On discretization schemes for stochastic differential equations with unbounded drift in the kinetic theory of polymer solutions

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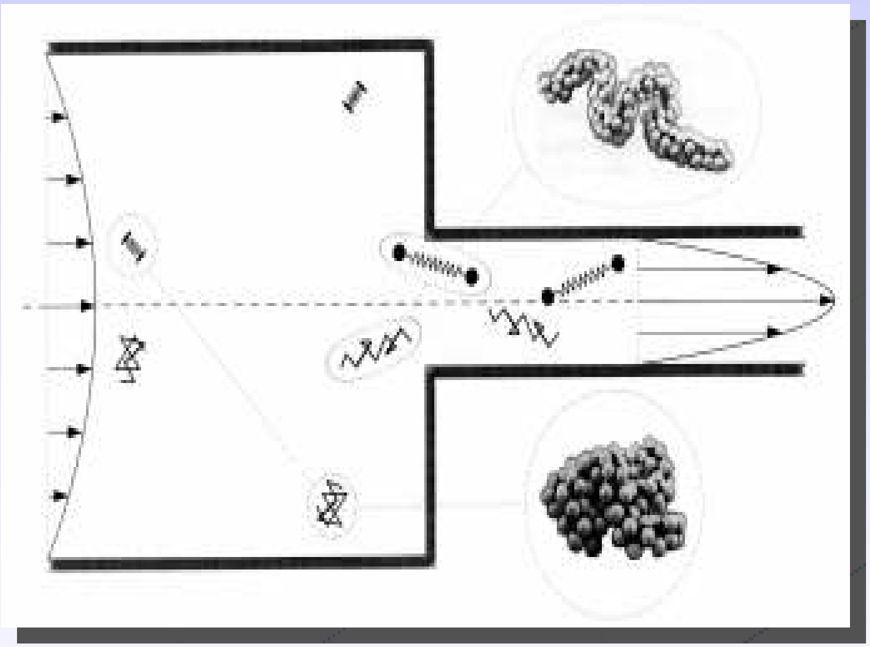
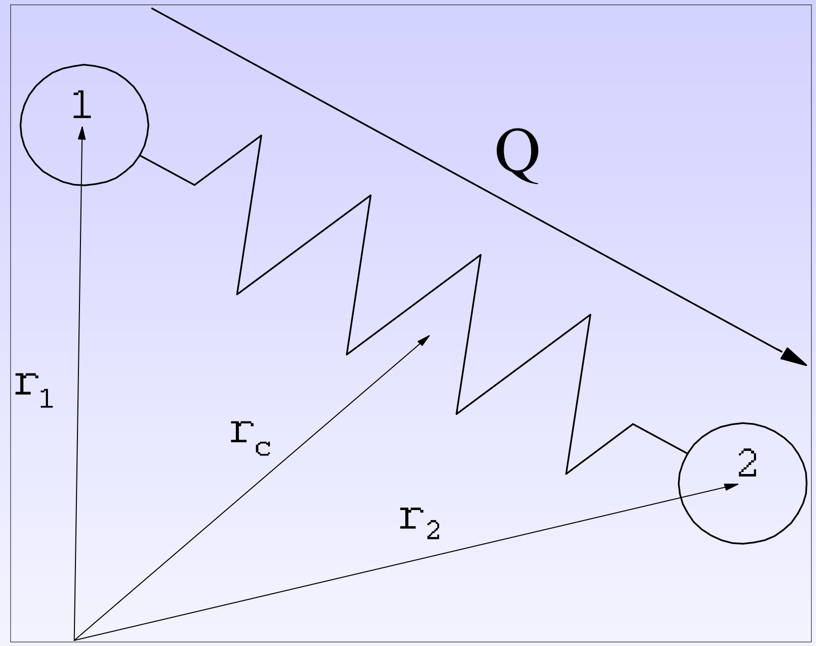
Outline

- Modelling polymer molecules by “dumbbells”
- A new force law: “Constrained Hookean” force leading to the Reflecting Stochastic Differential Equations
- Calculating the extra-stress tensor via penalization (theoretical results)
- 3 methods for the discretization in time: penalization, reflection and half-space approximation
- Numerical results for simple flows

Dumbbell models for polymer molecules





$$\mathbf{Q} = \mathbf{r}_2 - \mathbf{r}_1$$
$$\mathbf{r}_c = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$$

Governing SDE

$$dQ_t = \left(\kappa(t)Q_t - \frac{1}{2\lambda}F(Q_t)\right)dt + \sqrt{\frac{1}{\lambda}}dB_t,$$

Gradient of the velocity

Spring force

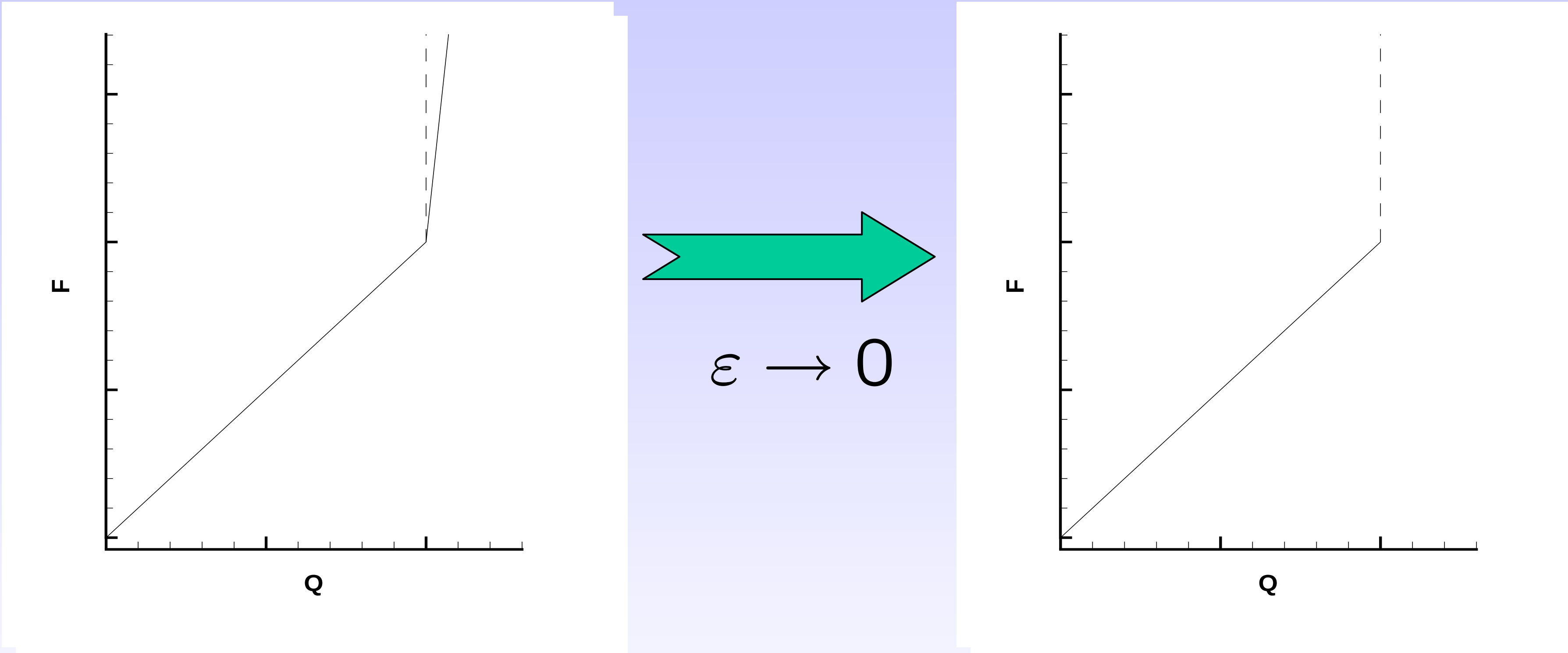
Brownian motion

Stress tensor : $\tau(t) = \mathbb{E}(Q_t \otimes F(Q_t))$

Hookean force → $\mathbf{F}(\mathbf{Q}) = H\mathbf{Q},$

FENE force → $\mathbf{F}(\mathbf{Q}) = \frac{H\mathbf{Q}}{1-|\mathbf{Q}|^2/b}$

“Constraned” Hookean forcce



$$F^{\varepsilon}(Q) = Q + \frac{1}{\varepsilon}\beta(Q) \qquad\qquad F(Q) = \partial \Pi$$

$\beta(Q) = Q - \Pi Q$ and Π is the projection on $\overline{B(0,R)}$ where $R = \sqrt{b}$

Reflecting SDE

Define $\mathbf{F}$ as the subdifferential of the potential

$$\Pi(Q) = \begin{cases} \frac{1}{2}|Q|^2, & \text{if } |Q| < R \\ +\infty, & \text{otherwise} \end{cases}$$

for some fixed R.

