shake your hips
an active particle with a fluctuating propulsion force

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Physical Review E 106, L012603, 2022

Math Colloquium
NJIT, 23 September 2022
Langevin equations for the 2D active Brownian particle (ABP) model:

\[
\begin{align*}
\dot{x} &= (U_{\text{swim}} + \sqrt{2D_{\parallel}} \dot{w}_{\parallel}) p_{\parallel}(\phi) + \sqrt{2D_{\perp}} p_{\perp}(\phi) \dot{w}_{\perp}, \\
\dot{\phi} &= \Omega + \sqrt{2D_{r}} \dot{w}_{r}.
\end{align*}
\]

- Translational noises \(\sqrt{2D_{\parallel}} \dot{w}_{\parallel}\) and \(\sqrt{2D_{\perp}} \dot{w}_{\perp}\) are respectively along \((p_{\parallel})\) and perpendicular \((p_{\perp})\) to the direction of swimming.
- The rotational noise \(\sqrt{2D_{r}} \dot{w}_{r}\) affects the swimming direction.
- \(w_{i}(t)\) are independent standard Wiener processes.

[Peruani & Morelli (2007); van Teeffelen & Löwen (2008); Baskaran & Marchetti (2008); Romanczuk & Schimansky-Geier (2011); Romanczuk et al. (2012); Kurzthaler et al. (2016); Kurzthaler & Franosch (2017); Ai et al. (2013); Solon et al. (2015); Zöttl & Stark (2016); Wagner et al. (2017); Redner et al. (2013); Stenhammar et al. (2014); Chen & Thiffeault (2021)]
How do we derive the ABP model? Easy enough (it seems).

Particle subjected to a fluctuating force (e.g. flagellum)

\[ f(\phi, t) = (F_\parallel + \sqrt{2E_\parallel} \dot{w}_\parallel) \mathbf{p}_\parallel(\phi) + (F_\perp + \sqrt{2E_\perp} \dot{w}_\perp) \mathbf{p}_\perp(\phi) \]

acting at the point \( \ell \mathbf{p}_\parallel \) with respect to the center of reaction [Happel & Brenner (1983)] satisfies, after neglecting some terms,

\[ m \ddot{\mathbf{u}} = -K \cdot \mathbf{u} + f, \quad I \ddot{\omega} = -\sigma_\mathbf{r} \omega + \tau, \]

where \( K = Q \cdot \text{diag}(\sigma_\parallel, \sigma_\perp) \cdot Q^\top \) is the resistance matrix, with \( Q(\phi) \) a 2 × 2 rotation matrix.

The force exerts a torque \( \tau(t) = \ell (F_\perp + \sqrt{2E_\perp} \dot{w}_\perp) \).
A sample trajectory

**standard ABP with independent rotational noise:**

\[ U_{\text{swim}} = 1, \quad \Omega = 0, \quad m = I = .05, \]
\[ \sigma_\parallel = 0.5, \quad \sigma_\perp = E_\perp = \sigma_r = \ell = 1, \]
\[ E_\parallel = 0. \]

play movie
We rewrite the system in the standard SDE form drift + noise:

\[
\begin{align*}
\frac{d\hat{x}}{dt} &= \hat{u}, \\
\frac{d\hat{u}}{dt} &= \hat{B} \cdot (\hat{U} - \hat{u}) + \hat{\Sigma}(\hat{x}) \cdot \dot{w}
\end{align*}
\]

where

\[
\hat{x} = (x, \phi), \quad \hat{u} = (u, \omega), \quad \dot{w} = (\dot{w}_\parallel, \dot{w}_\perp)
\]

\[
\hat{B} = \text{diag}(\frac{K}{m}, \frac{\sigma_r}{I}), \quad \hat{U} = (U_{\text{swim}}, \Omega) = (\frac{K^{-1}}{} \cdot F, \ell F_\perp / \sigma_r),
\]

\[
\hat{\Sigma} = \begin{pmatrix}
(\sqrt{2}E_\parallel / m) p_\parallel & (\sqrt{2}E_\perp / m) p_\perp \\
0 & \sqrt{2}E_\perp \ell / I
\end{pmatrix}.
\]

