

# General Kernel Spectral Methods for Equilibrium Measures

Seminar Talk at the University of Graz



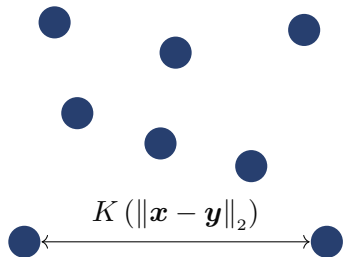
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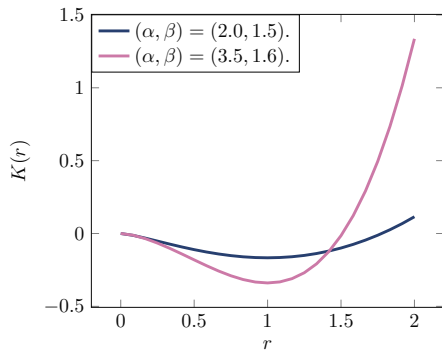
supervised by  
Dr. Timon Gutleb and Prof. José Carrillo

9<sup>th</sup> of November, 2023

- Find the Equilibrium Distribution  $\rho(\mathbf{x})$  of a Many-Particle-System.



$N_p = 8$  particles interacting with one another through the potential  $K(r)$ .



Plot of attractive-repulsive potential functions  $K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$  for different  $\alpha, \beta$ .

- Model interactions through (power law) attraction-repulsion potentials<sup>1</sup>

for example,  $K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$  with parameters  $\alpha, \beta \in \mathbb{R} \setminus \{0\}$ .

- Each particle  $i = 1, \dots, N$  at position  $\mathbf{x}_i \in \mathbb{R}^d$  and time  $t \in \mathbb{R}^+$  follows

$$\frac{d^2 \mathbf{x}_i}{dt^2} = f \left( \left\| \frac{d\mathbf{x}_i}{dt} \right\|_2 \right) \frac{d\mathbf{x}_i}{dt} - \frac{1}{N} \sum_{j=1, i \neq j}^N \nabla K(\|\mathbf{x}_i - \mathbf{x}_j\|_2),$$

for reference see, for example, [1, 2]. For now, we only consider the case without an external potential  $V(\mathbf{x})$ .

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<sup>1</sup>If the repulsive term is stronger (so  $\beta > \alpha$ ), there is no equilibrium distribution as particles simply continue repelling each other out to infinity.

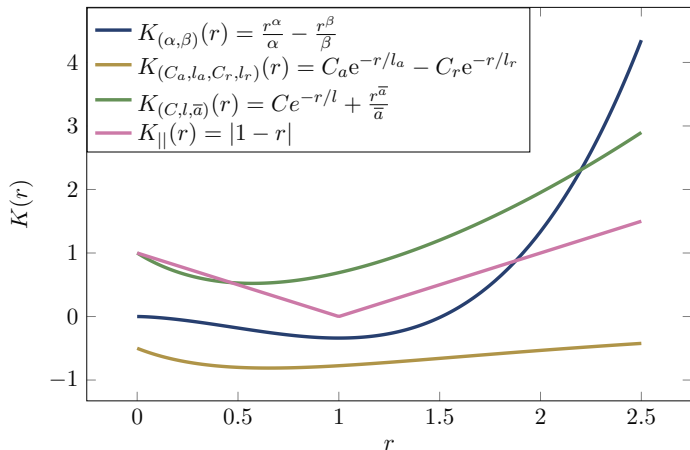


Figure: Comparison of different interaction potentials.

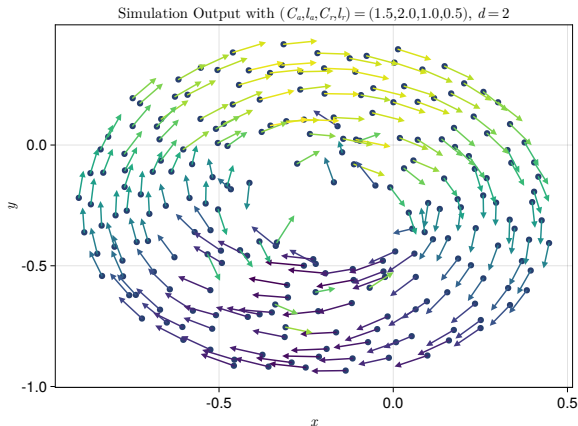


Figure:  $N_p = 120$  particles in  $d = 2$  dimensions. Morse potential, friction and self-propulsion parameters are as given in [3], reproducing their results.

