From point particles to rigid bodies in MCell

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Definition of the problem

To capture the behavior of particles with spatial extent based on their rigid body features, dynamics, diffusion and hydrodynamic interactions

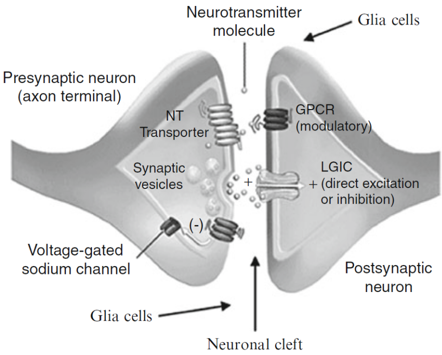

Fig: Schuss Z., Brownian Dynamics at Boundaries and Interfaces, Springer, 2013.

Our proposal

- Coarse-graining the structure of molecules as a series of subunits connected by linkers.
- Each subunit will contain a rigid cluster of C^{α} atoms, possibly determined based on SPECTRUS algorithm[a].
- If the molecule is small enough, it may be modeled either as a single ellipsoid ((a)symmetric top) with minimum volume, or as connected spheres.
- Otherwise, it can be represented by multiple rigid bodies, connected by linkers (e.g. springs).

[a] Ponzoni et al., Structure 2015.

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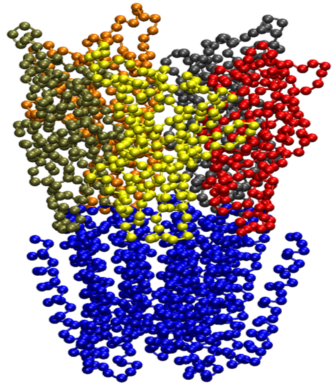
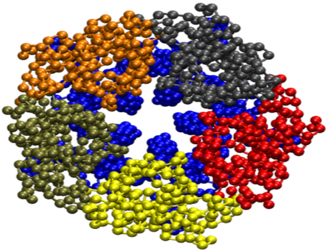
Example: GLIC – ligand-gated ion channel

6-domain dynamical decomposition by SPECTRUS + RTB[1](Rotation Translation Blocks)





[1] Tama et al., Proteins 2000.

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Stochastic Differential Equations (SDEs)

- A Wiener type stochastic differential equation is given by

$$dX_t = \underbrace{a(X_t, t)dt}_{deterministic} + \underbrace{b(X_t, t)dW_t}_{stochastic},$$

  where X_t, W_t are a stochastic variable and a Wiener process, respectively.

- A Wiener process can be defined as a limit of an unbiased random walk with independent Gaussian increments such that

$$W_{t+s} - W_t \approx \mathcal{N}(0, s).$$

Stochastic Differential Equations (SDEs)

- Non-differentiable with probability 1, albeit continuous.

$$\begin{aligned} \langle W_t^i W_s^j \rangle &= \sigma_j^2 \delta_{ij} \min(t, s)\,, \\ \langle dW_t^i, dW_s^j \rangle &\sim \delta_{ij} \delta(t - s)\,, \\ dt^2 &= dt\, dW_t = 0\,, \\ (dW_t)^2 &= dt \Leftrightarrow dW_t \sim \sqrt{\Delta t}\,. \end{aligned}$$

- A formal solution of a SDE is given by

$$X_t = X_0 + \int_0^t ds\, a(X_s, s) + \int_0^t dW_s\, b(X_s, s)\,,$$

where the last integral is taken in the Itô sense.

- Leibniz's product rule for stochastic differential:

$$d(X_t\, Y_t) = Y_t dX_t + X_t dY_t + dX_t dY_t\,.$$

- Ito Lemma:

$$dF_t = f'(X_t)dX_t + \frac{1}{2}f''(X_t)(dX_t)^2\,,$$

where $F_t = f(X_t)$.

