SYSTEMATIC UPSCALING:

Linear Scaling

And Beyond

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($\Rightarrow$ survey paper)

Linear Scaling ?

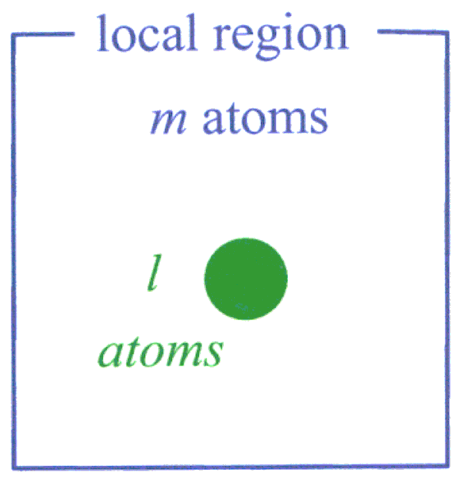
N atoms, electrons, …

O(N) computer operations?

Localization:

$\mathcal{F}(m)$ operations

per l atoms



⇓

Total operations: $N \frac{\mathcal{F}(m)}{l} \approx N m^2$

$N m^2$

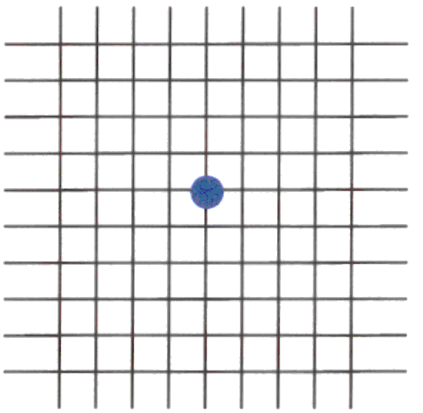
Needed: O(CN), C independent of m

(or $C \sim \log m$)

hypersparsity

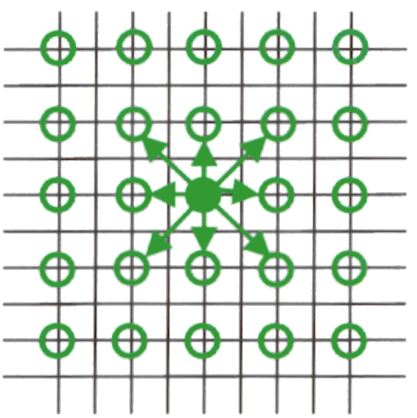
Actually needed: # operations << N

A solution value is NOT
generally determined just
by few local equations



BC

A coarse equation IS
generally determined just
by few local equations



$\Rightarrow$ O(N) operations

The coarse equation can be derived ONCE

for all similar neighborhoods

$\Rightarrow$ # operations << N

Renormalization + Multigrid (RMG)

⇓

Systematic Upscaling

I. Choice of coarse variables

- Small coarsening ratio

  ⇒ avoiding large volumes
  and computational slowdown

- General criterion

II. Derivation of coarse "equations"

- In the form of numerical tables

  ⇒ accuracy unlimited

- General method

Slowdown

of local processing in large domains

- Slow convergence (or sampling)

  of large-scale features

  ⇒ Bad scaling

Multigrid ⇒ Linear scaling: O(N)

- Attraction basins:

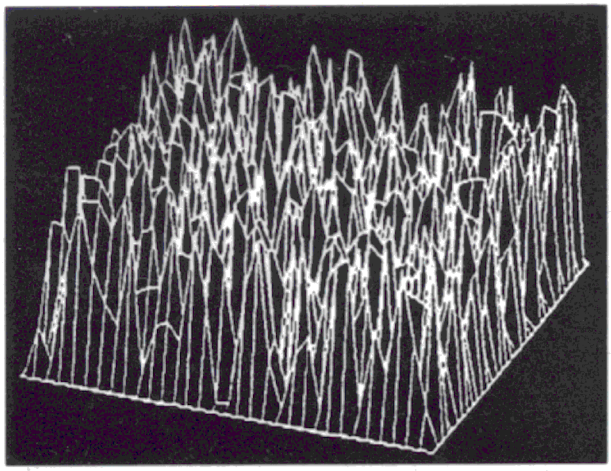
  Multiscale, nested energy barriers

  ⇒ Very bad (e.g., exponential) scaling

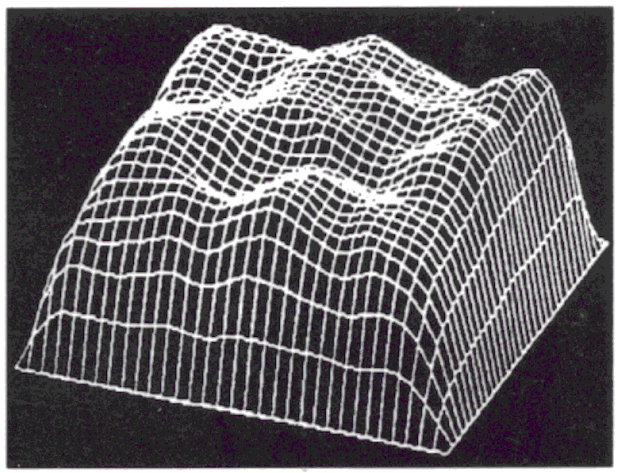
RMG ⇒ sublinear scaling: << N

Influence of (pointwise) Gauss-Seidel relaxation on the error

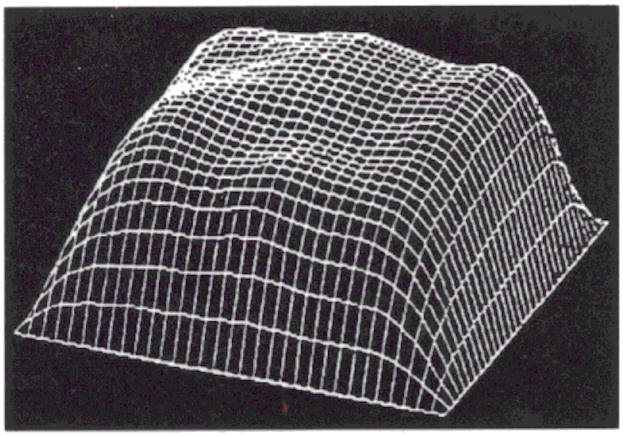
Poisson equation, *uniform grid*



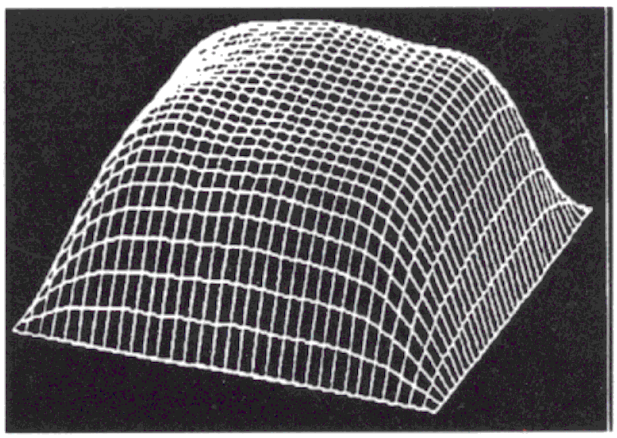
Error of initial guess



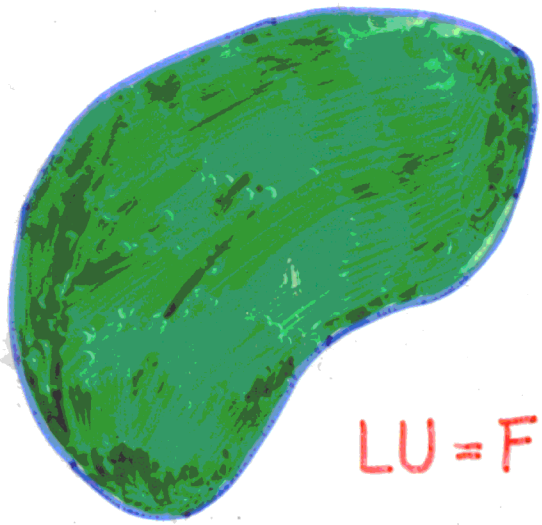
Error after 5 relaxations



Error after 10 relaxations

