Explicitly computable flock and mill states of self-propelled particles systems

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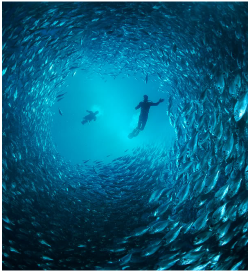
"Emergent behavior in multi-particle systems with non-local interactions"

Collective animal behavior

- Motivation: Understand the dynamics of emerging patterns in animal groups, such as swarms of birds, schools of fish, herds of sheep and many other.
- Similarity: Macroscopic structures arise from seemingly local interactions of individuals and in absence of leaders or global information.
- Our model type: Newtonian particles, pairwise interaction, short-range repulsion vs. long-range attraction. Able to reproduce aligned flocks and rotating mills.
- In this talk: Introduce *Quasi-Morse* interaction potentials, whose stationary states are explicitly computable up to linear coefficients



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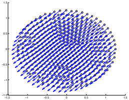
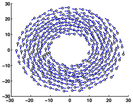
Self-propelled second-order interacting particle model

$$\frac{dx_i}{dt} = v_i \,,$$
$$\frac{dv_i}{dt} = \alpha v_i - \beta v_i |v_i|^2 - \nabla_{x_i} \sum_{i \neq j} W(x_i - x_j)\,.$$

$i \in \{1, \ldots, N\}$, α: propulsion force , β: friction force
$W(r) = U(|r|)$ interaction potential (with a local minimum)

- Standard choice: Morse potential $U(r) = -C_A e^{-r/l_A} + C_R e^{-r/l_R}$
  C_A, C_R attractive / repulsive strengths, l_A, l_R resp. length scales
- Aligned flocks and rotating mills are obtained





Kinetic equations

- Letting $N \to \infty$, with the weak-coupling scaling, the associated mean-field equation reads

Vlasov-like kinetic equation

$$\partial_t f + v \cdot \nabla_x f + F[\rho] \cdot \nabla_v f + \operatorname{div}\left(\left(\alpha - \beta |v|^2\right) v f\right) = 0\,,$$

$f(t,x,v) : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$: (one-particle) probability distribution function
$\rho(t,x) := \int f(t,x,v)\,\mathrm{d}v$.: macroscopic density
$F[\rho] = -\nabla_x W \star \rho$: interaction force

- Monokinetic ansatz: $f(t,x,v) = \rho(t,x)\,\delta(v - u(t,x))$, leads to

Hydrodynamic equations

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \operatorname{div}_x(\rho u) = 0, \\ \rho\,\dfrac{\partial u}{\partial t} + \rho\,(u \cdot \nabla_x) u = \rho\,(\alpha - \beta |u|^2) u - \rho\,(\nabla_x W \star \rho). \end{cases}$$

Characteristic equations

- Relevant radially symmetric stationary states of the system are written as

$$\text{Flock: } f_F(t,x,v) = \rho_F(x - tu_0)\,\delta(v - u_0)\,,\ |u_0| = \sqrt{\frac{\alpha}{\beta}}$$

$$\text{Mill: } f_M(t,x,v) = \rho_M(x)\,\delta\left(v - \pm\sqrt{\frac{\alpha}{\beta}}\frac{x^\perp}{|x|}\,,\right)$$

- Inserting into kinetic equations, we get the characteristic equations

$$\text{Flock: } W \star \rho_F = C \quad \text{in } B(0,R_F) = \operatorname{supp}(\rho_F)$$

$$\text{Mill: } W \star \rho_M = D + \frac{\alpha}{\beta}\log|x| \quad \text{in } B(R_m,R_M) = \operatorname{supp}(\rho_M)\,,$$

  where the support is a-priori unknown.

- Bertozzi, A.L. et. al.: State transitions and the continuum limit for a 2D interacting, self-propelled particle system.
  Carrillo, J.A. et. al. : Double milling in self-propelled swarms from kinetic theory.
  Levine, H. et. al. : Self-organization in systems of self-propelled particles.

  D'Orsogna et. al. Self-propelled particles with soft-core interactions.

