General Kernel Spectral Methods for Equilibrium Measures

Seminar Talk at the University of Graz

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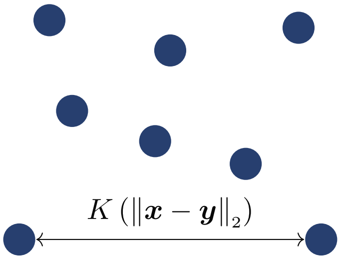
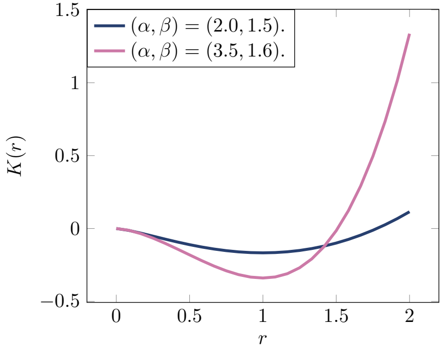
- Find the Equilibrium Distribution $\rho(\boldsymbol{x})$ of a Many-Particle-System.



$N_p = 8$ 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 α, β.

- Interactions through (power law) attraction-repulsion potentials[1]

$$K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta} \quad \text{with parameters} \quad \alpha, \beta \in \mathbb{R}\backslash\{0\}\,.$$

- Each particle $i = 1, ..., N$ at position $\boldsymbol{x_i} \in \mathbb{R}^d$ and time $t \in \mathbb{R}^+$ follows

$$\frac{\mathrm{d}^2\boldsymbol{x_i}}{\mathrm{d}t^2} = f\left(\left\|\frac{\mathrm{d}\boldsymbol{x_i}}{\mathrm{d}t}\right\|_2\right)\frac{\mathrm{d}\boldsymbol{x_i}}{\mathrm{d}t} - \frac{1}{N}\sum_{j=1, i\neq j}^{N} \nabla K\left(\|\boldsymbol{x_i} - \boldsymbol{x_j}\|_2\right)\,,$$

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

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

Leapfrog Integration

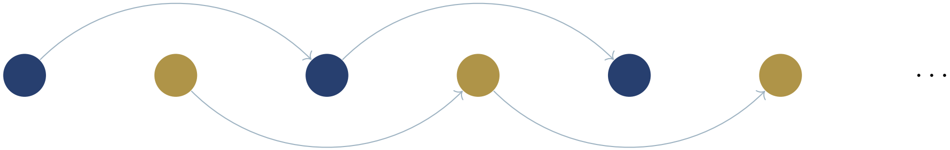
Every particle i at position $\boldsymbol{x_i} \in \mathbb{R}^d$ with velocity $\boldsymbol{v_i} \in \mathbb{R}^d$ is updated using

$$
\begin{aligned}
\boldsymbol{x_i}(t+\tau) &= \boldsymbol{x_i}(t) + \tau \cdot \boldsymbol{v_i}(t+\tau/2), && \text{for } t = 0, \tau, \dots\,, \\
\boldsymbol{v_i}(t+\tau/2) &= \boldsymbol{v_i}(t-\tau/2) + \tau \cdot \boldsymbol{f}[\boldsymbol{x_i}(t), t], && \text{for } t = \tau, 2\tau, \dots\,, \\
\boldsymbol{v_i}(\tau/2) &= \boldsymbol{v_i}(0) + \frac{\tau}{2} \cdot \boldsymbol{f}[\boldsymbol{x_i}(0), 0], && \text{for } t = 0\,,
\end{aligned}
$$

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

Leapfrog Integration

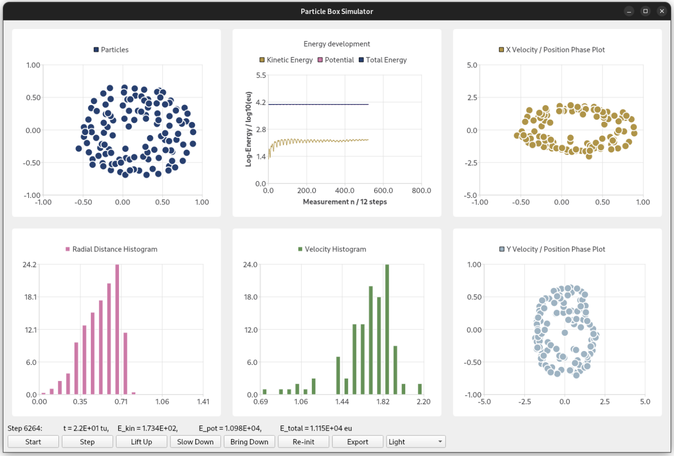
In fewer words... a particle at position $\boldsymbol{x} \in \mathbb{R}^d$ with velocity $\boldsymbol{v} \in \mathbb{R}^d$



