Load Balancing

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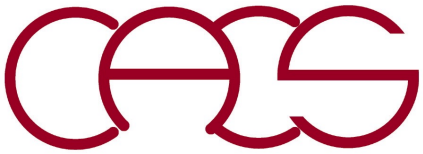
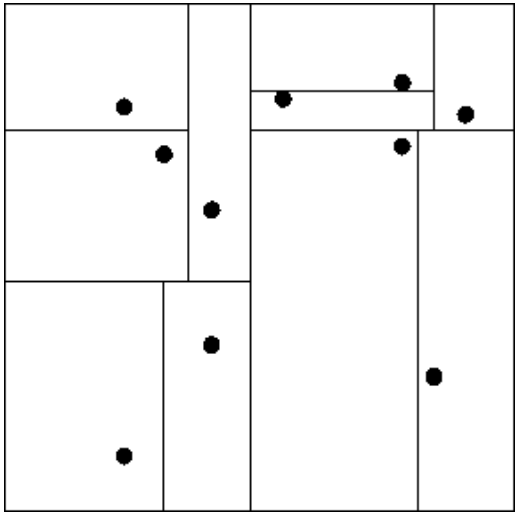


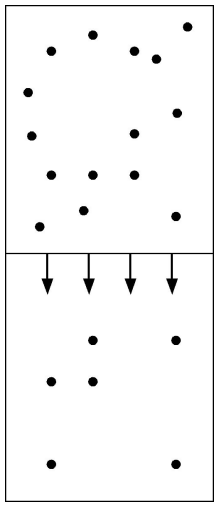
Load Imbalance

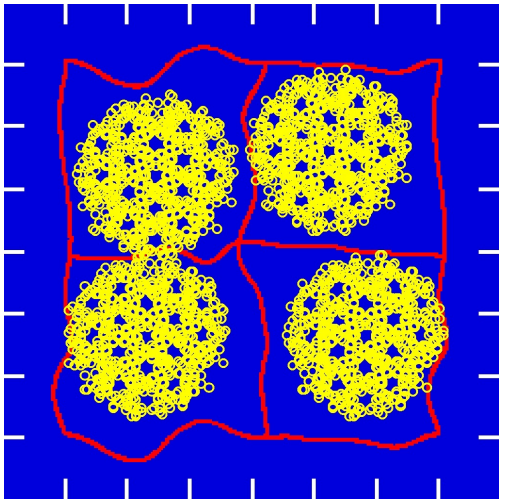
- It is difficult to keep all processors equally busy

