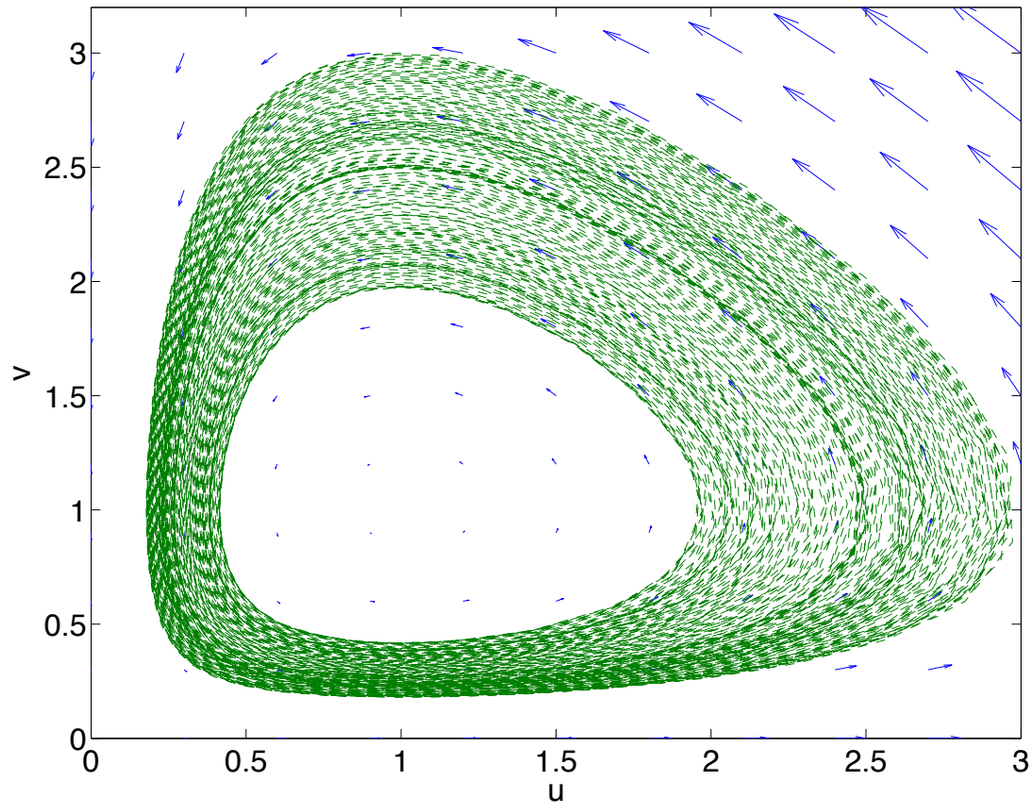
Splitting methods and rigid body integration

Ralf Banisch



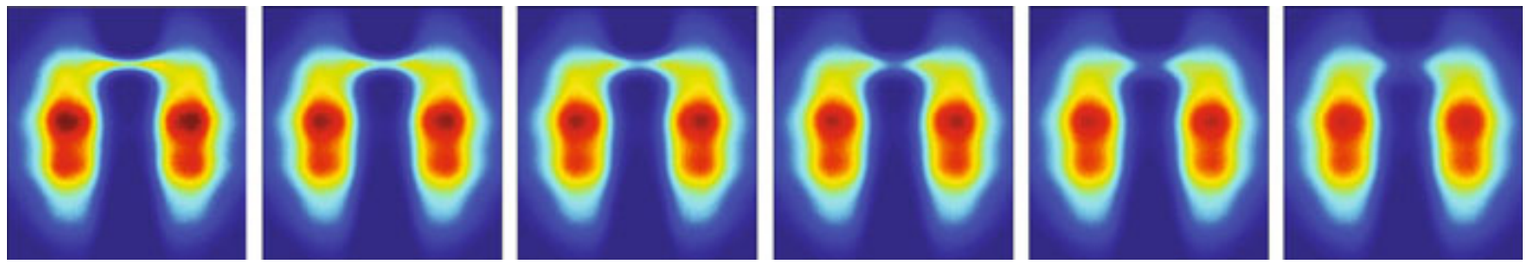
Outline

- Langevin Dynamics
- Numerical integration, splitting strategies
- The Mercedes Benz potential as a model for water like particles
- Rigid bodies
- The DLM algorithm