- Integration by parts:

$$\int_a^b dW_t f(t) g'(W_t) = f(t)g(W_t)\big|_a^b - \int dt f'(t) g(W_t) - \frac{1}{2}\int_a^b dt f(t_g''(W_t)\,.$$

Ornstein-Uhlenbeck process

One dimensional diffusion of a point particle

- One-dimensional Langevin equation is an Ornstein-Uhlenbeck process:

$$dx_t = v_t dt \,,$$
$$m dv_t = -\xi v_t dt + b dW_t \,,$$

  where m and ξ are the mass and the friction constant, respectively.
- Let's define $\tau = m/\xi$,

$$v_t = v_0 e^{-t/\tau} + \frac{b}{m}\int_0^t dW_s e^{-(t-s)/\tau} \,.$$

- Equipartion theorem allows us to relate the long-time diffusion process to its average energy over as ensemble as a thermodynamic limit.

$$\langle v_t^2 \rangle_{eq} = \frac{k_B T}{m} \Rightarrow b^2 = 2\xi k_B T \,.$$

Ornstein-Uhlenbeck process

- Similarly for the x_t process:

$$x_t = x_0 + v_0\tau\left(1 - e^{-t/\tau}\right) + \frac{\tau b}{m}\int_0^t dW_s\left[1 - e^{-(t-s)/\tau}\right] .$$

- Let's look at the mean square displacement:

$$\langle (x_t - x_0)^2\rangle_{eq} = \frac{2\tau k_B T}{m}\left[t - \tau(1 - e^{-t/\tau})\right] ,$$

$$\lim_{t\to 0}\langle (x_t - x_0)^2\rangle_{eq} = \frac{k_B T}{m^2}t^2 ,$$

$$\lim_{t\to \infty}\langle (x_t - x_0)^2\rangle_{eq} = \frac{2k_B T}{\xi}t = 2Dt ,$$

where D is the diffusion constant.(Fluctuation-dissipation theorem[2]).

[2] Kubo, Rep. Prog. Phys. 1966.

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- Diffusion D and friction ζ tensors of a 3-dimensional rigid body[3]:

$$D = \begin{pmatrix} {}^{tt}D_{3\times3} & {}^{tr}D^T_{3\times3} \\ {}^{rt}D_{3\times3} & {}^{rr}D_{3\times3} \end{pmatrix}_{6\times6} = \frac{k_B T}{\mu}\xi^{-1},$$

  μ being the viscosity of the fluid.
- The coupling term ${}^{tr}D$ is symmetric only at center of diffusion, which is unique for a body.
- It is zero at the center of hydrodynamic stress if such a point exist.
- They do not need to coincide with the center of mass.

[3] Brener, J. Coll. Inter. Sci. 1967.

- For spherically isotropic particles (spheres, tetrahedra, cubes, octahedra, dodecahedra and icosahedra) ${}^{tr}D = 0$ far away a boundary.
- Even for a sphere near a wall, ${}^{tr}D \neq 0$!
- Triaxial ellipsoids possess three mutually orthogonal planes of reflection symmetry so that

$$ {}^{tr}D = 0 \,. $$

- **Caveat:** A general ellipsoid cannot always as a model for the rotational features of arbitrarily shaped rigid molecules due to Wegener[4].

[4] Wegener et al., PNAS 1979.

Diffusion properties of rigid bodies

Example: Diffusion tensor of an ellipsoid

Diffusion constants of an ellipsoid[5], defined by $\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \frac{x_3^2}{a_3^2} = 1$:

$$ {}^{\mathbf{tt}}\mathbf{D} = \frac{k_B T}{16\pi\mu} \left[\mathbf{e_1 e_1}(\chi + a_1^2\alpha_1) + \mathbf{e_2 e_2}(\chi + a_2^2\alpha_2) + \mathbf{e_3 e_3}(\chi + a_3^2\alpha_3) \right] , $$

$$ {}^{\mathbf{rr}}\mathbf{D} = \frac{3k_B T}{16\pi\mu} \left(\mathbf{e_1 e_1} \frac{a_2^2\alpha_2 + a_3^2\alpha_3}{a_2^2 + a_3^2} + \mathbf{e_2 e_2} \frac{a_3^2\alpha_3 + a_1^2\alpha_1}{a_3^2 + a_1^2} + \mathbf{e_3 e_3} \frac{a_1^2\alpha_1 + a_2^2\alpha_2}{a_1^2 + a_2^2} \right) , $$

where e_β are unit vectors parallel to the principal axes of the ellipsoid, and

$$ \alpha_\beta = \int_0^\infty \frac{d\lambda}{(a_\beta^2 + \lambda)\Delta(\lambda)} , \qquad (\beta = 1, 2, 3) , $$

$$ \chi = \int_0^\infty \frac{d\lambda}{\Delta(\lambda)} , $$

$$ \Delta(\lambda) = \left[(a_1^2 + \lambda)(a_2^2 + \lambda)(a_3^2 + \lambda) \right]^{1/2} . $$

[5] Brener, J. Coll. Inter. Sci. 1967.

