Temporal integrators for Langevin equations arising in Fluctuating Hydrodynamics

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Light-Activated Diffusion/Osmophoresis

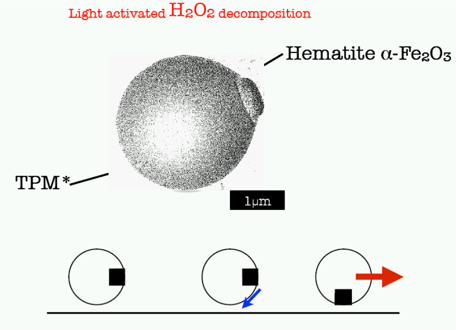
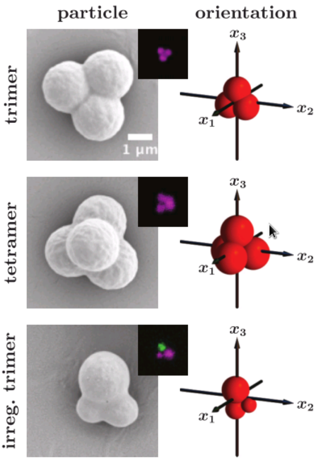


Figure: From Jeremie Palacci, Paul Chaikin lab (NYU Physics) [1]

Non-Spherical Colloids near Boundaries



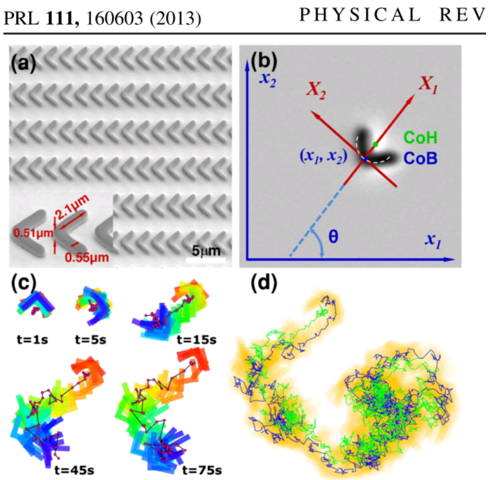


Figure: (Left) Cross-linked spheres; Kraft et al. [2]. (Right) Lithographed boomerangs; Chakrabarty et al. [3].

Immersed Spherical Particles

- For simplicity, we first consider the dynamics of several immersed spherical particles with positions given by $\boldsymbol{x} = \{\boldsymbol{x}_i\}$.
- For now we will ignore the orientation of the particles.
- We assume that inertia evolves much faster than particle position, and consider the **overdamped** equations for particle motion.

Brownian Dynamics

- We write the overdamped Langevin equation for the Brownian dynamics of the particles.

$$\partial_t \boldsymbol{x} = -\boldsymbol{M}\partial_{\boldsymbol{x}} U(\boldsymbol{x}) + \sqrt{2k_B T}\boldsymbol{M}_{\frac{1}{2}}\boldsymbol{\mathcal{W}} + k_B T \partial_{\boldsymbol{x}} \cdot (\boldsymbol{M})$$

- $\boldsymbol{M}$ is the mobility operator, $\boldsymbol{M}_{\frac{1}{2}}\boldsymbol{M}^{\star}_{\frac{1}{2}} = \boldsymbol{M}$, U is the potential energy, $k_B T$ is the temperature, and $\boldsymbol{\mathcal{W}}$ is a vector of independent white noise.
- The thermal drift term $\partial_{\boldsymbol{x}} \cdot (\boldsymbol{M})$ can be written as $\sum_{j=1}^{N} \partial_{x_j} M_{ij}(\boldsymbol{x})$.
- These equations of motion are time reversible w.r.t the Gibbs Boltzmann distribution

