UDC 004.94, 519.6

SIMULATION OF JANUS PARTICLES ON SPARSE GRIDS

A. Pliushchai[1,a], M. Neumann[2,b], S. Gemming[2,c]

[1] Institute of Physics and Technology

[2] Institute of Physics, Chemnitz University of Technology, D-09107, Chemnitz, Germany

Abstract

Characteristic of Janus particles is that one half of their surface is modified such that the two sides of the particle exhibit different properties. In this study we will formulate of the problem of Janus particles with an interaction potential due to magnetic caps and simulate their energy, presenting theoretical ground work and implementation for two approaches to tackling this problem, namely incremental approach and its modification involving sparse grids. We will compare those two approaches, their significance for further research and potential for future improvements.

Keywords: magnetic colloids, simulations, sparse grids, approximation

1. Introduction

Rapid development of innovative approaches in machine learning and numerical methods and their consequent adoption in various fields of study, has created a fruitful interplay between generation of novel insights via employing more and more sophisticated methods for solving previously seemingly unfeasible problems and conversely incentivize further refinement of existing approaches and invention of the new ones to push the boundaries of what is possible even further. Density Functional Theory calculation in solid state physics, machine learned potential, Monte Carlo simulations are only few examples out of many. One of the problems that we encounter frequently is efficiently approximating a function that is otherwise hard to evaluate. It occurs in variety of fields and applications ranging from finance[1] to cosmological parameters sampling [2]. In this work we are going to attempt to tackle the problem of approximating a surrogate function for relative potential energy level of different arrangements of two Janus Particles,[3] using sparse grids[4].

2. Theory

2.1. Overview of Janus particles

Janus particles represent a specialized class of colloidal particles characterized by their asymmetric structure with two distinct regions on their surface having different properties. The most common configuration consists of spherical particles with two hemispheres possessing contrasting properties. In this study we focus on spherical particles are coated with a magnetic metal layer on one hemisphere, they become magnetically anisotropic with a permanent magnetization that points perpendicular to the cap surface. Magnetically capped Janus particles demonstrate complex assembly behaviour.[5] Additionally, Janus particles respond uniquely to external stimuli such as magnetic fields, light, or solvents. Their compartmentalized structure makes them particularly valuable for pharmaceutical applications and drug delivery systems.

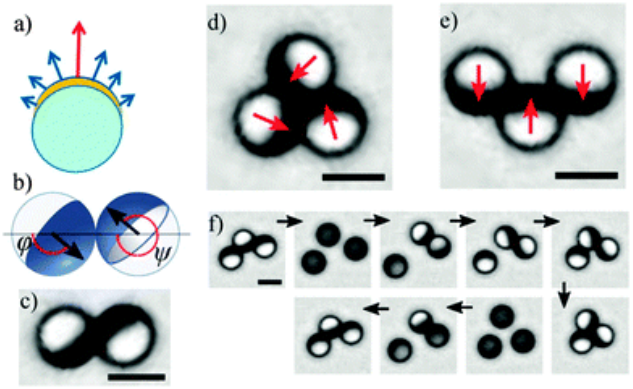

Figure 1. Janus Particles. Bistable self-assembly in homogeneous colloidal systems for flexible modular architectures.

2.2. Overview of sparse grids

2.2.1. Motivation of the sparse grids method

Sparse grids method is a surrogate modelling techniques that addresses the problems of representing, approximating and computing weighted integrals of a function $f : \mathbb{R}^N \to \mathbb{R}^V$ given some samples of f whose location we are free to choose.[4] Sparse grids were

[a] annplu-ipt25@lll.kpi.ua
[b] maximilian.neumann@physik.tu-chemnitz.de
[c] sibylle.gemming@physik.tu-chemnitz.de

developed to address the fundamental computational challenge known as the "curse of dimensionality" that plagues traditional numerical methods when dealing with high-dimensional problems.[6] It attempts to stem exponential growth of data points needed to employ full grid methods via obtaining a hierarchical combination of tensor grids where all the relevant information is represented by as few of them as possible.