Reflecting SDE for Q_t

$$dQ_t = \left(\kappa(t)Q_t - \frac{1}{2\lambda}Q_t\right) dt - n d\eta_t + \sqrt{\frac{1}{\lambda}} dB_t,$$

where η_t is an unknown stochastic process imposing to the process to remain in the ball $\overline{B(0,R)}$.

Stress tensor for the constrained Hookean force

The Kramers expression for the stress (for a nice force law)

$$\tau(t) = \mathbb{E}(Q_t \otimes F(Q_t))$$

In the case of the reflected diffusion the force is (something like)

$$F_t dt = Q_t dt + \frac{2\lambda}{R} Q_t d\eta_t$$

The Kramers stress is (something like)

$$\tau(t) \sim \frac{\eta_p}{\lambda} \left(\mathbb{E}(Q_t \otimes Q_t) + \frac{2\lambda}{R} \frac{\mathbb{E}(Q_t \otimes Q_t d\eta_t)}{dt} - I \right) \qquad ???$$

The sensible way to define the stress is rather

$$\tau(t) = \frac{\eta_p}{\lambda} \lim_{\epsilon \longrightarrow 0} \left(\mathbb{E} \left(Q_t^\varepsilon \otimes Q_t^\varepsilon + Q_t^\varepsilon \otimes \frac{1}{\varepsilon} \beta(Q_t^\varepsilon) \right) - I \right).$$

Main result, calculation of the stress

Let
$q \in B(0, R)$ be an initial condition,
$\kappa \in \mathbb{R}^{d \times d}$,
$\lambda > 0$, $\eta_p > 0$,

$$dQ_t^\varepsilon = \left(\kappa(t) Q_t^\varepsilon - \frac{1}{2\lambda} Q_t^\varepsilon - \frac{1}{2\lambda\varepsilon} \beta(Q_t^\varepsilon)\right) dt + \sqrt{\frac{1}{\lambda}} dB_t, \;\; Q_0^\varepsilon = q$$

$$\tau_\varepsilon(t) = \frac{\eta_p}{\lambda} \left(\mathbb{E}\left(Q_t^\varepsilon \otimes Q_t^\varepsilon + Q_t^\varepsilon \otimes \frac{1}{\varepsilon} \beta(Q_t^\varepsilon)\right) - I\right).$$

Then

$$\tau(t) = \lim_{\varepsilon \to 0} \tau_\varepsilon(t) \in \mathcal{C}^0([0, T]; \mathbb{R}^{d \times d})$$

and the limit above exists for all $t \in [0, T]$. Moreover,

$$\tau(t) = -\eta_p \frac{d}{dt}(Q_t \otimes Q_t) t + \eta_p \mathbb{E}((Q_t \otimes Q_t) \kappa(t)^T + \kappa(t)(Q_t \otimes Q_t))$$

a.e. in $[0, T]$.

Known properties of reflected diffusions

Menaldi (82)

For each $1 \leq p < \infty$, there exists a constant C independent of ε such that

$$\left(\sup_{t \in [0,T]} |Q_t^\varepsilon|^p \right) \leq C \tag{1}$$

and for each $1 \leq p < \infty$, $0 < T < \infty$ we have

$$\lim_{\varepsilon \to 0} \left(\sup_{0 \leq t \leq T} |Q_t - Q_t^\varepsilon|^p \right) = 0. \tag{2}$$

Proof of our main result in a weak form

Apply Itô's rule to $Q_t^\varepsilon \otimes (Q_t^\varepsilon)$ and take the expectation :

$$\frac{1}{\lambda}\mathbb{E}\int_0^t \left(Q_s^\varepsilon \otimes Q_s^\varepsilon + \frac{1}{\varepsilon} Q_s^\varepsilon \otimes \beta(Q_s^\varepsilon)\right) ds = -\mathbb{E}\Big(Q_t^\varepsilon \otimes Q_t^\varepsilon\Big) + q \otimes q$$
$$+ \int_0^t \mathbb{E}(Q_s^\varepsilon \otimes Q_s^\varepsilon)\kappa(s)^T + \kappa(s)(Q_s^\varepsilon \otimes Q_s^\varepsilon))ds + \frac{1}{\lambda} tI.$$

By known results, the limits of all the terms in the RHS as $\varepsilon \to 0$ exist, hence

$$\frac{1}{\lambda}\lim_{\varepsilon\to 0}\mathbb{E}\int_0^t \left(Q_s^\varepsilon \otimes Q_s^\varepsilon + \frac{1}{\varepsilon} Q_s^\varepsilon \otimes \beta(Q_s^\varepsilon)\right) ds$$
$$= -\mathbb{E}\Big(Q_t \otimes Q_t\Big) + q \otimes q$$
$$+ \int_0^t \mathbb{E}(Q_s \otimes Q_s)\kappa(s)^T + \kappa(s)(Q_s \otimes Q_s))ds_{ij} + \frac{1}{\lambda} tI.$$

Proof of our main result pointwise in time

We need

- Boundedness uniform in ε: $\mathbb{E}(Q_t^\varepsilon \cdot \frac{1}{\varepsilon}\beta(Q_t^\varepsilon)) \le C$,
- Continuity in t uniformly in ε :

$$\lim_{h\to 0} \sup_{\varepsilon} \left| \mathbb{E}(Q_{t+h}^\varepsilon \cdot \frac{1}{\varepsilon}\beta(Q_{t+h}^\varepsilon)) - \mathbb{E}(Q_t^\varepsilon \cdot \frac{1}{\varepsilon}\beta(Q_t^\varepsilon)) \right| = 0.$$

The desired result is then obtained by the lemma:

Let $f_\varepsilon(x)$ ($\varepsilon \in \mathbb{R}$) be a family of functions $[0,T] \to \mathbb{R}$ such that

$$\lim_{h\to 0} \sup_{\varepsilon} |f_\varepsilon(t+h) - f_\varepsilon(t)| = 0, \forall t \in [0,T]$$

and the limit $\lim_{\varepsilon\to 0} \int_0^t f_\varepsilon(s)ds$ exists for all $t \in [0,T]$. Then the limit $f(t) = \lim_{\varepsilon\to\infty} f_\varepsilon(t)$ exists for all $t \in [0,T]$, $f(t)$ is continuous and

$$\lim_{\varepsilon\to 0} \int_0^t f_\varepsilon(s)ds = \int_0^t f(s)ds.$$

The Fokker-Planck equation

$\psi(t,\mathbf{Q})$, $\mathbf{Q} \in B$ $(B = (0,\sqrt{b}))$ – the probability density to find a dumbbell with end-to-end vector $\mathbf{Q}$ at time t

$$\frac{\partial \psi}{\partial t} + \mathrm{div}_{\mathbf{Q}}\left(\left(\kappa \mathbf{Q} - \frac{1}{2\lambda}\mathbf{Q}\right)\psi\right) = \frac{1}{2\lambda}\Delta_{\mathbf{Q}}\psi.$$

Boundary conditions at ∂B (vanishing of the probability flux):

$$\left(-\kappa \mathbf{Q}\psi + \frac{1}{2\lambda}\mathbf{Q}\psi + \frac{1}{2\lambda}\nabla_{\mathbf{Q}}\psi\right)\cdot n = 0$$

