Global optimization using smoothed potentials

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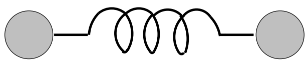
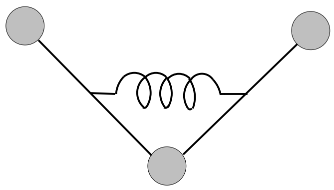
Empirical potential (AMBER 4.1)

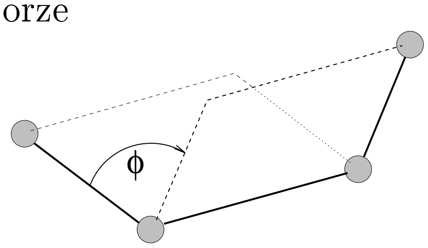
$$H(x) = \sum_{\text{vazby}} S_k(b_k(x) - b_{k,0})^2$$



$$+ \sum_{\substack{\text{vazebné}\\ \text{úhly}}} B_\ell(\theta_\ell(x) - \theta_{\ell,0})^2$$



$$+ \sum_{\text{torze}} T_m[1 + \cos(n_m \phi_m(x) - \delta_m)]$$



$$+ \sum_{\substack{\text{nevázané}\\ \text{dvojice atomů}}} \left[\frac{A_{ij}}{r_{ij}^{12}(x)} - \frac{C_{ij}}{r_{ij}^{6}(x)} + \frac{q_i q_j}{D_{ij}(x) r_{ij}(x)} \right]$$

Minimization of $H(x)$ is a NP-hard problem (Hendrickson 1991, Ngo and Marks 1991, 1992).

Piela, Scheraga 1989: Diffusion equation method

$$\forall \lambda > 0: \quad \langle h \rangle_\lambda (x) = \frac{1}{\lambda^n \pi^{n/2}} \int_{\mathbb{R}^n} h(x-u)\, e^{-\frac{\|u\|^2}{\lambda}}\, du$$

$$\langle h_1 + h_2 \rangle_\lambda = \langle h_1 \rangle_\lambda + \langle h_2 \rangle_\lambda$$

Algorithm GMIN:

1. Select a sequence $\lambda_0 > \lambda_1 > \ldots \lambda_k = 0$.
   Select x_0 randomly.
2. **for** i:=0 **to** k **do**
   x_{i+1}:= Min($\langle f \rangle_{\lambda_i}$, x_i)

We have used Min = SA.

Simulated Annealing (SA):

1. $T := T_0$
2. Do a Monte Carlo step.
3. **If** too many steps have been done/accepted **then** $T := 0.9\,T$
4. **If** $T < T_{\min}$ **then** terminate **else** goto 2.