$$\rho_{eq}(\boldsymbol{x}) = Z^{-1} \exp\left(-U(\boldsymbol{x})/k_B T\right)$$

Difficulties in Integration

- The mobility $\boldsymbol{M}$ includes all particle interaction and boundary effects. Constructing this operator is non trivial (Aleksandar Donev will talk more on this).
- Calculating just the application of $\boldsymbol{M}$ and $\boldsymbol{M}_{\frac{1}{2}}$ is an expensive process.
- More complicated objects such as $\partial_{\boldsymbol{x}} \cdot \boldsymbol{M}$ and $\boldsymbol{M}^{-1}$ may not be directly computable.
- This talk focuses on the thermal drift. Our goal is to develop schemes that use only only application of $\boldsymbol{M}$ and $\boldsymbol{M}_{\frac{1}{2}}$.

Fixman's Method

- A standard way to handle the themal drift is with Fixman's midpoint method

$$\begin{aligned} x^{n+\frac{1}{2}} =& x^n - \frac{\Delta t}{2} M^n \partial_x U(x^n) + \sqrt{\frac{k_B T \Delta t}{2}} M^n_{\frac{1}{2}} W^n \\ x^{n+1} =& x^n - \Delta t M^{n+\frac{1}{2}} \partial_x U(x^{n+\frac{1}{2}}) \\ &+ \sqrt{2 k_B T \Delta t} M^{n+\frac{1}{2}} \left(M^n_{\frac{1}{2}} \right)^{-1} W^n., \end{aligned}$$

  where W^n is a vector of independent $\mathcal{N}(0,1)$ variables.
- While this achieves the correct drift, it requires knowledge of $\left(M^n_{\frac{1}{2}} \right)^{-1} = M^{-1} M_{\frac{1}{2}}$, which we recall is not easy to obtain.

Random Finite Difference

- We can also generate the drift with $\left(\boldsymbol{M}(\boldsymbol{x}^n + \delta\widetilde{\boldsymbol{W}}) - \boldsymbol{M}^n\right)\widetilde{\boldsymbol{W}}/\delta$, where $\widetilde{\boldsymbol{W}}$ is a vector of independent $\mathcal{N}(0,1)$ variables.
- This leads to the Random Finite Difference (RFD) scheme

$$\begin{aligned}\boldsymbol{x}^{n+1} =& \boldsymbol{x}^n - \Delta t \boldsymbol{M}^n \partial_{\boldsymbol{x}} U + \sqrt{2k_B T \Delta t}\boldsymbol{M}^n_{\frac{1}{2}} \boldsymbol{W}^n \\ &+ \frac{k_B T}{\delta}\left(\boldsymbol{M}(\boldsymbol{x}^n + \delta\widetilde{\boldsymbol{W}}) - \boldsymbol{M}^n\right)\widetilde{\boldsymbol{W}}.\end{aligned}$$

- This scheme makes an error of order δ. Fixman takes $\delta \sim \Delta t$, but this is not neccessary.
- We need to apply $\boldsymbol{M}^n$, $\boldsymbol{M}^n_{\frac{1}{2}}$, and $\boldsymbol{M}\left(\boldsymbol{x}^n + \delta\widetilde{\boldsymbol{W}}\right)$, but *not* $\left(\boldsymbol{M}^n_{\frac{1}{2}}\right)^{-1}$.

Bodies with rotation

- We can extend our work to simulate bodies with **rotational DOFs** by formulating the appropriate Langevin equation and using a RFD approach to for temporal integration.
- For simplicity, first we consider a single body with only rotational degrees of freedom.
- Orientation is an element of SO(3) so we need to parameterize it: we use **normalized quaternion** (point on the unit 4-sphere)

$$\boldsymbol{\theta} \in \mathbb{R}^4, \quad \|\boldsymbol{\theta}\|_2 = \boldsymbol{\theta} \cdot \boldsymbol{\theta} = 1.$$

- This offers several advantages over several other common approaches, such as rotation angles, rotation matrices, and Euler angles[4].