Every particle  $i$  at position  $\mathbf{x}_i \in \mathbb{R}^d$  with velocity  $\mathbf{v}_i \in \mathbb{R}^d$  is updated using

$$\begin{aligned}\mathbf{x}_i(t + \tau) &= \mathbf{x}_i(t) + \tau \cdot \mathbf{v}_i(t + \tau/2), & \text{for } t = 0, \tau, \dots, \\ \mathbf{v}_i(t + \tau/2) &= \mathbf{v}_i(t - \tau/2) + \tau \cdot \mathbf{f}[\mathbf{x}_i(t), t], & \text{for } t = \tau, 2\tau, \dots, \\ \mathbf{v}_i(\tau/2) &= \mathbf{v}_i(0) + \frac{\tau}{2} \cdot \mathbf{f}[\mathbf{x}_i(0), 0], & \text{for } t = 0,\end{aligned}$$

where  $\mathbf{f}_i[\mathbf{x}_i(t), t] \in \mathbb{R}^d$  denotes the acceleration (sum of contributions of all forces divided by particle mass  $m_i$ ) at time  $t$ .

In fewer words... a particle at position  $\mathbf{x} \in \mathbb{R}^d$  with velocity  $\mathbf{v} \in \mathbb{R}^d$

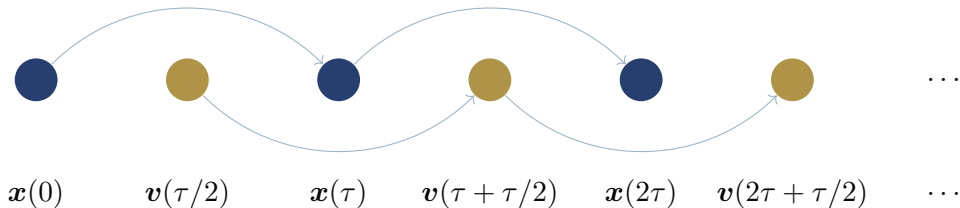
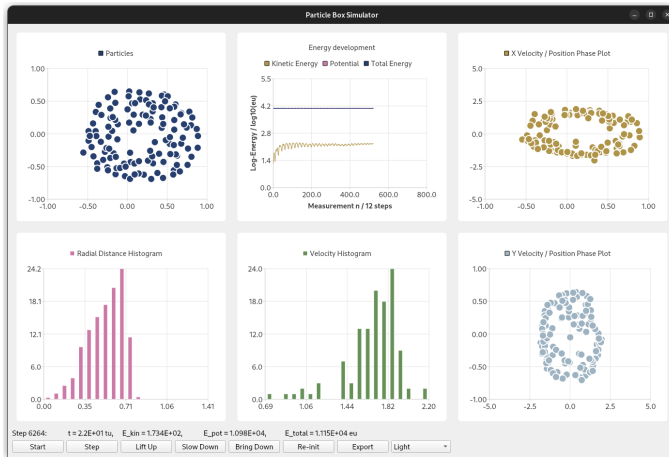


Figure: Visualisation of the Leapfrog integration method, position and velocity are updated at times shifted by  $\tau/2$ , half the timestep.



The positional distribution approached by  $N_p = 250$  particles.



The total potential energy of an  $N_p$ -particle system is then given by

$$E = \sum_{i=1}^{N_p} \sum_{j=1, j \neq i}^{N_p} K(\|\mathbf{x}_i - \mathbf{x}_j\|_2) ,$$

which, in the continuous limit as  $N_p \rightarrow \infty$ , becomes

$$E = \frac{1}{2} \iint K(\|\mathbf{x} - \mathbf{y}\|_2) \, \mathrm{d}\rho(\mathbf{x}) \, \mathrm{d}\rho(\mathbf{y}) ,$$

where  $\mathrm{d}\rho = \rho(\mathbf{x})\mathrm{d}\mathbf{x}$  is a measure (the equilibrium distribution) chosen such that

$$M = \int \mathrm{d}\rho = \int_{\text{supp}(\rho)} \rho(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 1 .$$