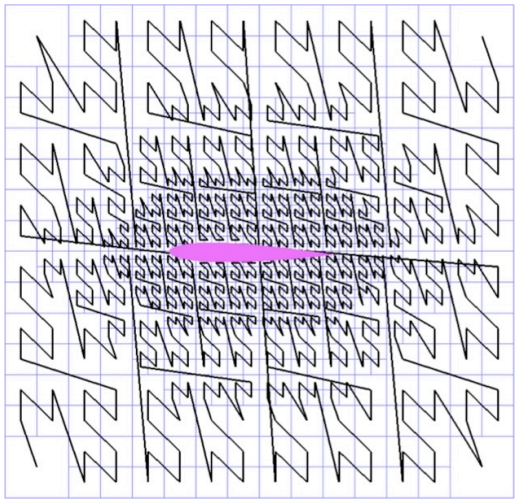
Load Balancing

- **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





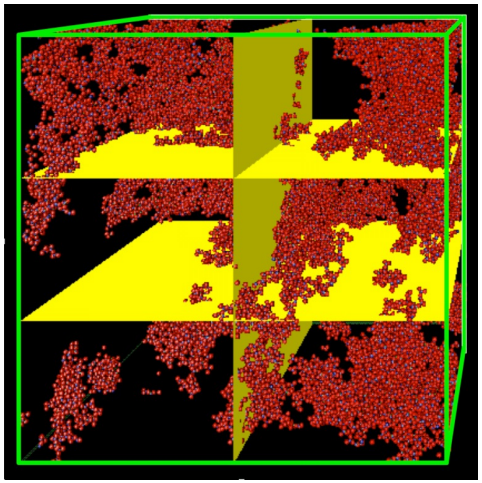




Data Locality in Parallelization

Challenge: Load balancing for irregular data structures

Irregular data-structures/ processor-speed

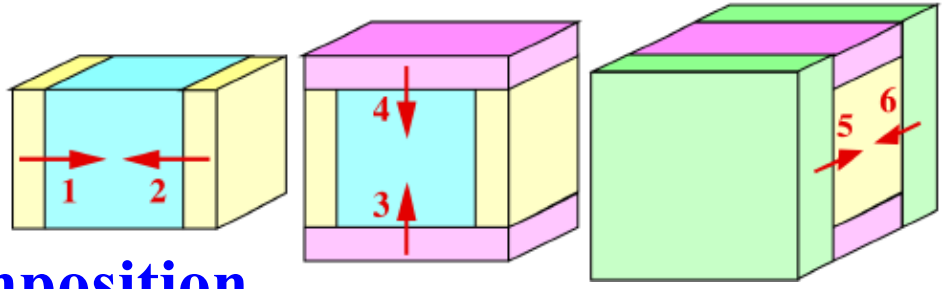


Map

Parallel computer

Optimization problem:

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



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

Computational-Space Decomposition

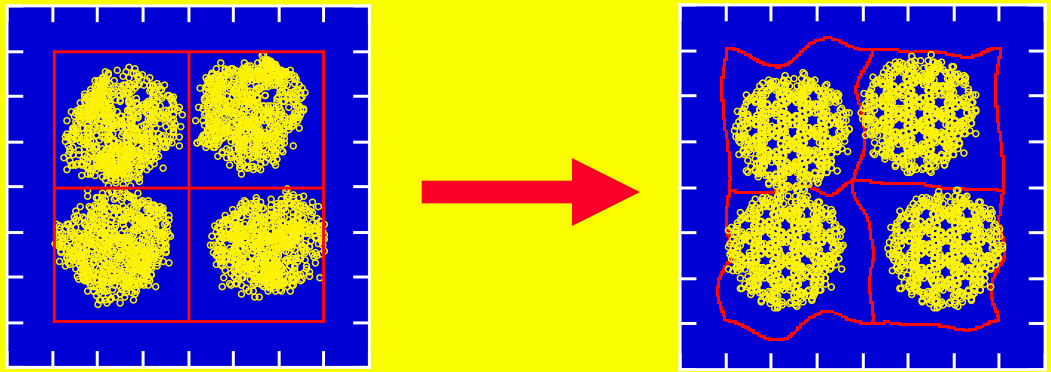
Topology-preserving "computational-space" decomposition in curved space