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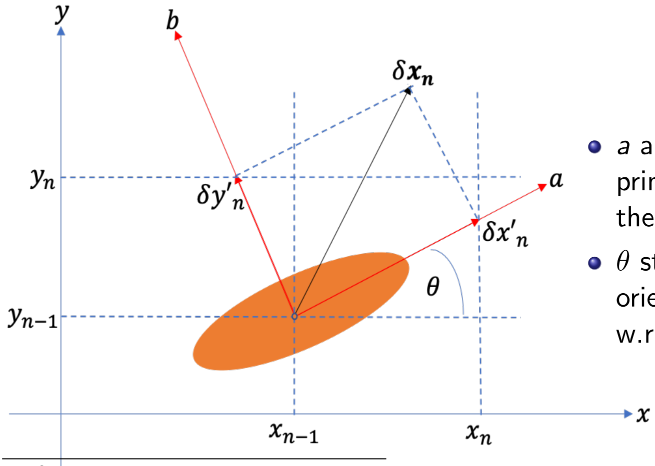
Uniaxial ellipsoids under strong quasi-2d confinement (Brownian case)[6]

- (x, y) and (x', y') are the lab and body frames coords., respectively.



- a and b denote the principal directions of the ellipse.
- θ stands for the orientation of the ellipse w.r.t. the inertial frame.

[6] Y. Han et al., Science 314 (2006) 626.

Uniaxial ellipsoids under strong quasi-2d confinement (Brownian case)

- Diffusion tensor in the body frame is diagonal:

$$D' = \begin{pmatrix} D_{x'} & 0 & 0 \\ 0 & D_{y'} & 0 \\ 0 & 0 & D_\theta \end{pmatrix} .$$

- Equations of motion in the lab frame:

$$\begin{aligned} dx &= \cos\theta\sqrt{2D_{x'}}dW^1 - \sin\theta\sqrt{2D_{y'}}dW^2 , \\ dy &= \sin\theta\sqrt{2D_{x'}}dW^1 + \cos\theta\sqrt{2D_{y'}}dW^2 , \\ d\theta &= \sqrt{2D_\theta}dW^3 . \end{aligned}$$

- Diffusion tensor is no longer diagonal in the lab frame.

Uniaxial ellipsoids under strong quasi-2d confinement (Brownian case)

- The time dependent diffusion coefficients for fixed θ_0 in the lab frame is given by

$$D_{xx} = \bar{D} + \Delta D \cos 2\theta_0 \frac{1 - e^{-4D_\theta t}}{8 D_\theta t},$$

$$D_{yy} = \bar{D} - \Delta D \cos 2\theta_0 \frac{1 - e^{-4D_\theta t}}{8 D_\theta t},$$

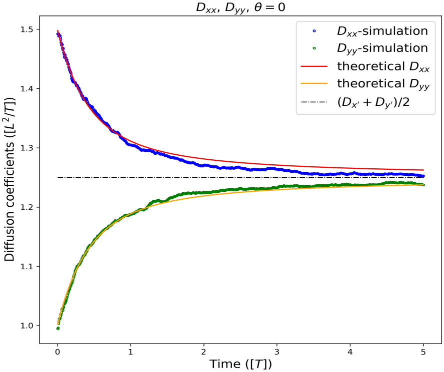
$$D_{xy} = \Delta D \sin 2\theta_0 \frac{1 - e^{-4D_\theta t}}{8 D_\theta t},$$

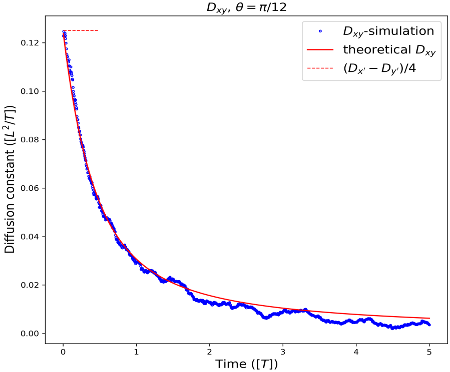
where $\bar{D} = (D_{x'} + D_{y'})/2$ and $\Delta D = D_{x'} - D_{y'}$.