## Definition (Equilibrium Measure)

For a given pairwise interaction potential  $K : \mathbb{R} \rightarrow \mathbb{R}$ , the equilibrium measure  $\hat{\rho} : D \rightarrow \mathbb{R}$  with  $D \subseteq \mathbb{R}^d$  is a measure chosen such that

$$U_K[\hat{\rho}] := \frac{1}{2} \iint K(\|\hat{\mathbf{x}} - \hat{\mathbf{y}}\|_2) \, \mathrm{d}\hat{\rho}(\hat{\mathbf{x}}) \, \mathrm{d}\hat{\rho}(\hat{\mathbf{y}}),$$

is minimised, where  $\mathrm{d}\hat{\rho} = \hat{\rho}(\hat{\mathbf{x}})\mathrm{d}\hat{\mathbf{x}}$  [2].

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For example: in a two-particle system,  $\hat{\rho}(\hat{\mathbf{x}}) = \delta(\hat{\mathbf{x}} - \hat{\mathbf{p}}_1) + \delta(\hat{\mathbf{x}} - \hat{\mathbf{p}}_2)$  to see that  $U_K[\hat{\rho}] = K(0) + K(\|\hat{\mathbf{p}}_1 - \hat{\mathbf{p}}_2\|_2)$ , and hence, the total energy becomes

$$E = \frac{m}{2} \left( \|\hat{\mathbf{v}}_1\|_2^2 + \|\hat{\mathbf{v}}_2\|_2^2 \right) + K(0) + K(\|\hat{\mathbf{p}}_1 - \hat{\mathbf{p}}_2\|_2).$$

- ▶ In order to find  $\rho(\mathbf{x})$ , we consider an ansatz of the following form:

$$\rho(\mathbf{x}) = \sum_{n=0}^{\infty} c_n \varphi_n(\mathbf{x}), \quad c_n \in \mathbb{R},$$

with which we construct a spectral method for the numerical solution of the above integral equation.

- ▶ Minimization routine of  $E$  over coefficients in  $\rho$ , as a subroutine of outer minimisation over the bounds of the box (simpler case: use  $[-r, r]$ ,  $r \in \mathbb{R}^+$ ).
- ▶ By construction, we find that we do not need an iterative approach for the inner optimisation routine.
- ▶ The outer minimisation can be performed using known methods from continuous optimisation.

Jacobi polynomials  $P_n^{(a,b)}(x)$  are orthogonal on  $[-1, 1]$  w.r.t. the weight function

$$w^{(a,b)}(x) = (1-x)^a(1+x)^b,$$

so they satisfy

$$\int_{-1}^1 (1-x)^a(1+x)^b P_n^{(a,b)} P_m^{(a,b)} dx = \frac{2^{a+b+1} \Gamma(a+n+1) \Gamma(b+n+1)}{n!(a+b+2n+1) \Gamma(a+b+n+1)} \delta_{n,m},$$

with  $a, b > -1$ , which uniquely determines  $P_n^{(a,b)}(x)$ . The special case of  $a = b$  corresponds to the ultraspherical or Gegenbauer polynomials, while the case  $a = b = 0$  corresponds to the Legendre polynomials [4].

- This basis yields a **sparse**, and in particular, **banded** operator.

### Definition (Particle Density Distribution Problem)

Given an interaction kernel  $K : \mathbb{R}^+ \rightarrow \mathbb{R}$ , the density distribution problem is to find the equilibrium measure  $\hat{\rho} : B_R(\mathbf{0}) \rightarrow \mathbb{R}$  of mass  $M = 1$  on a  $d$ -dimensional ball of radius  $R \in \mathbb{R}^+$  that minimises the total potential  $U_K[\hat{\rho}]$ .

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As mentioned above, we will consider a **spectral method** to solve this problem. More precisely, using the following ansatz:

$$\rho(\mathbf{x}) := \left(1 - \|\mathbf{x}\|_2^2\right)^{m - \frac{\alpha+d}{2}} \sum_{k=0}^{N-1} \rho_k P_k^{\left(m - \frac{\alpha+d}{2}, \frac{d-2}{2}\right)} \left(2 \|\mathbf{x}\|_2^2 - 1\right), \quad (1)$$

with  $P_k^{(a,b)}$  the  $k$ th Jacobi polynomial and  $\rho_k$  its corresponding coefficient.

