (<{node}, {hyperedge = a group of nodes})
2. More expressive power for computation-communication relation compared with graphs



U. V. Catalyurek *et al.*, “Hypergraph-based dynamic load balancing for adaptive scientific computations,” in *Proc. IPDPS* (IEEE, ’07)

M. Kunaseth *et al.*, “A scalable parallel algorithm for dynamic range-limited  $n$ -tuple computation in many-body molecular dynamics simulation,” in *Proc. SC* (ACM/IEEE, ’13)

# Hybrid Decomposition

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Who does what?



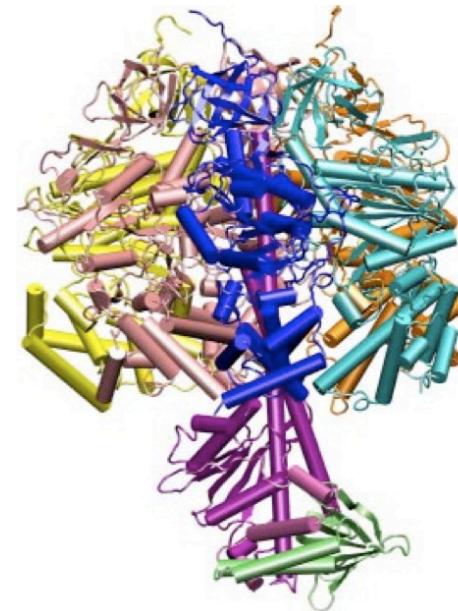
# Fine-Grained Parallel MD

## Pathways to a Protein Folding Intermediate Observed in a 1-Microsecond Simulation in Aqueous Solution

Yong Duan and Peter A. Kollman\*

An implementation of classical molecular dynamics on parallel computers of increased efficiency has enabled a simulation of protein folding with explicit representation of water for 1 microsecond, about two orders of magnitude longer than the longest simulation of a protein in water reported to date. Starting with an unfolded state of villin headpiece subdomain, hydrophobic collapse and helix formation occur in an initial phase, followed by conformational readjustments. A marginally stable state, which has a lifetime of about 150 nanoseconds, a favorable solvation free energy, and shows significant resemblance to the native structure, is observed; two pathways to this state have been found.

*Science 282, 740 ('98)*

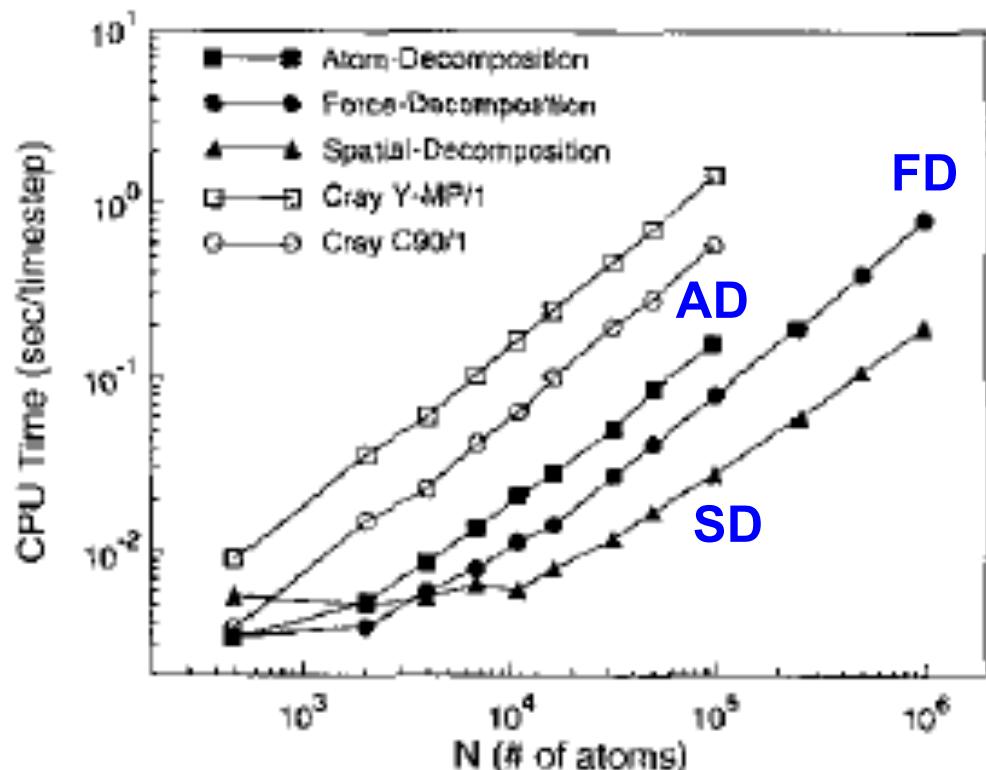
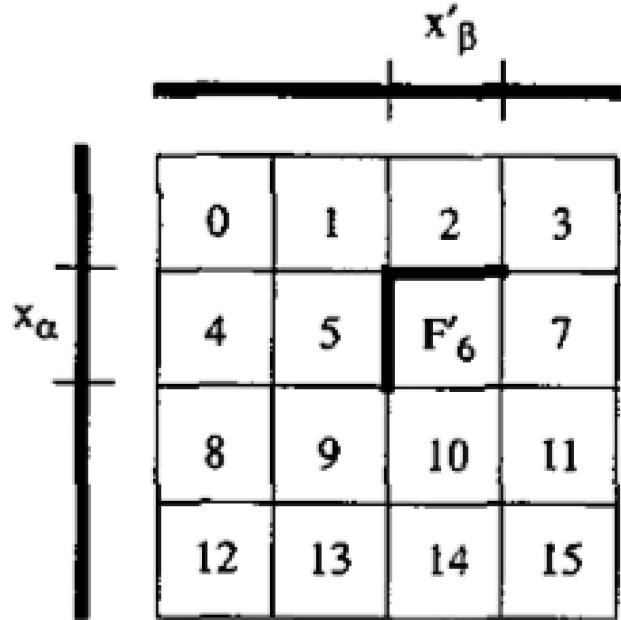


