Brownian dynamics simulations with hard-body interactions: Exact numerical treatment

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Hard-wall interactions in soft matter systems: Exact numerical treatment

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Brownian dynamics simulations with hard-body interactions: Spherical particles

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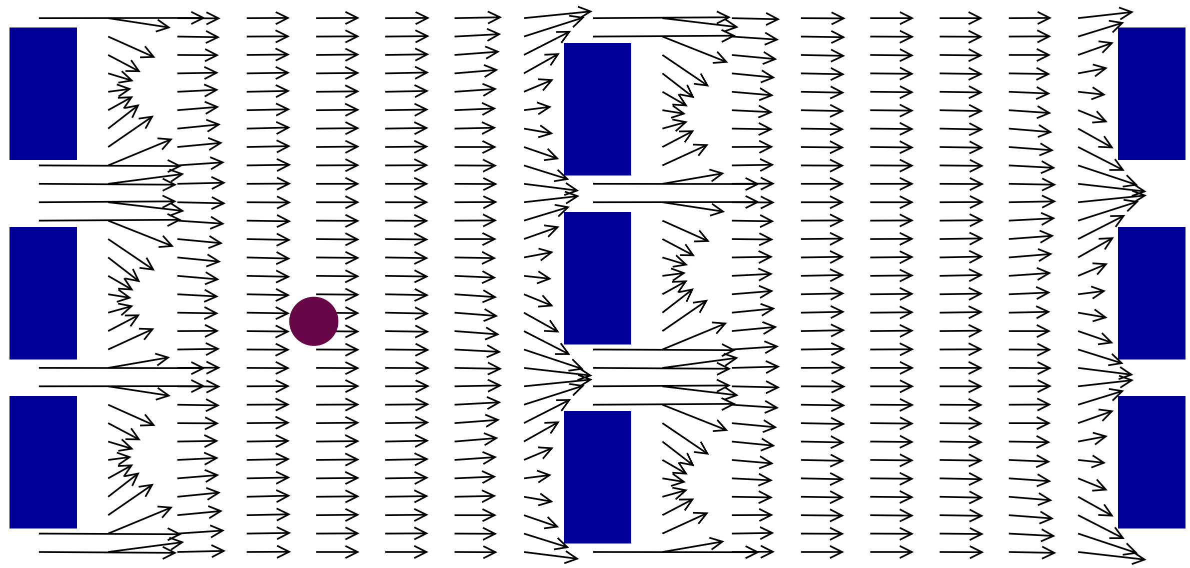
Brownian motion

- interacting particles in a suspension (e.g. colloids)
- driven by external forces
- in a structured environment
- **solvent**: viscous friction and thermal fluctuations



microfluidics, biomolecules in the cell, self-assembly, polymers, ...

$\hookrightarrow$ **numerical simulation** of particle interaction with **hard walls**

Langevin equation

$$\dot{\vec{r}}(t) = \frac{1}{\eta}\vec{F}(\vec{r}(t), t) + \sqrt{2D}\,\vec{\xi}(t)$$

two common idealizations/approximations:

- overdamped limit ("$m = 0$")
- hard-body interactions (singular!)

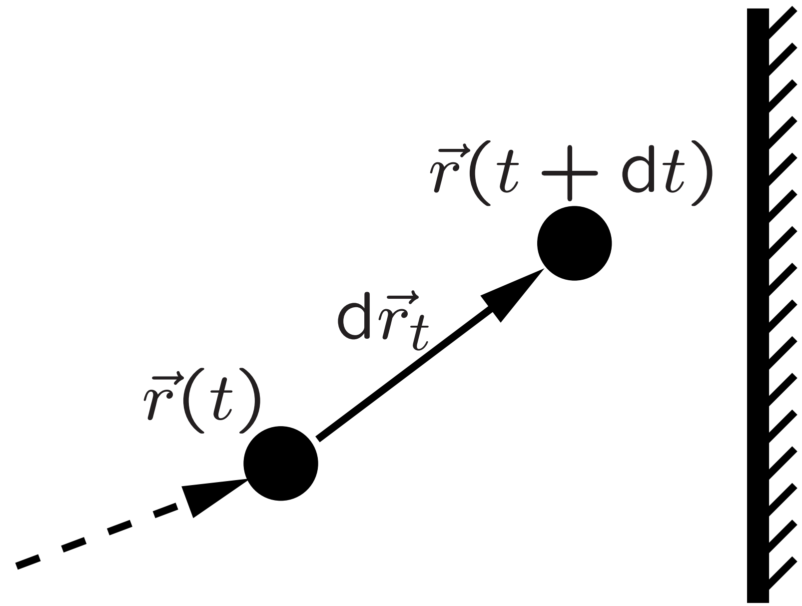
  to represent the extremely short-ranged and strong repulsive contact forces

  not included in $\vec{F}(\vec{r}(t), t)$

Euler algorithm

$$\boxed{\mathrm{d}\vec{r}_t = \vec{v}_t\,\mathrm{d}t + \sqrt{2D\,\mathrm{d}t}\,\vec{G}_t\,, \qquad \vec{r}(t+\mathrm{d}t) = \vec{r}(t) + \mathrm{d}\vec{r}_t}$$

with $\vec{v}_t = \frac{1}{\eta}\vec{F}(\vec{r}(t),t)$, and $\vec{G}_t \in \mathcal{N}(0,1)^d$