Uniaxial ellipsoids under strong quasi-2d confinement (Brownian case)

The vertical axes are the time evolution of diffusion tensor in the lab frame.

$$D_{x'} = 1.5\,, \quad D_{y'} = 1.0\,, \quad D_\theta = 1.0\,, \quad n_{step} = 10^3\,, \quad n_{sim} = 10^5$$





$$\bar{D}_{theo} = 1.25\,, \quad \bar{D}_{sim} = 1.26$$

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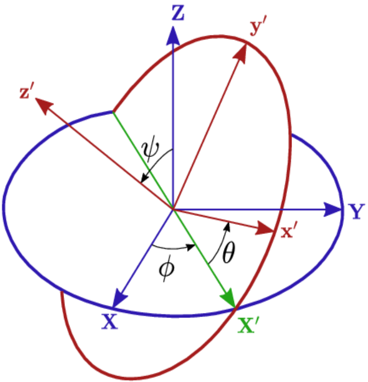
Rigid body dynamics

Euler angles in ZXZ convention



- $\mathbf{X}$ and $\mathbf{x}'$ are the space-fixed and body-fixed frames, respectively.
- The rotation matrix transforming from the space-fixed to body-fixed frame is given by:

$$\mathbf{x}' = \mathbf{A}\mathbf{X}\,.$$

$$A = \begin{pmatrix} c\psi c\phi - c\theta s\phi s\psi & c\psi s\phi + c\theta c\phi s\psi & s\psi s\theta \\ -s\psi c\phi - c\theta s\phi c\psi & -s\psi s\phi + c\theta c\phi c\psi & c\psi s\theta \\ s\theta s\phi & -s\theta c\phi & c\theta \end{pmatrix},$$

where c and s stand for cos and sin, respectively.

- Equations of motion:

$$I_1\dot{\omega}_1 - (I_2 - I_3)\omega_2\omega_3 = \tau_1\,,$$
$$I_2\dot{\omega}_2 - (I_3 - I_1)\omega_3\omega_1 = \tau_2\,,$$
$$I_3\dot{\omega}_3 - (I_1 - I_2)\omega_1\omega_2 = \tau_3\,,$$

where ω_α is the angular velocity about the principal axis α, I_α is the moment of inertia, and τ_α is the external torque.

- The moment of inertia:
$I_{\alpha\beta} = \sum_i m_i \left(r_i^2 \delta_{\alpha\beta} - r_{i\alpha} r_{i\beta} \right)\,, \quad i = 1, \ldots, N, \quad \alpha, \beta = 1, 2, 3\,.$
- Euler angles:

$$\dot{\theta} = \omega_1 \cos\psi - \omega_2 \cos\psi\,,$$
$$\dot{\psi} = (\omega_1 \sin\psi + \omega_2 \cos\psi) / \sin\theta\,,$$
$$\dot{\phi} = \omega_3 - \cot\theta(\omega_1 \sin\psi + \omega_2 \cos\psi)\,.$$

Rigid body dynamics

Euler's equations

- Euler's equations are singular for small θ values, not ideal for numerical simulations.
- If two rotations become coplanar, then we lose one rotational degree of freedom, known as Gimbal lock.
- Rigid body motion is an example of a constrained dynamical system. Therefore, appropriate constraint schemes should be implemented for numerical simulations (SHAKE, RATTLE).
- Instead, we can use quaternions not only to represent rotations but also to describe the rigid body dynamics.

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Rigid body dynamics

Quaternions

- Quaternions are an (algebraic) extension of complex numbers.

$$q = q_0 + iq_1 + jq_2 + kq_3\,, \quad -1 = i^2 = j^2 = k^2 = ijk\,,$$
$$q^* = q_0 - iq_1 - jq_2 - kq_3\,, \quad \|q\|^2 = q \star q^*\,, \quad q^{-1} = \frac{q^*}{\|q\|^2}\,.$$

- They have a noncommutative multiplication:

$$q \star p = (q_0 p_0 - \mathbf{q} \cdot \mathbf{p}, q_0 \mathbf{p} + p_0 \mathbf{q} + \mathbf{q} \times \mathbf{p})\,.$$

- The multiplication of unit quaternions can preserve their unit length.
- Unit quaternions represent rotations in $\mathbb{R}^3$ and are nonsingular.

$$q = \cos\frac{\|\mathbf{\Phi}\|}{2} + \frac{\mathbf{\Phi}}{\|\mathbf{\Phi}\|}\sin\frac{\|\mathbf{\Phi}\|}{2}\,.$$

- Pure quaternions represent vectors: $v = (0, v_x, v_y, v_z)$.
- Rotation of a vector via a quaternion: $v' = q \star v \star q^*$.