The third components of vectors and matrices wearing a hat pertain to angular quantities. ("grand")
Typically, in the overdamped limit (small mass, or large drag) the term $d\hat{u}/dt$ is neglected,

\[
\frac{d\hat{x}}{dt} = \hat{u}, \quad \frac{d\hat{u}}{dt} = \hat{B} \cdot (\hat{U} - \hat{u}) + \hat{\Sigma} \cdot \hat{w}
\]

resulting in

\[
\frac{d\hat{x}}{dt} = \hat{U} + (\hat{B}^{-1} \cdot \hat{\Sigma}) \cdot \hat{w}.
\]

Close to the standard ABP model, except that here there are only two ($\dot{\mathbf{w}}||, \dot{\mathbf{w}}_\perp$) rather than three ($\dot{\mathbf{w}}||, \dot{\mathbf{w}}_\perp, \dot{\mathbf{w}}_r$) independent noises:

The rotational noise is correlated to the translational noise, since the former is caused by the torque of the latter. We will see the consequences of this correlation later.
But first note that taking the overdamped limit in this way is suspicious, since the original noise is additive:

\[
\frac{d\hat{x}}{dt} = \hat{u}, \quad \frac{d\hat{u}}{dt} = \hat{B} \cdot (\hat{U} - \hat{u}) + \hat{\Sigma}(\hat{x}) \cdot \dot{w}
\]

in the sense that there is no Itô vs Stratonovich ambiguity in interpretation, whereas

\[
\frac{d\hat{x}}{dt} = \hat{U} + \hat{B}^{-1} \cdot \hat{\Sigma}(\hat{x}) \cdot \dot{w}.
\]

has a multiplicative noise.

[Kupferman et al. (2004); Lau & Lubensky (2007); Farago (2017)]

Care is thus required in taking the overdamped limit...
Fokker–Planck equation

\[
\frac{d\hat{x}}{dt} = \hat{u}, \quad \frac{d\hat{u}}{dt} = \hat{B} \cdot (\hat{U} - \hat{u}) + \hat{\Sigma}(\hat{x}) \cdot \hat{w}
\]

Safer approach: we take the overdamped limit of the Fokker–Planck equation for the probability density \( p(\hat{x}, \hat{u}, t) \) corresponding to our SDE [Kupferman et al. (2004); Bo & Celani (2013); Pavliotis (2014); Hottovy et al. (2014)]:

\[
\varepsilon^2 \partial_t p + \varepsilon \nabla \hat{x} \cdot (\hat{u} p) + \varepsilon \nabla \hat{u} \cdot (\hat{B} \cdot \hat{U} p) = \mathcal{L} p
\]

where \( \varepsilon \to 0 \) is the overdamped limit, and

\[
\mathcal{L} p := \nabla \hat{u} \cdot (\hat{B} \cdot \hat{u} p) + \nabla \hat{u} \otimes \nabla \hat{u} : (\hat{E} p)
\]

with \( \hat{E} := \frac{1}{2} \hat{\Sigma} \cdot \hat{\Sigma}^\top \).

Now we proceed order-by-order with an expansion \( p = p_0 + \varepsilon p_1 + \cdots \).
At leading order we have

\[ \mathcal{L}p_0 = 0, \quad \text{with solution} \quad p_0 = P(\hat{x}, t) \varphi(\hat{x}, \hat{u}) \]

where \( P \) is yet to be determined and \( \varphi(\hat{x}, \hat{u}) \) is the invariant density for an Ornstein–Uhlenbeck process [Risken (1996)]:

\[
\varphi = (2\pi)^{-3} (\det \hat{A})^{-1/2} \exp \left( -\frac{1}{2} \hat{u} \cdot \hat{A}^{-1} \cdot \hat{u} \right).
\]

Here the symmetric positive-definite matrix \( \hat{A}(\hat{x}) \) is the unique solution to the continuous-time Lyapunov (Sylvester) equation

\[
\hat{B} \cdot \hat{A} + \hat{A} \cdot \hat{B}^\top = 2\hat{E}.
\]

For us \( \hat{B} = \hat{B}^\top \). When \( \hat{B} \) commutes with \( \hat{E} \), as occurs for thermal fluctuations, the solution is \( \hat{A} = \hat{E} \cdot \hat{B}^{-1} \); this is not the case here.
Covariance matrix $\hat{A}$

$$\hat{B} \cdot \hat{A} + \hat{A} \cdot \hat{B}^\top = 2\hat{E}$$

The solution of this matrix problem is implemented as `LyapunovSolve` in Mathematica, `sylvester` in Matlab, and `solve_continuous_lyapunov` in Python.