Quasi-Morse potentials

Definition

Let $C, l, \lambda, k \in \mathbb{R}$ be positive parameters, then the Quasi-Morse potential is

$$U(r) := \lambda \left(V(r) - C\, V\left(\frac{r}{l}\right)\right) ,$$

where V is chosen dependent of the space dimension as

$$\begin{cases} n = 1: & V(r) = -\frac{1}{2k} e^{-kr} \\ n = 2: & V(r) = -\frac{1}{2\pi} K_0(kr) \\ n = 3: & V(r) = -\frac{1}{4\pi} \frac{e^{-kr}}{r} \end{cases}$$

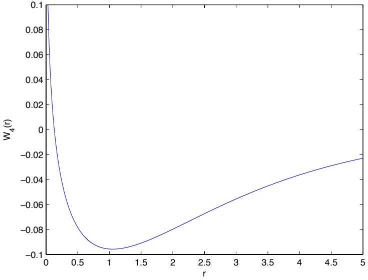
K_0 is the modified Bessel function of second kind. V are chosen as the radially symmetric, monotone fundamental solution of the *screened Poisson equation*

$$\boxed{\Delta u - k^2 u = \delta_0} ,$$

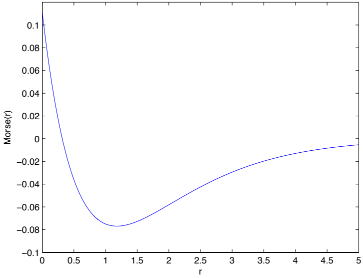
that vanish at infinity. For $n = 1$, we re-obtain the Morse potential.

An exemplary configuration

We illustrate the Quasi-Morse potential in comparison to Morse potential for $n = 2$:



(a) Quasi-Morse potential,
$C = \frac{10}{9}, l = 0.75, k = \frac{1}{2}, \lambda = 4$



(b) Morse potential,
$C = \frac{10}{9}, l = 0.75, k = 1, \lambda = 2$

$\Rightarrow$ Attraction-repulsion setting in both potentials. Different singularity at zero.
$\Rightarrow$ From modeling point-of-view, there is no reason to prefer one over the other.

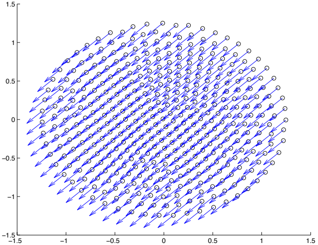
Properties

- The Quasi-Morse potential is H-stable for $Cl^n > 1$ and catastrophic for $Cl^n < 1$.
- Biologically relevant shapes, i.e. a unique minimum of the potential, are obtained for the following range of parameters:

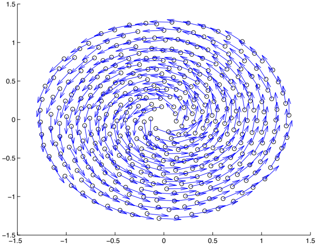
$$\begin{cases} n = 1 : & l < 1, l < C \\ n = 2 : & l < 1, C > 1 \\ n = 3 : & l < 1, Cl > 1 \end{cases}$$

Emerging patterns (2D)

Quasi-Morse potentials have the ability to produce coherent patterns just as the standard Morse potential:



Example 1: Flock, $N = 400$



Example 2: Mill, $N = 400$

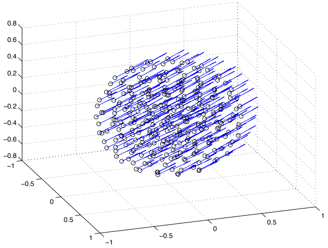
Movies will be available on my website

$C = \frac{10}{9}$	$k = \frac{1}{2}$	$l = \frac{3}{4}$
$\alpha = 1$	$\beta = 5$	$\lambda = 1000$

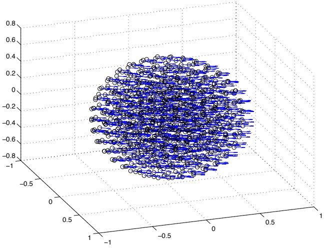
N = number of particles

Emerging patterns (3D)

We observe the emergence of aligned flocks for the three-dimensional Quasi-Morse potential:



Example 1: Flock, $N = 200$



Example 2: Flock, $N = 1000$

Movies will be available on my website

$C = 1.255$	$k = 0.2$	$l = 0.8$
$\alpha = 1$	$\beta = 5$	$\lambda = 1000$

N = number of particles

Computation

Define the operators $\mathcal{L}_1 := \Delta - k^2 I$, $\mathcal{L}_2 := \Delta - \frac{k^2}{l^2} I$ and consider the characteristic equation $(W \star \rho)(r) = s(r)$ on $\operatorname{supp}(\rho)$ with some radial $s(r)$. Then

$$\begin{aligned}
\mathcal{L}_2\mathcal{L}_1(W \star \rho) &= (\mathcal{L}_2\mathcal{L}_1 W) \star \rho = \lambda \left(-C\, \mathcal{L}_1\mathcal{L}_2 V\left(\frac{r}{l}\right) + \mathcal{L}_2\mathcal{L}_1 V(r) \right) \star \rho \\
&= \lambda \left(-Cl^{n-2}\Delta\delta + Ck^2 l^{n-2}\delta + \Delta\delta - \frac{k^2}{l^2}\delta \right) \star \rho \\
&= \lambda(1 - Cl^{n-2})\Delta\rho + \lambda \left(Ck^2 l^{n-2} - \frac{k^2}{l^2} \right) \rho = \mathcal{L}_2\mathcal{L}_1 s.
\end{aligned}$$

Hence, ρ should satisfy the following equation in its support

$$\Delta\rho \pm a^2\rho = \frac{1}{\lambda}\frac{1}{1 - Cl^{n-2}}\mathcal{L}_2\mathcal{L}_1 s$$

must hold with $a^2 = |A|$ and $A = \dfrac{Ck^2 l^{n-2} - \frac{k^2}{l^2}}{1 - Cl^{n-2}} = k^2 \dfrac{Cl^n - 1}{l^2 - Cl^n}$.
This is the Helmholtz equation for $A > 0$, the screened Poisson equation for $A < 0$ and the Poisson equation for $A = 0$.

Computations (II)

Right-hand side:

- Flock in any dimension: $s(r) = D \Rightarrow \frac{1}{\lambda(1-Cl^{n-2})}\mathcal{L}_2\mathcal{L}_1 D = \tilde{D}$

  $\Rightarrow$ inhomogeneous solution : $\rho(r) = \frac{\tilde{D}}{A} = \bar{D}$ for $A \neq 0$
- Mill in 2D: $s(r) = D + \frac{\alpha}{\beta}\log(r)$

  $\Rightarrow \frac{1}{\lambda(1-C)}\mathcal{L}_2\mathcal{L}_1\left[D + \frac{\alpha}{\beta}\log(r)\right] = \frac{k^4}{\lambda l^2(1-C)}\frac{\alpha}{\beta}\log(r) + \tilde{D}$

  $\Rightarrow$ inhomogeneous solution: $\rho_{\text{inhom},A}(r) = \frac{k^4}{\lambda A l^2(1-C)}\frac{\alpha}{\beta}\log(r) + \frac{\tilde{D}}{A}$ for $A \neq 0$.

Homogeneous & fundamental solutions:

- Helmholtz equation: $\begin{cases} n=1: & \sin(ar),\ \cos(ar) \\ n=2: & J_0(ar),\ Y_0(ar) \\ n=3: & \frac{\sin(ar)}{r},\ \frac{\cos(ar)}{r} \end{cases}$
- Screened Poisson equation: $\begin{cases} n=1: & \exp(ar),\ \exp(-ar) \\ n=2: & I_0(ar),\ K_0(ar) \\ n=3: & \frac{\sinh(ar)}{r},\ \frac{\cosh(ar)}{r} \end{cases}$
- Poisson equation: (in)-homogeneous solution explicitly known

Explicit solution space

Given that flock/mill densities are radially symmetric and flock solutions do not posses a singularity at zero, we get that if stationary solutions to $W \star \rho = s$ exist, they have to be of the following form:

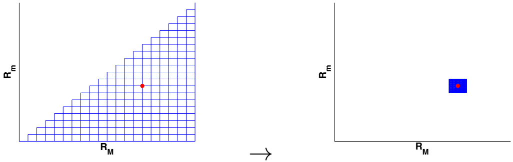
Theorem: Quasi-Morse potential solution space