Euler algorithm

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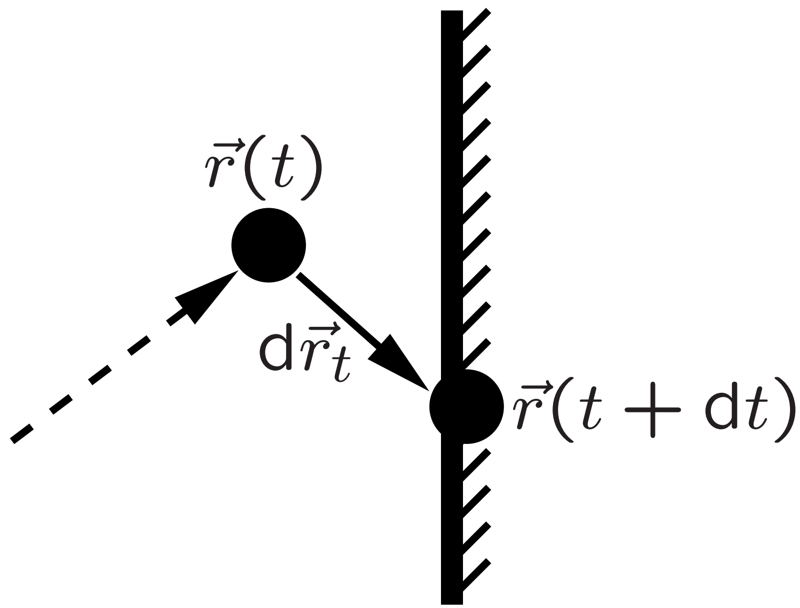

Euler algorithm

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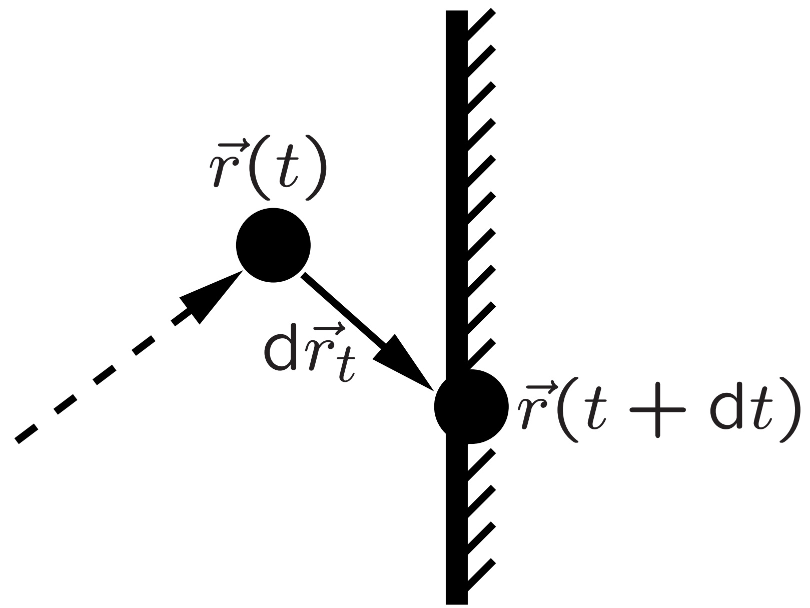
with $\vec{v}_t = \frac{1}{\eta}\vec{F}(\vec{r}(t), t)$, and $\vec{G}_t \in \mathcal{N}(0,1)^d$

algorithm:

1) detect unphysical configurations
("collisions")

2) **rule** to generate physically valid configuration



Heuristic methods (prominent examples)

- **rejection scheme**
  discard unphysical configurations
  (advance time or not???)
  [B. Cichocki and K. Hinsen, Physica A **166**, 473 (1990)]