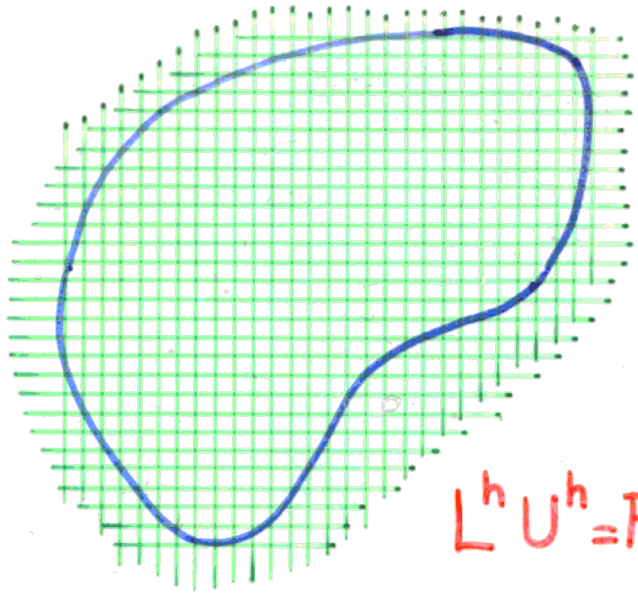


Error after 15 relaxations



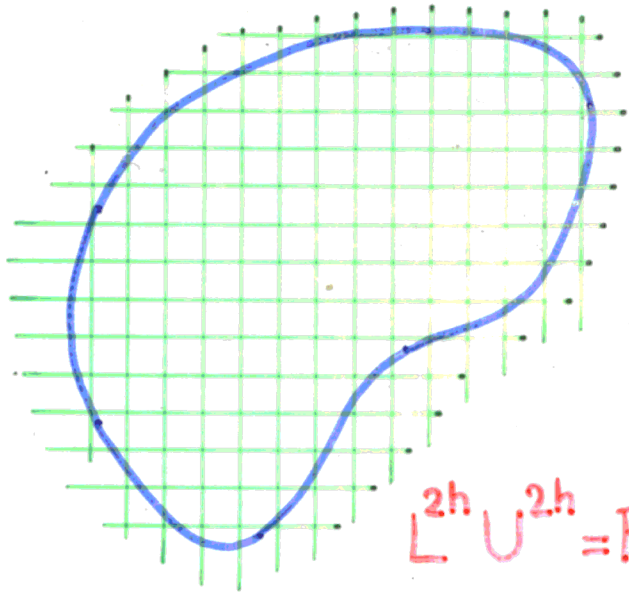
$LU = F$

h



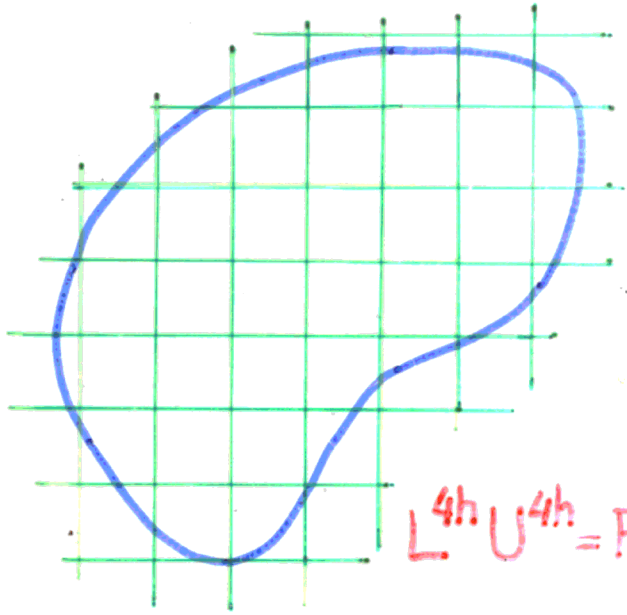
$L^h U^h = F^h$

2h



$L^{2h} U^{2h} = F^{2h}$

4h



$L^{4h} U^{4h} = F^{4h}$

⋮

Poisson equation

$$-\Delta V(x) = \rho(x)$$

Multigrid solver on **3** - dimensional

grid with **N** gridpoints

and **p** - order accuracy

Costs **18pN** computer operations

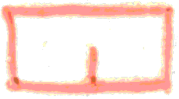
(15pN additions, 3pN multiplications)