Book ‘Molecular Dynamics’ by
Ben Leimkuhler & Charles Matthews

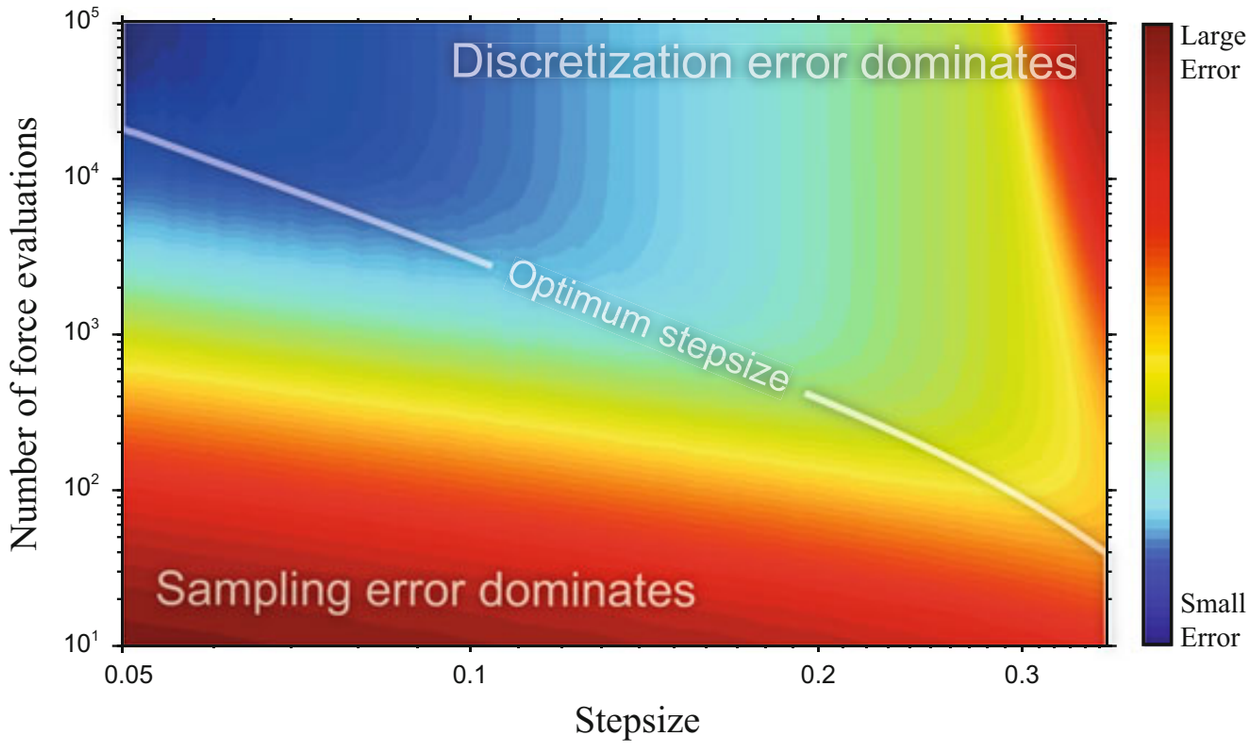
Numerical integration in MD: Sampling error vs discretisation error

- Discretisation error due to introduction of discretisation time step h:



Picture from
[Leimkuhler, Matthews '15]

- Sampling error vs. discretisation error:



Picture from
[Leimkuhler, Matthews '15]

Langevin dynamics

- Langevin dynamics

$$\mathrm{d}\boldsymbol{q} = \boldsymbol{M}^{-1}\boldsymbol{p}\mathrm{d}t,$$

$$\mathrm{d}\boldsymbol{p} = -\nabla U(\boldsymbol{q})\mathrm{d}t - \gamma\boldsymbol{p}\mathrm{d}t + \sqrt{2\gamma \mathrm{k_B T}}\boldsymbol{M}^{1/2}\mathrm{d}\mathbf{W}.$$