We find

$$\hat{A} = \hat{Q} \cdot \begin{pmatrix} \frac{E_\parallel}{m\sigma_\parallel} & 0 & 0 \\ 0 & \frac{E_\perp}{m\sigma_\perp} & \frac{2E_\perp \ell}{m\sigma_r + I\sigma_\perp} \\ 0 & \frac{2E_\perp \ell}{m\sigma_r + I\sigma_\perp} & \frac{E_\perp \ell^2}{I\sigma_r} \end{pmatrix} \cdot \hat{Q}^\top$$

where $\hat{Q}(\phi) = \text{diag}(Q, 1)$ is a $3 \times 3$ rotation matrix about the third axis.
\[ \mathcal{L} p_1 = \nabla \hat{x} \cdot (\hat{u} \varphi P) - \hat{u} \cdot \hat{A}^{-1} \cdot \hat{B} \cdot \hat{U} \varphi P. \]

The solution can be written in two pieces \( p_1 = p_1^{(1)} + p_1^{(2)} \), with

\[
\begin{align*}
p_1^{(1)} &= (\nabla \hat{x} P - \hat{U} \cdot \hat{B}^\top \cdot \hat{A}^{-1} P) \cdot \hat{\chi}^{(1)} \\
p_1^{(2)} &= -\frac{1}{2} P \nabla \hat{x} \hat{A}^{-1} : \hat{\chi}^{(2)},
\end{align*}
\]

where \( \hat{\chi}^{(1)} \) and \( \hat{\chi}^{(2)} \) satisfy

\[
\mathcal{L} \hat{\chi}^{(1)} = \hat{u} \varphi, \quad \mathcal{L} \hat{\chi}^{(2)} = \hat{u} \hat{u} \hat{u} \varphi.
\]

It is easy to solve for \( \hat{\chi}^{(1)} = -\hat{A} \cdot \hat{B}^{-\top} \cdot \hat{A}^{-1} \cdot \hat{u} \varphi \);

\( \hat{\chi}^{(2)} \) is harder to solve for in general.

However, we shall not need its precise expression in our derivation.
Order $\varepsilon^2$ (the last one)

\[ \mathcal{L}_p^2 = \nabla \hat{x} \cdot (\hat{u}_p^1) + \nabla \hat{u} \cdot (\hat{B} \cdot \hat{U}_p^1) + \partial_t p_0, \]
to which we need only apply a solvability condition by integrating over $\hat{u}$ (denoted by angle brackets):

\[ \partial_t P = -\nabla \hat{x} \cdot \langle \hat{u} p_1 \rangle. \]

There is a trick based on the adjoint of $\mathcal{L}$ that can be used to evaluate the averages

\[ \langle \hat{u} \hat{\chi}^{(1)} \rangle = -\hat{B}^{-1} \cdot \langle \hat{u} \hat{u} \varphi \rangle = -\hat{B}^{-1} \cdot \hat{A} \]

\[ \langle \hat{u} \hat{\chi}^{(2)} \rangle = -\hat{B}^{-1} \cdot \langle \hat{u} \hat{u} \hat{u} \varphi \rangle \]

where the fourth moment for the Gaussian $\varphi$

\[ \langle \hat{u} \hat{u} \hat{u} \hat{u} \varphi \rangle_{ijkl} = \hat{A}_{ij} \hat{A}_{kl} + \hat{A}_{ik} \hat{A}_{jl} + \hat{A}_{il} \hat{A}_{jk}. \]

We have thus evaluated the required average $\langle \hat{u} \hat{\chi}^{(2)} \rangle$ without needing to solve for $\hat{\chi}^{(2)}$. 
The overdamped Fokker–Planck equation

