Course 14/2

Constraints in MD (2/2): general method and SHAKE algorithm

- General method
- SHAKE algorithm

General method

Constraints

$$\sigma_k(\{\vec{r}_i(t)\}) = 0 \qquad k = 1, \dots M$$

Lagrange parameters

Evolution by position Verlet

$$\vec{r}_i(t+\Delta t) = \underbrace{2\,\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \frac{\Delta t^2}{m_i}\vec{F}_i}_{\vec{r}_i{}'(t+\Delta t)} - \frac{\Delta t^2}{m_i}\sum_{k=1}^{M}\gamma_k \left.\frac{\partial \sigma_k}{\partial \vec{r}_i}\right|_{\{\vec{r}_i(t)\}}$$

Verlet evolution without constraints

Exact enforcement of constraint

The Lagrange parameters γ_k are determined by exactly imposing the constraints at $t + \Delta t$:

$$\sigma_k(\{\vec{r}_i(t+\Delta t)\}) = 0 \qquad k = 1, \dots M$$

Linearization

$$\sigma_k(\{\vec{r}_i(t+\Delta t)\}) = \sigma_k(\{\vec{r}_i{}'(t+\Delta t) + [\vec{r}_i(t+\Delta t) - \vec{r}_i{}'(t+\Delta t)]\})$$

$$= \sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) + \sum_{i=1}^{N} \underbrace{[\vec{r}_i(t+\Delta t) - \vec{r}_i{}'(t+\Delta t)]}_{\text{linear in } \Delta t^2\gamma_k} \left.\frac{\partial \sigma_k}{\partial \vec{r}_i}\right|_{\{\vec{r}_i{}'(t+\Delta t)\}}$$

$$+ \underbrace{B_k(\{\Delta t^2 \gamma_k\})}_{\text{higher order in } \Delta t^2\gamma_k}$$

Using the Verlet evolution

$$= \sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) + \sum_{i=1}^{N} \frac{-\Delta t^2}{m_i} \sum_{k'=1}^{M} \gamma_{k'} \left.\frac{\partial \sigma_{k'}}{\partial \vec{r}_i}\right|_{\{\vec{r}_i(t)\}} \left.\frac{\partial \sigma_k}{\partial \vec{r}_i}\right|_{\{\vec{r}_i{}'(t+\Delta t)\}}$$

$$+ B_k(\{\Delta t^2 \gamma_k\})$$

$$= \sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) + \underbrace{\sum_{k'} A_{kk'} \Delta t^2 \gamma_{k'}}_{\text{linear in } \Delta t^2\gamma_k} + \underbrace{B_k(\{\Delta t^2 \gamma_k\})}_{\text{higher order in } \Delta t^2\gamma_k}$$

Linearized equation to be solved

Constraints to be imposed

$$\sigma_k(\{\vec{r}_i(t+\Delta t)\}) = 0 \qquad k = 1, \ldots M$$

Linearized equation

$$\sigma_k(\{\vec{r}_i(t+\Delta t)\}) = \sigma_k(\{\vec{r}_i'(t+\Delta t)\}) + \sum_{k'=1}^{M} A_{kk'}\Delta t^2\gamma_{k'} + B_k(\{\Delta t^2\gamma_k\}) = 0$$

where $$A_{kk'} = \sum_{i=1}^{N} -\frac{1}{m_i} \left.\frac{\partial\sigma_k}{\partial\vec{r}_i}\right|_{\{\vec{r}_i'(t+\Delta t)\}} \left.\frac{\partial\sigma_{k'}}{\partial\vec{r}_i}\right|_{\{\vec{r}_i(t)\}}$$

$$B_k(\{\Delta t^2\gamma_k\}) = \sigma_k(\{\vec{r}_i(t+\Delta t)\}) - \sigma_k(\{\vec{r}_i'(t+\Delta t)\}) - \sum_{k'} A_{kk'}\Delta t^2\gamma_{k'}$$

Solution by iteration

Equation to be solved

$$\sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) + \sum_{k'=1}^{M} A_{kk'} \Delta t^2 \gamma_{k'} + B_k(\{\Delta t^2 \gamma_k\}) = 0$$

$$\{\Delta t^2 \gamma_k{}^{(\ell+1)}\} \qquad \{\Delta t^2 \gamma_k{}^{(\ell)}\}$$