2.2.2. Components of sparse grids

The first step to build a sparse grid is to define a set of collocation knots for each variable y_n. We thus introduce the univariate discretization level i_n in $\mathbb{N}_+$ and a so-called level-to-knots function that specifies the number of collocation knots to be used for each random variable, i.e.,

$$m : \mathbb{N}_+ \to \mathbb{N}_+, i_n \mapsto m\left(i_n\right).$$

Then, we denote by $\mathcal{T}_{n,i_n}$ the set of $m(i_n)$ discretization knots along y_n, i.e.,

$$\mathcal{T}_{n,i_n} = \left\{ y_{n,m(i_\infty)}^{(j_n)} : j_n = 1, \dots, m\left(i_n\right) \right\}$$

for $n = 1, \dots, N$.

Such sequence is usually chosen according to the probability distribution of the random variablesρ_n for efficiency reasons. Furthermore, for efficiency purposes it is beneficial if the sequences of knots are nested, i.e., if $\mathcal{T}_{n,i_n} \subset \mathcal{T}_{n,j_n}$ when $j_n \geq i_n$.

Next, we introduce the N-dimensional tensor grids, that are obtained by taking the Cartesian product of the N univariate sets of knots just introduced. For this purpose we collect the discretization levels i_n in a multi-index $\mathbf{i} = [i_1, \dots, i_N] \in \mathbb{N}_+^N$ and denote the corresponding tensor grid by $\mathcal{T}_i = \bigotimes_{n=1}^N \mathcal{T}_{n,i_n}$. Using standard multi-index notation, we can then write

$$\mathcal{T}_{\mathrm{i}} = \left\{ \mathbf{y}_{m(\mathrm{i})}^{(\mathrm{j})} \right\}_{\mathrm{j} \leq m(\mathrm{i})},$$

with

$$\mathbf{y}_{m(\mathrm{i})}^{(\mathrm{j})} = \left[y_{1,m(i_1)}^{(\mathrm{j}1)}, \dots, y_{N,m(i_N)}^{(\mathrm{GN}_N)} \right] \text{ and } \mathbf{j} \in \mathbb{N}_+^N,$$

where $m(\mathbf{i}) = \left[m\left(i_1\right), m\left(i_2\right), \dots, m\left(i_N\right)\right]$ and $\mathbf{j} \leq m(\mathbf{i})$ means that $j_n \leq m\left(i_n\right)$ for every $n = 1, \dots, N$.

2.2.3. Interpolation on the sparse grids

To explain how approximation is carried out on sparse grid, let us first consider regular full tensor grid scenario. A tensor grid approximation of $f(\mathbf{y})$ based on global Lagrangian interpolants collocated at these grid knots can then be written in the following form

$$\mathcal{U}_{\mathrm{i}}(\mathbf{y}) := \sum_{\mathrm{j} \leq m(\mathrm{i})} f\left(\mathbf{y}_{m(\mathrm{i})}^{(\mathrm{j})}\right) \mathcal{L}_{m(\mathrm{j})}^{(\mathrm{j})}(\mathbf{y}),$$

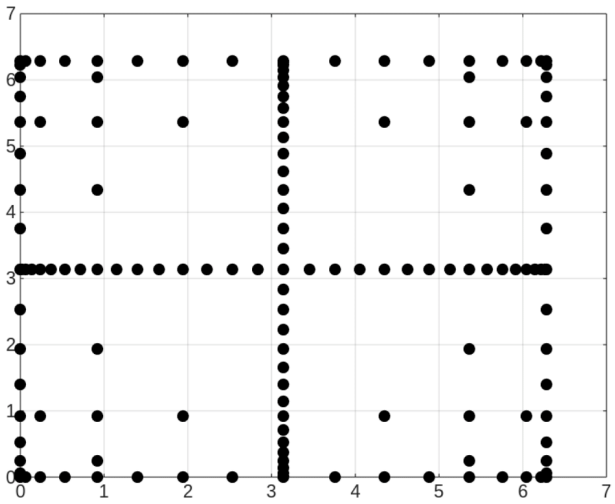

Figure 2. Example of a sparse grid.