- Map between Euler angles in ZXZ convention and quaternions

$$q_0 = \cos\frac{\theta}{2}\cos\frac{\phi+\psi}{2}, \quad q_1 = \sin\frac{\theta}{2} cos \frac{\phi-\psi}{2},$$
$$q_2 = \sin\frac{\theta}{2}\sin\frac{\phi-\psi}{2}, \quad q_3 + \cos\frac{\theta}{2}\sin\frac{\phi+\psi}{2}.$$

- Rotation matrix in terms of a quaternion is given by

$$A(q) = 2\begin{pmatrix} q_0^2+q_1^2-\frac{1}{2} & q_1q_2+q_0q_3 & q_1q_3-q_0q_2 \\ q_1q_2-q_0q_3 & q_0^2+q_2^2-\frac{1}{2} & q_2q_3+q_0q_1 \\ q_1q_3+q_0q_2 & q_2q_3-q_0q_1 & q_0^2+q_3^2-\frac{1}{2} \end{pmatrix}.$$

Rigid body dynamics

Rigid body Hamiltonian in terms of quaternions[7,8]

- The Hamiltonian of n rigid bodies with center of mass coordinates $r = (r^{1T}, \ldots, r^{n^T})^T \in \mathbb{R}^{3n}$, and orientations given by unit quaternions $q = (q^{1T}, \ldots, q^{nT})^T, q^i = (q_0^i, q_1^i, q_2^i, q_3^i) \in \mathbb{S}^3$.

$$H(r,p,q,\pi) = \sum_{i=1}^{n} \frac{p^{iT} p^i}{2m_i} + \sum_{i=1}^{n} \sum_{l=1}^{3} \frac{1}{I_l^i} V_l(q^i, \pi^i) + U(\mathbf{r}, \mathbf{q}),$$

  where p and π are, respectively, the center of mass momenta conjugate to r and the angular momenta conjugate to q such that $q^{iT}\pi^i = 0$, i.e. $\pi^i \in T^*_{q^i}\mathbb{S}^3$.

- The rotational kinetic energy is given by

$$V_l(q,\pi) = \frac{1}{8}[\pi^T S_l q]^2, \quad \frac{V_l(q^i,\pi^i)}{I_l^i} = \frac{1}{2} I_l^i \omega_l^{i^2},$$

where S_l are three 4×4 constant projection matrices.

[7] Miller et al. J. Chem. Phys. 2002

[8] Davidchack et al. J. Chem. Phys. 2017

Rigid body dynamics

Symplectic integrator

- Hamilton's equations of motions for (r, p):

$$\begin{pmatrix} \dot{r} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{pmatrix}$$

- The matrix in the middle above Ω roles as a metric tensor of the phase space. Any canonical transformations leaving this metric invariant preserves the volume of the phase space (Liouville's theorem):

$$J \Omega J^T = \Omega \, ,$$

  where J is the Jacobian of the canonical transformations. If $\det J = 1$, then it is called symplectic.

- Symplectic integrators enjoy similar features, especially when the Hamiltonian is separable.

- Each step of the numerical integration in this picture corresponds to an action of an evolution operator, known as Liouville operator.
- Separability of the Hamiltonian allows us to split the Liouville operator into pieces.
- Harmonic oscillator as an example: $H(x,p) = \frac{p^2}{2} + \frac{x^2}{2}$.
- Corresponding operators: $i\mathcal{L}_k = \frac{\partial H_k}{\partial p}\frac{\partial}{\partial x} - \frac{\partial H_k}{\partial x}\frac{\partial}{\partial p}$.
- The full operator: $e^{i\mathcal{L}t} = \prod_{k=1}^{N}\left[e^{i\mathcal{L}_1 \Delta t/2} e^{i\mathcal{L}_2 \Delta t} e^{i\mathcal{L}_1 \Delta t/2}\right] + \mathcal{O}(t\Delta t^2)$.
- The conserved Hamiltonian with $\alpha = 1 - (\Delta t/2)^2$:
  $\tilde{H}(x,p,\Delta t) = \left[\frac{p^2}{2\alpha^{1/2}} + \frac{x^2\alpha^{1/2}}{2}\right]\frac{\arccos\left(1 - \frac{\Delta t^2}{2}\right)}{|\Delta t|}$.
- The integrator has closed orbits for $\Delta t/2 \ll 1$,
  $\lim_{\Delta t \to 0}\tilde{H}(x,p,\Delta t) = H(x,p)$.