Quaternions

- Successive rotations can be accumulated by **quaternion multiplication.**
- In three dimensions, there exists a 4×3 matrix $\boldsymbol{\Psi}(\boldsymbol{\theta})$ such that, given a conservative potential $U(\boldsymbol{\theta})$,

$$\dot{\boldsymbol{\theta}} = \boldsymbol{\Psi}\boldsymbol{\omega}, \quad \boldsymbol{\tau} = \boldsymbol{\Psi}^T \partial_{\boldsymbol{\theta}} U(\boldsymbol{\theta}).$$

  Here $\boldsymbol{\tau}$ is the torque applied to the body, and $\boldsymbol{\omega}$ is the angular velocity.
- One can also rotate a body by an oriented angle ϕ, denoted as

$$\boldsymbol{\theta}^{n+1} = \text{Rotate}\left(\boldsymbol{\theta}^n, \, \phi\right).$$

Equations for Rotation

- We assume now that we know the mobility tensor $\boldsymbol{M}_{\boldsymbol{\omega}\boldsymbol{\tau}}$,

$$\boldsymbol{\omega} = \boldsymbol{M}_{\boldsymbol{\omega}\boldsymbol{\tau}}\boldsymbol{\tau}.$$

- Given $\boldsymbol{M}_{\boldsymbol{\omega}\boldsymbol{\tau}}$ and a potential $U(\boldsymbol{\theta})$, the Langevin Equation for orientation is

$$\partial_t \boldsymbol{\theta} = -\left(\boldsymbol{\Psi}\boldsymbol{M}_{\boldsymbol{\omega}\boldsymbol{\tau}}\boldsymbol{\Psi}^T\right)\partial_{\boldsymbol{\theta}} U + \sqrt{2k_B T}\boldsymbol{\Psi}\boldsymbol{M}^{\frac{1}{2}}_{\boldsymbol{\omega}\boldsymbol{\tau}}\boldsymbol{\mathcal{W}} + k_B T \partial_{\boldsymbol{\theta}} \cdot \left(\boldsymbol{\Psi}\boldsymbol{M}_{\boldsymbol{\omega}\boldsymbol{\tau}}\boldsymbol{\Psi}^T\right).$$

- This equation preserves the unit norm constraint and is time reversible w.r.t. the Gibbs Boltzmann distribution

$$P_{\text{eq}}\left(\boldsymbol{\theta}\right) = Z^{-1}\exp\left(-U\left(\boldsymbol{\theta}\right)/k_B T\right)\delta\left(\boldsymbol{\theta}^T\boldsymbol{\theta} - 1\right).$$

Random Finite Difference for Orientation

- We construct a RFD scheme for timestepping the quaternion orientation

$$
\begin{aligned}
\boldsymbol{\theta}^{\star} =& \text{Rotate}\left(\boldsymbol{\theta}^{n},\, \delta\widetilde{\boldsymbol{W}}\right) \\
\boldsymbol{\omega}^{n} =& -\left(\boldsymbol{M}\boldsymbol{\Psi}^{T}\frac{\partial U}{\partial \boldsymbol{\theta}}\right)^{n} + \left(\frac{2k_B T}{\Delta t}\boldsymbol{M}^{n}\right)^{\frac{1}{2}} \boldsymbol{W}^{n} \\
& + \left(\frac{k_B T}{\delta}\right)\left(\boldsymbol{M}^{\star} - \boldsymbol{M}^{n}\right)\widetilde{\boldsymbol{W}} \\
\boldsymbol{\theta}^{n+1} =& \text{Rotate}\left(\boldsymbol{\theta}^{n},\, \boldsymbol{\omega}^{n}\Delta t\right).
\end{aligned}
$$

Algorithm with Translation

- To include translation, we introduce the matrix $\boldsymbol{\Xi}$, letting $\boldsymbol{u} = \dot{\boldsymbol{q}}$ where $\boldsymbol{q}$ is the location of the body.