- Langevin dynamics is ergodic:

$$(q, p) \sim Z^{-1}e^{-H(q,p)}$$

- Splitting strategy:

$$\mathrm{d}\begin{bmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{bmatrix} = \underbrace{\begin{bmatrix}\boldsymbol{M}^{-1}\boldsymbol{p}\\ \mathbf{0}\end{bmatrix}\mathrm{d}t}_{\mathrm{A}} + \underbrace{\begin{bmatrix}\mathbf{0}\\ -\nabla U(\boldsymbol{q})\end{bmatrix}\mathrm{d}t}_{\mathrm{B}} + \underbrace{\begin{bmatrix}\mathbf{0}\\ -\gamma\boldsymbol{p}\mathrm{d}t + \sigma\boldsymbol{M}^{1/2}\mathrm{d}\mathbf{W}\end{bmatrix}}_{\mathrm{O}},$$

Splitting strategies

- Splitting strategy:

$$\mathrm{d}\begin{bmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{bmatrix} = \underbrace{\begin{bmatrix}\boldsymbol{M}^{-1}\boldsymbol{p}\\ \mathbf{0}\end{bmatrix}\mathrm{d}t}_{\mathrm{A}} + \underbrace{\begin{bmatrix}\mathbf{0}\\ -\nabla U(\boldsymbol{q})\end{bmatrix}\mathrm{d}t}_{\mathrm{B}} + \underbrace{\begin{bmatrix}\mathbf{0}\\ -\gamma\boldsymbol{p}\mathrm{d}t + \sigma\boldsymbol{M}^{1/2}\mathrm{d}\mathbf{W}\end{bmatrix}}_{\mathrm{O}},$$

- Update maps for the individual pieces (O part is solved exactly):

$$\begin{aligned}
\mathscr{U}_h^{\mathrm{A}}(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{q} + h\boldsymbol{M}^{-1}\boldsymbol{p}, \boldsymbol{p}),\\
\mathscr{U}_h^{\mathrm{B}}(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{q}, \boldsymbol{p} - h\nabla U(\boldsymbol{q})),\\
\mathscr{U}_h^{\mathrm{O}}(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{q}, e^{-\gamma h}\boldsymbol{p} + \sqrt{\mathrm{k_B T}\,(1 - e^{-2\gamma h})}\boldsymbol{M}^{1/2}\mathbf{R}),
\end{aligned}$$

- We can define a family of schemes codified as strings with the alphabet “ABO”, e.g.

$$\mathscr{U}_h^{[\![\mathrm{ABO}]\!]} = \mathscr{U}_h^{\mathrm{O}} \circ \mathscr{U}_h^{\mathrm{B}} \circ \mathscr{U}_h^{\mathrm{A}}. \qquad \mathscr{U}_h^{[\![\mathrm{BABO}]\!]} = \mathscr{U}_h^{\mathrm{O}} \circ \mathscr{U}_{h/2}^{\mathrm{B}} \circ \mathscr{U}_h^{\mathrm{A}} \circ \mathscr{U}_{h/2}^{\mathrm{B}}.$$

Splitting strategies

- Symmetric schemes like “ABOBA” typically have more favourable properties compared to non-symmetric ones, e.g. “ABAO”

- Some schemes and explicit maps:

$$
\begin{aligned}
&[\![\text{BAOAB}]\!]\\
\boldsymbol{p}_{n+1/2} &= \boldsymbol{p}_n - (h/2)\nabla U(\boldsymbol{q}_n),\\
\boldsymbol{q}_{n+1/2} &= \boldsymbol{q}_n + (h/2)\boldsymbol{M}^{-1}\boldsymbol{p}_{n+1/2},\\
\hat{\boldsymbol{p}}_{n+1/2} &= e^{-h\gamma}\boldsymbol{p}_{n+1/2} + \zeta_2\boldsymbol{M}^{1/2}\mathbf{R}_n,\\
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_{n+1/2} + (h/2)\boldsymbol{M}^{-1}\hat{\boldsymbol{p}}_{n+1/2},\\
\boldsymbol{p}_{n+1} &= \hat{\boldsymbol{p}}_{n+1/2} - (h/2)\nabla U(\boldsymbol{q}_{n+1}),
\end{aligned}
\qquad
\begin{aligned}
&[\![\text{OBABO}]\!]\\
\boldsymbol{p}_{n+1/2} &= e^{-h\gamma/2}\boldsymbol{p}_n + \zeta_1\boldsymbol{M}^{1/2}\mathbf{R}_n,\\
\hat{\boldsymbol{p}}_{n+1/2} &= \boldsymbol{p}_{n+1/2} - (h/2)\nabla U(\boldsymbol{q}_n),\\
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_n + h\boldsymbol{M}^{-1}\hat{\boldsymbol{p}}_{n+1/2},\\
\hat{\boldsymbol{p}}_{n+1} &= \hat{\boldsymbol{p}}_{n+1/2} - (h/2)\nabla U(\boldsymbol{q}_{n+1}),\\
\boldsymbol{p}_{n+1} &= e^{-h\gamma/2}\hat{\boldsymbol{p}}_{n+1} + \zeta_1\boldsymbol{M}^{1/2}\mathbf{R}_{n+1/2},
\end{aligned}
\qquad
\begin{aligned}
&[\![\text{ABOBA}]\!]\\
\boldsymbol{q}_{n+1/2} &= \boldsymbol{q}_n + (h/2)\boldsymbol{M}^{-1}\boldsymbol{p}_n,\\
\boldsymbol{p}_{n+1/2} &= \boldsymbol{p}_n - (h/2)\nabla U(\boldsymbol{q}_{n+1/2}),\\
\hat{\boldsymbol{p}}_{n+1/2} &= e^{-h\gamma}\boldsymbol{p}_{n+1/2} + \zeta_2\boldsymbol{M}^{1/2}\mathbf{R}_n,\\
\boldsymbol{p}_{n+1} &= \hat{\boldsymbol{p}}_{n+1/2} - (h/2)\nabla U(\boldsymbol{q}_{n+1/2}),\\
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_{n+1/2} + (h/2)\boldsymbol{M}^{-1}\boldsymbol{p}_{n+1},
\end{aligned}
$$

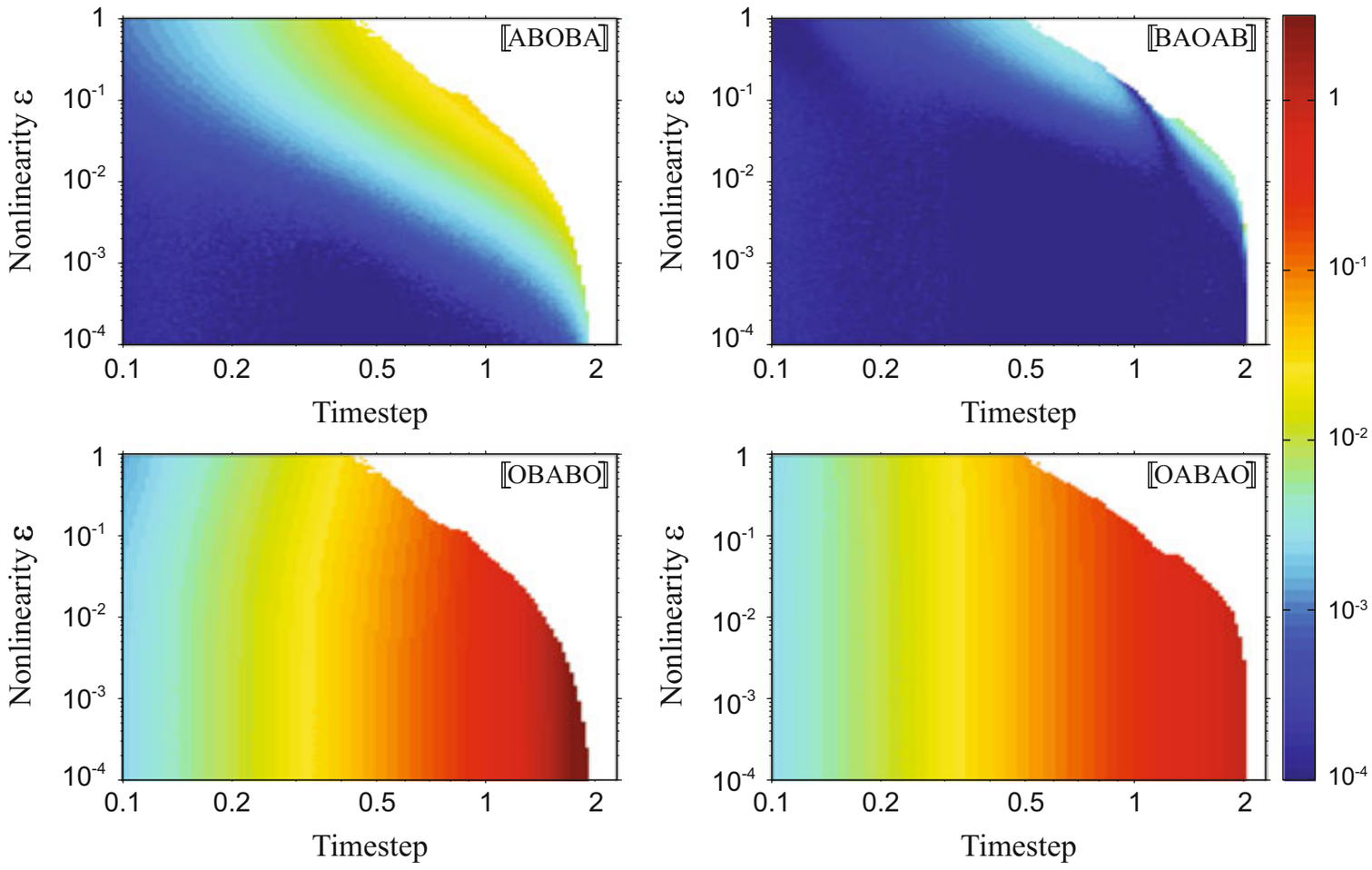
$\zeta_j = \left[\mathrm{k_B T}\left(1 - e^{-j\gamma h}\right)\right]^{1/2}$, $\mathbf{R}_n, \mathbf{R}_{n+1/2}$ are N(0,1) random variables