- Similar technique can be applied to rotational motion of a rigid body. The corresponding map $\Psi_{t,l}(q,\pi):(q,\pi)\mapsto(Q,\Pi)$

$$e^{i\mathcal{L}_l\Delta t}q = \cos(\zeta_l\Delta t)q + \sin(\zeta_l\Delta t)S_l q\,,$$
$$e^{i\mathcal{L}_l\Delta t}\pi = \cos(\zeta_l\Delta t)\pi + \sin(\zeta_l\Delta t)S_l \pi\,.$$

  where $\zeta_l = \frac{1}{4I_l}\pi^T S_l q$.

- The composite map for the whole integration at each step consist of

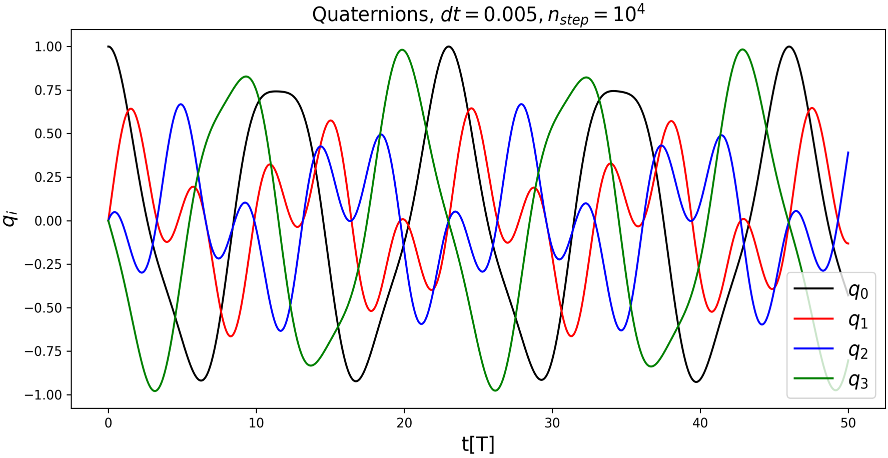
$$\Psi_t^- = \Psi_{t,3}\circ\Psi_{t,2}\circ\Psi_{t,1}\,,$$
$$\Psi_t^+ = \Psi_{t,1}\circ\Psi_{t,2}\circ\Psi_{t,3}\,,$$

  where $\circ$ denotes function composition, i.e. $(g\circ f) = g(f(x))$.

Rigid body dynamics

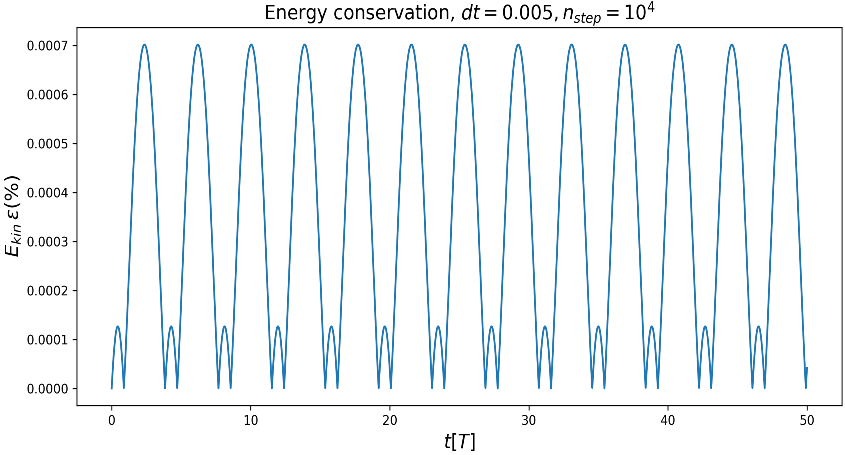
Simulation of a prolate spheroid (ellipsoid of revolution / symmetric top)

$I_x = I_y < I_z$



Rigid body dynamics

Simulation of a free prolate spheroid (ellipsoid of revolution / symmetric top)