- Same count with local refinements
- Much faster than FMM, Ewald, …
- Much simpler, more parallizable
- Integrated into the KS-system multigrid

  $\Rightarrow$ negligible work

Multigrid Solvers

Cost: 25 - 100 operations per unknown

- Linear scalar elliptic equation (~1971) *
- Nonlinear — FAS (1975)
- Grid adaptation — τ — within solver
- General boundaries, BCs * —  ABC
- Discontinuous coefficients — $\nabla(a\nabla u)=f$
- Disordered: coefficients, grid (FE) — AMG
- Several coupled PDEs * — (1984)
- Non-elliptic: high-Reynolds flow
- Highly indefinite: waves — $\Delta u + k^2 u = f$
- Many eigenfunctions (N) — $O(N \log N)$
- Near zero modes
- Gauge topology: Dirac eq.
- Inverse problems — unkown a — Data assimilation
- Integral equations

Massive parallel processing

Even for initial value ODE; PDE (1980)

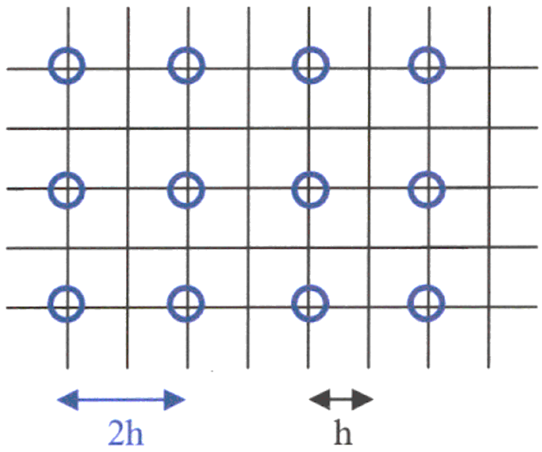
Rigorous quantitave analysis (1986)

Nonlinear Equation   LU = F

FAS: $L^{2h} U^{2h} = F^{2h} + \tau_h^{2h}$

Fine-to-coarse correction

Calculated by relaxation on grid h



One-shot solver: no linearization

e.g. CFD

Kohn-Sham system

$$[-\Delta + V_{LOC}(x, \rho(x)) + V_{ELC}(x)]\ \psi_i(x) = \varepsilon_i \psi_i(x)$$

$$i = 1, \ldots, N_{ELC}$$

$$-\Delta\ V_{ELC}(x) = \rho(x) = \sum_i |\psi_i(x)|^2$$

One shot solver:

No self-consistency iterations

No nuclear-positioning iterations

Goedecker Elasticity

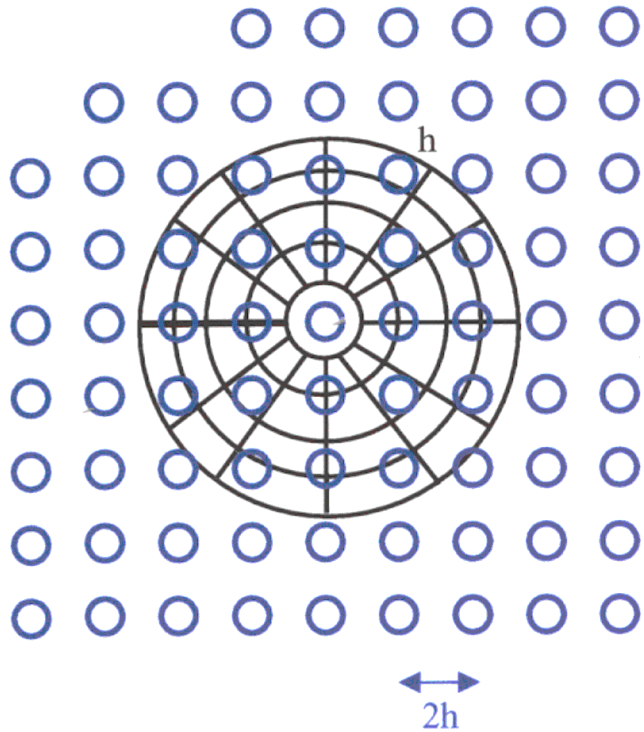
ברמות O(a)
ווריאציות קוונטיות בבסיס יותר.