- One derives error bounds by considering perturbative expansions of e.g.

$$
e^{h\hat{\mathcal{L}}^\dagger} = e^{\frac{h}{2}\mathcal{L}_{\mathrm{X}}^\dagger} e^{\frac{h}{2}\mathcal{L}_{\mathrm{Y}}^\dagger} e^{h\mathcal{L}_{\mathrm{Z}}^\dagger} e^{\frac{h}{2}\mathcal{L}_{\mathrm{Y}}^\dagger} e^{\frac{h}{2}\mathcal{L}_{\mathrm{X}}^\dagger},
$$

Splitting strategies

- Different schemes can have very different discretisation error!



Picture from
[Leimkuhler, Matthews '15]

Fig. 7.3 *Each pixel* in the above grids marks the result of a numerical experiment using one of the four second order (in stepsize) symmetric Langevin discretization schemes. A *pixel's color* denotes the absolute error of $\langle q^2 \rangle_h$ from an experiment conducted at the given stepsize h (*horizontal*) and nonlinearity parameter ε (*vertical*) defining the potential energy in (7.13), with *white pixels* indicating instability. Experiments were taken over a sufficiently long time interval such that the observed errors are the result of discretization error, rather than sampling error

Ergodicity

Langevin dynamics (friction parameter $\gamma > 0$)

$$\begin{cases} dq_t = M^{-1} p_t \, dt, \\ dp_t = -\nabla V(q_t) \, dt - \gamma M^{-1} p_t \, dt + \sqrt{\dfrac{2\gamma}{\beta}} \, dW_t. \end{cases}$$

- Unique invariant measure μ
- Convergence of ergodic averages over one trajectory

$$\lim_{t \to \infty} \frac{1}{t} \int_0^t \varphi(q_s, p_s) ds = \mathbb{E}_\mu(\varphi) = \int_{\mathcal{E}} \varphi(q,p) \; d\mu(q,p), \text{ a.s.}$$

- Rate of convergence $\rightarrow$ Central limit theorem : define $\Pi\varphi := \varphi - \mathbb{E}_\mu(\varphi)$

$$\sqrt{t} \left(\frac{1}{t} \int_0^t \Pi\varphi(q_t, p_t) dt \right) \xrightarrow[t \to +\infty]{\text{law}} \mathcal{N}(0, \sigma^2)$$

with asymptotic variance $\sigma^2(\varphi) = 2 \displaystyle\int_0^{+\infty} \mathbb{E}\left(\Pi\varphi(q_t, p_t) \Pi\varphi(q_0, p_0)\right) dt$

Ergodicity

- Need to check for ergodicity by computing trajectory averages of observables whose exact ergodic averages are known.

