General Kernel Spectral Methods for Equilibrium Measures

Seminar Talk at the University of Graz

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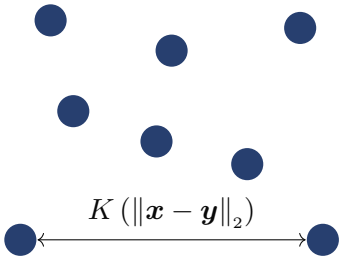
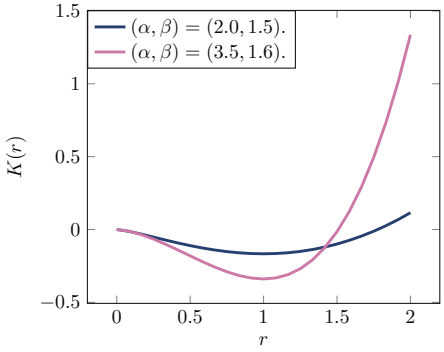
Problem Setting

- 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.

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

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

- 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.

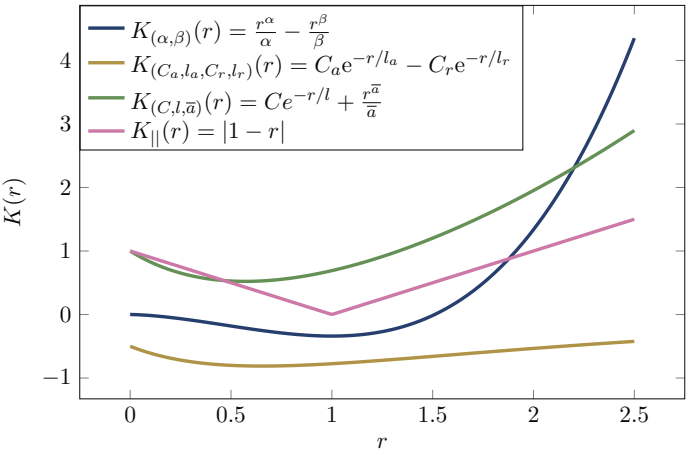


Figure: Comparison of different interaction potentials.

Connection to Swarming Behaviour

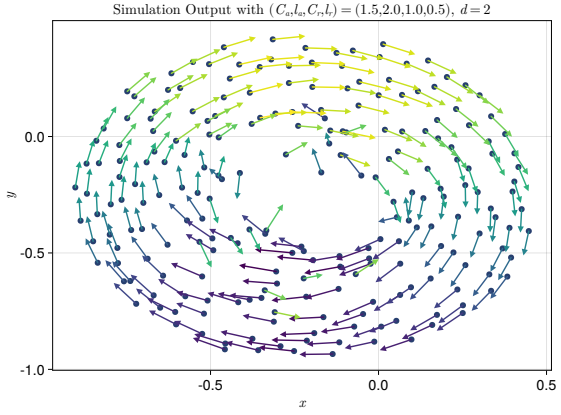


Figure: $N_p = 120$ particles in $d = 2$ dimensions.

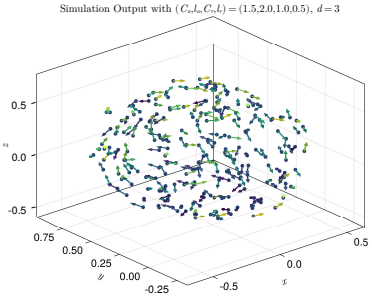


Figure: Self-propelled particles in a reflective box $[-1, 1]^3$.

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.

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

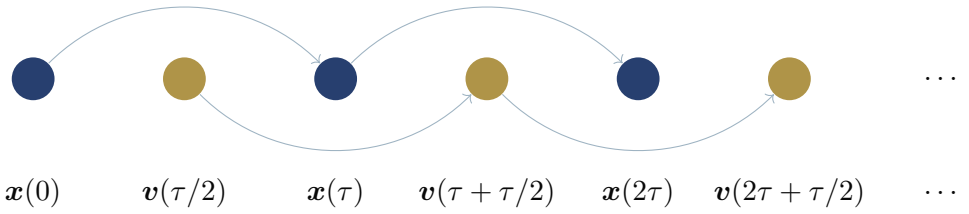
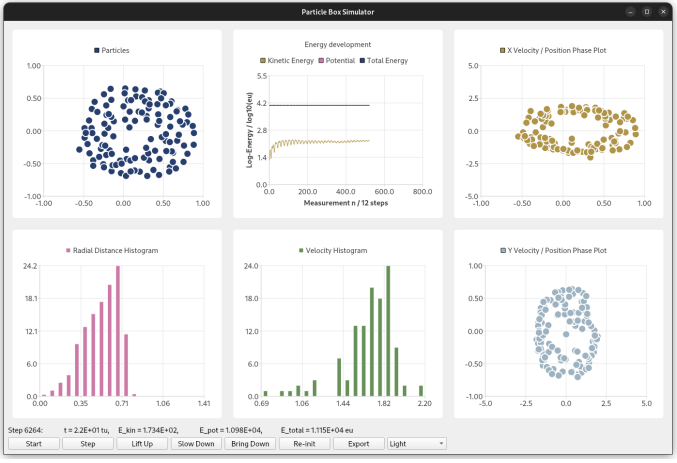


Figure: Visualisation of the Leapfrog integration method, position and velocity are updated at times shifted by $\tau/2$, half the timestep.