where $\left\{ \mathcal{L}_{m(i)}^{(j)}(\mathbf{y}) \right\}_{j \leq m(i)}$ are the N-variate Lagrange basis polynomials, defined as tensor products of univariate Lagrange polynomials, i.e.

$$\mathcal{L}_{m(i)}^{(j)}(\mathbf{y}) = \prod_{n=1}^{N} l_{n,m(i_n)}^{(j_n)}\left(y_n\right)$$

with

$$l_{n,m(i_n)}^{(j_n)}\left(y_n\right) = \prod_{k=1, k \neq j_n}^{m(i_n)} \frac{y_n - y_{n,m(i_\infty)}^{(k)}}{y_{n,m(i_n)}^{(j_0)} - y_{n,m(i_\infty)}^{(k)}}.$$

Finally, building upon the concepts just introduced, the sparse grid approximation of $f(\mathbf{y})$, can be written as:

$$f(\mathbf{y}) \approx \mathcal{U}_I(\mathbf{y}) = \sum_{i \in I} c_{\mathrm{i}} \mathcal{U}_{\mathrm{i}}$$

$$c_{\mathrm{i}} := \sum_{\substack{\mathrm{j} \in \{0,1\}^N \\ i+j \in I}} (-1)^{\|\mathrm{j}\|_2} \int_\Gamma f(\mathbf{y}) \rho(\mathbf{y}) \mathrm{d}\mathbf{y} \approx \mathcal{Q}_I(\mathbf{y}) = \sum_{\mathrm{i} \in I} c_i \mathcal{Q}_{\mathbf{i}},$$

with $\mathcal{I} \subset \mathbb{N}_+^N$ denoting the multi-index set collecting the multi-indices in the sum. The sparse grid is then defined as

$$\mathcal{T}_I = \bigcup_{\substack{1 \in I \\ c \neq 0}} \mathcal{T}_{\mathrm{i}}.$$

For more details on derivation see references.[4]

3. Methodology

3.1. Original iterative approach

3.1.1. Parameters to define two particle arrangement:

The model particles are represented by hard spheres; magnetic field induced by them is simulated via an encapsulated ring coil with a current. The sphere with

radius R is centred at x_0. The centre of the coil located with a shift v from x_0 along radius vector of the sphere r_1, to which the coil is positioned perpendicular. It further is assigned a constant current I. [3] As we have already established our goal is to approximate the relative potential energy level of two particles arrangements, therefore the target function is going to have the following parameters:

1. coil shift;
2. coil radius;
3. distance between two particles' centres;
4. angle between normal vector of the first particle's coil plane and x axis;
5. angle between normal vector of the second particle's coil plane and x axis.

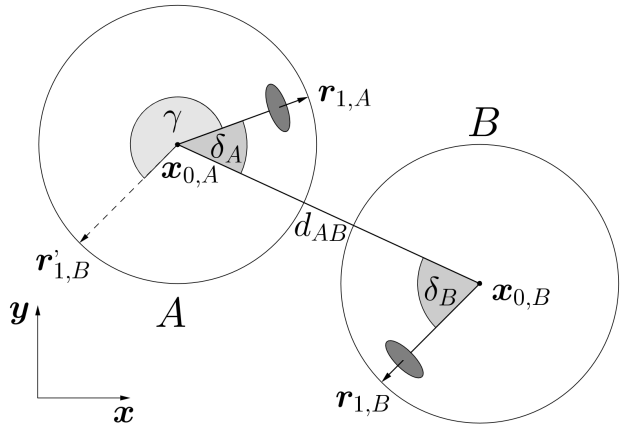

Figure 3. Parameters describing the interaction of two identical Janus particles.