- **event-driven scheme**
  propagate fraction of time step $\epsilon \mathrm{d}t$ until "collision point"
  use rejection scheme for remaining time step $(1-\epsilon)\mathrm{d}t$
  [Y.-G. Tao et al., J. Chem. Phys. **124**, 134906 (2006)]

lack thorough justification

Euler algorithm

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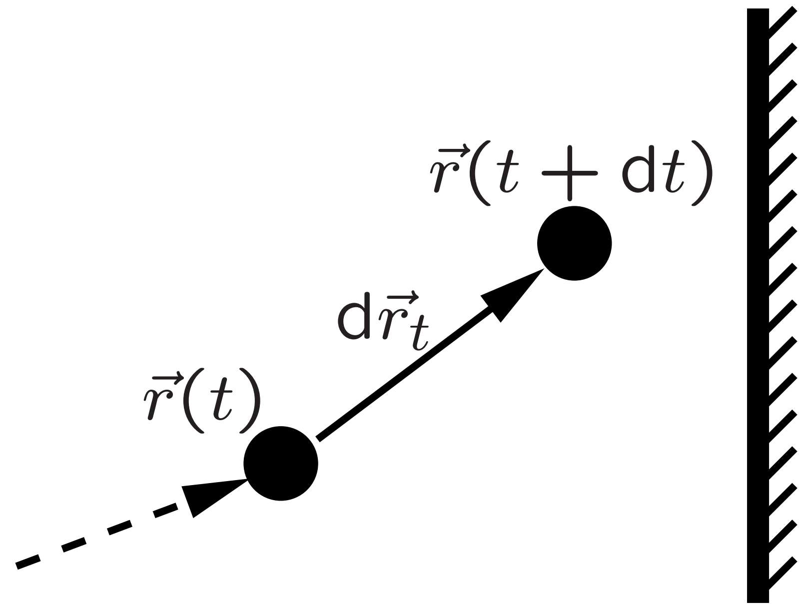
with $\vec{v}_t = \frac{1}{\eta}\vec{F}(\vec{r}(t),t)$, and $\vec{G}_t \in \mathcal{N}(0,1)^d$

$$p(\mathrm{d}\vec{r}_t) = \frac{1}{\sqrt{4\pi D\,\mathrm{d}t}^{\,d}} \exp\left(-\frac{[\mathrm{d}\vec{r}_t - \vec{v}_t\,\mathrm{d}t]^2}{4D\,\mathrm{d}t}\right)$$



Euler algorithm

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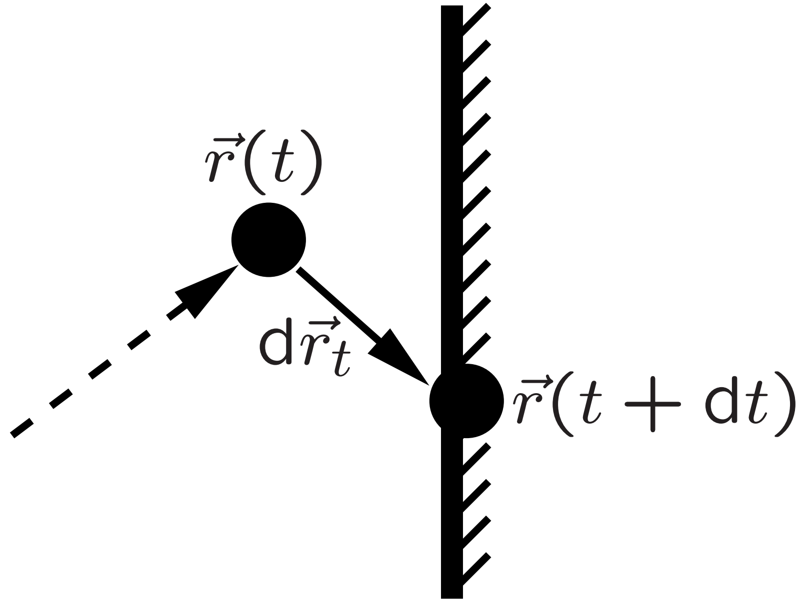
algorithm:

1) detect unphysical configurations
   (“collisions”)

2) **rule** to generate physically valid configuration

$$p(\mathrm{d}\vec{r}_t) = ???$$



Euler algorithm

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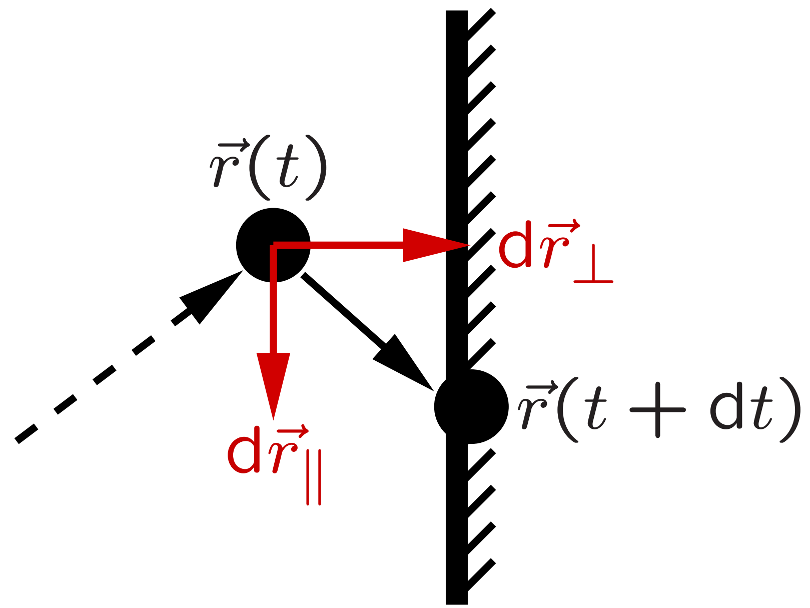