Kinetic temperature

$$\mathrm{T} = \mathrm{Av}_\beta\left(\frac{p^2}{m\mathrm{k_B}}\right).$$

configurational temperature

$$\frac{\mathrm{Av}_\beta(\|\nabla U\|^2)}{\mathrm{Av}_\beta(\Delta U)} = k_\mathrm{B}\mathrm{T}.$$

- Av_β is the average with respect to the canonical density exp(-βH(q,p))

- Special cases of general result:

Proposition 6.1 *Let H be a Hamiltonian defined on the phase space $\mathbb{R}^{2N_c}$ and suppose $\boldsymbol{G} : \mathbb{R}^{2N_c} \to \mathbb{R}^{2N_c}$ is a smooth (C^1) vector field with the following properties:*

- $0 < |\mathrm{Av}_\beta(\boldsymbol{G}\cdot\nabla H)| < \infty$,
- $0 < \mathrm{Av}_\beta(\nabla\cdot\boldsymbol{G}) < \infty$,
- $|\boldsymbol{G}e^{-\beta H}| < \infty$

Then

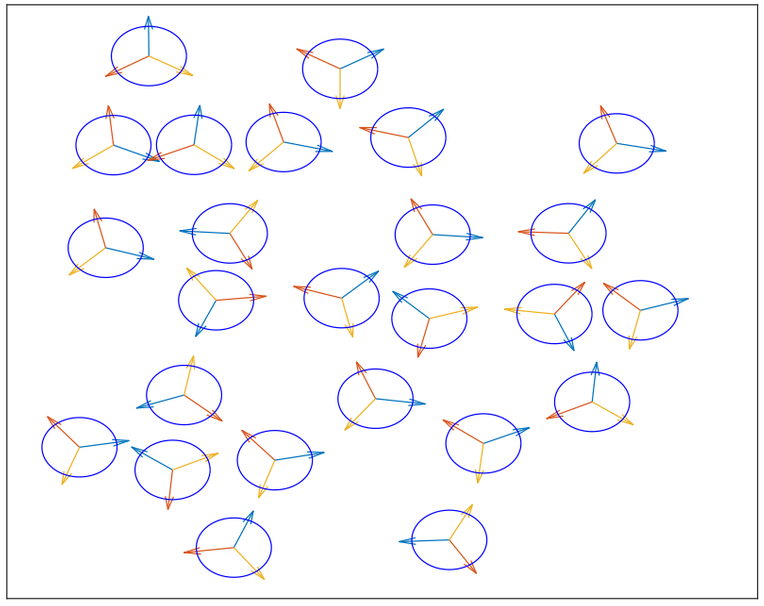
$$\mathrm{k_B T} = \frac{\mathrm{Av}_\beta(\boldsymbol{G}\cdot\nabla H)}{\mathrm{Av}_\beta(\nabla\cdot\boldsymbol{G})}.$$

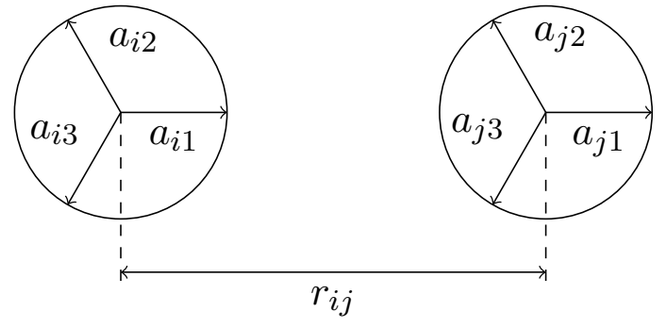
[Leimkuhler, Matthews '15]

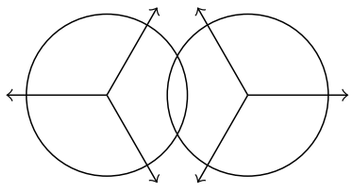
The Mercedes Benz potential

- Model for water like particles

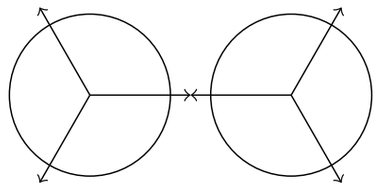
- Each particle has three arms originating from its center of mass. Thus particles are **anisotropic rigid bodies**.