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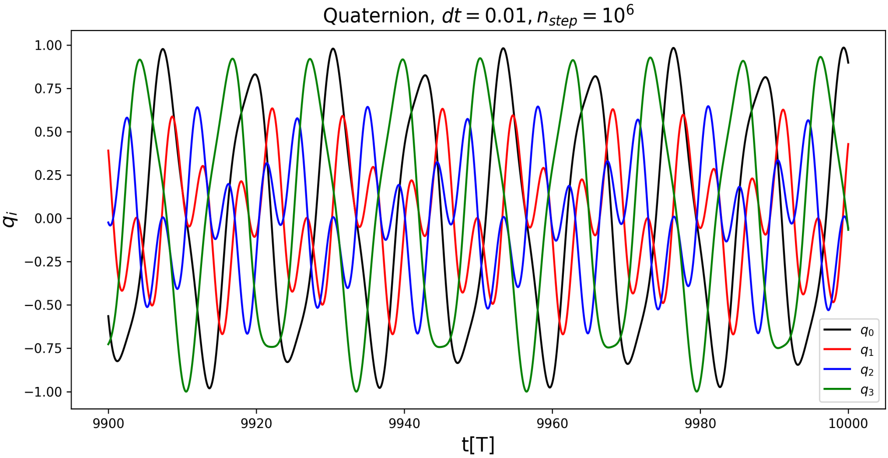

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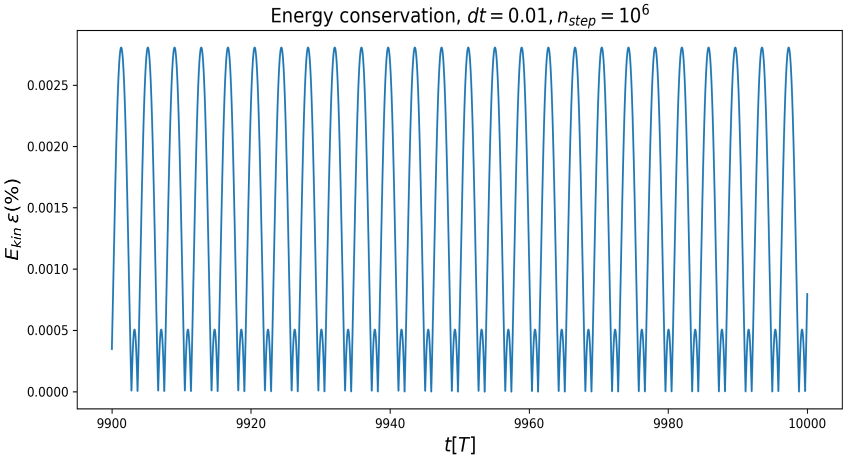
Simulation of a prolate spheroid (ellipsoid of revolution / symmetric top)



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Rigid body dynamics with diffusion & hydrodynamic interactions[9]

The Langevin type equations in the form of Itô of rigid bodies under the influence of conservative forces, hydrodynamic interactions, and thermal noise is given by

$$
\begin{aligned}
dR^i &= \frac{P^i}{m^i}dt, \quad R^i(0) = r^i\,, \quad P^i(0) = p^i\,, \quad i = 1, \ldots, n\,, \\
dP^i &= f^i(\mathbf{R}, \mathbf{Q})dt - \sum_{j=1}^{n} {}^{tt}\xi^{(i,j)}(\mathbf{R}, \mathbf{Q})\frac{P^j}{m^j}dt \\
&\quad - \frac{1}{2}\sum_{j=1}^{n} {}^{tr}\xi^{(i,j)}(\mathbf{R}, \mathbf{Q})A^T(Q^j)\hat{D}^j\hat{S}^T(Q^j)\Pi^j dt \\
&\quad + \sum_{j=1}^{n} {}^{tt}b^{(i,j)}(\mathbf{R}, \mathbf{Q})dw^j(t) + \sum_{j=1}^{n} {}^{tr}b^{(i,j)}(\mathbf{R}, \mathbf{Q})dW^j(t)\,,
\end{aligned}
$$

[9] Davidchack et al. J. Chem. Phys. 2017.