Curvilinear coordinate transformation

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

Particle-processor mapping: regular 3D mesh topology

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



Regular mesh topology in computational space, ξ

Curved partition in physical space, x

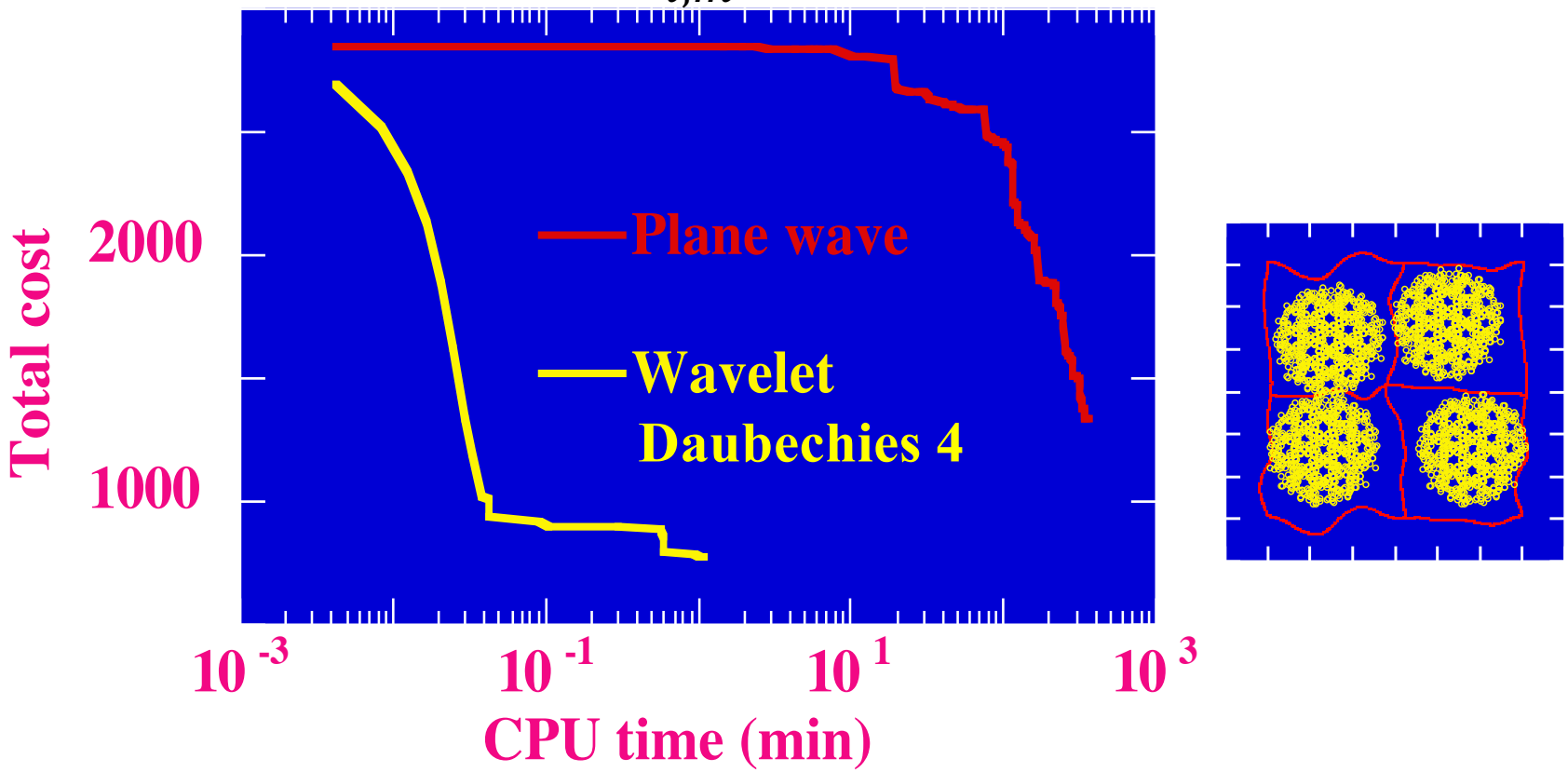
A. Nakano & T. J. Campbell, *Parallel Comput.* **23**, 1461 ('97)

cf. Coordinate transformation in Boltzmann generator, F. Noe *et al*., *Science* **365**, 1001 ('19)