Local Refinements

$$L^{2h} U^{2h} = F^{2h} + \tau_h^{2h}$$

τ_h^{2h} calculated on

local patch of grid h



- e.g., atomic core
- Nested refinements

$$\tau_h^{2h} = \tau_{2h}^{h}\left(U^{2h}\right)$$

- Table calculated once for all U^{2h}
- Or by rare additional h-level relaxation
- $\Rightarrow$ Numerical "pseudo potentials"

Many eigenfunctions

Quantum chemistry

Kohn-Sham equation:

$$[-\Delta + V(x)]\psi_i(x) = \lambda_i \psi_i(x)$$
$$i = 1, \ldots, N = \#\text{ electrons}$$

O(N) gridpoints per ψ_i

$\Rightarrow$ $O(N^2)$ storage

Orthogonalization

$\Rightarrow$ $O(N^3)$ operations

Multiscale eigenbase — 1D: Livne

O(N *log* N) storage & operations

$V = V_{nuclear} + V(\psi)$

One shot solver

Eigenfunction Structure

$L\,U_\alpha(x) = \lambda_\alpha\,U_\alpha(x)$ e.g. $L = -\Delta + V$

$\alpha = 1,\ldots,N$ U_α **complex**

$U_\alpha(x) = A_\alpha(x)\,\varphi_{\ell(\alpha)}(x)$

$L\,\varphi_\ell(x) \approx \lambda\,\varphi_\ell(x)$ $\ell = 1,\ldots,\ell_{max} = O(1)$

