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Published: unpublished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 eigenfunctions of the Laplace-Beltrami operator on the unit sphere, have been widely used in various fields of science and engineering. While numerous software packages exist for standard three-dimensional spherical harmonics, many modern scientific challenges require working with hyperspherical harmonics, which are spherical harmonics in higher dimensions. Hyperspherical harmonics have been widely used for various applications, including 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). However, there is a barrier for researchers to implement spherical harmonics and hyperspherical harmonics methods in their work, as the implementation is often specific to the dimension and coordinate system used, requiring significant effort to adapt the code for different dimensions or coordinate systems. To address this, we have developed a software package for implementing spherical harmonics techniques in arbitrary dimensions and coordinate systems. Our packages would allow researchers to easily implement and 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). Built on top of `ultrasphere`, `ultrasphere-harmonics` implements hyperspherical harmonics methods for any type of polyspherical coordinates. While spherical harmonics in 3D itself have been widely implemented in various software packages, such as Scipy (Virtanen et al., 2020) and SphericalFunctions.jl (Boyle, 2025), hyperspherical harmonics are rarely implemented, and software packages which supports arbitrary VKS polyspherical coordinates are not known. To remedy this, our packages allow to convert between Cartesian coordinates and VKS polyspherical coordinates, compute hyperspherical harmonics, elementary solutions to the Helmholtz equation, hyperspherical expansion of a function, and the translational coefficients of elementary solutions of the Helmholtz equation under arbitrary VKS polyspherical coordinates and dimensions. The underlying implementation leverages the "method of trees" (Cohl, 2012; Vilenkin & Klimyk, 1993), the rooted tree

representation of VKS coordinates with the help of NetworkX (Hagberg et al., 2008). A command-line application that solves for acoustic scattering from a sound-soft sphere using arbitrary VKS polyspherical coordinates is included to illustrate a practical use case.

Spherical expansion methods are sometimes computationally expensive, especially in higher dimensions. To utilize modern high-performance computing resources, which environment is recently diversified, our api is made to be compatible with the array API standard (Meurer et al., 2023), ensuring that the same code can run 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 array 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

Boyle, M. (2025). *SphericalFunctions.jl*. Zenodo. https://doi.org/10.5281/zenodo.15263415

Cohl, H. (2012). Fourier, gegenbauer and jacobi expansions for a power-law fundamental solution of the polyharmonic equation and polyspherical addition theorems. *Symmetry, Integrability and Geometry: Methods and Applications (SIGMA)*, *9*. https://doi.org/10.3842/SIGMA.2013.042

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

Hagberg, A. A., Schult, D. A., & Swart, P. J. (2008). Exploring network structure, dynamics, and function using NetworkX. In G. Varoquaux, T. Vaught, & J. Millman (Eds.), *Proceedings of the 7th python in science conference* (pp. 11–15).

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