$$\boldsymbol{\Xi} = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Psi} \end{bmatrix}, \quad \left[\dot{\boldsymbol{q}}, \dot{\boldsymbol{\theta}}\right]^T = \boldsymbol{\Xi}\left[\boldsymbol{u}, \boldsymbol{\omega}\right]^T$$

- The equations of motion in this case are

$$\boldsymbol{\upsilon} = \frac{d\boldsymbol{x}}{dt} = -\left(\boldsymbol{\Xi N \Xi}^{\star}\right)\partial_{\boldsymbol{x}} U + \sqrt{2k_B T}\,\boldsymbol{\Xi N}^{\frac{1}{2}}\boldsymbol{\mathcal{W}} + \left(k_B T\right)\partial_{\boldsymbol{x}} \cdot \left(\boldsymbol{\Xi N \Xi}^{\star}\right),$$

where $\boldsymbol{x} = \left(\boldsymbol{q}, \boldsymbol{\theta}\right)^T$, $\boldsymbol{\upsilon} = \left(\boldsymbol{u}, \dot{\boldsymbol{\theta}}\right)^T$, and $\boldsymbol{N}$ is the grand mobility tensor, such that given force $\boldsymbol{F}$ on the body, we have.

$$\left[\boldsymbol{u}, \boldsymbol{\omega}\right]^T = \boldsymbol{N}\left[\boldsymbol{F}, \boldsymbol{\tau}\right]^T.$$

Random Finite Difference with Translation

- We can also write a RFD scheme that works with translation

$$
\begin{aligned}
\tilde{\boldsymbol{v}} &= \widetilde{\boldsymbol{W}} \\
\tilde{\boldsymbol{q}} &= \boldsymbol{q}^n + \delta \tilde{\boldsymbol{u}} \\
\tilde{\boldsymbol{\theta}} &= \text{Rotate}\left(\boldsymbol{\theta}^n, \delta \tilde{\boldsymbol{\omega}}\right) \\
\boldsymbol{v}^n &= -\left(\boldsymbol{N}\boldsymbol{\Xi}^T \partial_{\boldsymbol{x}} U\right)^n + \sqrt{\frac{2k_B T}{\Delta t}} \left(\boldsymbol{N}^{\frac{1}{2}}\right)^n \boldsymbol{W}^n + \frac{k_B T}{\delta}\left(\widetilde{\boldsymbol{N}} - \boldsymbol{N}^n\right) \widetilde{\boldsymbol{W}} \\
\boldsymbol{q}^{n+1} &= \boldsymbol{q}^n + \Delta t \boldsymbol{u}^n \\
\boldsymbol{\theta}^{n+1} &= \text{Rotate}\left(\boldsymbol{\theta}^n, \Delta t \boldsymbol{\omega}^n\right).
\end{aligned}
$$

Computing Mobilty

- There are different ways to obtain $\boldsymbol{M}$ (more in talk by Aleksandar Donev):
  - In unbounded domains we can just use the **Rotne-Prager-Yamakawa tensor** (RPY) (always SPD!).
  - In simple geometries such as a single wall we can use a generalization of RPY;
    We use the analytical mobility for a **single wall** (Swan&Brady [5]).
  - In more general cases we can use a fluctuating **FEM/FVM fluid Stokes solver** combined with an immersed-boundary representation of the particles [6].
- In [6] we develop an RFD scheme that requires only one Stokes solve per time step for spherical particles.

Simulation: particles in a channel

- For the single particle case, we can write down the biased distribution that we expect when no drift is present (Euler Maruyama).