3.1.2. Relative potential energy level calculation procedure

Janus particle is represented by a sphere of a certain radius; the magnetic field is modelled by a current running through a coil within particle's sphere. The moment of particle is restricted in 2 dimensions. The scale is large enough that we can limit ourselves to only considering macroscopic forces, e. i. the Lorentz force. With the coils centre being used as reference, in addition to its discretisation in p sections ($\varphi \to \varphi_i = i\frac{2\pi}{p}$), follows for the magnetic induction:

$$\boldsymbol{B}(\boldsymbol{x}) = \frac{\mu_0 I u}{2p} \sum_{i=0}^{p-1} \frac{\boldsymbol{e}_{\varphi_i} \times \left(\boldsymbol{x} - \boldsymbol{x}'\left(\varphi_i\right)\right)}{\left|\boldsymbol{x} - \boldsymbol{x}'\left(\varphi_i\right)\right|^3}.$$

The interaction between two modelled particles A and B is described by the Lorentz force F_L,

$$\boldsymbol{F}_L = \frac{2\pi I u}{p} \sum_{i=0}^{p-1} \left(\boldsymbol{e}_{\varphi_i} \times \boldsymbol{B}\left(\boldsymbol{x}_{\varphi_i}\right)\right)$$

induced by the influence of the magnetic stray field exerted by A on the electric current in B, and the resulting torque M_L :

$$\boldsymbol{M}_L = \frac{2\pi I u}{p} \sum_{i=0}^{p-1} \left(\boldsymbol{e}_{\varphi_i} \times \boldsymbol{B}\left(\boldsymbol{x}_{\varphi_i}\right)\right) \times \left(\boldsymbol{x}_{\varphi_i} - \boldsymbol{x}_0\right).$$

Energy in the system is calculated as sum work necessary to incrementally move particles with given parameters form one arrangement to another with or against torque. For more detailed derevation see references. [3]

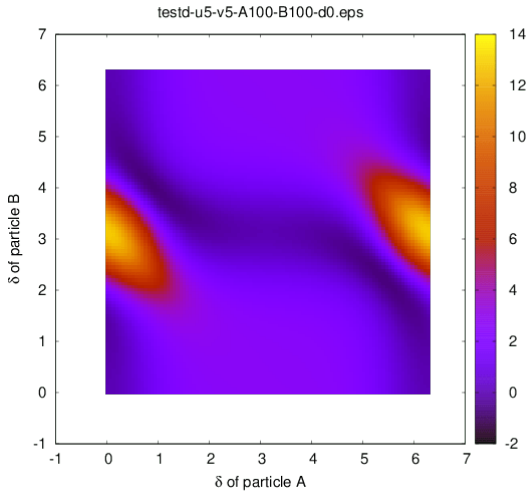

Figure 4. Example plot of relative potential energy level simulation using incremental approach, with varying angles and fixed distance, coil shift and radius.

3.2. Sparse grid approach

3.2.1. Generation of sparse grids

As discussed, sparse grid is a linear combination of many tensor grids on R^N (parameter space).

Each of the tensor grids included has relatively few points.

With suitable linear combinations of such grids, it is possible to achieve good accuracy in quadrature and interpolation, with a computational cost lower than using a single tensor grid.

Each of the tensor grids in the sparse grid is built by taking cartesian products of 1D distribution of points.

For purposes of this study, we are going to employ «vanilla» grid that is provided by implementation[4].

3.2.2. Evaluation on sparse grids

To evaluate the target function on sparse grid's knots we employ a modification of the original iterative approach.

We choose a starting point on the sparse grid assigning it a relative potential energy level of zero(we can do it since potential energy is defined up to an arbitrary constant).

Then we find the closest point of sparse grid that has not yet been evaluated and employing the same procedure as in initial approach. We connect two point by a path, which allows us to obtain the value of the target function.

We repeat these steps until all the points are evaluated (not unlike Prim's algorithm).

3.2.3. Interpolation on sparse grid

After generating the sparse grid and obtained the target function values at each point we utilize built-in procedure to interpolate the target function. Note since the sparse grid is a linear combination of several tensor grid interpolants, the interpolation error at a given point of the sparse grid is not necessarily zero, unless all tensor interpolates include that point.

4. Discussion

Up to this point we discussed two ways of tackling the problem of Janus particles relative potential energy level approximation.