Expression for the stress tensor:

$$\begin{aligned} \tau &= -\eta_p \frac{\partial}{\partial t}\int_B \mathbf{Q}\otimes\mathbf{Q}\psi d\mathbf{Q} + \eta_p \int_B \left(\kappa \mathbf{Q}\otimes\mathbf{Q} + \mathbf{Q}\otimes\mathbf{Q}\kappa^T\right)\psi d\mathbf{Q} \\ &= \frac{\eta_p}{\lambda}\int_B \mathbf{Q}\otimes\mathbf{Q}\psi d\mathbf{Q} + \frac{\eta_p}{\lambda R}\int_{\partial B}\mathbf{Q}\otimes\mathbf{Q}\psi ds - \frac{\eta_p}{\lambda}I \end{aligned}$$

Numerical algorithm with penalization

Algorithm by penalization

$$Q_0^{\varepsilon,h} = q$$

$$Q_{t_{n+1}}^{\varepsilon,h} + \frac{1}{2\lambda\varepsilon}\beta(Q_{t_{n+1}}^{\varepsilon,h})h = Q_{t_n}^{\varepsilon,h} + \left(\kappa Q_{t_n}^{\varepsilon,h} - \frac{1}{2\lambda}Q_{t_n}^{\varepsilon,h}\right)h + \sqrt{\frac{1}{\lambda}}(B_{t_{n+1}} - B_{t_n}).$$

$$\tau^h(t_n) = \frac{\eta_p}{\lambda}\mathbb{E}\left(Q_{t_n}^{\varepsilon,h} \otimes Q_{t_n}^{\varepsilon,h} + \frac{1}{\varepsilon}Q_{t_n}^{\varepsilon,h} \otimes \beta(Q_{t_n}^{\varepsilon,h})\right) - \frac{\eta_p}{\lambda}I.$$

Weak convergence of $Q_t^{\varepsilon,h}$ to Q_t with order $\sqrt{h}$ is known for the choice $\varepsilon = h$ (*Pettersson, 1997*).

Convergence of τ^h?

Auxiliary lemma: A comparison principle

Let

$$\gamma = \sup_{Q\in\mathbb{R}^d,\ |Q|=1} Q\cdot\left(\kappa - \frac{1}{2\lambda}\right)Q.$$

Let $|q| \le |y|$ and consider

$$Y^{\varepsilon,h}_{t_{n+1}} + \frac{1}{2\lambda\varepsilon}\beta(Y^{\varepsilon,h}_{t_{n+1}})h = Y^{\varepsilon,h}_{t_n} + h\gamma Y^{\varepsilon,h}_{t_n} + \sqrt{\frac{1}{\lambda}}(B_{t_{n+1}} - B_{t_n}), \qquad Y^{\varepsilon}_0 = y,$$

Then, for any nondecreasing function $g : [0,\infty[\to \mathbb{R}$

$$\mathbb{E}^q(g(|Q^{\varepsilon,h}_{t_n}|)) \le \mathbb{E}^y(g(|Y^{\varepsilon,h}_{t_n}|)),\ \forall n \in \mathbb{N}.$$

I: Uniform boundedness

The process $Q_{t_n}^{\varepsilon,h}$ with any initial condition $q \in B(0,1)$ and any $t \in [0,T]$ satisfies

$$\mathbb{E}^q(Q_{t_n}^{\varepsilon,h} \cdot \frac{1}{\varepsilon}\beta(Q_{t_n}^{\varepsilon,h})) \leq C$$

Proof. Let $\pi_{\varepsilon,h}$ be the stationary distribution of $Q_{t_n}^{\varepsilon,h}$ and $I_+ = \{z \in \mathbb{R}^d : |z| > |x|\}$. The comparison principle with with $h(Q) = Q \cdot \frac{1}{\varepsilon}\beta(Q)$ entails

$$\begin{aligned}
\mathbb{E}^q(Q_{t_n}^{\varepsilon,h} \cdot \frac{1}{\varepsilon}\beta(Q_{t_n}^{\varepsilon,h})) &\leq \mathbb{E}^{\pi_{\varepsilon,h} \cap I_+}(Y_{t_n}^{\varepsilon,h} \cdot \frac{1}{\varepsilon}\beta(Y_{t_n}^{\varepsilon,h})) \\
&\leq \frac{\mathbb{E}^{\pi_{\varepsilon,h}}(Y_{t_n}^{\varepsilon,h} \cdot \frac{1}{\varepsilon}\beta(Y_{t_n}^{\varepsilon,h}))}{\pi_{\varepsilon,h}(I_+)} \leq \frac{\mathbb{E}^{\pi_{\varepsilon,h}}|Y_{t_n}^{\varepsilon,h}|^2}{\pi_{\varepsilon,h}(I_+)}
\end{aligned}$$

II: Equi-continuity

Let $\phi : \mathbb{R}^d \to \mathbb{R}$ *such that* $\phi(z) = 0$ *for all* $z \in B(0,1)$ and *suppose that for all* $n \in \mathbb{N}$ *it holds*

$$\mathbb{E}^q \left| \frac{1}{\varepsilon} \phi(Q^{\varepsilon,h}_{t_n}) \right| \leq C(|q|).$$

Then we have for any $\pm > 0$

$$\sup_{\varepsilon>0} \left| \mathbb{E}^q \left(\frac{1}{\varepsilon} (\phi(Q^{\varepsilon,h}_{t_{n+1}}) - \phi(Q^{\varepsilon,h}_{t_n})) \right) \right| \leq C h^{1/2-\pm}. \tag{1}$$

Proof. Fix any r such that $|q| < r < 1$ and $\alpha \in (0,1)$

$$\begin{aligned} \mathbb{E}^q \left(\frac{1}{\epsilon} \phi(Q^{\varepsilon,h}_{t_n}) \right) &= \int_{B(0,r)} p^{Q^{\varepsilon,h}}_{h^\alpha}(z) \mathbb{E}^z \left(\frac{1}{\varepsilon} \phi(Q^{\varepsilon,h}_{t-h^\alpha}) \right) dz \\ &\quad + \int_{\mathbb{R}^d \setminus B(0,r)} p^{Q^{\varepsilon,h}}_{h^\alpha}(z) \mathbb{E}^q \left(\frac{1}{\varepsilon} \phi(Q^{\varepsilon,h}_{t-h^\alpha}) \right) dz \end{aligned} \tag{2}$$

Consider also the unconstrained process $Q^h_{t_n}$

$$Q^h_{t_{n+1}} = Q^h_{t_n} + \left(\kappa Q^h_{t_n} - \frac{1}{2\lambda} Q^h_{t_n}\right) h + \sqrt{\frac{1}{\lambda}} (B_{t_{n+1}} - B_{t_n}).$$

and the stopping time $\sigma = \inf\{s : |Q^{\varepsilon,h}_s| = r\} = \inf\{s : |Q^h_s| = r\}$.