After a lengthy but straightforward calculation we find

\[
\frac{\partial}{\partial t} P + \nabla_x \cdot \left( (U_{\text{swim}} + V_{\text{noise}}) P \right) + \partial \phi(\Omega P) = \nabla \hat{x} \otimes \nabla \hat{x} : (\hat{D} P)
\]

where the noise-induced drift [Grassia et al. (1995); Lau & Lubensky (2007); Hottovy et al. (2012a,b, 2014); Volpe & Wehr (2016); Farago (2017)] is

\[
V_{\text{noise}} = \frac{2\ell E_\perp (\sigma^{-1}_\parallel - \sigma^{-1}_\perp)}{\sigma_r (1 + I \sigma_\perp / m \sigma_r)} \mathbf{p}_\parallel
\]

and the translational-rotational grand diffusion tensor is

\[
\hat{D} = \hat{Q} \cdot \begin{pmatrix} D_\parallel & 0 & 0 \\ 0 & D_\perp & \sqrt{D_\perp D_r} \\ 0 & \sqrt{D_\perp D_r} & D_r \end{pmatrix} \cdot \hat{Q}^\top
\]

with \(D_\parallel = E_\parallel / \sigma^2_\parallel\), \(D_\perp = E_\perp / \sigma^2_\perp\), and \(D_r = E_\perp \ell^2 / \sigma^2_r\).
The noise-induced drift $V_{\text{noise}}$

$$V_{\text{noise}} = \frac{2\ell E_{\perp}(\sigma_{\parallel}^{-1} - \sigma_{\perp}^{-1})}{\sigma_{r}(1 + I\sigma_{\perp}/m\sigma_{r})} p_{\parallel}$$

$V_{\text{noise}} \neq 0$ implies that the particle appears to swim at a constant speed, even for $U_{\text{swim}} = 0$ (no net propulsion), and even for small mass.

$V_{\text{noise}}$ is only present when the fluctuating force exerts a torque; it is an inertial effect that vanishes for isotropic particles ($\sigma_{\parallel} = \sigma_{\perp}$).

Péclet numbers based on the advective time $a/|V_{\text{noise}}|$ and diffusive times $a^2/D_{\perp}$ and $1/D_{r}$, with $a$ the particle size:

$$\text{Pe}_{\perp} = \frac{|V_{\text{noise}}|a}{D_{\perp}} \sim \frac{\ell}{a}, \quad \text{Pe}_{r} = \frac{|V_{\text{noise}}|}{D_{r}a} \sim \frac{a}{\ell}.$$

$\text{Pe}_{\perp}$ is not large, but also not necessarily small. $\text{Pe}_{r}$ is a dimensionless correlation length that diverges as $\ell \to 0$, since the rotational diffusivity $D_{r}$ then vanishes.
The long-time effective diffusivity

There are two new effects compared to standard ABP:

- The noise-induced drift $V_{\text{noise}}$ (for $\sigma_\parallel \neq \sigma_\perp$);
- The coupling terms $\sqrt{D_\perp D_r}$ in the grand diffusion tensor $\hat{D}$.

One way to see their repercussion is to compute the long-time effective diffusivity of the active particle.

Recall the overdamped Fokker–Planck equation for $P(\hat{x}, t)$ is

$$\partial_t P + W_i \partial_{x_i} P + \Omega \partial_{\phi} P =$$

$$\partial_{x_i} \partial_{x_j} (D_{ij} P) + 2\partial_{x_i} \partial_{\phi} (\hat{D}_{i3} P) + \partial_{\phi}^2 (D_r P)$$

where $W = U_{\text{swim}} + V_{\text{noise}} = W p_\parallel$ is the total drift, and indices are summed over 1, 2.
To find the effective diffusivity, we focus on large scales $\delta^{-1} \sim \ell^{-1}$ and long times $\delta^{-2}$, with $\delta$ a small parameter.

We let

$$\partial_t \to \partial_t + \delta^2 \partial_T, \quad \partial_x \to \partial_x + \delta \partial_X$$

and expand

$$P = \mathcal{P}(X, T) + \delta P_1(\phi; X, T) + \delta^2 P_2(\phi; X, T) + \cdots,$$

where we anticipated the functional dependencies to abridge the derivation.