$n=2$:	flock	$A>0$	$\rho_F = \mu_1 J_0(ar) + \mu_2$
		$A=0$	$\rho_F = \mu_1 r^2 + \mu_2$
		$A<0$	$\rho_F = \mu_1 I_0(ar) + \mu_2$
	mill	$A>0$	$\rho_M = \rho_{\text{inhom}} + \mu_1 J_0(ar) + \mu_2 Y_0(ar) + \mu_3$
		$A=0$	$\rho_M = \frac{\alpha}{\beta}\frac{k^4}{4\lambda l^2(1-C)} r^2(\log(r)-1) + \mu_1 r^2 + \mu_2 \log(r) + \mu_3$
		$A<0$	$\rho_M = \rho_{\text{inhom}} + \mu_1 I_0(-ar) + \mu_2 \cdot K_0(ar) + \mu_3$
$n=3$:	flock	$A>0$	$\rho_F = \mu_1 \sin(ar)\frac{1}{r} + \mu_2$
		$A=0$	$\rho_F = \mu_1 r^2 + \mu_2$
		$A<0$	$\rho_F = \mu_1 \sinh(ar)\frac{1}{r} + \mu_2$

Ref: A. Bernoff and C. Topaz: "A primer of swarm equilibria"

Numerical challenge

- Task: Find supp ρ and coefficients μ_i, such that $\int \rho \, \mathrm{d}x = 1$, $\rho > 0$.
- Remark: Multi-d convolution of radially symmetric functions are a linear operator of radial functions: $(W \star \bar{\rho})(r) = \int_{\mathbb{R}^+} \Psi(r,s)\bar{\rho}(s)\,\mathrm{d}s$, where Ψ has to be computed.
- Strategy: support optimization
  Vary support $\Rightarrow$ "inverse" best fit approximation for ρ $\Rightarrow$ positivity and unit mass hard constraints for feasability $\Rightarrow$ penalize $(W \star \rho)(r) - s(r)$ select support with minimal penalty
- Discretization refinement:



Search algorithm (for mills)

Input : fixed support $B(R_m, R_M)$, discretization size Δr

(0): Define radial grid $\bar{r} = \{r_0, \dots, r_N\}$ s.t. $r_0 = r_l, r_N = R_r, r_{i+1} - r_i = \Delta r \, \forall i$
Denote $\bar{\rho}$ the approximation of ρ on $\bar{r}$ (likewise for other functions).
Compute a matrix H s.t. $\overline{W \star \rho} = H\bar{\rho}$

(1): Evaluate $\rho_{\text{inhom},A}$ on $\operatorname{supp}\rho$ and convolve $\bar{s}_{\text{inhom}} := H\bar{\rho}_{\text{inhom},A}$.
Define $\bar{s}_{\text{rem}} := \bar{s} - \bar{s}_{\text{inhom}}$.

(2): Evaluate $J_0(ar), Y_0(ar), 1$ on $\operatorname{supp}\rho$ and convolve
$g^1 := H\bar{J}_0, g^2 := H\bar{Y}_0, g^3 := H\bar{1}$.

(3): Fix three points r_1, r_j, r_N ($j = \lfloor N/2 \rfloor$) and interpolate $\bar{s}_{\text{rem}}$ with $g_1, g_2, g_3 \Rightarrow$.

$$\text{Solve } \mu_{\text{rem}} := \begin{pmatrix} g_1^1 & g_1^2 & g_1^3 \\ g_j^1 & g_j^2 & g_j^3 \\ g_N^1 & g_N^2 & g_N^3 \end{pmatrix} \Big\backslash \begin{pmatrix} \bar{s}_{\text{rem},1} \\ \bar{s}_{\text{rem},j} \\ \bar{s}_{\text{rem},N} \end{pmatrix} \text{ with } j := \lfloor N/2 \rfloor.$$

(4) : Likewise, interpolate the constant $D = 1$ temp. choice . $\Rightarrow$

$$\text{Solve } \mu_{\text{const}} := \begin{pmatrix} g_1^1 & g_1^2 & g_1^3 \\ g_j^1 & g_j^2 & g_j^3 \\ g_N^1 & g_N^2 & g_N^3 \end{pmatrix} \Big\backslash \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

(5) : Set $\bar{\rho}_{\text{rem}} := \mu_{\text{rem},1}\bar{J}_0 + \mu_{\text{rem},2}\bar{Y}_0 + \mu_{\text{rem},3}$ and $\bar{\rho}_{\text{const}} := \mu_{\text{const},1}\bar{J}_0 + \mu_{\text{const},2}\bar{Y}_0 + \mu_{\text{const},3}$.