$$\boldsymbol{x}(0) \quad \boldsymbol{v}(\tau/2) \quad \boldsymbol{x}(\tau) \quad \boldsymbol{v}(\tau + \tau/2) \quad \boldsymbol{x}(2\tau) \quad \boldsymbol{v}(2\tau + \tau/2) \quad \cdots$$

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

Simulation Demo



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

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

$$E = \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} K\left(\|\boldsymbol{x_i} - \boldsymbol{x_j}\|_2\right) \,,$$

which, in the continuous limit as $N \to \infty$, becomes

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

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

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

- In order to find $\rho(\hat{\boldsymbol{x}})$, we consider the following ansatz

$$\rho(\boldsymbol{x}) = \sum_{n=0}^{\infty} c_n P_n^{(a,b)}(\boldsymbol{x}) \,, \quad c_n \in \mathbb{R} \,,$$

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

- Minimization routine of E over coefficients in ρ, 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

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

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 [3].

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

Connection to Swarming Behaviour

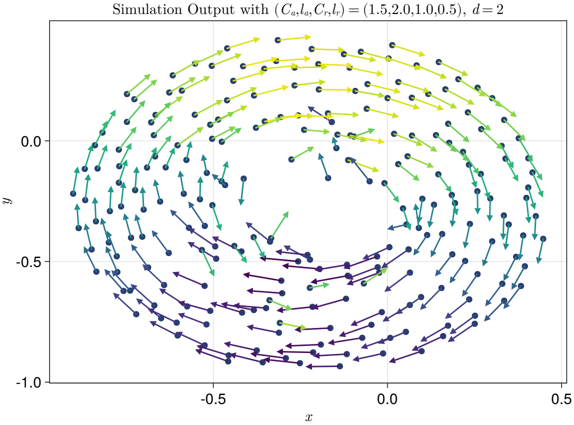


Figure: $N_p = 120$ particles in $d = 2$ dimensions. Morse potential, friction and self-propulsion parameters are as given in [4], reproducing their results.

Definition (Equilibrium Measure)

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

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

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

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For example: in a two-particle system, $\hat{\rho}(\hat{\boldsymbol{x}}) = \delta(\hat{\boldsymbol{x}} - \hat{\boldsymbol{p}}_{\mathbf{1}}) + \delta(\hat{\boldsymbol{x}} - \hat{\boldsymbol{p}}_{\mathbf{2}})$ to see that $U_K[\hat{\rho}] = K(0) + K(\|\hat{\boldsymbol{p}}_{\mathbf{1}} - \hat{\boldsymbol{p}}_{\mathbf{2}}\|_2)$, and hence, the total energy becomes

$$E = \frac{m}{2}\left(\|\hat{\boldsymbol{v}}_{\mathbf{1}}\|_2^2 + \|\hat{\boldsymbol{v}}_{\mathbf{2}}\|_2^2\right) + K(0) + K(\|\hat{\boldsymbol{p}}_{\mathbf{1}} - \hat{\boldsymbol{p}}_{\mathbf{2}}\|_2).$$

Problem Formulation

Definition (Particle Density Distribution Problem)

Given an interaction kernel $K : \mathbb{R}^+ \to \mathbb{R}$, the density distribution problem is to find the equilibrium measure $\hat{\rho} : B_R(\mathbf{0}) \to \mathbb{R}$ 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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We then consider a spectral method with the following ansatz

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

with $P_k^{(a,b)}$ the kth Jacobi polynomial and ρ_k its corresponding coefficient.