Wavelet-based Adaptive Load Balancing

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

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

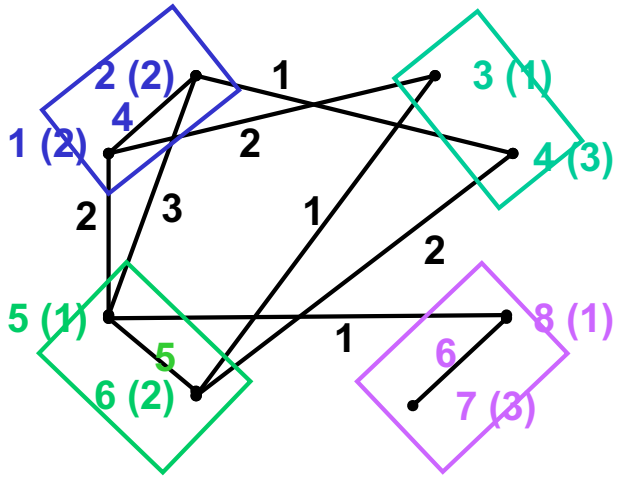


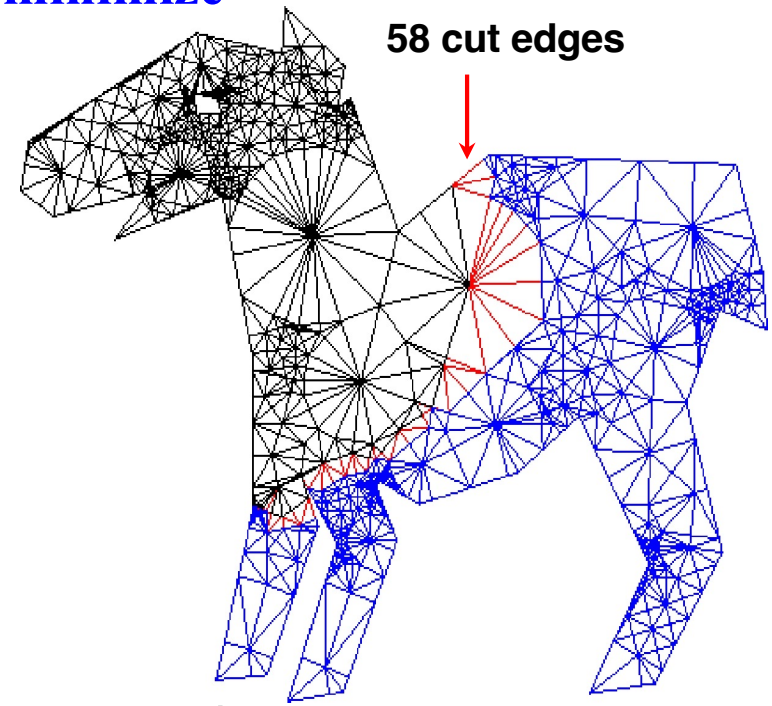
A. Nakano, *Concurrency: Practice and Experience* **11**, 343 ('99)

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 = $\{w_N(j)$: task costs$\}$**
  - **E: edge set = $\{(j,k) \mid$ messages from j to $k\}$**
  - **W_E: edge weights = $\{w_E(j,k)$: message sizes$\}$**

  choose a partition $N = N_1 \cup N_2 \cup \ldots \cup N_P$ to minimize
  - **$\max_p\{\sum_{j \in Np} w_N(j)\}$**
  - **$\max_{(p,q)}\{\sum_{j \in Np, k \in Nq} w_E(j,k)\}$**
- **Graph bisection: Special case of $N = N_1 \cup N_2$**
- **Choosing optimal partitioning is known to be NP-complete → need heuristics**