The second integral above is estimated as

$$\mathbb{E}^q \left(\frac{1}{\epsilon}\phi(Q^{\varepsilon,h}_{t_n}) 1_{|Q_{h^\alpha}| \geq r}\right) \leq \mathbb{E}^q \left(\frac{1}{\epsilon}\phi(Q^{\varepsilon,h}_{t_n}) 1_{\sigma < h^\alpha}\right) =$$

$$= \mathbb{E}\left(\mathbb{E}^{Q^{\varepsilon,h}_\sigma}\left(\frac{1}{\epsilon}\phi(Q^\varepsilon_{t-\sigma})\right) 1_{\sigma<h^\alpha}\right) \leq C(r)\mathcal{P}(\sigma < h^\alpha).$$

Hence

$$\mathbb{E}^q \left(\frac{1}{\epsilon}\phi(Q^{\varepsilon,h}_{t_n})\right) \;=\; \int_{B(0,r)} p^{Q^{\varepsilon,h}}_{h^\alpha}(z) \mathbb{E}^z \left(\frac{1}{\varepsilon}\phi(Q^{\varepsilon,h}_{t-h^\alpha})\right) dz + O(h^{1/2-\pm}).$$

End of the proof

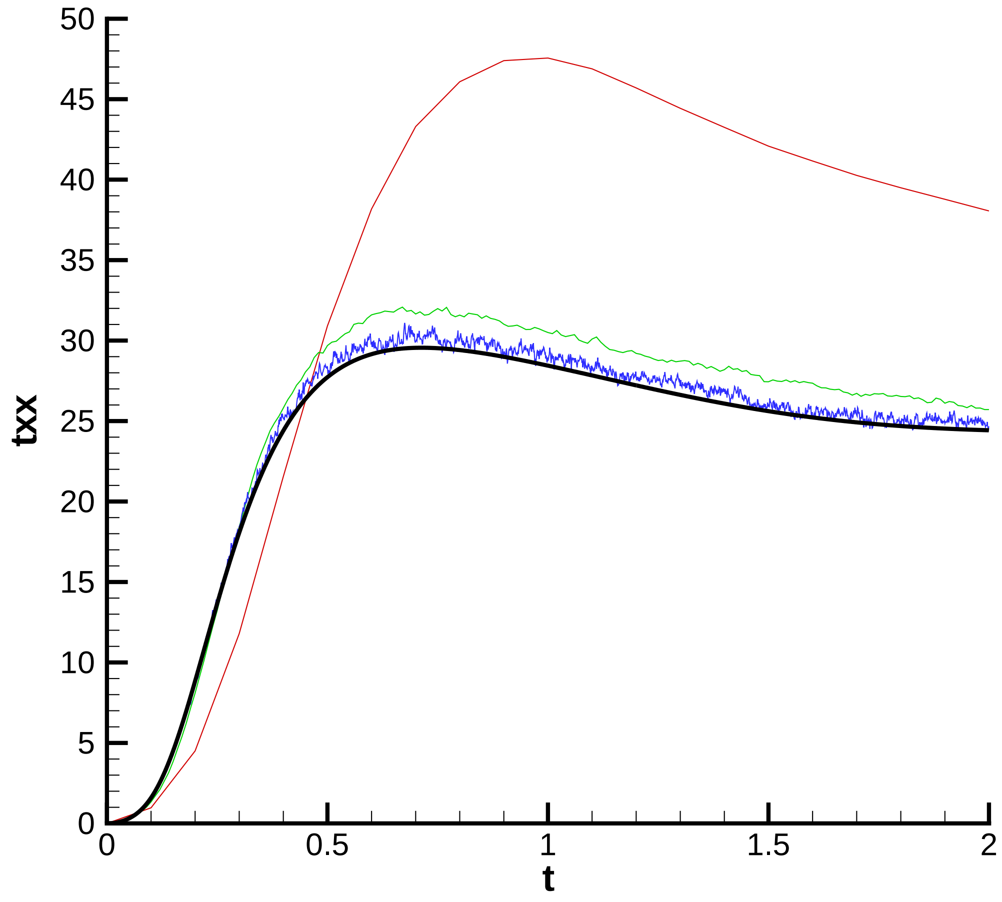
By similar calculations

$$\int_{B_r^+} p_{h^\alpha}^{Q^{\varepsilon,h}}(z)\mathbb{E}^z\left(\frac{1}{\varepsilon}\phi(Q^{\varepsilon,h}_{t-h^\alpha})\right)dz = \int_{B_r^+} p_{h^\alpha}^{Q^h}(z)\mathbb{E}^z\left(\frac{1}{\varepsilon}\phi(Q^{\varepsilon,h}_{t-h^\alpha})\right)dz + O(h^{1/2-\pm})$$

We can now compare the result at times t_n and $t_{n+1} = t_n + h$

$$\begin{aligned}
&\left|\mathbb{E}^q\left(\frac{1}{\epsilon}\phi(Q^{\varepsilon,h}_{t_n+h})\right) - \mathbb{E}^q\left(\frac{1}{\epsilon}\phi(Q^{\varepsilon,h}_{t_n})\right)\right| \\
&\qquad = \left|\int_{B(0,r)}(p^{Q^h}_{h^\alpha+h}(z) - p^{Q^h}_{h^\alpha}(z))\mathbb{E}^z\left(\frac{1}{\varepsilon}\phi(Q^{\varepsilon,h}_{t-h^\alpha})\right)dz\right| + O(h^{1/2-\pm}) \\
&\qquad \leq C\int_{B(0,r)}|p^{Q^h}_{h^\alpha+h}(z) - p^{Q^h}_{h^\alpha}(z)|dz + O(h^{1/2-\pm})
\end{aligned}$$

Convergence of the stochastic simulations by penalization



$\lambda = \eta_p = 1$

$b = 20$

$\kappa(t) = \begin{pmatrix} 0 & 10 \\ 0 & 0 \end{pmatrix}$

$M = 25000$

Red $-$ $\Delta t = 0.1$

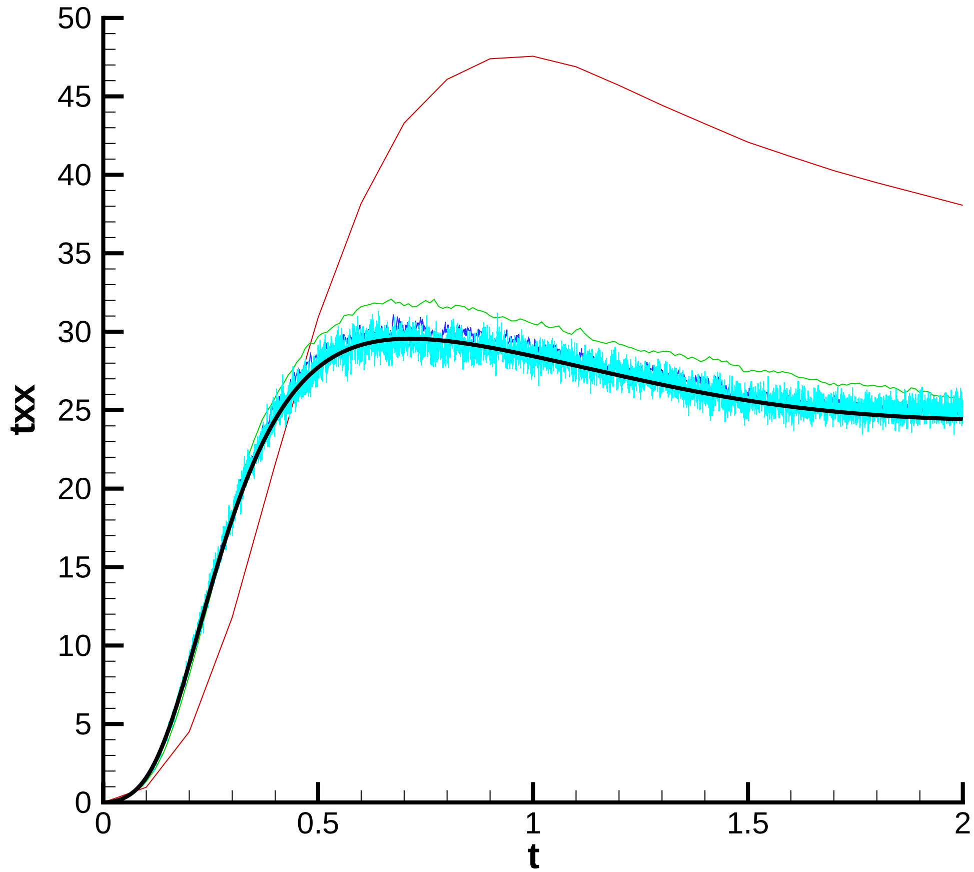
Green $-$ $\Delta t = 0.01$

Blue $-$ $\Delta t = 0.001$

Black - FP

Good convergence

Convergence of the stochastic simulations by penalization



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Cyan $-$ $\Delta t = 0.0001$