In comparison with incremental approach sparse grids provide the following advantages:

- Sparse grid approach aprroximation is suitable for standard gradient-based optimization methods. [7]
- It also requires less storage capacity in comparison with incremental approach. As the sparse grid approximation involves fewer points than the incremental approach, as well as addressing curse of dimensionality for the multi-parametric model in question.
- Finally, the sparse grids approach is more computationally efficient, since while employing it we need to evaluate the target function of relative potential energy level only at the subset of points for which we would have to carry out evaluation in case of incremental approach.

This novel approach is well-suited for exploration of multiple Janus particles assembles (finding stable arrangements which correspond to low energy levels). Additionally, sparse grid modification approach lends itself well to further optimization such as parallelization and evaluation recycling pushing the horizons of our computational capacities even more.

5. Conclusion

In this work we formulated the problem of two Janus particles arrange relative potential energy level simulation. We have presented theoretical ground work and implementation for two approaches to tackling this problem, namely incremental approach and its modification involving sparse grids. Compared to incremental approach sparse grid provide a number of advantages, e. i. applicability of gradient based optimization methods, storage and computational efficiency, at a moderate cost to precision. Our findings provide a modification of incremental approach that allows for application gradient based optimization technique in subsequent simulations of multi-particles assembly as well as further optimization via parallelization and evaluation recycling.

References

1. Sparse grids for dynamic economic models / J. Brumm, C. Krause, A. Schaab, S. Scheidegger // SSRN Electronic Journal. — 2021. — ISSN 1556-5068. — DOI: 10.2139/ssrn.3979412. — URL: https://www.ssrn.com/abstract=3979412 (visited on 05/05/2025).
2. *Lewis A.* Efficient sampling of fast and slow cosmological parameters // Physical Review D. — 2013. — May. — Vol. 87, no. 10. — P. 103529. — ISSN 1550-7998, 1550-2368. — DOI: 10.1103/PhysRevD.87.103529. — URL: https://link.aps.org/doi/10.1103/PhysRevD.87.103529 (visited on 05/02/2025).
3. A Two-Parameter Model for Colloidal Particles with an Extended Magnetic Cap / M. Neumann, A. Strobel, Y. Al-Saadawi, G. Steinbach, A. Erbe, S. Gemming // physica status solidi (a). — 2019. — Oct. — Vol. 216, no. 19. — P. 1900506. — ISSN 1862-6300, 1862-6319. — DOI: 10.1002/pssa.201900506. — URL: https://onlinelibrary.wiley.com/doi/10.1002/pssa.201900506 (visited on 05/02/2025).
4. *Piazzola C., Tamellini L.* Algorithm 1040: The Sparse Grids Matlab Kit - a Matlab implementation of sparse grids for high-dimensional function approximation and uncertainty quantification // ACM Transactions on Mathematical Software. — 2024. — Mar. — Vol. 50, no. 1. — P. 1–22. — ISSN 0098-3500, 1557-7295. — DOI: 10.1145/3630023. — URL: https://dl.acm.org/doi/10.1145/3630023 (visited on 04/22/2025).
5. Bistable self-assembly in homogeneous colloidal systems for flexible modular architectures / G. Steinbach, D. Nissen, M. Albrecht, E. V. Novak, P. A. Sánchez, S. S. Kantorovich, S. Gemming, A. Erbe // Soft Matter. — 2016. — Vol. 12, no. 10. — P. 2737–2743. — ISSN 1744-683X, 1744-6848. — DOI: 10.1039/C5SM02899J. — URL: https://xlink.rsc.org/?DOI=C5SM02899J (visited on 05/02/2025).
6. *Garcke J.* Sparse Grids in a Nutshell // Sparse Grids and Applications. Vol. 88 / ed. by J. Garcke, M. Griebel. — Berlin, Heidelberg : Springer Berlin Heidelberg, 2012. — P. 57–80. — DOI: 10.1007/978-3-642-31703-3_3. — URL: https://link.springer.com/10.1007/978-3-642-31703-3_3 (visited on 04/22/2025) ; Series Title: Lecture Notes in Computational Science and Engineering.
7. *Pflüger D.* Spatially adaptive sparse grids for high-dimensional problems. — 1. Aufl. — München : Verl. Dr. Hut, 2010. — ISBN 978-3-86853-555-6.