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

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

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

which, in the continuous limit as $N_p \to \infty$, 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

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

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

For example: in a two-particle system, $\hat{\rho}(\hat{\boldsymbol{x}}) = \delta(\hat{\boldsymbol{x}} - \hat{\boldsymbol{p_1}}) + \delta(\hat{\boldsymbol{x}} - \hat{\boldsymbol{p_2}})$ to see that $U_K[\hat{\rho}] = K(0) + K(\|\hat{\boldsymbol{p_1}} - \hat{\boldsymbol{p_2}}\|_2)$, and hence, the total energy becomes

$$E = \frac{m}{2}\left(\|\hat{\boldsymbol{v_1}}\|_2^2 + \|\hat{\boldsymbol{v_2}}\|_2^2\right) + K(0) + K(\|\hat{\boldsymbol{p_1}} - \hat{\boldsymbol{p_2}}\|_2).$$

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

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

  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.

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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As mentioned above, we will consider a spectral method to solve this problem. More precisely, using 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

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

Theorem (Power Law Potential of the nth 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 nth weighted radial Jacobi polynomial $(1-\|\boldsymbol{y}\|_2^2)^{m-\frac{\alpha+d}{2}} P_n^{\left(m-\frac{\alpha+d}{2},\frac{d-2}{2}\right)}\left(2\|\boldsymbol{y}\|_2^2-1\right)$ reduces to a Gaussian hypergeometric function as follows:

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

Lemma (Mass of the Solution)

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

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

so solely depending on the first coefficient ρ_0.

Analysis: The Attractive-Repulsive Operator

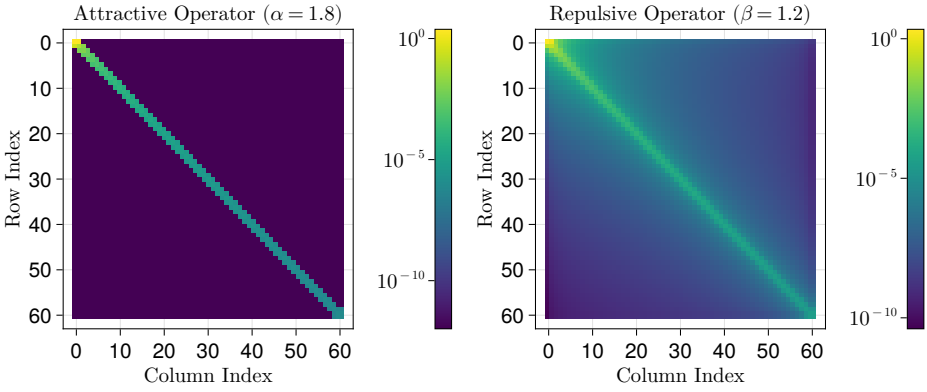

Figure: The attractive and repulsive operators (matrices), the (absolute) matrix values are shown in a $\log_{10}$ colour scale. Due to the choice of basis, the attractive operator is exactly banded.

Analysis: Comparison with Analytical Solution

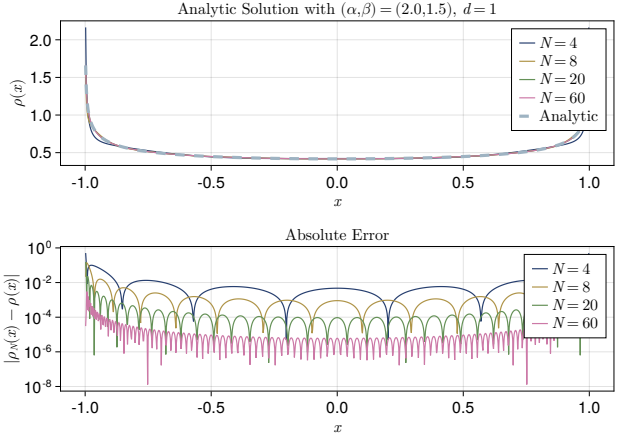

Figure: The analytical solution $\rho(x)$ compared to the (spectral method) solutions $\rho_N(x)$ of different order.