Smoluchowski solution

[M. V. Smoluchowski, Phys. Z. **17**, 557 (1916)]

driven diffusion on a half-line $q \in [0, \infty)$ $$\frac{\partial}{\partial t} p = D_q \frac{\partial^2}{\partial q^2} p - v_q \frac{\partial}{\partial q} p$$

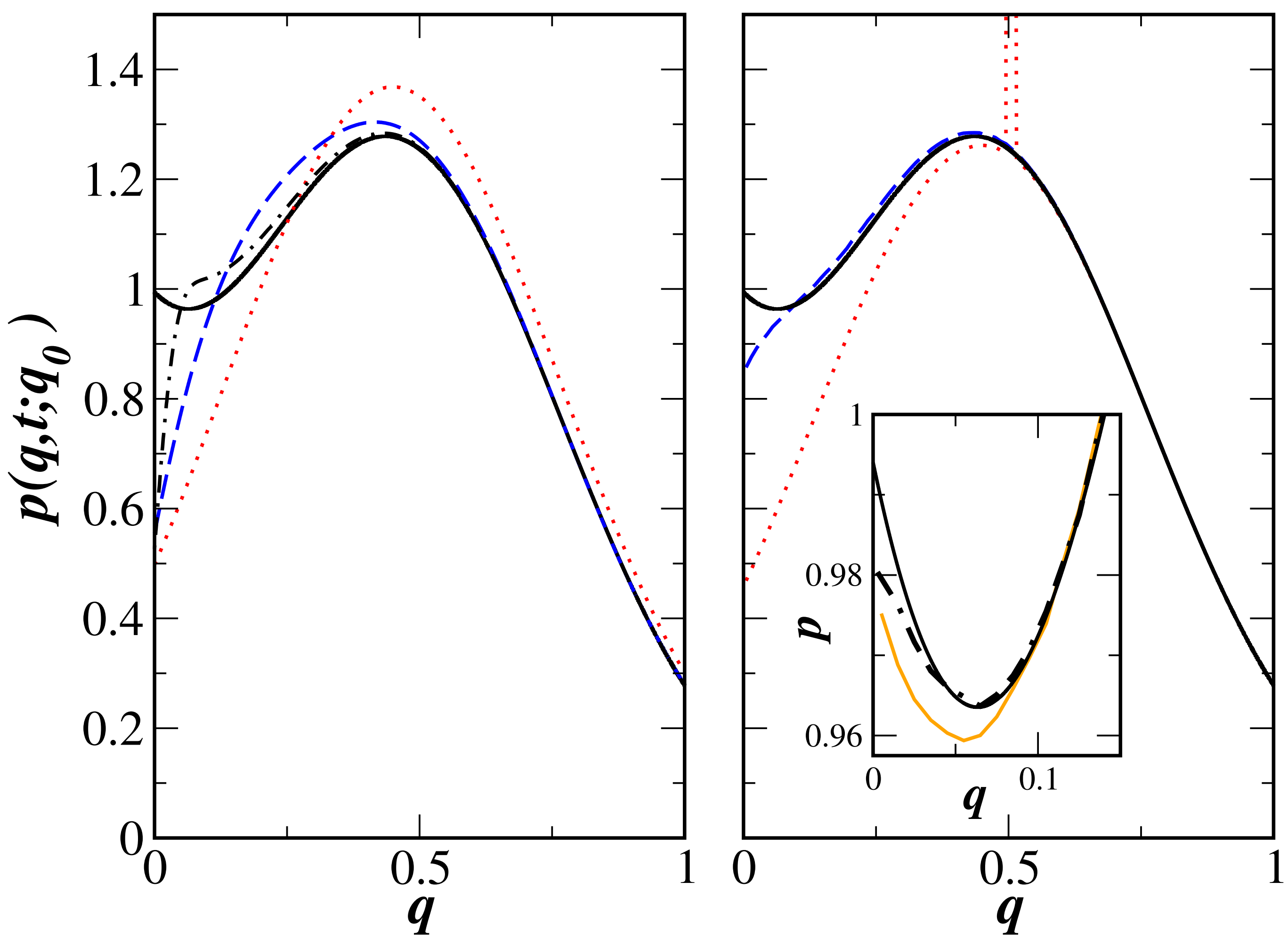
reflecting boundary at $q = 0$ $$-\left[D_q \frac{\partial}{\partial q} p - v_q p \right]_{q=0} = 0$$