$A_\alpha(x)$ smooth

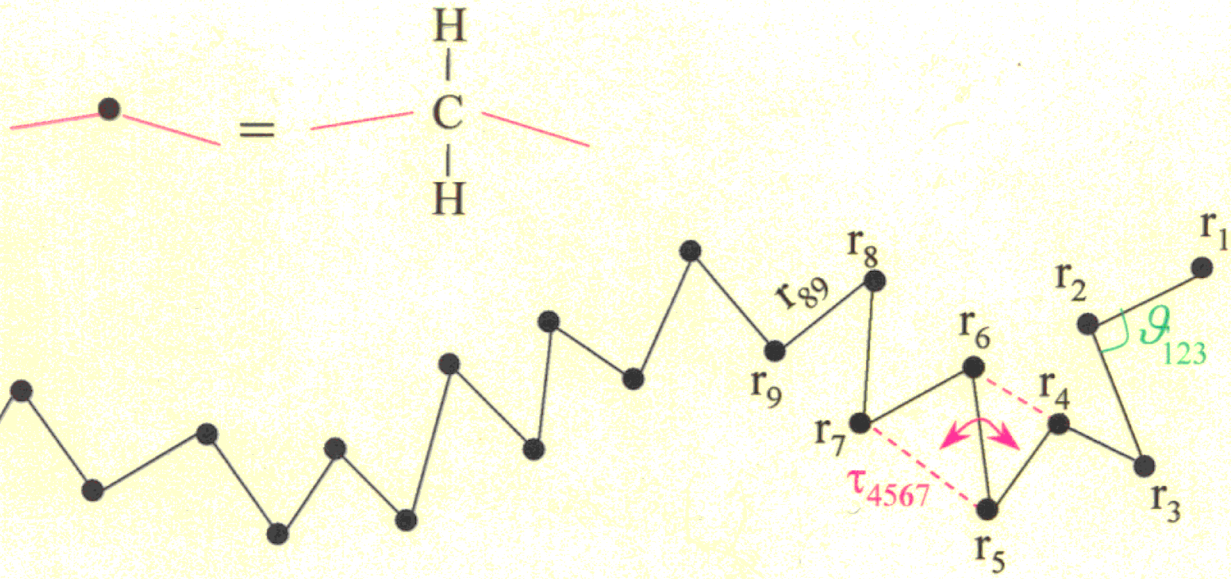
$\varphi_\ell(x)$ found by relaxation

$A_\alpha(x)$ represented on a coarser grid

Objective: **O(N log m)** operations, storage

Feasibility studies: 1D Kohn-Sham

2D Helmholz

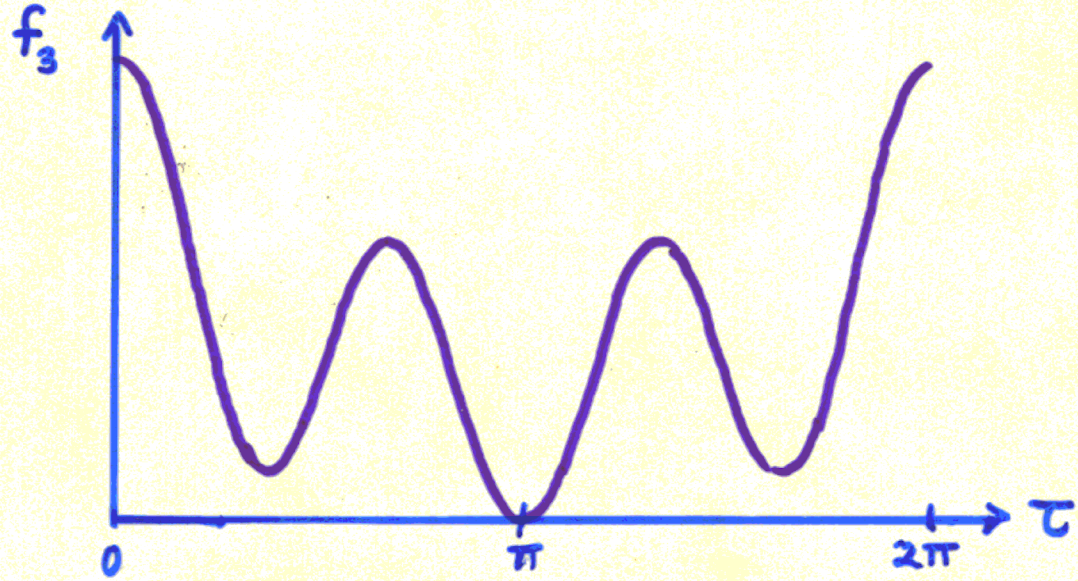


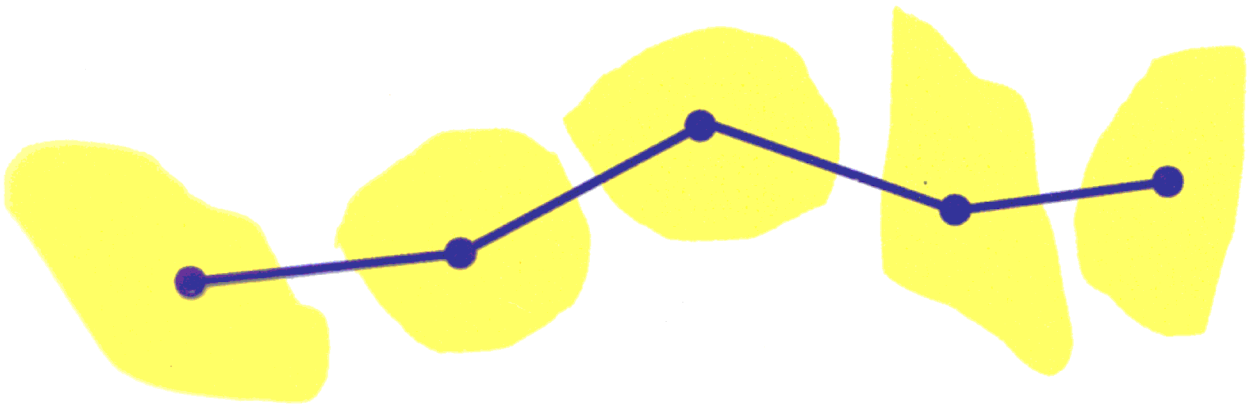
Fine: $\mathrm{P}(\mathrm{r}_1,\ldots,\mathrm{r}_n) \equiv \mathbf{P(r)} \sim e^{-\mathrm{H(r)}}$