Definition (Power Law Operator  $\mathcal{Q}^\beta$ )

The power law operator  $\mathcal{Q}^\beta : \mathcal{L} \rightarrow \mathcal{L}$  is given by

$$\mathcal{Q}^\beta[\rho](\mathbf{x}) := \int \|\mathbf{x} - \mathbf{y}\|_2^\beta \, \mathrm{d}\rho(\mathbf{y}) = \int_{\text{supp}(\rho)} \|\mathbf{x} - \mathbf{y}\|_2^\beta \rho(\mathbf{y}) \, \mathrm{d}\mathbf{y}.$$

Applied to the ansatz given in (1), we can evaluate the appearing integrals **explicitly**. For the attractive-repulsive interaction kernel  $K_{\alpha,\beta}(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$ , the matrix representation of the operator becomes

$$Q_{\alpha,\beta} := \frac{R^{\alpha+d}}{\alpha} Q^\alpha - \frac{R^{\beta+d}}{\beta} Q^\beta. \quad (2)$$



## Theorem (Power Law Potential of the $n$ th Jacobi Polynomial)

On the  $d$ -dimensional unit ball  $B_1(\mathbf{0})$  the power law potential, with power  $\alpha \in (-d, 2 + 2m - d)$ ,  $m \in \mathbb{N}_0$  and  $\beta > -d$ , of the  $n$ th weighted radial Jacobi polynomial  $(1 - \|\mathbf{y}\|_2^2)^{m - \frac{\alpha+d}{2}} P_n^{(m - \frac{\alpha+d}{2}, \frac{d-2}{2})} (2\|\mathbf{y}\|_2^2 - 1)$  reduces to a Gaussian hypergeometric function as follows:

$$\begin{aligned} I_{m,n}^{\alpha,\beta}(\mathbf{x}) &= \int_{B_1(\mathbf{0})} \|\mathbf{x} - \mathbf{y}\|_2^\beta (1 - \|\mathbf{y}\|_2^2)^{m - \frac{\alpha+d}{2}} P_n^{(m - \frac{\alpha+d}{2}, \frac{d-2}{2})} (2\|\mathbf{y}\|_2^2 - 1) d\mathbf{y} \\ &= \frac{\pi^{d/2} \Gamma(1 + \frac{\beta}{2}) \Gamma(\frac{\beta+d}{2}) \Gamma(m+n - \frac{\alpha+d}{2} + 1)}{\Gamma(\frac{d}{2}) \Gamma(n+1) \Gamma(\frac{\beta}{2} - n + 1) \Gamma(\frac{\beta-\alpha}{2} + m+n+1)} {}_2F_1 \left( n - \frac{\beta}{2}, -m - n + \frac{\alpha-\beta}{2}; \frac{d}{2}; \|\mathbf{x}\|_2^2 \right). \end{aligned}$$

## Lemma (Mass of the Solution)

*For a given solution  $\rho : B_1(\mathbf{0}) \rightarrow \mathbb{R}$ , its mass  $M \in \mathbb{R}$  can be evaluated explicitly, provided the appropriate ansatz, an expansion of weighted radial Jacobi polynomials with coefficients  $\rho_k$ . The mass is given by*

$$M[\rho[\boldsymbol{\rho}]] = \int_{\text{supp}(\rho)} \rho(y) \, dy = \frac{\pi^{d/2} \Gamma(a+1)}{\Gamma(a+d/2+1)} \rho_0,$$

*so solely depending on the first coefficient  $\rho_0$ .*

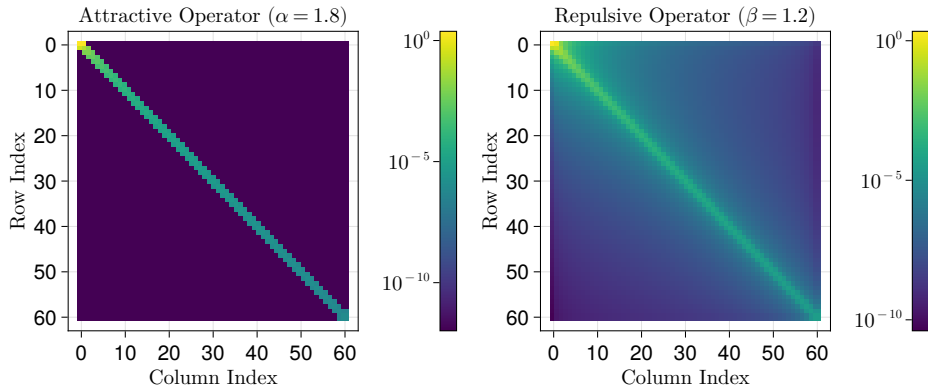


Figure: The attractive and repulsive operators (matrices), the (absolute) matrix values are shown in a  $\log_{10}$  colour scale. Due to the choice of basis, the attractive operator is exactly banded.