Black FP

Noise gets bigger when refining in time

Algorithm by symmetric reflection

M. Bossy et al, 2004,

Weak convergence of order Δt

- Update the stochastic process without taking into account the reflecting force

$$Y^{\Delta t}_{n+1} - Q^{\Delta t}_{n} = \left(\kappa(t_n) Q^{\Delta t}_{n} - \frac{1}{2\lambda} Q^{\Delta t}_{n} \right) \Delta t + \sqrt{\frac{1}{\lambda}} (B_{t_{n+1}} - B_{t_n})$$

- If a reflection occurs ($|Y^{\Delta t}_{n+1}| > R$), set

$$Q^{\Delta t}_{n+1} = \frac{2R - |Y^{\Delta t}_{n+1}|}{|Y^{\Delta t}_{n+1}|} Y^{\Delta t}_{n+1}$$

Approximations for the stress tensor

$$\tau = \frac{\eta_p}{\lambda}\int_B \mathbf{Q}\otimes\mathbf{Q}\psi d\mathbf{Q} + \frac{\eta_p}{\lambda R}\int_{\partial B}\mathbf{Q}\otimes\mathbf{Q}\psi ds - \frac{\eta_p}{\lambda}I$$

We can use

$$\psi(R,\theta) = \frac{1}{aR}\int_{R-a}^{R} r\psi(r)dr + O(a)$$

to write

$$\int_{\partial D} Q\otimes Q\psi ds = \frac{1}{aR}\int_{R-a<|Q|<R}\frac{R^2}{|Q|^2}Q\otimes Q\psi(Q)dQ + O(a)$$

The first idea for the stochastic approximation ($a = h$)

$$\tau^h(t_n) = \frac{\eta_p}{\lambda}\mathbb{E}\left(\mathbf{Q}^h_{t_n}\otimes\mathbf{Q}^h_{t_n}\left(1 + 1_{|Q^h_{t_n}|>R-h}\frac{R}{h|Q^h_{t_n}|^2}\right) - I\right)$$

A better approximation for the stress

If we know that $\frac{\partial\psi}{\partial r}(R,\theta) = b(\theta)\psi(R,\theta)$ then we can write (for example)

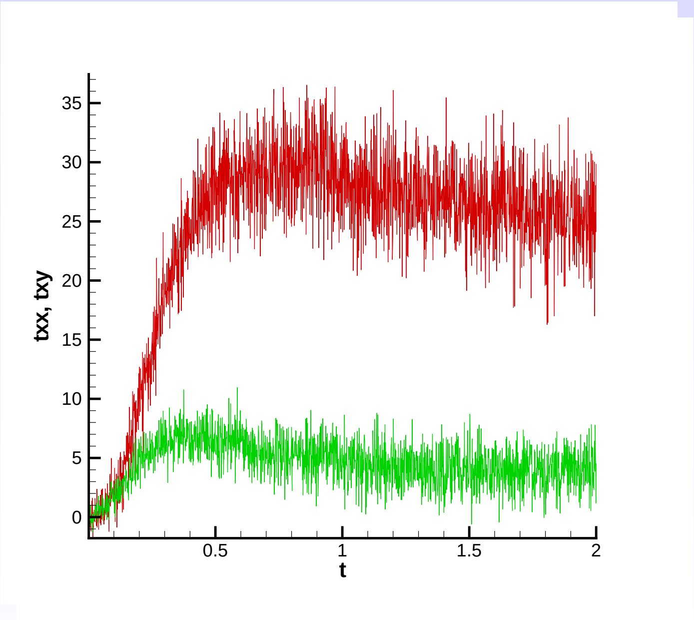
$$\int_{\partial D} Q \otimes Q\psi ds = \int_{R-a<|Q|<R} \frac{R^2}{|Q|^2} Q \otimes Q \frac{2(R-|Q|)}{a^2(R-a/2-b(\theta)aR/2)}\psi(Q)dQ$$
$$+O(a^2)$$

Take $a = \sqrt{h}$ and approximate the stress by

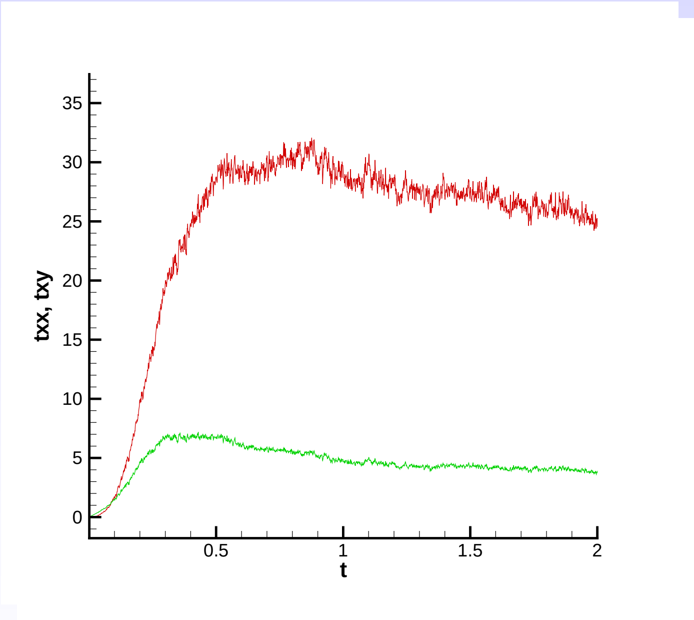
$$\tau^h(t_n) = \frac{{}'\,p}{\lambda}\mathbb{E}\Big(\mathbf{Q}^h_{t_n} \otimes \mathbf{Q}^h_{t_n}$$
$$\Big(1 + 1_{|Q^h_{t_n}|>R-\sqrt{h}} \frac{2(R-|Q^h_{t_n}|)}{h(R-\sqrt{h}/2-b(Q^h_{t_n})\sqrt{h}R/2)} \frac{R^2}{|Q^h_{t_n}|^2}\Big) - I\Big)$$

Results of simulations

$$\lambda = {}'_p = 1,\ b = 20,\ \kappa(t) = \begin{pmatrix} 0 & 10 \\ 0 & 0 \end{pmatrix}, \Delta t = 0.001, M = 5000$$