**Article $\varepsilon^3$ of Geneva convention:** “Only one asymptotic expansion is allowed in a talk, and it shall be limited to second order.” So I will skip the details.
Cut to the chase: at order $\delta^2$ we have the solvability condition

$$
\partial_T \mathcal{P} = \left\langle W_i \left( W_j - 2 \partial_\phi \hat{D}_{j3} \right)/D_r + D_{ij} \right\rangle \partial_{X_i} \partial_{X_j} \mathcal{P} =: D_{\text{eff}} \nabla^2_X \mathcal{P} \quad \text{(isotropic)}
$$

where angle brackets are repurposed for angular averaging, and the effective diffusivity is (recall: $W = U_{\text{swim}} + V_{\text{noise}}$)

$$
D_{\text{eff}} = \frac{1}{2} (D_\parallel + D_\perp) + \tilde{D}
$$

$$
\tilde{D} := \frac{WD_r}{2(D_r^2 + \Omega^2)} \left( W + \frac{2E_\perp \ell}{\sigma_\perp \sigma_r} \right).
$$

Compare to $\tilde{D}$ for the standard ABP model,

$$
\frac{U_{\text{swim}}^2 D_r}{2(D_r^2 + \Omega^2)}
$$

[Howse et al. (2007); Peruani & Morelli (2007); Lindner & Nicola (2008); Golestanian (2009); Fodor et al. (2016); Caprini & Marconi (2021)].
Effective diffusivity for wiggler (non-swimmer)

The new diffusivity \( \tilde{D} \) combines contributions from the propulsion \( U_{\text{swim}} \), the noise-induced drift \( V_{\text{noise}} \), and from the coupling terms in \( \hat{D} \).

To best see these new effects, we set \( U_{\text{swim}} = \Omega = D_\parallel = 0 \): the particle is “shaking its hips” but would be a non-swimmer if not for the noise-induced drift.

A wiggler? But maybe the field has enough cute names.

[Similar to a “treadmiller” or reciprocal swimmer that doesn’t strictly swim, but only diffuses; see Crowdy & Or (2010); Lauga (2011); Obuse & Thiffeault (2012).]

For the wiggler:

\[
\tilde{D}_0 = \frac{2D_\perp(1 + I\sigma_\parallel/m\sigma_r)}{(1 + I\sigma_\perp/m\sigma_r)^2} \frac{\sigma_\perp}{\sigma_\parallel} \left( \frac{\sigma_\perp}{\sigma_\parallel} - 1 \right).
\]

Negative for particles with \( \sigma_\perp < \sigma_\parallel \) (oblate), so that it hinders diffusion.
A prolate wiggler ($\sigma_\parallel < \sigma_\perp$) has an enhanced diffusivity compared to a passive particle. [Possibly related to an effect observed by Lauga (2011)].

Wiggler ($\mathbf{U}_{\text{swim}} = \Omega = 0$); $m = I = 0.05$, $\sigma_\parallel = 0.5$, $\sigma_\perp = E_\perp = \sigma_r = \ell = 1$, $E_\parallel = 0$. 
An oblate wiggler ($\sigma_\parallel > \sigma_\perp$) has a **reduced** diffusivity compared to a passive particle.

Similar reduced diffusivity observed for ABP with $\Omega \neq 0$, due to “over-rotating.” [See also the flipping rod of Takagi et al. (2013)].

Wiggler ($U_{\text{swim}} = \Omega = 0$); $m = I = .05$, $\sigma_\parallel = 2$, $\sigma_\perp = E_\perp = \sigma_r = \ell = 1$, $E_\parallel = 0$. 
$D_{\text{eff}}$ for the wiggler: The neutral wiggler

With $U_{\text{swim}} = D_{\parallel} = 0$, the effective diffusivity is

$$D_{\text{eff}0} = \tilde{D}_0 + \frac{1}{2}D_{\perp} = D_{\perp} \left(\frac{\sigma_{\parallel} - 2\sigma_{\perp} - I\sigma_{\parallel}\sigma_{\perp}/m\sigma_r}{2\sigma_{\parallel}^2(1 + I\sigma_{\perp}/m\sigma_r)^2}\right)^2 \geq 0.$$  

$D_{\text{eff}0}$ attains a minimum of zero for

$$\sigma_{\perp} = \sigma_{\parallel}/(2 + I\sigma_{\parallel}/m\sigma_r) < \sigma_{\parallel} \quad \text{(oblate)}.$$  

A particle satisfying this relation is a **neutral active particle** that can only diffuse via $D_{\parallel}$ and thermal noise.

Note that swimmers are rarely oblate, but perhaps synthetic active particles can be manufactured this way.
The neutral wiggler

Indeed, we can see that a neutral wiggler is going nowhere, though it may “diffuse” on very long timescales:

Wiggler \((U_{\text{swim}} = \Omega = 0)\).