Solution of linear equation

$$\Delta t^2 \gamma_{k'}{}^{(\ell+1)} = -\sum_{k=1}^{M} (A^{-1})_{k'k} \left[\sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) + B_k(\{\Delta t^2 \gamma_k{}^{(\ell)}\}) \right]$$

matrix inversion: only once per time step

Sequence: from ℓ to $\ell+1$

$$\Delta t^2 \gamma_k^{(\ell)} \xrightarrow{(*)} \vec{r}_i^{(\ell)}(t+\Delta t) \xrightarrow{(**)} B_k(\{\Delta t^2 \gamma_k^{(\ell)}\}) \xrightarrow{(***)} \Delta t^2 \gamma_k^{(\ell+1)}$$

$$(*) \qquad \vec{r}_i^{(\ell)}(t+\Delta t) = \vec{r}_i{}'(t+\Delta t) - \frac{\Delta t^2}{m_i} \sum_{k=1}^{M} \gamma_k^{(\ell)} \left. \frac{\partial \sigma_k}{\partial \vec{r}_i} \right|_{\{\vec{r}_i(t)\}}$$

Verlet evolution

$$(**) \qquad B_k(\{\Delta t^2 \gamma_k^{(\ell)}\}) = \sigma_k(\{\vec{r}_i^{(\ell)}(t+\Delta t)\}) - \sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) - \sum_{k'=1}^{M} A_{kk'} \Delta t^2 \gamma_{k'}^{(\ell)}$$

$$(***) \qquad \Delta t^2 \gamma_{k'}^{(\ell+1)} = - \sum_{k=1}^{M} (A^{-1})_{k'k} \left[\sigma_k(\{\vec{r}_i{}'(t+\Delta t)\}) + B_k(\{\Delta t^2 \gamma_k^{(\ell)}\}) \right]$$

Starting point

$$\Delta t^2 \gamma_k^{(\ell)} \xrightarrow{(*)} \vec{r}_i^{\,(\ell)}(t+\Delta t) \xrightarrow{(**)} B_k(\{\Delta t^2 \gamma_k^{(\ell)}\}) \xrightarrow{(***)} \Delta t^2 \gamma_k^{(\ell+1)}$$

$\Delta t^2 \gamma_k^{(0)} = 0$ | $\vec{r}_i^{\,(0)}(t+\Delta t) = \vec{r}_i^{\,\prime}(t+\Delta t)$ | $B_k(\{\Delta t^2 \gamma_k^{(0)}\}) = 0$ | $\Delta t^2 \gamma_k^{(1)}$

$$(*) \quad \vec{r}_i^{\,(\ell)}(t+\Delta t) = \vec{r}_i^{\,\prime}(t+\Delta t) - \frac{\Delta t^2}{m_i} \sum_{k=1}^{M} \gamma_k^{(\ell)} \left. \frac{\partial \sigma_k}{\partial \vec{r}_i} \right|_{\{\vec{r}_i(t)\}}$$

Verlet evolution

$$(**) \quad B_k(\{\Delta t^2 \gamma_k^{(\ell)}\}) = \sigma_k(\{\vec{r}_i^{\,(\ell)}(t+\Delta t)\}) - \sigma_k(\{\vec{r}_i^{\,\prime}(t+\Delta t)\}) - \sum_{k'=1}^{M} A_{kk'} \Delta t^2 \gamma_{k'}^{(\ell)}$$

$$(***) \quad \Delta t^2 \gamma_{k'}^{(\ell+1)} = - \sum_{k=1}^{M} (A^{-1})_{k'k} \left[\sigma_k(\{\vec{r}_i^{\,\prime}(t+\Delta t)\}) + B_k(\{\Delta t^2 \gamma_k^{(\ell)}\}) \right]$$

Convergence

$$\lim_{\ell \to \infty} \vec{r}_i^{\,(\ell)}(t + \Delta t) = \vec{r}_i(t + \Delta t)$$

- Convergence is generally rapid.
- Convergence can be controlled by reducing the MD time step.

Constraints in MD

General method

- Derivatives calculated in two points per timestep.
- Higher orders are considered.
- All constraints are treated concurrently.

SHAKE algorithm

- Derivatives continuously recalculated as convergence proceeds.
- Only linear order is retained.
- One constraint at the time is treated.