Double Bond



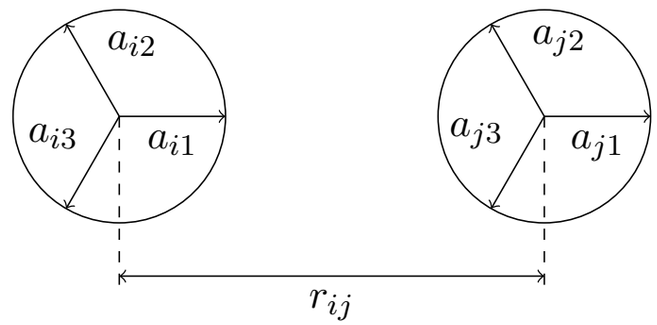
Single Bond

Tutorial sheet ‘Mercedes Benz potential’ by Anton Martinsson

The Mercedes Benz potential

- Model for water like particles

- Each particle has three arms originating from its center of mass. Thus particles are **anisotropic rigid bodies**.



- MB pair potential:

$$V(x_i, x_j, Q_i, Q_j) = 4\varepsilon_{LJ}\left(\left(\frac{\sigma_{LJ}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{LJ}}{r_{ij}}\right)^{6}\right)$$
$$+ \varepsilon_{HB} G(r_{ij} - r_{HB}) \sum_{k,l=1}^{3} G(\left(Q_i^T a_{ik}\right)^T u_{ij} - 1) G(\left(Q_i^T a_{ik}\right)^T u_{ij} + 1)$$
$$= V_{LJ}(x_i, x_j) + V_{HB}(x_i, x_j, Q_i, Q_j).$$

$$G(x) = \exp\left(-\frac{x^2}{2\sigma_{HB}}\right)$$

center of mass

rotation matrix

Rigid bodies

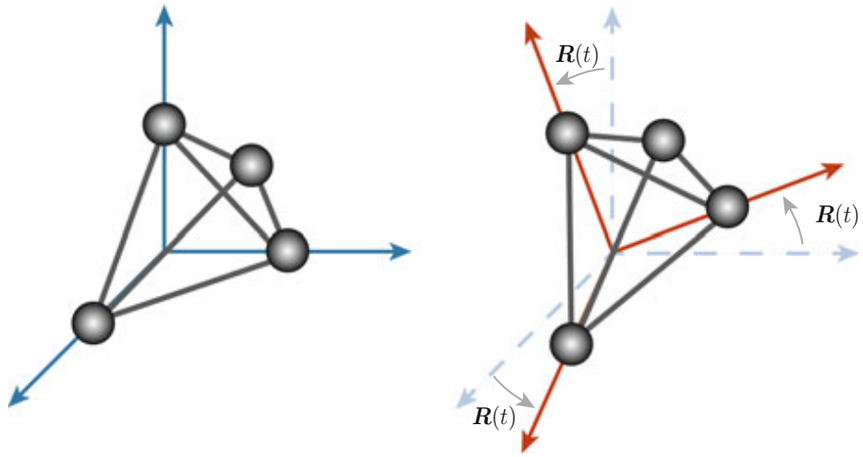


Fig. 4.7 A rigid rotation can be viewed as premultiplication by an orthogonal matrix $\boldsymbol{\Theta}$. In this way the orientation of the position vectors of points in the rigid body at any time t are described by a trajectory in the space of 3×3 orthogonal matrices, $\boldsymbol{\Theta}(t), t \in \mathbb{R}$

Two alternatives for representing rotational motion:

1. The rotation matrix $\boldsymbol{\Theta}(t)$ describing the rotation of each particle in global reference frame is the dynamical quantity, and we solve for $\boldsymbol{\Theta}(t)$. Need to enforce orthogonality constraints.

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{q}_{\mathrm{cm}} = \boldsymbol{p}_{\mathrm{cm}}/M, \quad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Theta} = \boldsymbol{\Pi}\boldsymbol{R}^{-1},$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p}_{\mathrm{cm}} = -\nabla_{\boldsymbol{q}_{\mathrm{cm}}} U, \quad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Pi} = -\nabla_{\boldsymbol{\Theta}} U - \boldsymbol{\Theta}\boldsymbol{\Lambda},$$
$$\boldsymbol{I} = \boldsymbol{\Theta}^T\boldsymbol{\Theta}.$$

2. Use the orthogonality to perform reduction to angular momentum representation $\boldsymbol{\pi}$ with respect to body frame of reference.