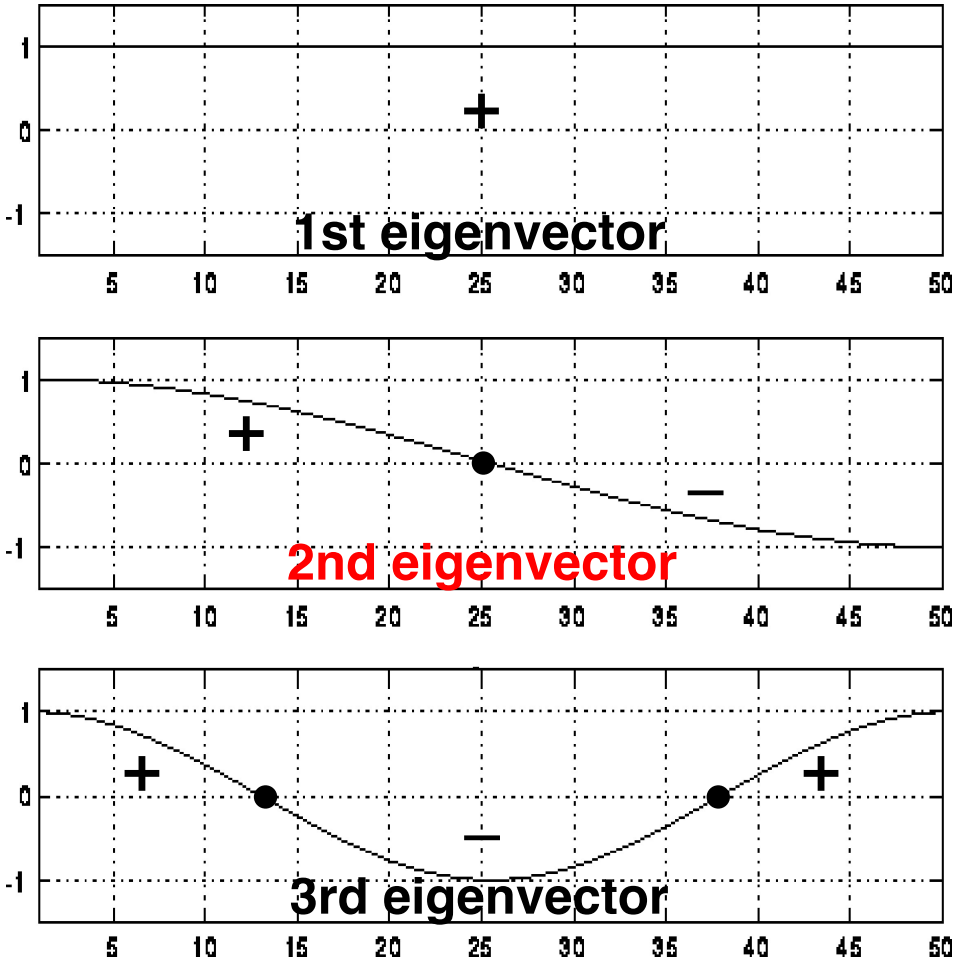


https://sites.google.com/lbl.gov/cs267-spr2022/
Prof. James Demmel (UC Berkeley)