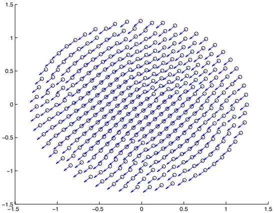
(6): Set $\bar{\rho} := \bar{\rho}_{\text{inhom},A} + \bar{\rho}_{\text{rem}} + \gamma\bar{\rho}_{\text{const}}$ with $\gamma := \frac{1 - m(\bar{\rho}_{\text{rem}}) - m(\bar{\rho}_{\text{inhom},A})}{m(\bar{\rho}_{\text{temp}})}$ (unit mass).

(7) : Measure deviation from $\bar{s}$: $e_1 := \frac{1}{R_M - R_m} \int \left[H\bar{\rho} - \bar{s} - \frac{1}{R_M - R_m} \int (H\bar{\rho} - \bar{s}) \, \mathrm{d}\bar{r} \right] \mathrm{d}\bar{r}$.

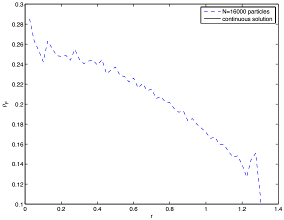
(8) : Penalize convexity of $\bar{s}$ by $e_2 := \int \chi_{[\bar{s}'' > 0]} \, \bar{s} \, \mathrm{d}\bar{r}$

Output : $e = e_1 + e_2, \bar{\rho}, \bar{s}$ if $\bar{\rho} \geq 0$

Results: 2D flock



Flock, N=400

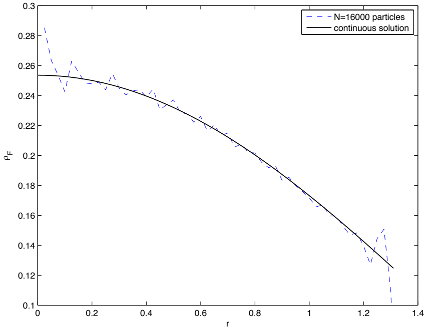


Empirical radial density, N=16000 $\rho(r)$

$C = \frac{10}{9}$	$k = \frac{1}{2}$	$l = \frac{3}{4}$
$\alpha = 1$	$\beta = 5$	$\lambda = 100$

N = number of particles

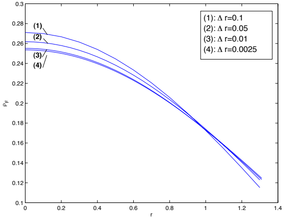
Results: 2D flock



Stationary flock solution: $\rho_F = \mu_1 J_0(ar) + \mu_2$
with $\mu_1 \approx 0.2356, \mu_2 \approx 0.018, A = 1.5, R_F \approx 1.31$

$C = \frac{10}{9}$	$k = \frac{1}{2}$	$l = \frac{3}{4}$
$\alpha = 1$	$\beta = 5$	$\lambda = 100$

Results: 2D flock

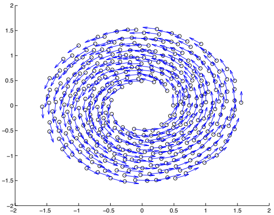


Continuous solution ρ_F for varying Δr

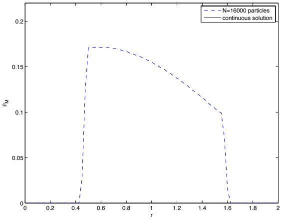
Δr	error e	computation time
0.1	3.54e-05	0.76s
0.05	1.36e-05	2.85s
0.01	3.99e-06	69.1s
0.0025	9.97e-07	1125s