initial position q_0 at time $t = 0$

solution: $p(q, t; q_0) = p_1(q, t; q_0) + p_2(q, t; q_0) + p_3(q, t; q_0)$

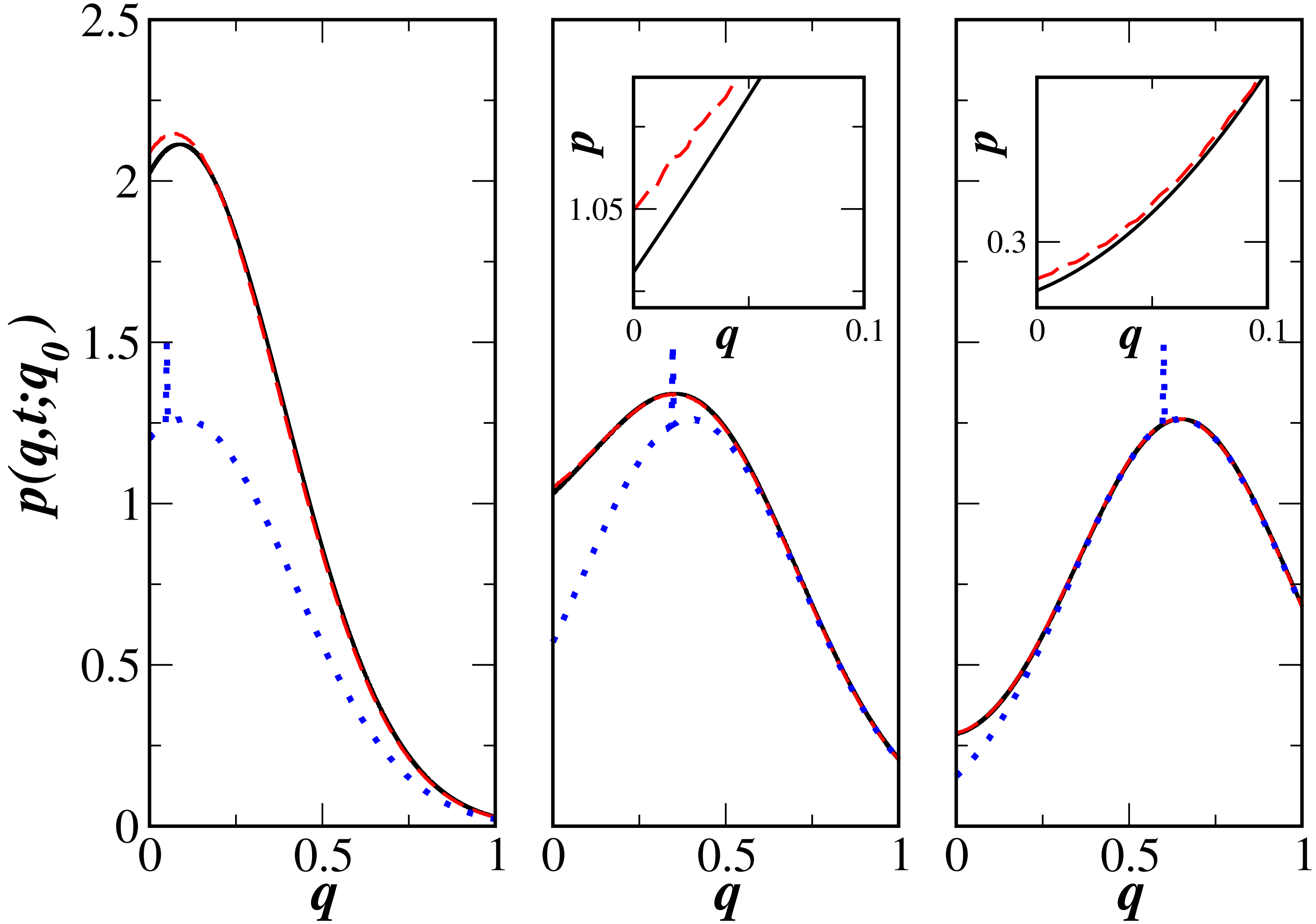
with
$$p_1(q, t; q_0) = \frac{1}{\sqrt{4\pi D_q t}} \exp\left(-\frac{(q - q_0 - v_q t)^2}{4 D_q t} \right)$$
$$p_2(q, t; q_0) = \frac{\exp\left(-\frac{v_q q_0}{D_q} \right)}{\sqrt{4\pi D_q t}} \exp\left(-\frac{(q + q_0 - v_q t)^2}{4 D_q t} \right)$$
$$p_3(q, t; q_0) = -\frac{v_q}{2 D_q} \exp\left(\frac{v_q q}{D_q} \right) \operatorname{erfc}\left(\frac{q + q_0 + v_q t}{\sqrt{4 D_q t}} \right)$$

Smoluchowski solution



$v_q = -1.0,\ D_q = 1.0,\ q_0 = 0.5,\ t = 0.05$

Smoluchowski solution



$q_0 = 0.05$ $q_0 = 0.35$ $q_0 = 0.6$

$v_q = 1.0,\ D_q = 1.0,\ t = 0.05$

Smoluchowski solution

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$$p_3(q, t; q_0) = -\frac{v_q}{2 D_q} \exp\left(\frac{v_q q}{D_q} \right) \mathrm{erfc}\left(\frac{q + q_0 + v_q t}{\sqrt{4 D_q t}} \right)$$