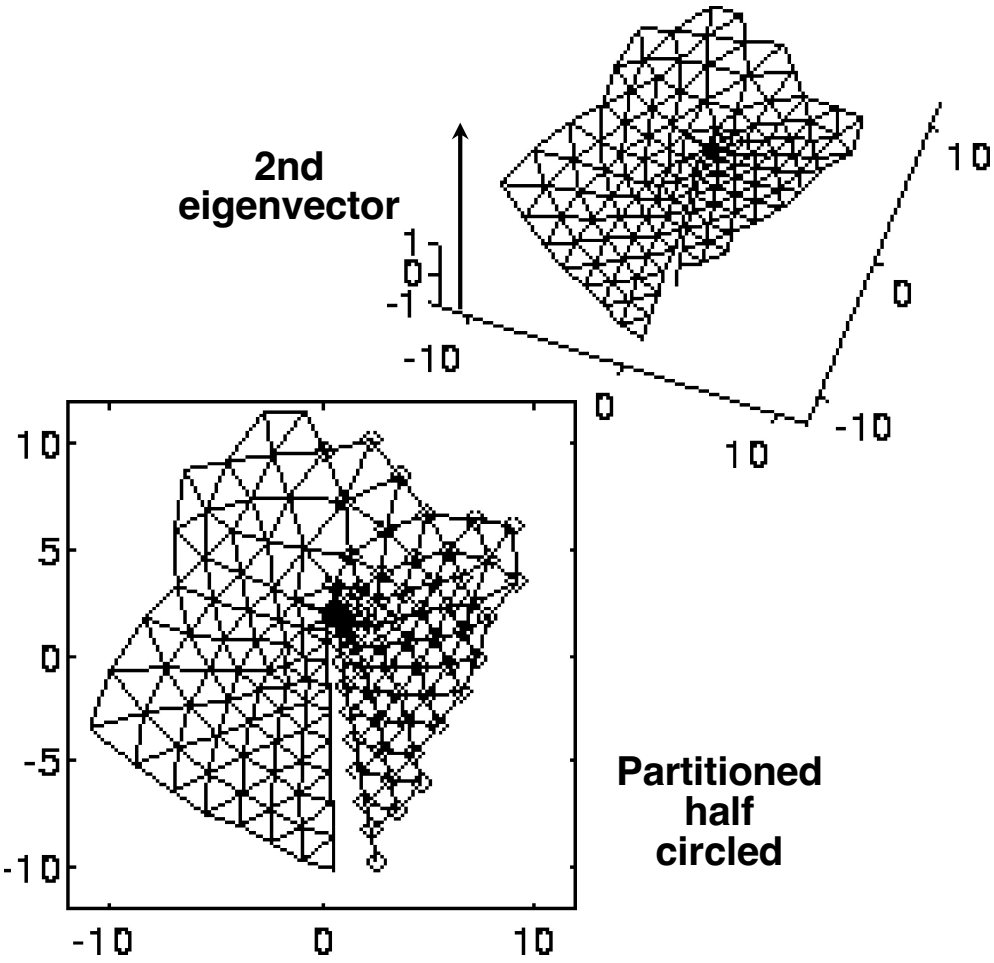
Spectral Bisection: Motivation

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

1D example



2D example



Spectral Bisection

Laplacian matrix:

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

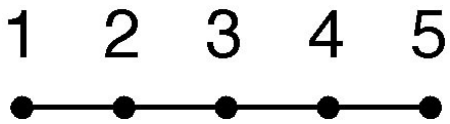
- **L(G)(i,i) = degree of node i (number of incident edges)**
- **L(G)(i,j) = –1 if $i \neq j$ and there is an edge (i,j)**
- **L(G)(i,j) = 0 otherwise**

$$\frac{\partial^2}{\partial x^2} f(x) \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta^2}$$

Theorems:

1. **The eigenvalues of L(G) are nonnegative:**
   $\lambda_1 = 0 \leq \lambda_2 \leq \bullet\bullet\bullet \leq \lambda_N$)
2. **λ_2(L(G)) ≠ 0 if and only if G is connected**

Example



	1	2	3	4	5
1	1	–1			
2	–1	2	–1		
3		–1	2	–1	
4			–1	2	–1
5				–1	1

Spectral bisection algorithm:

1. **Compute eigenvector v_2 corresponding to λ_2(L(G))**
2. **For each node i of G**
   a. **if $v_2(i) < 0$, put node i in partition N–**
   b. **else put node i in partition N+**

Solving eigenproblem costs $O(N^3)$

$O(N)$ λ_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
```

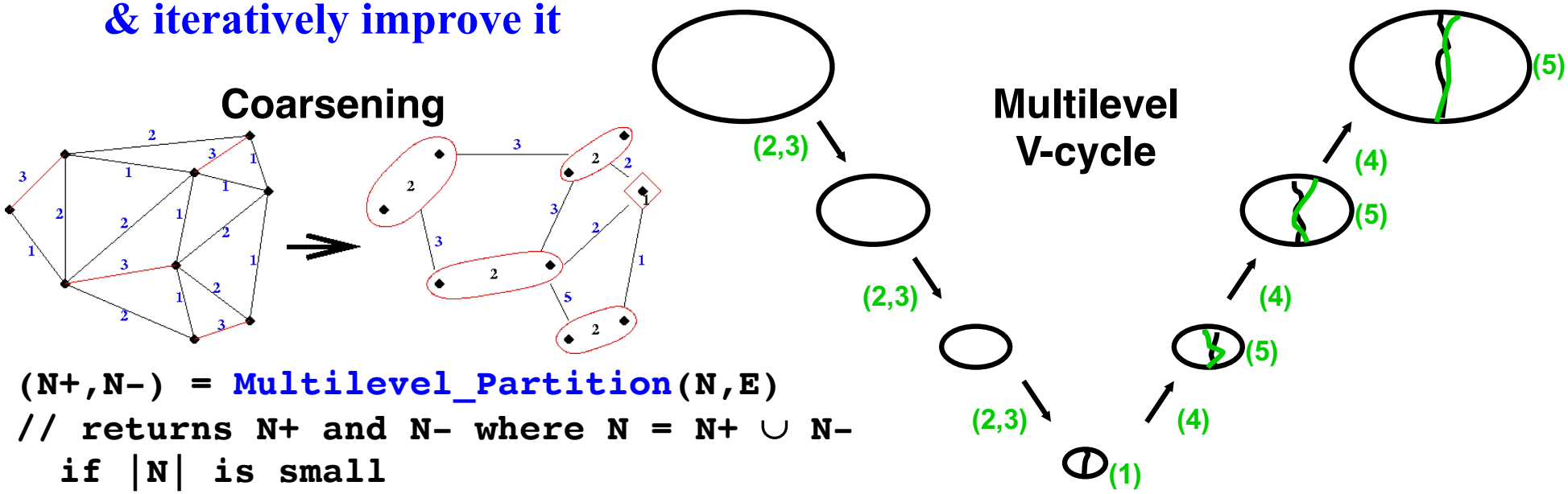
$$\mathbf{T} = \begin{bmatrix} a_1 & b_1 & & & \\ b_1 & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{K-2} & a_{K-1} & b_{K-1} \\ & & & b_{K-1} & a_K \end{bmatrix}$$

See the lecture slides on "Lanczos method for eigensystems"

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




