The Journal of Open Source Software

ultrasphere and ultrasphere-harmonics: Python packages for Vilenkin–Kuznetsov–Smorodinsky polyspherical coordinates and hyperspherical harmonics methods in array API

Hiromochi Itoh[1], **Kei Matsushima**[2], and **Takayuki Yamada**[3]

1 Department of Mechanical Engineering, Graduate School of Engineering, The University of Tokyo, Japan **2** Graduate School of Advanced Science and Engineering, Hiroshima University, Japan **3** Department of Strategic Studies, Institute of Engineering Innovation, Graduate School of Engineering, The University of Tokyo

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor: Open Journals

Reviewers:

- @openjournals

Submitted: 01 January 1970
Published: unpublished

Summary

Spherical harmonics, which are the solutions to the angular part of the laplace equation, have been widely used in various fields of science and engineering. Spherical harmonics in 3D are well-known and have various applications, and many software packages have been developed for them. Hyperspherical harmonics, which are spherical harmonics in higher dimensions, have been applied to many-body problems in quantum mechanics (Fock, 1935), representation of crystallographic textures (Bonvallet et al., 2007), description of 3D models (Bonvallet et al., 2007), representation of brain structures (Hosseinbor et al., 2013), representation of the Head-Related Transfer Function, which characterizes how an ear receives a sound from a point in space (Szwajcowski, 2023), and so on. However, an attempt to develop a framework which allows codes to work on both 3D and higher dimensions has not been made. Therefore, we aim to provide a unified framework for implementing spherical harmonics techniques in arbitrary dimensions and coordinate systems. Our packages would allow researchers to easily extend their work to higher dimensions, for example, from 2D to 3D and further to 4D, without having to duplicate code for each dimension.

Statement of need

`ultrasphere` is a Python package for Vilenkin–Kuznetsov–Smorodinsky (VKS) polyspherical coordinate systems (Vilenkin & Klimyk, 1993). `ultrasphere-harmonics` implements hyperspherical harmonics methods for any type of polyspherical coordinates based on `ultrasphere`. While spherical harmonics in 3D itself have been widely implemented in various software packages, such as Scipy (Virtanen et al., 2020), hyperspherical harmonics are rarely implemented, and software packages which supports arbitrary VKS polyspherical coordinates are not known. The main goal of out packages is to provide a unified framework for implementing spherical harmonics techniques in arbitrary VKS polyspherical coordinates and dimensions. To demonstrate this, code for solving acoustic scattering from a single sound-soft sphere using any type of polyspherical coordinates is implemented within `ultrasphere-harmonics` as a command-line application.

Spherical expansion methods are sometimes computationally expensive, especially in higher dimensions. To utilize HPC resources, which environment is recently diversified, our api is made to be compatible with the array API standard (Meurer et al., 2023), which enables writing code which runs on multiple array libraries (e.g., NumPy(Harris et al., 2020), PyTorch(Paszke et al., 2019)) and multiple hardware (e.g., CPU, GPU). Our packages fully support vectorization to leverage the performance of these libraries.

Acknowledgements

This work used computational resources Supermicro ARS-111GL-DNHR-LCC and FUJITSU Server PRIMERGY CX2550 M7 (Miyabi) at Joint Center for Advanced High Performance Computing (JCAHPC) and TSUBAME4.0 supercomputer provided by Institute of Science Tokyo through Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures and High Performance Computing Infrastructure in Japan (Project ID: jh240031).

References

Bonvallet, B., Griffin, N., & Li, J. (2007). A 3D shape descriptor: 4D hyperspherical harmonics "an exploration into the fourth dimension". *Proceedings of the IASTED International Conference on Graphics and Visualization in Engineering*, 113–116. ISBN: 9780889866270

Fock, V. (1935). Zur theorie des wasserstoffatoms. *Zeitschrift Für Physik*, *98*(3), 145–154. https://doi.org/10.1007/BF01336904

Harris, C. R., Millman, K. J., Walt, S. J. van der, Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., Kerkwijk, M. H. van, Brett, M., Haldane, A., Río, J. F. del, Wiebe, M., Peterson, P., … Oliphant, T. E. (2020). Array programming with NumPy. *Nature*, *585*(7825), 357–362. https://doi.org/10.1038/s41586-020-2649-2

Hosseinbor, A. P., Chung, M. K., Schaefer, S. M., Reekum, C. M. van, Peschke-Schmitz, L., Sutterer, M., Alexander, A. L., & Davidson, R. J. (2013). 4D hyperspherical harmonic (HyperSPHARM) representation of multiple disconnected brain subcortical structures. *Medical Image Computing and Computer-Assisted Intervention : MICCAI … International Conference on Medical Image Computing and Computer-Assisted Intervention*, *16*(0), 598–605. https://doi.org/10.1007/978-3-642-40811-3_75

Meurer, A., Reines, A., Gommers, R., Fang, Y.-L. L., Kirkham, J., Barber, M., Hoyer, S., Müller, A., Zha, S., Shanabrook, S., Gacha, S. J., Lezcano-Casado, M., Fan, T. J., Reddy, T., Passos, A., Kwon, H., Oliphant, T., & Standards, C. for P. D. A. (2023). Python array API standard: Toward array interoperability in the scientific python ecosystem. *Scipy*. https://doi.org/10.25080/gerudo-f2bc6f59-001

Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., Desmaison, A., Köpf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., … Chintala, S. (2019). PyTorch: An imperative style, high-performance deep learning library. In *Proceedings of the 33rd international conference on neural information processing systems* (pp. 8026–8037). Curran Associates Inc.

Szwajcowski, A. (2023). Continuous head-related transfer function representation based on hyperspherical harmonics. *Archives of Acoustics*, *48*(1), 127–139. https://doi.org/10.24425/aoa.2023.144267

Vilenkin, N. Ja., & Klimyk, A. U. (1993). *Representation of lie groups and special functions* (Vol. 74). Springer Netherlands. https://doi.org/10.1007/978-94-017-2883-6

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., … SciPy 1.0 Contributors. (2020). SciPy 1.0: Fundamental Algorithms for Scientific Computing in

Python. *Nature Methods*, *17*, 261–272. https://doi.org/10.1038/s41592-019-0686-2