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

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

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

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

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

Analysis: The Attractive-Repulsive Operator

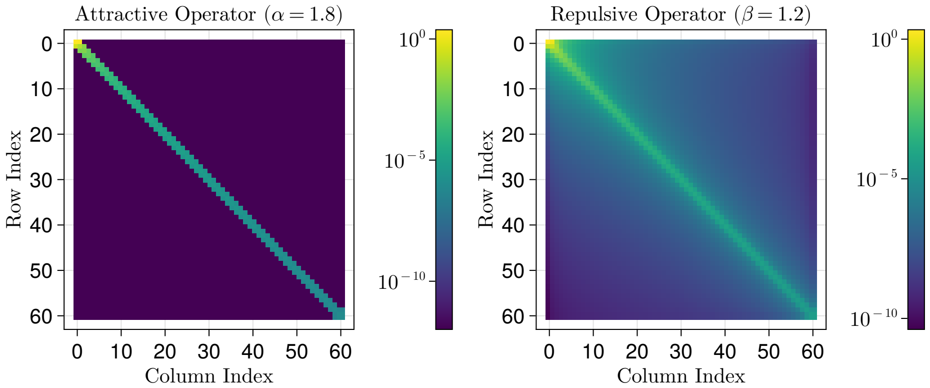

Figure: The attractive and repulsive operators (matrices), the (absolute) matrix values are shown in a $\log_{10}$ colour scale. Due to the choice of basis, the attractive operator is exactly banded.

Analysis: Comparison with Analytical Solution

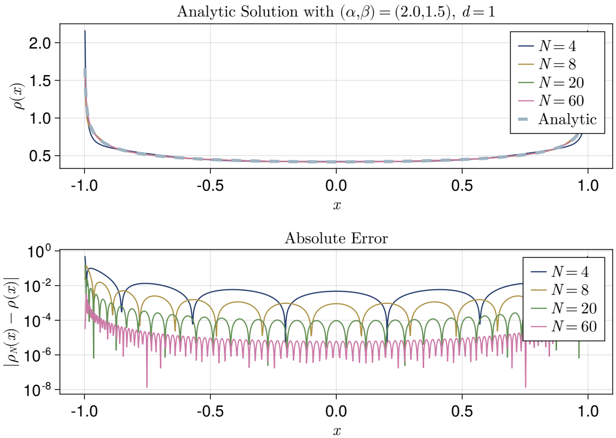

Figure: The analytical solution $\rho(x)$ compared to the (spectral method) solutions $\rho_N(x)$ of different order.

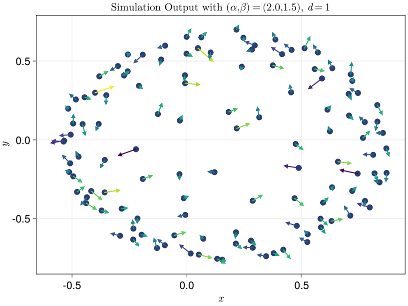

Figure: Simulation output with $N_p = 150$ particles using the same attractive-repulsive kernel $K_{\alpha,\beta}(r)$.

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

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

The operator can then be expressed as

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

Results: Simulation and Solver Comparison

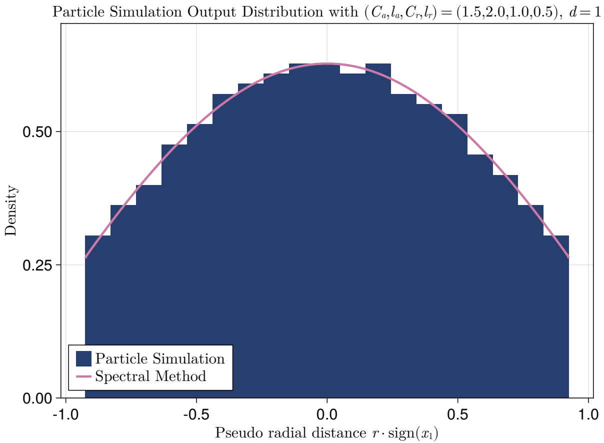

Figure: Comparison of simulation output with the $G = 8$ general kernel solver's equilibrium measure $\rho_{12}(r)$ at R given by the simulator.

Contributions, Challenges Faced & Future Work

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 4.2, 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.

[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.

[3] 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. (Visited on 18/08/2023).

[4] 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.

GUI	Graphical User Interface	20