Processors			Time/step		Speedup		GFLOPS	
	Total	Per Node	MPI	Elan	MPI	Elan	MPI	Elan
1	1	1	28.08 s	28.08 s	1	1	0.480	0.480
128	4	248.3 ms	234.6 ms	113	119	54	57	
256	4	135.2 ms	121.9 ms	207	230	99	110	
512	4	65.8 ms	63.8 ms	426	440	204	211	
510	3	65.7 ms	63.0 ms	427	445	205	213	
1024	4	41.9 ms	36.1 ms	670	778	322	373	
1023	3	35.1 ms	33.9 ms	799	829	383	397	
1536	4	35.4 ms	32.9 ms	792	854	380	410	
1536	3	26.7 ms	24.7 ms	1050	1137	504	545	
2048	4	31.8 ms	25.9 ms	883	1083	423	520	
1800	3	25.8 ms	22.3 ms	1087	1261	521	605	
2250	3	19.7 ms	18.4 ms	1425	1527	684	733	
2400	4	32.4 ms	27.2 ms	866	1032	416	495	
2800	4	32.3 ms	32.1 ms	869	873	417	419	
3000	4	32.5 ms	28.8 ms	862	973	414	467	

J.C. Phillips, G. Zheng, S. Kumar, & L.V. Kale,  
in *Proc. of IEEE/ACM SC2002*

Table 1: NAMD performance on 327K atom ATPase benchmark system with and multiple timesteping with PME every four steps for Charm++ based on MPI and Elan.

# Force Decomposition for Parallel MD



Runtime on 1,024-processor Intel Paragon

**FIG. 5.** The division of the permuted force matrix  $F'$  among 16 processors in the force-decomposition algorithm. Processor  $P_6$  is assigned a sub-block  $F'_6$  of size  $N/\sqrt{P}$  by  $N/\sqrt{P}$ . To compute its matrix elements it must know the corresponding  $N/\sqrt{P}$ -length pieces  $x_\alpha$  and  $x'_\beta$  of the position vector  $x$  and permuted position vector  $x'$ .