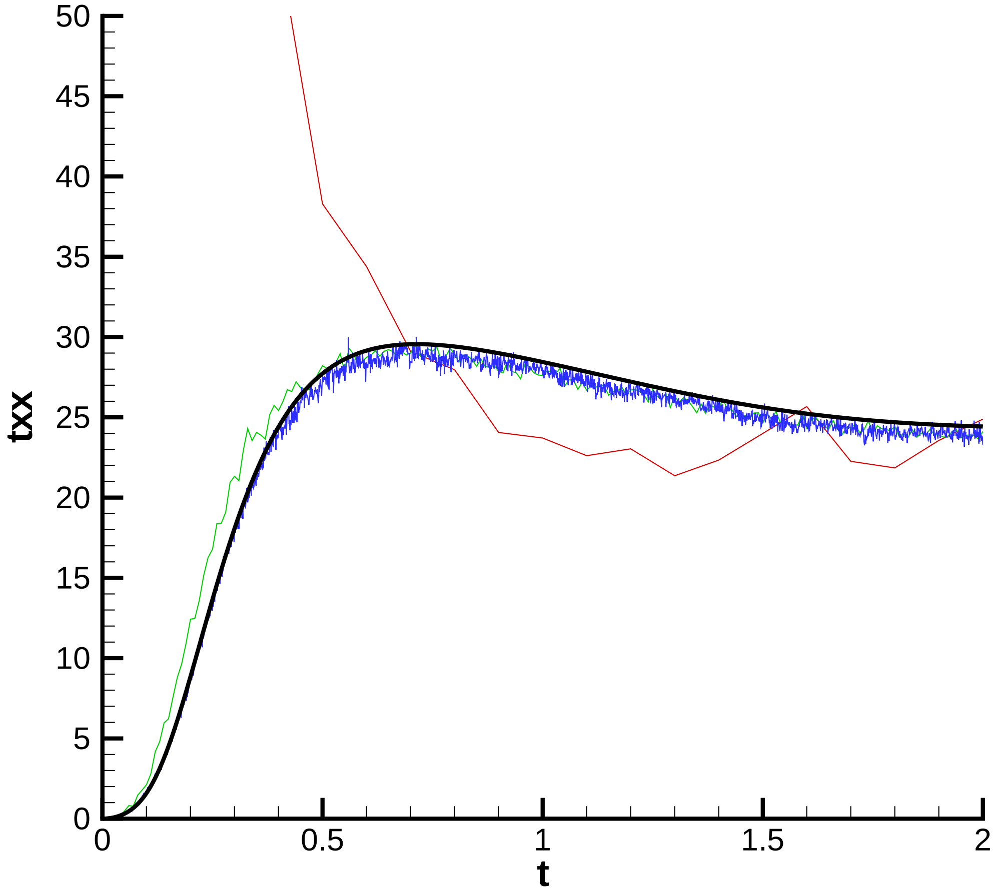


0th-order approximation



1st-order approximation

Convergence of the stochastic simulations by symmetric reflection



$\lambda = {}'_p = 1$

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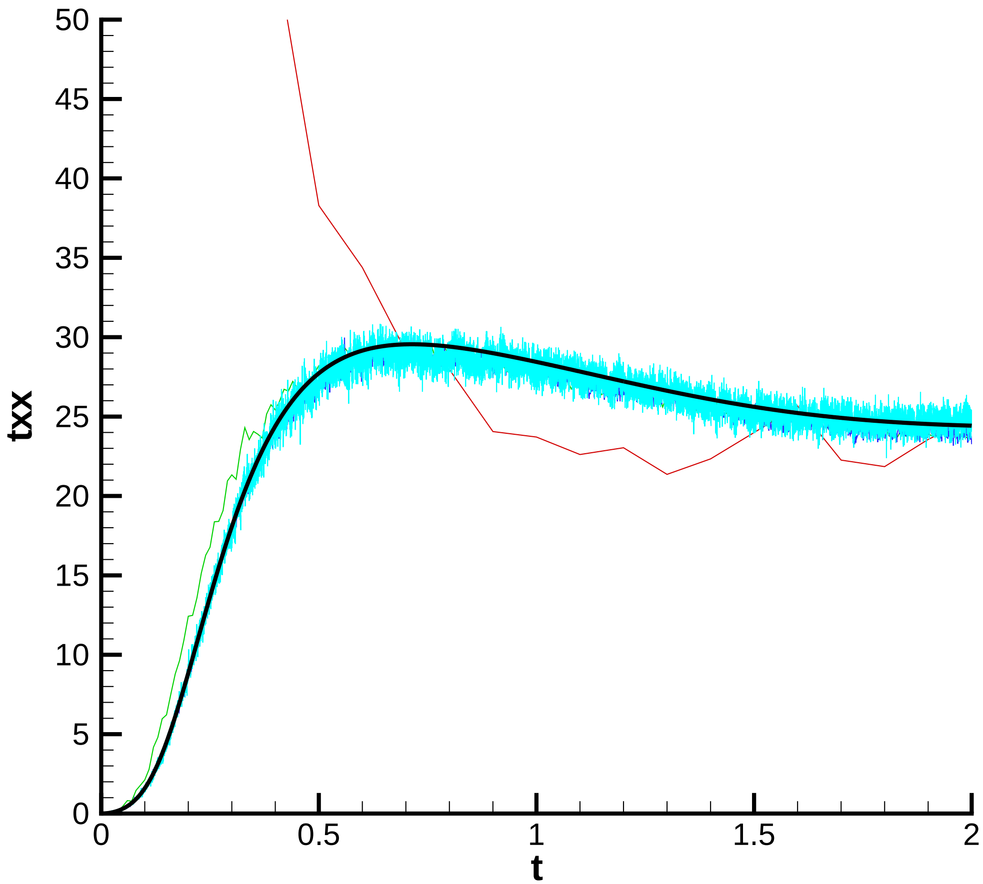
Convergence to the correct solution

Convergence of the stochastic simulations by symmetric reflection



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Too much noise with small Δt

An algorithm by half-space approximation

D. Lepingle (1995), E. Gobet (2001)

Going from $Q^h_{t_n}$ to $Q^h_{t_{n+1}}$:

• Set $\Pi_n = \pi_{\partial D}(Q^h_{t_n})$ and approximate the domain D by the half-space $\{z \in \mathbb{R}^d : (z - \Pi_n) \cdot \mathbf{n}(\Pi_n) < 0\}$

• Use the exact solution for the diffusion reflected in the half-space

$$\tilde{Q}^h_{t_{n+1}} - Q^h_{t_n} = \left(\kappa Q^h_{t_n} - \frac{1}{2\lambda} Q^h_{t_n}\right) h + \sqrt{\frac{1}{\lambda}}(B_{t_{n+1}} - B_{t_n}) - (\eta^h_{t_{n+1}} - \eta^h_{t_n})\mathbf{n}$$

where the increment of the local time is

$$\eta^h_{t_{n+1}} - \eta^h_{t_n} = \max\Bigg(0,$$
$$\sup_{0 \le s \le h} \left(Q^h_{t_n} + \left(\kappa Q^h_{t_n} - \frac{1}{2\lambda} Q^h_{t_n}\right) s + \sqrt{\frac{1}{\lambda}}(B_{t_n+s} - B_{t_n})\right) \cdot \mathbf{n} - R\Bigg)$$

The algorithm (continued)

the supremum is equivalent in law to

$$\sup_{0 \leq s \leq h} a \cdot \widetilde{B}_s + cs \sim \frac{1}{2}(a \cdot B_h + ch + \sqrt{|a|^2 V + (a \cdot \widetilde{B}_h + ch)^2}$$

where $\widetilde{B}_s = B_{t_n+s} - B_{t_n}$ and V is an random variable exponentially distributed with rate $\frac{1}{2h}$ and independent of $\widetilde{B}_h$.

• If the half-space approximation was not accurate enough, i.e. $|\widetilde{Q}^h_{t_{n+1}}| > R$, set

$$Q^h_{t_{n+1}} = \frac{R}{|Y^{\Delta t}_{n+1}|} \widetilde{Q}^h_{t_{n+1}},$$

otherwise $Q^h_{t_{n+1}} = \widetilde{Q}^h_{t_{n+1}}$.

Approximation of the stress

We have the convergence of order h for the functionals of Q_t and η_t

$$\mathbb{E}(f(Q_t) + \int_0^t g(Q_t) d\eta_t) =$$
$$\mathbb{E}(f(Q^h_{t_n}) + \sum_{i=0}^{n-1} g(\pi_{\partial D}(Q^h_{t_i}))(\eta^h_{t_{i+1}} - \eta^h_{t_i} + |\tilde{Q}^h_{t_{i+1}} - Q^h_{t_{i+1}}|) + O(h)$$

