A Stochastic Quasi Newton Method for molecular simulations
Chun Dong Chau

A STOCHASTIC QUASI NEWTON METHOD

for molecular simulations

FSN: $J_{k+1}J_{k+1}^T = V_k V_{k-1} \cdots V_{k-m+1} J_0 J_0^T V_{k-m+1}^T \cdots V_{k-1}^T V_k^T$

$$V_k = \left(1 - \frac{1}{h_k^T y_k}\left(h_k - \frac{s_k}{\alpha_k}\right) y_k\right)$$

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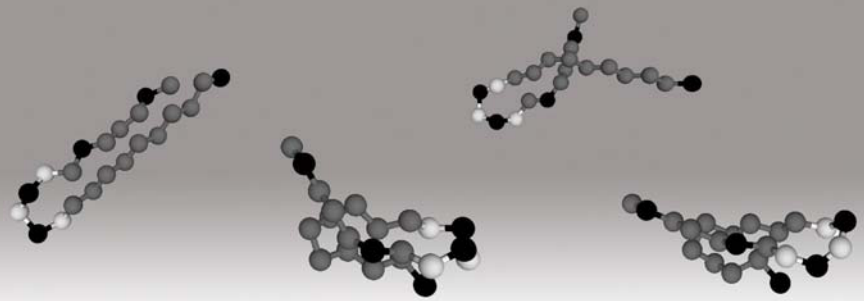

FSU sampled different parts of the energy landsape!

Constant mobility sampled small part of energy landscape, same local minima?!