The DLM rigid body integration algorithm

- Idea: Use splitting strategy
    - Solve for translational motion of center of masses,
    - Integrate torques due to rotational interactions
    - Solve Euler equations, recover rotation matrix

The DLM rigid body integration algorithm

1. "Kick": update the momenta and angular momentum vectors with known forces and torques for a half step:

$$\boldsymbol{p}^k := \boldsymbol{p}^k + \frac{h}{2}\boldsymbol{F}^k, \qquad \boldsymbol{\pi}^k := \boldsymbol{\pi}^k + \frac{h}{2}\boldsymbol{\tau}^k.$$

2. "Drift": step forward a whole step in positions

$$\boldsymbol{q}^k := \boldsymbol{q}^k + h\boldsymbol{p}^k.$$

3. "Spin": update the rotational state of the kth rigid body by the sequence of steps

$$\begin{aligned}
&\boldsymbol{\Theta} := \boldsymbol{\Theta}^x\left(\tfrac{h}{2}\pi_1^k/I_1\right);\ \boldsymbol{\pi}^k := \boldsymbol{\Theta}\boldsymbol{\pi}^k;\ \boldsymbol{\Theta}^k := \boldsymbol{\Theta}^k\boldsymbol{\Theta}^T\\
&\boldsymbol{\Theta} := \boldsymbol{\Theta}^y\left(\tfrac{h}{2}\pi_2^k/I_2\right);\ \boldsymbol{\pi}^k := \boldsymbol{\Theta}\boldsymbol{\pi}^k;\ \boldsymbol{\Theta}^k := \boldsymbol{\Theta}^k\boldsymbol{\Theta}^T\\
&\boldsymbol{\Theta} := \boldsymbol{\Theta}^z\left(h\pi_3^k/I_3\right);\ \boldsymbol{\pi}^k := \boldsymbol{\Theta}\boldsymbol{\pi}^k;\ \boldsymbol{\Theta}^k := \boldsymbol{\Theta}^k\boldsymbol{\Theta}^T\\
&\boldsymbol{\Theta} := \boldsymbol{\Theta}^y\left(\tfrac{h}{2}\pi_2^k/I_2\right);\ \boldsymbol{\pi}^k := \boldsymbol{\Theta}\boldsymbol{\pi}^k;\ \boldsymbol{\Theta}^k := \boldsymbol{\Theta}^k\boldsymbol{\Theta}^T\\
&\boldsymbol{\Theta} := \boldsymbol{\Theta}^x\left(\tfrac{h}{2}\pi_1^k/I_1\right);\ \boldsymbol{\pi}^k := \boldsymbol{\Theta}\boldsymbol{\pi}^k;\ \boldsymbol{\Theta}^k := \boldsymbol{\Theta}^k\boldsymbol{\Theta}^T
\end{aligned}$$

The notation $\boldsymbol{\Theta}^x(\phi)$ refers to a rotation around the x-axis by an angle ϕ, that is

$$\boldsymbol{\Theta}^x(\phi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & -\sin(\phi) \\ 0 & \sin(\phi) & \cos(\phi) \end{bmatrix},$$

with corresponding formulae for $\boldsymbol{\Theta}^y$ and $\boldsymbol{\Theta}^z$.

4. "Kick": update the momenta and angular momentum vectors (as in Step 1) with a half step using new forces $\boldsymbol{F}^k$ and torques $\boldsymbol{\tau}^k$ evaluated at the current $\boldsymbol{q}$, $\boldsymbol{\Theta}$.

Forces

$$\boldsymbol{F}^k = -\frac{\partial U}{\partial \boldsymbol{q}^k},$$

Torques

$$\boldsymbol{\tau}^k = -\mathrm{rot}\left(\left[\boldsymbol{\Theta}^k\right]^T \frac{\partial U}{\partial \boldsymbol{\Theta}^k}\right).$$

$$\mathrm{rot}(\boldsymbol{A}) = \mathrm{skew}^{-1}(\boldsymbol{A} - \boldsymbol{A}^T).$$

$$\mathrm{skew}(\boldsymbol{\omega}) \equiv \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix}$$

Steps to perform the tutorial

- Read Mercedes Benz tutorial sheet
- Take the BAOAB integrator in MIST as a starting point
- Find a way to store the angular momentum of each particle in the system (hint: there is only one rotation in 2D)
- Modify the BAOAB integrator by incorporating the DLM algorithm
- Set up the force evaluations by calculating the derivatives of the MB potential

Thank you for your attention