The algorithm

1. Perform standard integration as long as the displacements $\mathrm{d}\vec{r}_t$ do not lead to unphysical configurations ("collisions")

2. If a suggested displacement $\mathrm{d}\vec{r}_t$ results in a "collision", replace its component along the "collision axis" by a new $\mathrm{d}q = q - q_0$ drawn from $\frac{p_2(q, \mathrm{d}t; q_0) + p_3(q, \mathrm{d}t; q_0)}{w}$

   with
$$\begin{aligned} w &= \int_0^\infty \mathrm{d}q \, [p_2(q, \mathrm{d}t; q_0) + p_3(q, \mathrm{d}t; q_0)] \\ &= 1 - \int_0^\infty \mathrm{d}q \, p_1(q, \mathrm{d}t; q_0) \\ &= \int_{-\infty}^0 \mathrm{d}q \, p_1(q, \mathrm{d}t; q_0) \end{aligned}$$

The algorithm

"collision axis" $\hat{=}$ **half-line** (with "collision point" at the origin)

random number created on the "collision axis":

$$Q = Q_{\mathsf{G}}\,\Theta(Q_{\mathsf{G}}) + Q_{\mathsf{C}}\,\Theta(-Q_{\mathsf{G}})$$

with $p_{\mathsf{G}}(q) = p_1(q)\ \ (q \in \mathbb{R})$ and $p_{\mathsf{C}}(q) = \dfrac{p_2(q) + p_3(q)}{w}\ \ (q \in \mathbb{R}_{>0})$

$$\begin{aligned}
\Rightarrow \quad p_{\mathsf{alg}}(q) &= \int_{-\infty}^{\infty} \mathrm{d}q_1 \int_0^{\infty} \mathrm{d}q_2\, p_{\mathsf{G}}(q_1) p_{\mathsf{C}}(q_2)\, \delta(q - [q_1\Theta(q_1) + q_2\Theta(-q_1)]) \\
&= \int_{-\infty}^{\infty} \mathrm{d}q_1 \int_0^{\infty} \mathrm{d}q_2\, p_{\mathsf{G}}(q_1) p_{\mathsf{C}}(q_2)\, [\Theta(q_1)\delta(q - q_1) \\
&\qquad\qquad + \Theta(-q_1)\delta(q - q_2)]) \\
&= \Theta(q) p_{\mathsf{G}}(q) + p_{\mathsf{C}}(q) \int_{-\infty}^{0} \mathrm{d}q_1\, p_{\mathsf{G}}(q_1) \\
&= p_1(q) + p_2(q) + p_3(q)
\end{aligned}$$

Euler algorithm for hard wall

$$\mathrm{d}\vec{r}_t = \vec{v}_t\,\mathrm{d}t + \sqrt{2D\,\mathrm{d}t}\,\vec{G}_t\,, \qquad \vec{r}(t+\mathrm{d}t) = \vec{r}(t) + \mathrm{d}\vec{r}_t^{\,*}$$

with $\vec{v}_t = \frac{1}{\eta}\vec{F}(\vec{r}(t),t)$, and $\vec{G}_t \in \mathcal{N}(0,1)^d$

algorithm:

1) "suggest" $\mathrm{d}\vec{r}_t$ using standard Euler scheme

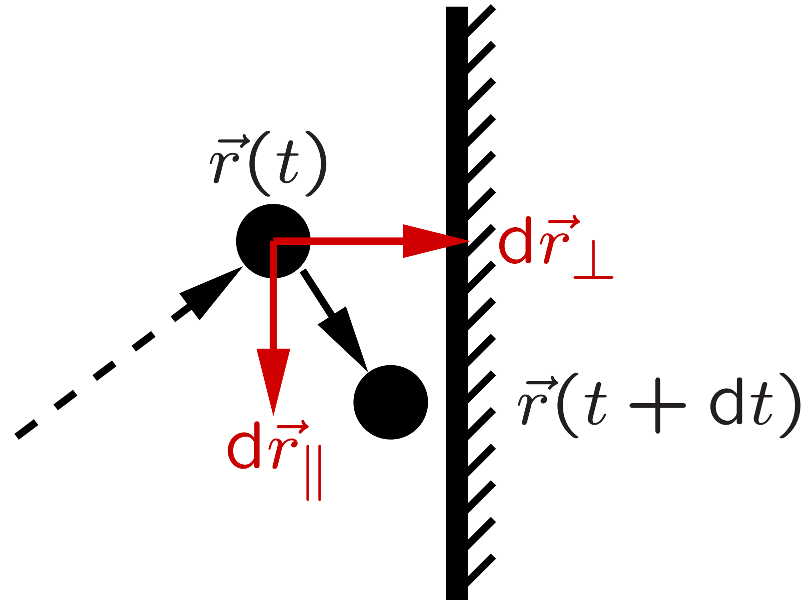
2a) **no "collision"**:

$\mathrm{d}\vec{r}_t^{\,*} = \mathrm{d}\vec{r}_t$

2b) **"collision"**:

$\mathrm{d}\vec{r}_t^{\,*} = \mathrm{d}\vec{r}_t + (q - q_0 - \vec{n}\cdot\mathrm{d}\vec{r}_t)\vec{n}$

with $\vec{n} = -\mathrm{d}\vec{r}_\perp / |\mathrm{d}\vec{r}_\perp|$



note: $\mathrm{d}\vec{r}_\perp$ and $\mathrm{d}\vec{r}_\parallel$ are uncorrelated

Euler algorithm for spherical particles

$$\mathrm{d}\vec{r}_1 = \vec{v}_1 \mathrm{d}t + \sqrt{2D_1 \mathrm{d}t}\,\vec{G}_1\,, \qquad \mathrm{d}\vec{r}_2 = \vec{v}_2\,\mathrm{d}t + \sqrt{2D_2\,\mathrm{d}t}\,\vec{G}_2$$

$$\vec{r}_1(t+\mathrm{d}t) = \vec{r}_1(t) + \mathrm{d}\vec{r}_1^{\,*}\,, \qquad \vec{r}_2(t+\mathrm{d}t) = \vec{r}_2(t) + \mathrm{d}\vec{r}_2^{\,*}$$

algorithm:

1) "suggest" $\mathrm{d}\vec{r}_1$, $\mathrm{d}\vec{r}_2$ using standard Euler scheme

2a) **no "collision"** :

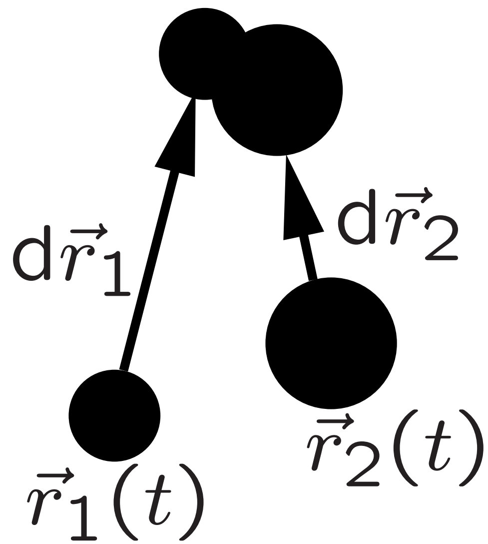
$\mathrm{d}\vec{r}_1^{\,*} = \mathrm{d}\vec{r}_1$ and $\mathrm{d}\vec{r}_2^{\,*} = \mathrm{d}\vec{r}_2$

2b) **"collision"** :

$$\mathrm{d}\vec{r}_1^{\,*} = \mathrm{d}\vec{r}_1 + \frac{\eta_2}{\eta_1+\eta_2}[(\mathrm{d}\vec{r}_2 - \mathrm{d}\vec{r}_1)\cdot\vec{e} - (q-q_0)]\vec{e}$$

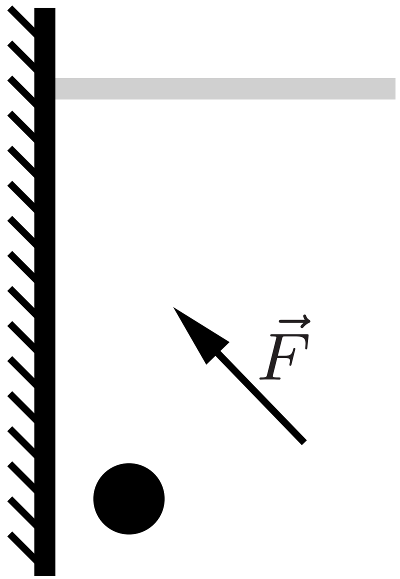
$$\mathrm{d}\vec{r}_2^{\,*} = \mathrm{d}\vec{r}_2 - \frac{\eta_1}{\eta_1+\eta_2}[(\mathrm{d}\vec{r}_2 - \mathrm{d}\vec{r}_1)\cdot\vec{e} - (q-q_0)]\vec{e}$$