SHAKE algorithm

Schematic flow chart of algorithm

1. Calculate $\vec{r}_i'(\, t + \Delta t\,)$, corresponding to the Verlet evolution without constraints.

2. Set $\vec{r}_i^{\,(0)}(\, t{+}\Delta t\,) = \vec{r}_i'(\, t{+}\Delta t\,)$.

3. Loop over successive refinements with iterations labeled by $\ell = 1,\ldots\infty$.

4. Inner loop over constraints: $k = 1, \ldots M$.

Partial update of $\vec{r}_i^{\,(\ell)}$ for a given constraint k .

Next k .

Next ℓ .

5. End when constraints are satisfied.

Partial update in SHAKE algorithm

Partial update of the coordinates at iteration step ℓ and at constraint k

$$\vec{r}_i^{\,\text{NEW}} = \vec{r}_i^{\,\text{OLD}} - \Delta t^2 \lambda_k^{(\ell)} \left. \frac{\partial \sigma_k}{\partial \vec{r}_i} \right|_{\{\vec{r}_i(t)\}}$$

where $\vec{r}_i(t)$ are the positions at the previous timestep t

and $\vec{r}_i^{\,\text{OLD}}$ / $\vec{r}_i^{\,\text{NEW}}$ are the positions before / after this partial update.

Enforcement of constraint k

linear term only

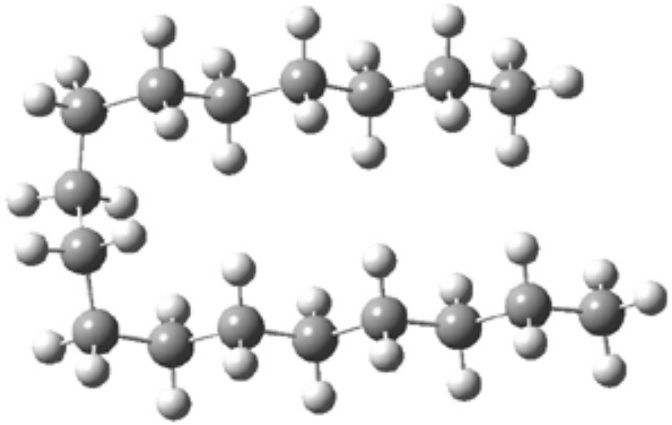
$$0 = \sigma_k(\{\vec{r}_i^{\,\text{NEW}}\}) = \sigma_k(\{\vec{r}_i^{\,\text{OLD}}\}) + \sum_{i=1}^{N} (\vec{r}_i^{\,\text{NEW}} - \vec{r}_i^{\,\text{OLD}}) \cdot \left. \frac{\partial \sigma_k}{\partial \vec{r}_i} \right|_{\{\vec{r}_i^{\,\text{OLD}}\}}$$

$$= \sigma_k(\{\vec{r}_i^{\,\text{OLD}}\}) - \Delta t^2 \lambda_k^{(\ell)} \sum_{i=1}^{N} \left. \frac{\partial \sigma_k}{\partial \vec{r}_i} \right|_{\{\vec{r}_i^{\,\text{OLD}}\}} \left. \frac{\partial \sigma_k}{\partial \vec{r}_i} \right|_{\{\vec{r}_i(t)\}}$$

Simple linear equation for $\lambda_k^{(\ell)}$

Considerations about SHAKE algorithm

$$\Delta t^2 \lambda_k^{(\ell)} = \frac{\sigma_k(\{\vec{r}_i^{\,\mathrm{OLD}}\})}{\sum_{i=1}^{N} \left.\frac{\partial \sigma_k}{\partial \vec{r}_i}\right|_{\{\vec{r}_i^{\,\mathrm{OLD}}\}} \left.\frac{\partial \sigma_k}{\partial \vec{r}_i}\right|_{\{\vec{r}_i(t)\}}}$$



- No matrix inversion is required. This contributes to the speed of the algorithm.
- Derivatives are recalculated as convergence proceeds. The linear expansion progressively becomes a better approximation as convergence approaches.
- Note the sum over particles $i = 1 \ldots N$: The SHAKE algorithm is particularly convenient when each of the various constraints does not depend on the positions of many different atoms. This makes the SHAKE algorithm particularly useful for bond constraints (just two particles involved).

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