S. Plimpton, *J. Comput. Phys.* 117, 1 ('95)

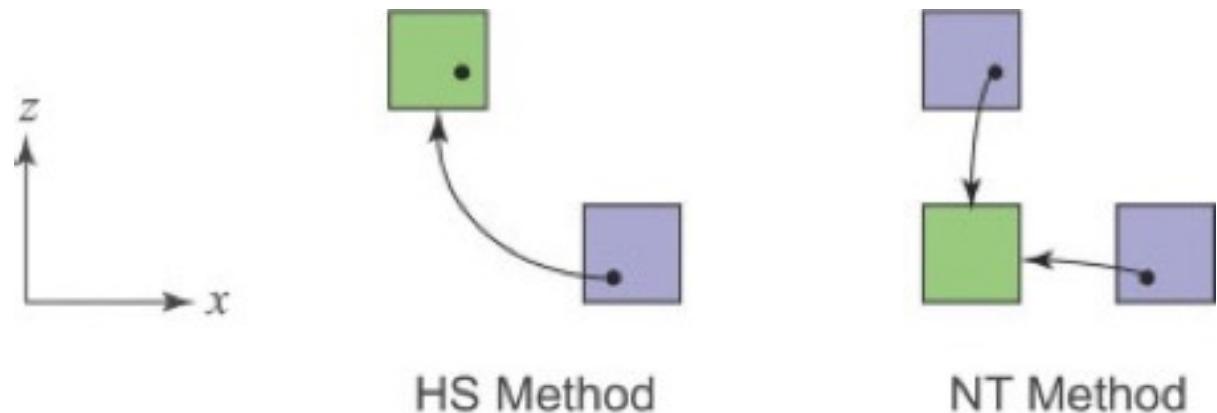
<https://www.lammps.org/cite.html>

# Neutral Territory Decomposition

D. E. Shaw,

“A fast, scalable method for the parallel evaluation of  
distance-limited pairwise particle interactions,”

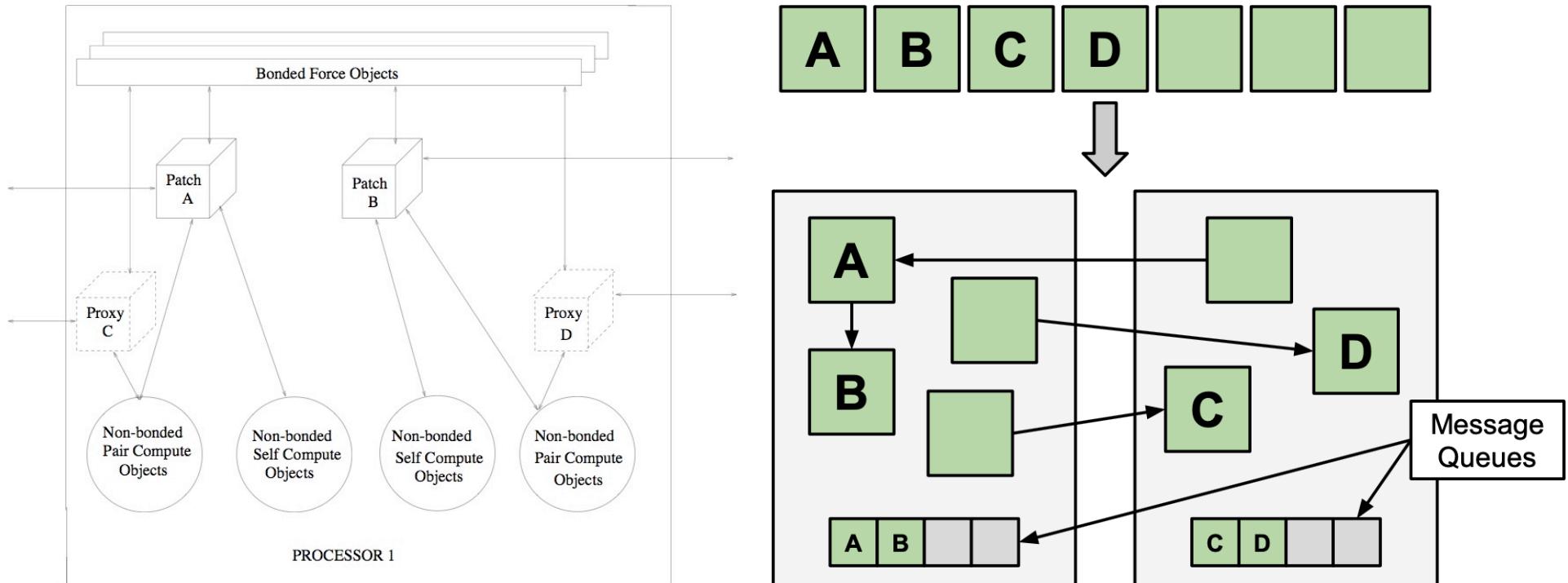
*J. Comput. Chem.* **26**, 1318 ('05)



*cf. Lecture note on “Shaw’s NT algorithm”*

# Hybrid Spatial+Force Decomposition

- Spatial decomposition of patches (localized spatial regions & atoms within)
- Inter-patch force computation objects assigned to any processor
- Message-driven object execution: computation-communication overlap



Kale *et al.*, *J. Comput. Phys.* **151**, 283 ('99); Phillips *et al.*, *SC02* (IEEE/ACM);  
Acun *et al.*, *SC14* (IEEE/ACM), Phillips *et al.*, *J. Chem. Phys.* **153**, 044130 ('20)