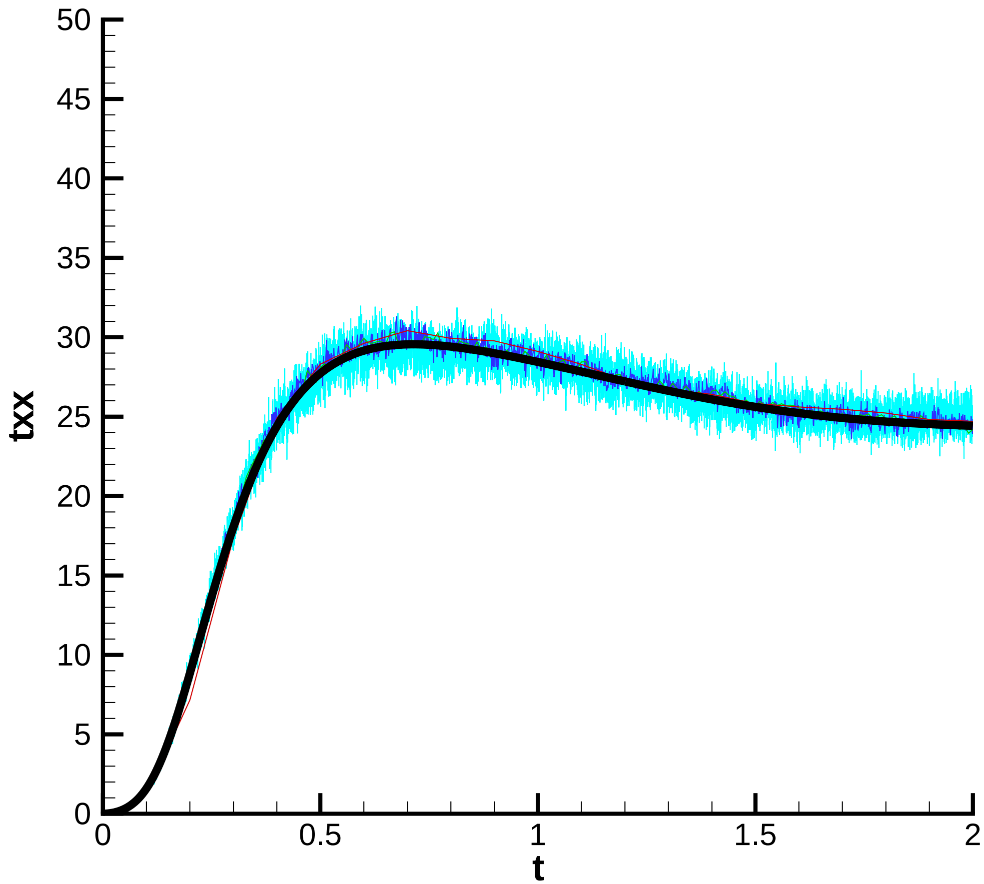
but the formula for the stress τ includes a derivative of the local time:

$$\tau(t) = \frac{\eta_p}{\lambda}\left(\mathbb{E}(Q_t \otimes Q_t) + \frac{2\lambda}{R}\frac{\mathbb{E}(Q_t \otimes Q_t d\eta_t)}{dt} - I\right)$$

We approximate the stress by

$$\tau^h(t_n) = \frac{\eta_p}{\lambda}\Big(\mathbb{E}(Q^h_{t_n} \otimes Q^h_{t_n})$$
$$+ \frac{2\lambda}{Rh}\mathbb{E}(\pi_{\partial D}(Q_t) \otimes \pi_{\partial D}(Q_t)(\eta^h_{t_n} - \eta^h_{t_{n-1}} + |\tilde{Q}^h_{t_n} - Q^h_{t_n}|) - I\Big)$$

Convergence of the stochastic simulations



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Convergence to the correct solution with less noise

Possible connection with FENE

Reminder:

$$dQ_t = \left(\kappa Q_t - \frac{1}{2\lambda}\frac{Q_t}{1-|Q_t|^2/b}\right)dt + \sqrt{\frac{1}{\lambda}}dB_t$$

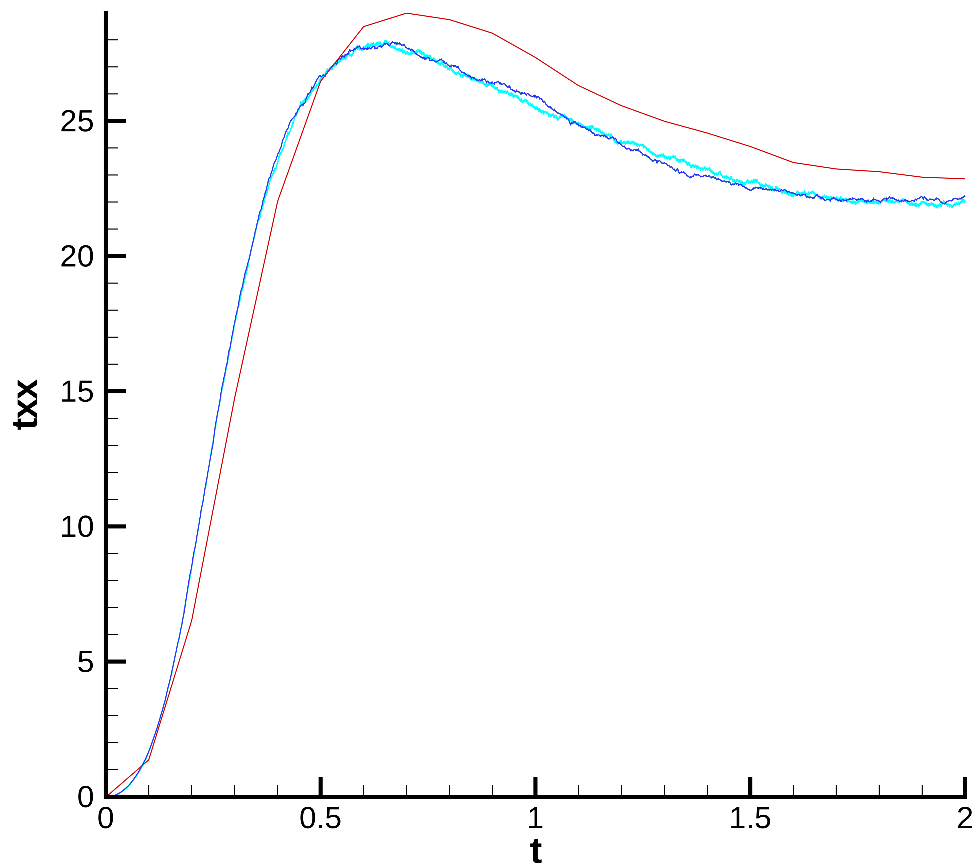
HC Ottinger discreization in time

$$Q^h_{t_{n+1}} + \frac{h}{2\lambda}\frac{Q^h_{t_{n+1}}}{1-|Q^h_{t_{n+1}}|^2/b} = \kappa Q^h_{t_n} h + \sqrt{\frac{1}{\lambda}}\Delta B_{t_n}$$

$$\tau^h(t_n) = \frac{'_p}{\lambda}\mathbb{E}(\left(Q^h_{t_n} \otimes \frac{Q^h_{t_{n+1}}}{1-|Q^h_{t_{n+1}}|^2/b}\right)$$

One can apply the same ideas as above to prove the boundedness of τ^h and possible the convergence of τ^h to τ