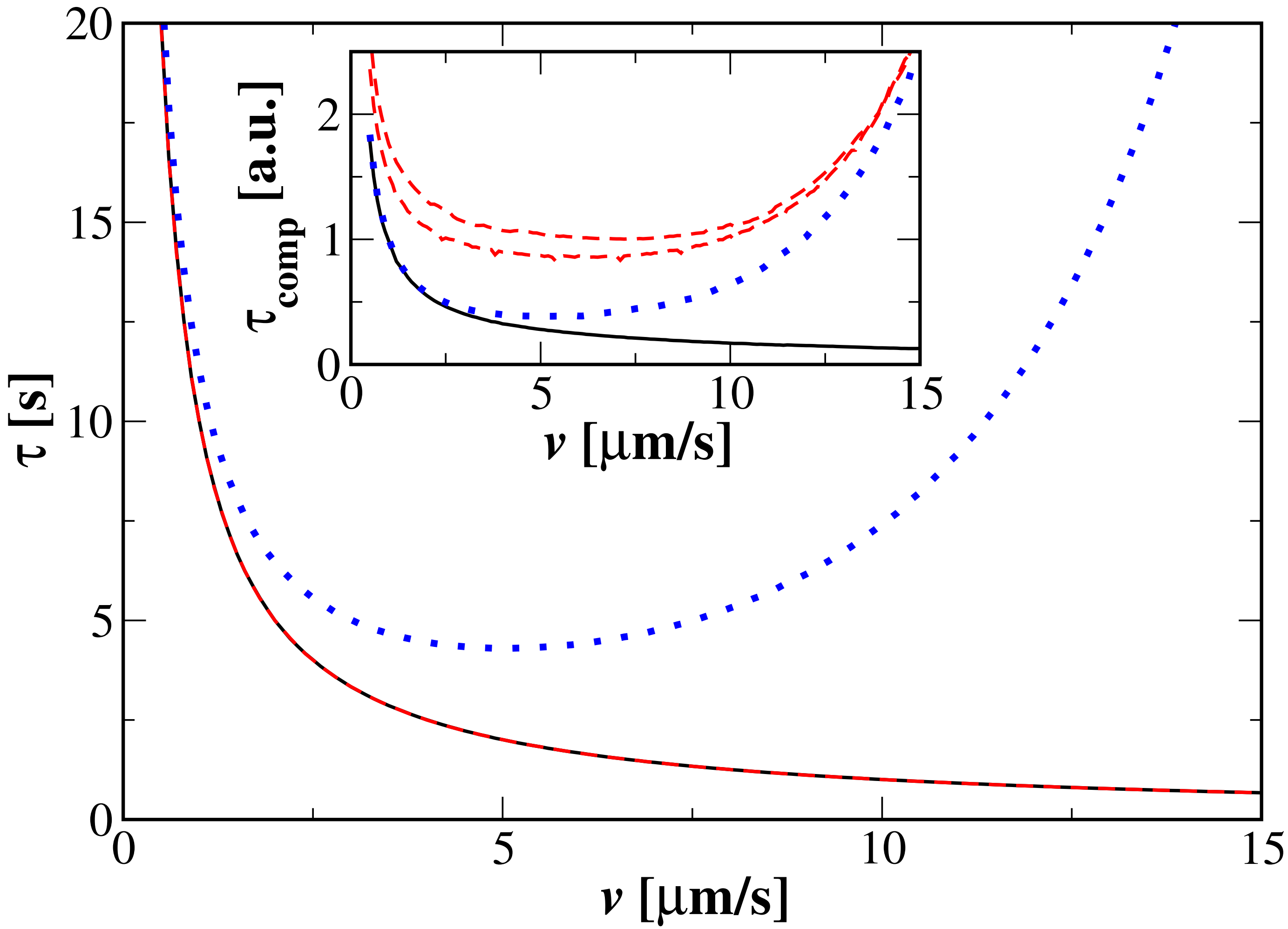
with $\vec{e} = (\vec{r}_2(t) - \vec{r}_1(t))/|\vec{r}_2(t) - \vec{r}_1(t)|$



note: **center of friction** and **relative motion** are uncorrelated

Example: Mean first passage time





$\vec{F} = (-f, f)$, $v = f/\eta$, particle radius 1 μm, d$t = 0.01$ s

In practice

- detection of "collisions"
  (any integration scheme)

- integration time step $\mathrm{d}t$ is determined by
  variations of $\vec{F}$ and **curvature of structures/particles**

- generation of random number q according to distribution
  $p_{\mathrm{C}}(q) = [p_2(q) + p_3(q)]/w$

$$F(q) = \int_0^q \mathrm{d}q'\, p_{\mathrm{C}}(q') = \frac{\mathrm{erfc}\left(\frac{q_0+v_q\mathrm{d}t}{\sqrt{4D_q\mathrm{d}t}}\right) - \exp\left(\frac{v_q q}{D_q}\right)\mathrm{erfc}\left(\frac{q+q_0+v_q\mathrm{d}t}{\sqrt{4D_q\mathrm{d}t}}\right)}{\mathrm{erfc}\left(\frac{q_0+v_q\mathrm{d}t}{\sqrt{4D_q\mathrm{d}t}}\right)}.$$

Then: $q = F^{-1}(x)$ with x uniformly distributed on $[0,1]$
is distributed according to $p_{\mathrm{C}}(q)$

numerical solution (Brent's scheme from the GNU scientific library)

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extensions:

non-spherical particles

corners & wedges

many particles (crowding)

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