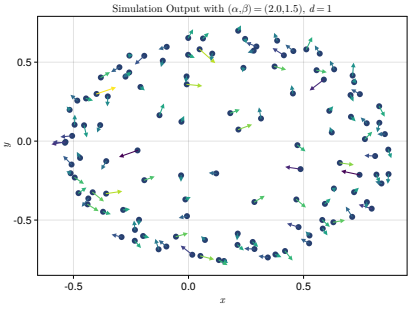

Figure: Simulation output with $N_p = 150$ particles using the same attractive-repulsive kernel $K_{\alpha,\beta}(r)$.

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

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

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

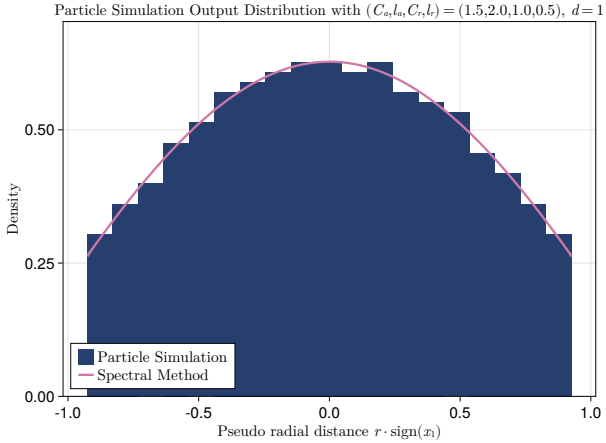

Figure: Comparison of simulation output with the $G = 8$ general kernel solver's equilibrium measure $\rho_{12}(r)$ at R given by the simulator.

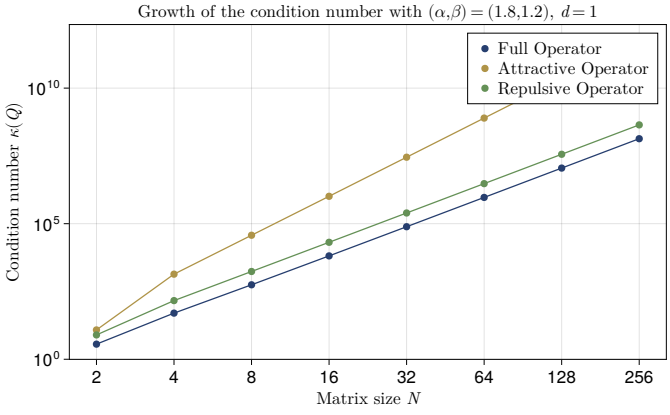

Figure: Growth of the 2-norm condition number $\kappa_2(Q)$ of the attractive-repulsive operators $Q^{(\alpha)}$, $Q^{(\beta)}$ and $Q_{\alpha,\beta}$ for growing system size N.

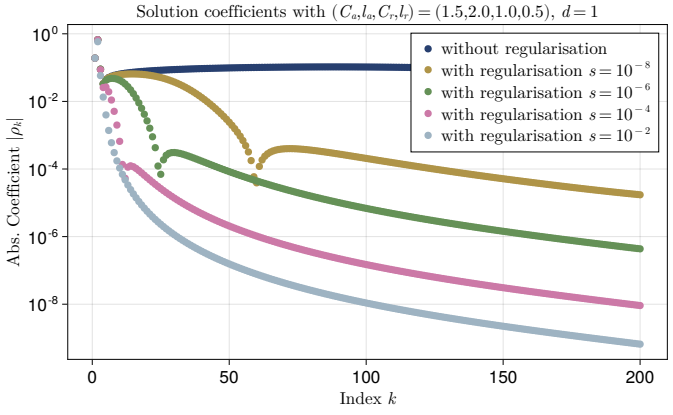

Figure: Absolute value of the solution coefficients ρ_k with and without Tikhonov regularisation after the solution of a 200×200 linear system.

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.

[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).

GUI Graphical User Interface 25

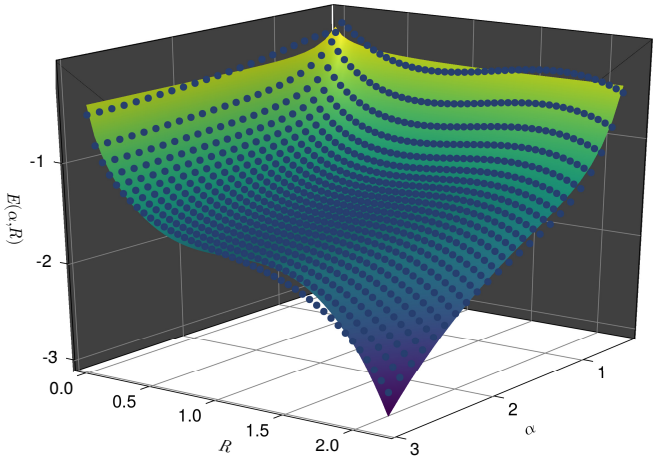

Figure: Surface plot of the total potential energy $E(\alpha, R)$, the blue scatter points represent the fit $E(\alpha, R; \boldsymbol{x}_{\min})$.