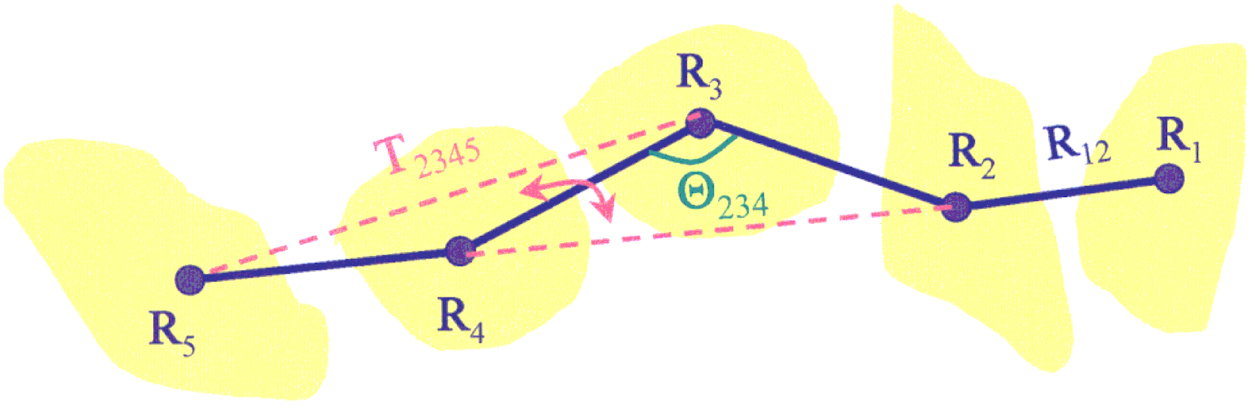
$$\mathbf{H(r)} = \sum_i \left[\mathrm{f}_1(\mathrm{r}_{i,i+1}) + \mathrm{f}_2(\vartheta_{i,i+1,i+2}) + \mathrm{f}_3(\tau_{i,i+1,i+2,i+3}) \right]$$

$$+ \sum_{|i-j|>3} \mathrm{f}_4(|\mathrm{r}_i - \mathrm{r}_j|) \qquad \mathrm{f}_4(\mathrm{r}) = \frac{a}{\mathrm{r}^{12}} - \frac{b}{\mathrm{r}^6}$$

$$+ \sum_{|i-j|>3} \mathrm{G}(\mathrm{r}_i,\mathrm{r}_j)\mathrm{q}_i\mathrm{q}_j \qquad \mathrm{G}(\mathrm{r}_i,\mathrm{r}_j) = \frac{1}{|\mathrm{r}_i - \mathrm{r}_j|^2}$$







Coarse: $\mathbf{P}^{c}(\mathbf{R}_1,\ldots,\mathbf{R}_{n/4}) \equiv \mathbf{P}^{c}(\mathbf{R}) \sim e^{-H^{c}(R)}$

$$\mathbf{H}^{c}(\mathbf{R}) = \sum_i \left[F_1(R_{i,i+1}) + F_2(\Theta_{i,i+1,i+2}) + F_3(T_{i,i+1,i+2,i+3})\right]$$

$$+ C_{AL} \sum_i \Theta_{i,i+1,i+2}(R_{i,i+1} + R_{i+1,i+2})$$

$$+ \sum F_4(|R_i - R_j|)$$

$$+ \sum G_{smooth}(R_i, R_j) Q_i Q_j, \qquad Q_i = \sum_{\nu=1}^{4} q_{i\nu}$$

- Iterative corrections to

$$H^c = \sum A_k H_k(R_1, R_2, \ldots)$$

$$\delta\langle o\rangle \approx \langle o\rangle\langle \delta H\rangle - \langle o \cdot \delta H\rangle$$

$\Rightarrow \{\delta A_k\}$ obtained by solving

$$\sum_l \left(\langle H_k\rangle\langle H_l\rangle - \langle H_k H_l\rangle\right) \delta A_l$$

$$= \langle H_k\rangle_f - \langle H_k\rangle_c$$

- If $\langle H_k H_l\rangle_f - \langle H_k H_l\rangle_c$ is large

  - add to H^c a new term: $A_{kl} H_k H_l$