Convergence of the stochastic simulations for FENE



$\lambda = {}'_p = 1$

$b = 20$

$\kappa(t) = \begin{pmatrix} 0 & 10 \\ 0 & 0 \end{pmatrix}$

$M = 25000$

Red $- \ \Delta t = 0.1$

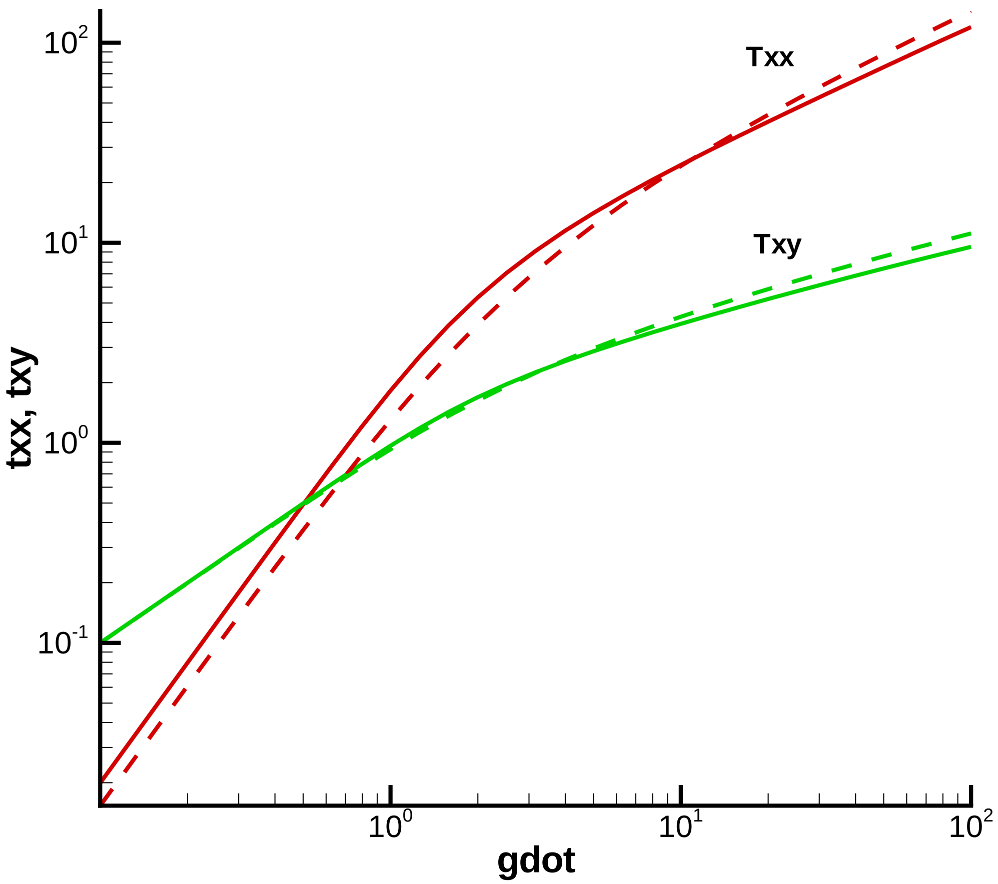
Green $- \ \Delta t = 0.01$

Blue $- \ \Delta t = 0.001$

Cyan $- \ \Delta t = 0.0001$

Convergence to the correct solution with less noise

Constrained Hookean vs FENE (steady state shear flow)



$\lambda = \eta_p = 1$

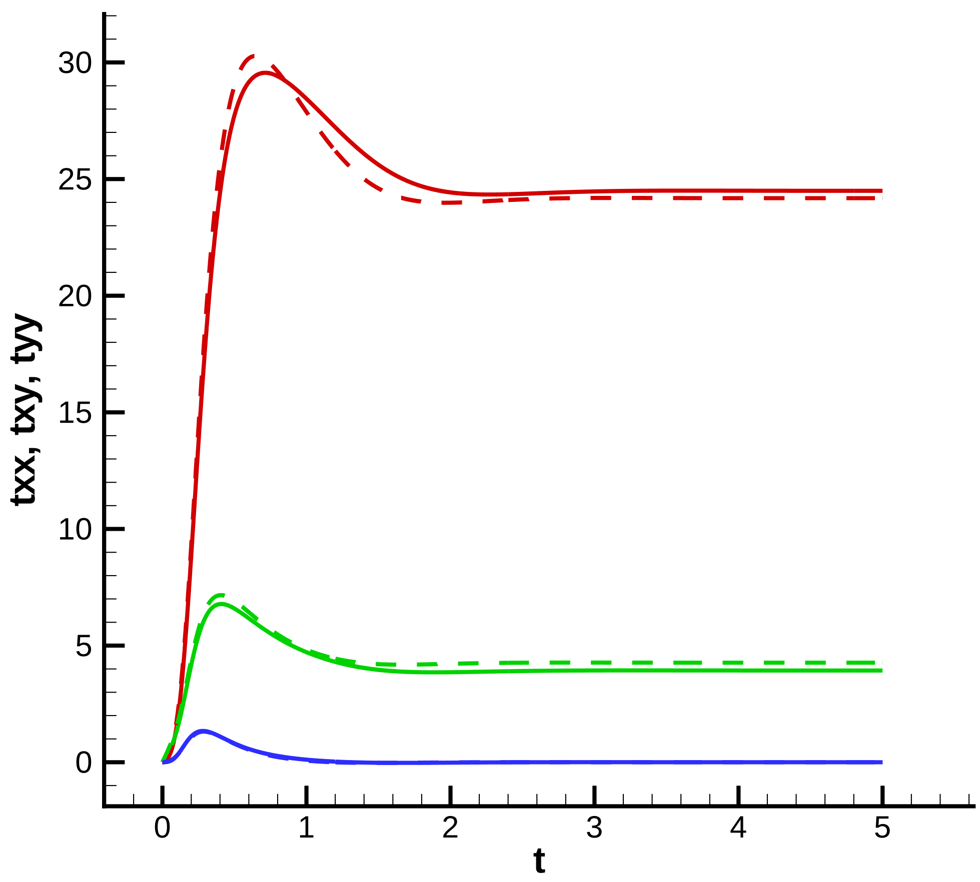
$b = 20$

$$\kappa(t) = \begin{pmatrix} 0 & \dot{\gamma} \\ 0 & 0 \end{pmatrix}$$

Solid - Cons. Hook.
Dashed - FENE

FP steady-state simulations

Constrained Hookean vs FENE (shear flow)



$\lambda = \eta_p = 1$

$b = 20$

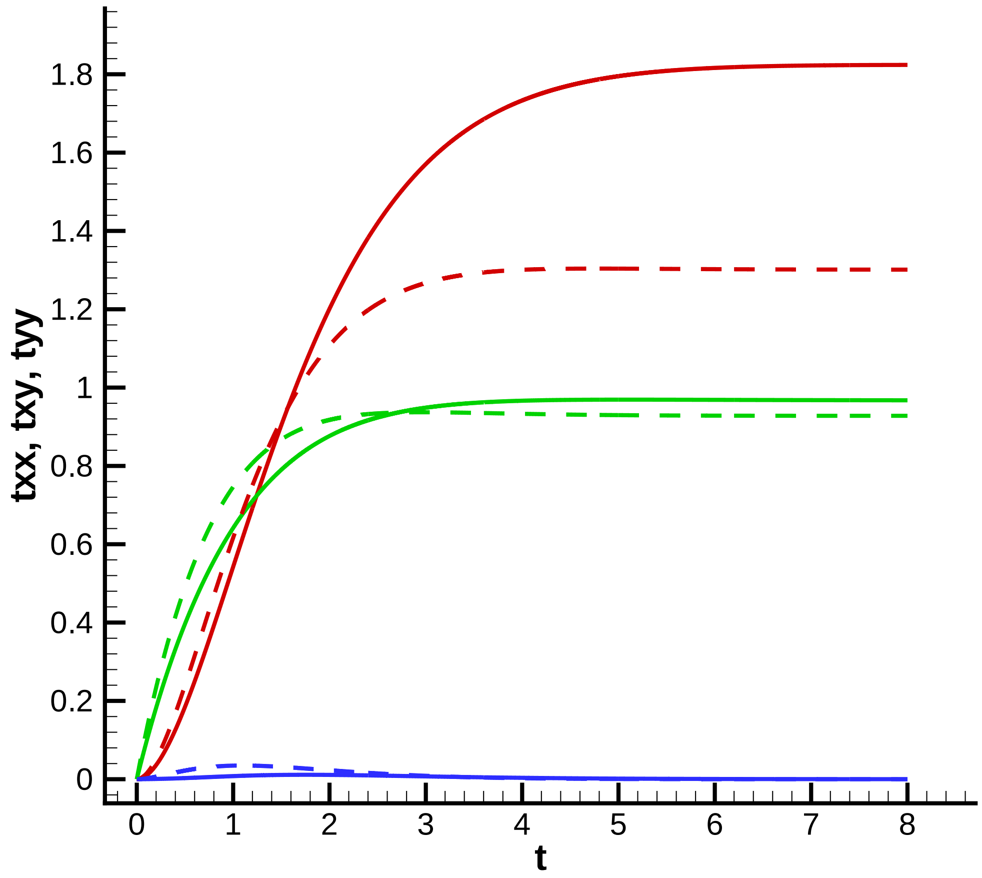
$$\kappa(t) = \begin{pmatrix} 0 & 10 \\ 0 & 0 \end{pmatrix}$$

Solid - Cons. Hook.

Dashed - FENE

FP transient simulations

Constrained Hookean vs FENE (shear flow)



$\lambda = \eta_p = 1$

$b = 20$

$\kappa(t) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

Solid - Cons. Hook.

Dashed - FENE

FP transient simulations