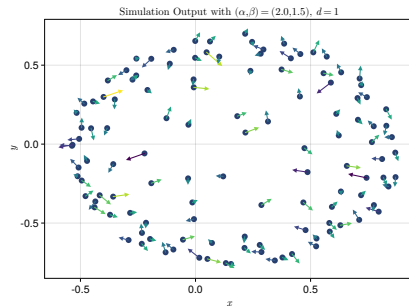
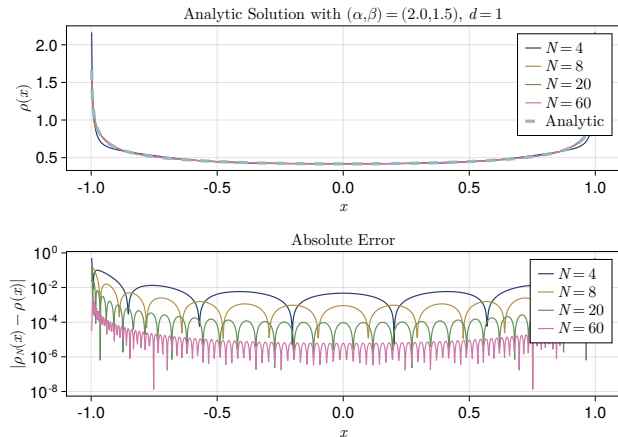


Figure: Simulation output with  $N_p = 150$  particles using the same attractive-repulsive kernel  $K_{\alpha, \beta}(r)$ .

Figure: The analytical solution  $\rho(x)$  compared to the (spectral method) solutions  $\rho_N(x)$  of different order.

We express the general kernel as a polynomial, through reprojection from the Jacobi polynomials,

$$K_G(r) = \sum_{l=0}^{G-1} g_l r^l \approx K(r), \quad \mathbf{g} := (g_0, \dots, g_{G-1})^T \in \mathbb{R}^G. \quad (3)$$

The operator can then be expressed as

$$\mathcal{Q}_G[\hat{\rho}](\hat{\mathbf{x}}) = \int_{B_R(\mathbf{0})} \sum_{l=0}^{G-1} g_l \|\hat{\mathbf{x}} - \hat{\mathbf{y}}\|_2^l \hat{\rho}(\hat{\mathbf{y}}) \, \mathrm{d}\hat{\mathbf{y}} = \sum_{l=0}^{G-1} g_l R^{l+d} \mathcal{Q}^l[\hat{\rho}](\mathbf{x}).$$

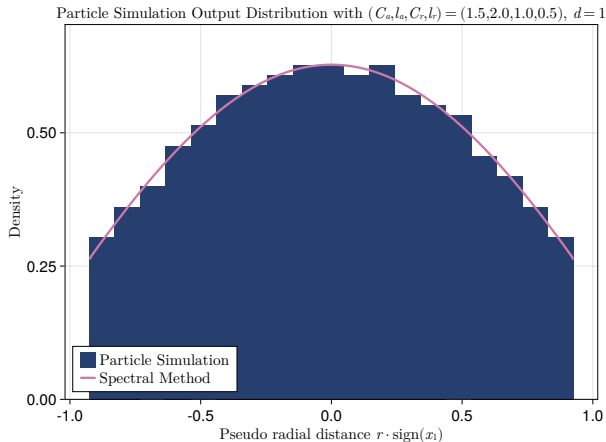


Figure: Comparison of simulation output with the  $G = 8$  general kernel solver's equilibrium measure  $\rho_{12}(r)$  at  $R$  given by the simulator.