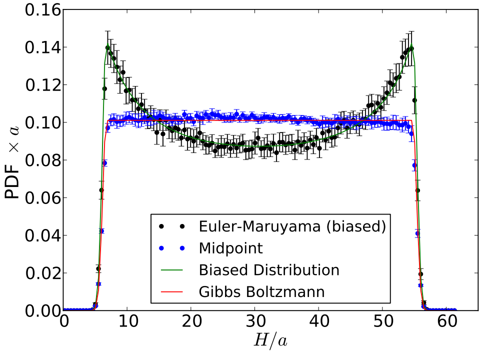
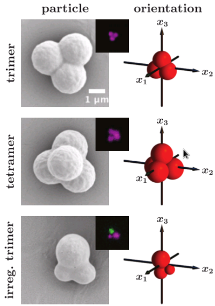


Figure: Distribution of a particle diffusing in a channel.

Importance of stochastic drift



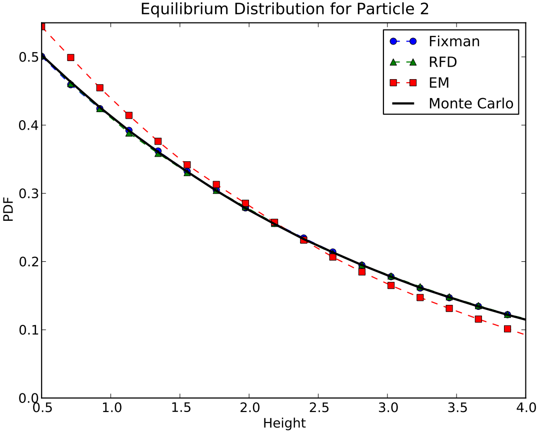
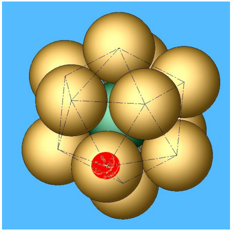


Figure: Height distribution of a vertex of a tetrahedron of spheres near a wall with one vertex tethered (**rotation only**).

Non-uniform Icosahedron



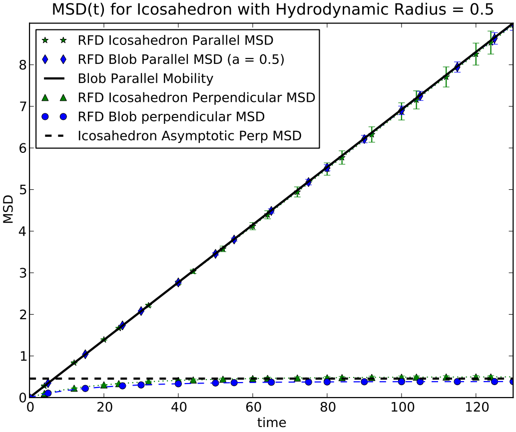
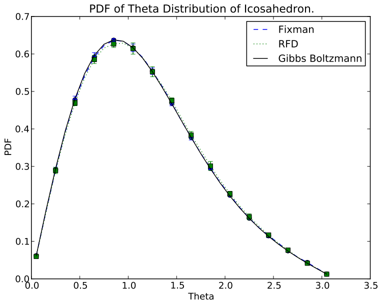


Figure: Translational Mean Square Displacement of a non-uniform Icosahedron.

Non-uniform Icosahedron



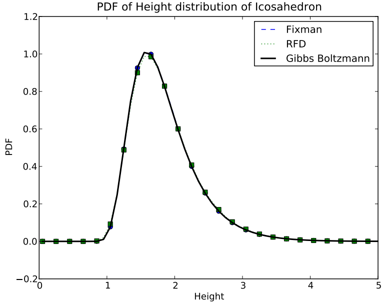


Figure: Height and Orientation distributions for a non-uniform icosahedron.

Conclusion

- We introduced the **Random Finite Difference (RFD)** scheme for timestepping the overdamped Langevin equations.
- This scheme requires only applications of M and $M_{\frac{1}{2}}$, and in particular we do **not** need to **invert the mobility**.
- We formulate an overdamped Langevin equation for angular degrees of freedom using **quaternions.**
- We can apply a specialized version of RFD to handle the thermal drift in the equations for orientation.

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