Rigid body dynamics with diffusion & hydrodynamic interactions

$$
\begin{aligned}
dQ^i &= \frac{1}{4}\hat{S}(Q^i)\hat{D}^i\hat{S}^T(Q^i)\Pi^i dt\,, \quad Q^i(0) = q^i, \quad |q^i| = 1\,, \quad i = 1, \dots, n\,, \\
d\Pi^i &= \frac{1}{4}\hat{S}(\Pi^i)\hat{D}^i\hat{S}^T(Q^i)\Pi^i dt + F(\mathbf{R},\mathbf{Q})dt \\
&\quad - \sum_{j=1}^{n}\check{S}(Q^i)^{rr}\xi^{(i,j)}(\mathbf{R},\mathbf{Q})A^T(Q^j)\hat{D}^j\hat{S}^T(Q^j)\Pi^j dt \\
&\quad - 2\sum_{j=1}^{n}\check{S}(Q^i)^{rt}\xi^{(i,j)}(\mathbf{R},\mathbf{Q})\frac{P^j}{m^j}dt \\
&\quad + 2\sum_{j=1}^{n}\check{S}(Q^i)^{rr}b^{(i,j)}(\mathbf{R},\mathbf{Q})dW^j(t) + 2\sum_{j=1}^{n}\check{S}(Q^i)^{tr}b^{(i,j)}(\mathbf{R},\mathbf{Q})dw^j(t)
\end{aligned}
$$

$$
\Pi^i(0) = \pi^i\,, \quad {q^i}^T\pi^i = 0, \quad i = 1, \dots, n\,.
$$

Rigid body dynamics with diffusion & hydrodynamic interactions

If the solution of these equation $X(t) = (\mathbf{R}^T(t), \mathbf{P}^T(t), \mathbf{Q}^T(t), \mathbf{\Pi}^T(t))$ is an ergodic process, then the invariant measure of $X(t)$ is Gibbsian with the density

$$\rho(r, p, q, \pi) \propto \exp(-\frac{1}{k_B T} H(r, p, q, \pi)),$$

if the following condition holds

$$b(r, q) b^T(r, q) = 2 k_B T \xi(r, q).$$

Rigid body dynamics with diffusion & hydrodynamic interactions

The numerical integrator for this set of equations combines the deterministic Hamiltonian system with Ornstein-Uhlenbeck-type and hydrodynamic interactions. Stochastic part can be converted into

$$dY = -\tilde{\xi}(r,q)Ydt + \tilde{b}(r,q)d\tilde{W} \, ,$$

where $Y = (\tilde{P}^T, \tilde{\Pi}^T)^T$ and $\tilde{W} = (w^T(t), W^T(t))^T$.

Rigid body dynamics with diffusion & hydrodynamic interactions

The solution is given by

$$Y(t) = e^{-\tilde{\xi}(r,q)t} Y(0) + \sigma(r,q,t)\chi(t)\,,$$

where χ is an $6n$-dimensional vector consisting of independent Gaussian random variables with zero mean and unit variance such that

$$\sigma(t,r,q)\sigma^T(t,r,q) = C(t,r,q)\,,$$

Here $C(t,r,q)$ is given by

$$C(t,r,q) = \frac{1}{\beta} G_1(q) K^{-1}(q) \left[\mathbf{1}_{6n} - e^{-2K(q)\xi(r,q)t} \right] G_1^T(q)\,,$$

where $G_1(q)$ and $K(q)$ are complicated matrices of the quaternion q.

Rigid body dynamics with diffusion & hydrodynamic interactions

Features of the geometric integrator

- In each time step, it performs half step of the Verlet-type integrator for Hamiltonian dynamics, followed by a full step of the Ornstein-Uhlenbeck process, and finally a second half step of the Verlet-type integrator.
- It is quasi-symplectic.
- It has a natural over-damped limit.
- It automatically preserves $|Q_k^i| = 1$ for all $t_k \geq 0$ since it is updated by an exact rotation at each step.
- It preserves $Q_k^{iT}\Pi = 0$ for all $t_k \geq 0$ via exact rotation.
- It requires a single computation of forces and the friction matrix per step.
- It is of weak order 2, i.e. $|\mathbb{E}f(\tilde{Y}) - \mathbb{E}f(\tilde{Y}_{\Delta t})| \leq C(\Delta t)^2$.

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Roadmap

- Implementation of the full integrator
- Simulations on unbounded domains (neglecting boundary effect) without hydrodynamical interactions
- Collision detection
- Spherical bodies with hydrodynamical interactions
- ...

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