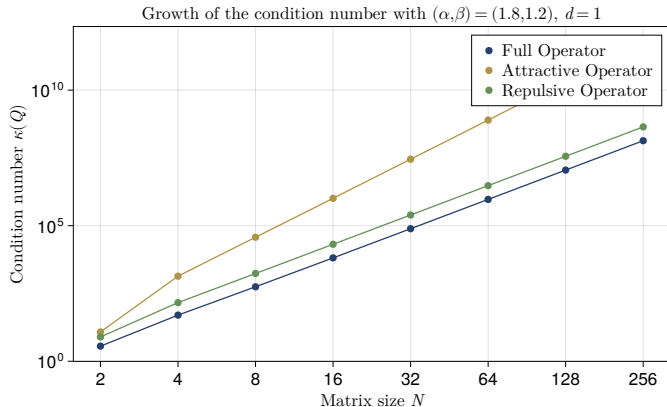


Figure: Growth of the 2-norm condition number  $\kappa_2(Q)$  of the attractive-repulsive operators  $Q^{(\alpha)}$ ,  $Q^{(\beta)}$  and  $Q_{\alpha, \beta}$  for growing system size  $N$ .

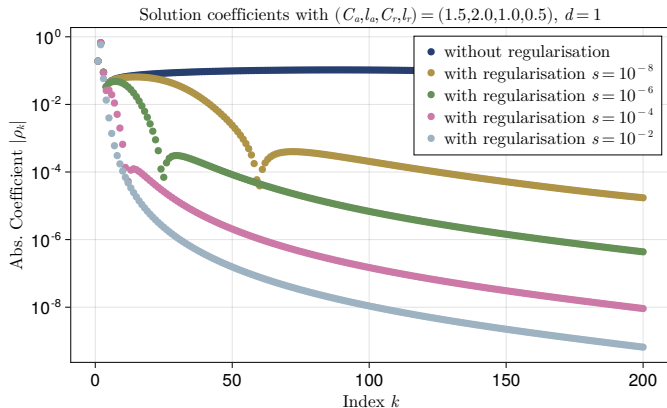


Figure: Absolute value of the solution coefficients  $\rho_k$  with and without Tikhonov regularisation after the solution of a  $200 \times 200$  linear system.



## Contributions:

- ▶ Original implementation of simulator (+GUI, in C++) and solver (in Julia).
- ▶ General kernel spectral method + implementation.
- ▶ Lemma for an initial guess of  $R$ .

## Challenges:

- ▶ Proving Theorem 4.3, the power law integral of the Jacobi polynomials.
- ▶ Synchronisation of simulation and solver (implementations).
- ▶ Correct parameter choices for the general kernel spectral method.

## Future Work:

- ▶ Describing phase-space distributions in a self-propulsion setup.
- ▶ Modelling (constrained) boundaries and boundary conditions.

Thank you.

- [1] Timon S. Gutleb, José Antonio Carrillo and Sheehan Olver. ‘Computing equilibrium measures with power law kernels’. In: *Math. Comput.* 91.337 (Sept. 2022), pp. 2247–2281. ISSN: 0025-5718. DOI: [10.1090/mcom/3740](https://doi.org/10.1090/mcom/3740).
- [2] Timon S. Gutleb, José Antonio Carrillo and Sheehan Olver. ‘Computation of Power Law Equilibrium Measures on Balls of Arbitrary Dimension’. In: *Constr. Approx.* (Dec. 2022), pp. 1–46. ISSN: 1432-0940. DOI: [10.1007/s00365-022-09606-0](https://doi.org/10.1007/s00365-022-09606-0).
- [3] M. R. D’Orsogna, Y. L. Chuang, A. L. Bertozzi and L. S. Chayes. ‘Self-Propelled Particles with Soft-Core Interactions: Patterns, Stability, and Collapse’. In: *Phys. Rev. Lett.* 96.10 (Mar. 2006), p. 104302. ISSN: 1079-7114. DOI: [10.1103/PhysRevLett.96.104302](https://doi.org/10.1103/PhysRevLett.96.104302).
- [4] F.W.J. Olver, A.B.O. Daalhuis, D.W. Lozier, B.I. Schneider, R.F. Boisvert, C.W. Clark, B.R. Miller and B. V. Saunders. *NIST Digital Library of Mathematical Functions*. <https://dlmf.nist.gov>. Dec. 2018. DOI: [10.1023/A:1022915830921](https://doi.org/10.1023/A:1022915830921). (Visited on 18/08/2023).

GUI Graphical User Interface

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