Parameter values: \(m = I = .05, \sigma_\parallel = 0.5, \sigma_\perp = 0.2, E_\perp = \sigma_r = \ell = 1, E_\parallel = 0\).
Another striking feature of the effective diffusivity $\tilde{D}_0$ is that it is independent of $\ell$, the position where the torque is applied:

$$\tilde{D}_0 = \frac{2D_\perp (1 + I\sigma_\parallel/m\sigma_r)}{(1 + I\sigma_\perp/m\sigma_r)^2} \frac{\sigma_\perp}{\sigma_\parallel} \left(\frac{\sigma_\perp}{\sigma_\parallel} - 1\right).$$

This is a paradox: for $\ell = 0$, we have $V_{\text{noise}} = 0$ and $\hat{D}_{i3} = 0$, so none of the effects mentioned here occur!

The resolution is that there is a transient of duration

$$D^{-1}_r = \sigma_r^2/E_\perp \ell^2 \sim \delta^{-2}$$

before the long-time form of $D_{\text{eff}}$ applies, and this transient becomes infinite as $\ell \rightarrow 0$. 

$D_{\text{eff}}$ for the wiggler as $\ell \to 0$

This transient can be seen in the simulations of the full inertial equations:

5,000 oblate wiggles ($U_{\text{swim}} = \Omega = 0$). Upper dotted line: $4 \times \frac{1}{2} (D_{\parallel} + D_{\perp})t$; Bottom dashed line: $4D_{\text{eff}}t$. As $\ell$ becomes smaller, there is a longer transient before the behavior begins to follow $D_{\text{eff}}$. Parameter values: $m = I = .05$, $\sigma_{\parallel} = 2$, $E_{\perp} = \sigma_{\perp} = \sigma_{r} = 1$, $E_{\parallel} = 0$. 

\[ \ell = 1/8 \]
\[ \ell = 1/4 \]
\[ \ell = 1 \]
$D_{\text{eff}}$ for the wiggler: relative size

$$\tilde{D}_0 = \frac{2D_\perp(1 + I\sigma_\parallel/m\sigma_r)}{(1 + I\sigma_\perp/m\sigma_r)^2} \frac{\sigma_\perp}{\sigma_\parallel} \left(\frac{\sigma_\perp}{\sigma_\parallel} - 1\right).$$

It is important to note that the ratio $\tilde{D}_0/D_\perp$ is rarely negligible: all the dimensionless ratios appearing on the right are typically of order one.

The transient time scale $D_r^{-1}$ can be estimated by $a^2/D_\perp$, where $a$ is the particle size; if $D_r^{-1}$ is very long, then $D_\perp$ was likely negligible to begin with.
Can these types of corrections be observed?

- Many authors simulate the ABP model directly, since the inertial equations are expensive to solve due the small step size required, in which case the new effects are ruled out.
- Particle anisotropy is seldom considered in the ABP model (though this is changing fast).
- Experimentally, diffusivities are measured directly from the distributions of displacements, and so any connection between the rotational and translational diffusivities is typically lost. One approach might be to measure the covariance matrix $\hat{A}$ directly. Do this in numerical simulations?
- Harder to observe if the swimmers are relatively fast, since the noise-induced effect is smaller.
A deterministic swimmer

Even easier to move forward if the fluctuating force is not random:

\[ A_0 = 0.5 \]

\[ A_0 = 1.0 \]

\[ A_0 = 1.8 \]

\[ A_0 = 5.3 \]

Some future work

- Arbitrary **three-dimensional** active particles, with the force not necessarily applied on an axis of symmetry. (Mostly done; quite messy. Is this why is the third Euler angle is rarely if ever considered?)
- There are several other possible extensions, such as the inclusion of multiple forces and torques acting on the body.
- Consequences to
  - swim pressure [Takatori et al. (2014); Takatori & Brady (2014)]
  - run-and-tumble dynamics [Subramanian & Koch (2009); Cates & Tailleur (2013)]
  - non-Newtonian swimming [Datt & Elfring (2019)]
  - velocity-dependent friction [Erdmann et al. (2000)]
  - and particle interactions [Fodor et al. (2016); Marath & Wettlaufer (2019)]?
- Deterministic version: Symmetry **14**, 620, 2022
References I