Computation times & error convergence

Results: 2D mill



Mill, N=400

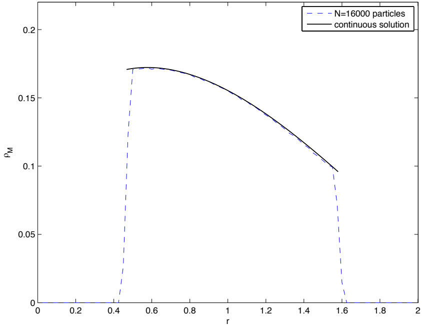


Empirical radial density, N=16000 $\rho(r)$

$$C = \frac{10}{9} \qquad k = \frac{1}{2} \qquad l = \frac{3}{4}$$
$$\alpha = 1 \qquad \beta = 5 \qquad \lambda = 100$$

N = number of particles

Results: 2D mill

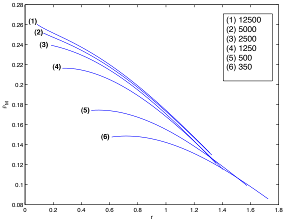


Stationary mill solution: $\rho_M = \frac{k^4}{\lambda a^2 l^2 (1-C)} \frac{\alpha}{\beta} \log(r) + \mu_1 J_0(ar) + \mu_2 Y_0(ar) + \mu_3$

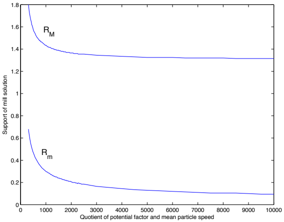
$\mu_1 \approx 0.1708, \mu_2 \approx 0.0468, \mu_3 = 0.0320, a^2 = A = 1.5, \mathrm{supp}_{\rho_M} \approx B(0.47, 1.57)$

$C = \frac{10}{9}$	$k = \frac{1}{2}$	$l = \frac{3}{4}$
$\alpha = 1$	$\beta = 5$	$\lambda = 100$

Result: 2D mill parameter dependence λ, α, β



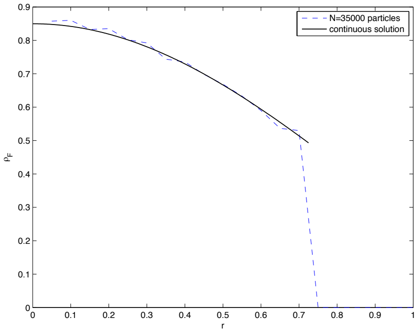
Density shapes



Support sizes

Mill solutions with identical shape parameters C, l, k and varying ratio $\beta\lambda/\alpha$.

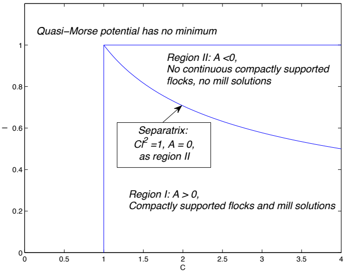
Results: 3D flock

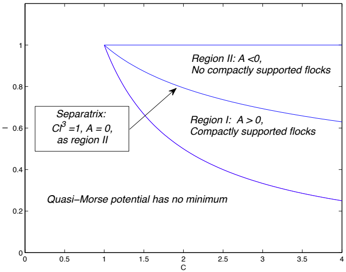


Stationary flock solution: $\rho_F = \mu_1 \cdot \sin(ar)\frac{1}{r} + \mu_2 \cdot 1$
with $\mu_1 \approx 0.3574, \mu_2 \approx 0.0052, R_F \approx 0.725, A = 5.585.$

$C = 1.255$	$k = 0.2$	$l = 0.8$
$\alpha = 1$	$\beta = 5$	$\lambda = 100$

Result: Parameter dependencies for Quasi-Morse





2D parameter phase diagram 3D parameter phase diagram

Region I: $A > 0$: compactly supported flocks (and mills in 2D) are found
Region II: $A < 0$: no compactly supported solutions are found
Separatrix: $A = 0$: no compactly supported solutions are found

Conclusions

- Introduced and defined Quasi-Morse potentials.
- All relevant coherent patterns of motions have been observed (micro).
- Flock and mill solutions have been explicitly derived.
- Numerical algorithm to determine linear coefficients has been introduced.
- Coherent match between our result and microscopics.
- Catastrophic potentials $A > 0$: compactly supported solutions are found, H-stable $A \leq 0$: no solutions are found (in accordance to microscopics).
- $\sum$: Quasi-Morse potentials allow computationally cheap explicit computation of stationary flock and mill solutions without simulating any time evolution, offering essentially the same modeling.

Thanks

Thank you for your attention!