```
(N+,N-) = Multilevel_Partition(N,E)
// returns N+ and N- where N = N+ ∪ N-
  if |N| is small
1   Partition G = (N,E) directly to get N = N+ ∪ N-
    Return (N+,N-)
  else
2   Coarsen G to get an approximation Gc = (Nc,Ec)
3   (Nc+,Nc-) = Multilevel_Partition(Nc,Ec)
4   Expand (Nc+,Nc-) to a partition (N+,N-) of N
5   Improve the partition (N+,N-)
    Return (N+,N-)
  endif
```

G. Karypis & V. Kumar, *SIAM J. Sci. Comput.* **20**, 359 (1998)

https://github.com/KarypisLab/ParMETIS

An Extra Lesson

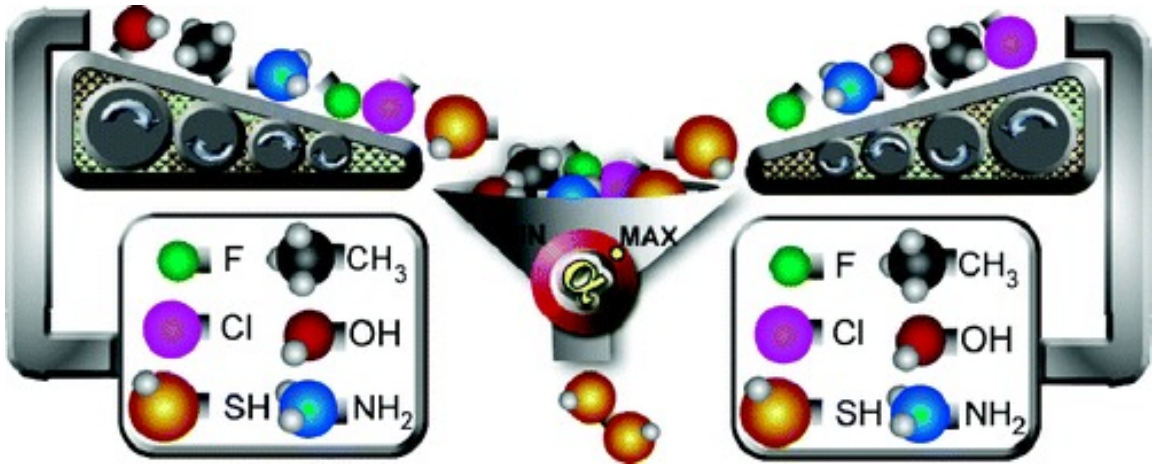
Continuous optimization is easier than discrete combinatorial optimization

cf. • **Linear combination of atomic potentials (LCAP)**

M. Wang *et al*., *J. Amer. Chem. Soc*. **128**, 3228 ('06)

• **Gradient-directed Monte Carlo (DGMC)**

X. Hu, *J. Chem. Phys*. **129**, 064102 ('08)



atom position

$$\text{LCAP: } v(\vec{r}) = \sum_{\vec{R},A} b_A^{\vec{R}} v_A^{\vec{R}}(\vec{r})$$

atom species