

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

Hiromochi Itoh¹, Kei Matsushima², and Takayuki Yamada³

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, Japan

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

Software

- [Review](#)
- [Repository](#)
- [Archive](#)

Editor: [Open Journals](#)

Reviewers:

- [@openjournals](#)

Submitted: 01 January 1970

Published: unpublished

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

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 shapes (Bonvallet et al., 2007), representation of brain structures (Hosseini et al., 2013), representation of the Head-Related Transfer Function, which characterizes how an ear receives a sound from a point in space (Szwajkowski, 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 software packages 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

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

44 Spherical expansion methods are sometimes computationally expensive, especially in higher
45 dimensions. To utilize modern high-performance computing resources, which environment is
46 recently diversified, our api is made to be compatible with the array API standard (Meurer
47 et al., 2023), ensuring that the same code can run on multiple array libraries (e.g., NumPy
48 (Harris et al., 2020), PyTorch (Paszke et al., 2019)) and multiple hardware (e.g., CPU, GPU).
49 Our packages fully support vectorization to leverage the performance of these array libraries.

50 Acknowledgements

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

56 References

- 57 Bonvallet, B., Griffin, N., & Li, J. (2007). A 3D shape descriptor: 4D hyperspherical harmonics
58 "an exploration into the fourth dimension". *Proceedings of the IASTED International*
59 *Conference on Graphics and Visualization in Engineering*, 113–116. ISBN: 9780889866270
- 60 Boyle, M. (2025). *SphericalFunctions.jl*. Zenodo. <https://doi.org/10.5281/zenodo.15263415>
- 61 Cohl, H. (2012). Fourier, gegenbauer and jacobi expansions for a power-law fundamental
62 solution of the polyharmonic equation and polyspherical addition theorems. *Symmetry,*
63 *Integrability and Geometry: Methods and Applications (SIGMA)*, 9. [https://doi.org/10.](https://doi.org/10.3842/SIGMA.2013.042)
64 [3842/SIGMA.2013.042](https://doi.org/10.3842/SIGMA.2013.042)
- 65 Fock, V. (1935). Zur theorie des wasserstoffatoms. *Zeitschrift Für Physik*, 98(3), 145–154.
66 <https://doi.org/10.1007/BF01336904>
- 67 Hagberg, A. A., Schult, D. A., & Swart, P. J. (2008). Exploring network structure, dynamics,
68 and function using NetworkX. In G. Varoquaux, T. Vaught, & J. Millman (Eds.), *Proceedings*
69 *of the 7th python in science conference* (pp. 11–15).
- 70 Harris, C. R., Millman, K. J., Walt, S. J. van der, Gommers, R., Virtanen, P., Cournapeau, D.,
71 Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., Kerkwijk,
72 M. H. van, Brett, M., Haldane, A., Río, J. F. del, Wiebe, M., Peterson, P., ... Oliphant,
73 T. E. (2020). Array programming with NumPy. *Nature*, 585(7825), 357–362. <https://doi.org/10.1038/s41586-020-2649-2>
- 74
- 75 Hosseinbor, A. P., Chung, M. K., Schaefer, S. M., Reekum, C. M. van, Peschke-Schmitz, L.,
76 Sutterer, M., Alexander, A. L., & Davidson, R. J. (2013). 4D hyperspherical harmonic
77 (HyperSPHARM) representation of multiple disconnected brain subcortical structures.
78 *Medical Image Computing and Computer-Assisted Intervention : MICCAI ... International*
79 *Conference on Medical Image Computing and Computer-Assisted Intervention*, 16(0),
80 598–605. https://doi.org/10.1007/978-3-642-40811-3_75
- 81 Meurer, A., Reines, A., Gommers, R., Fang, Y.-L. L., Kirkham, J., Barber, M., Hoyer, S.,
82 Müller, A., Zha, S., Shanabrook, S., Gacha, S. J., Lezcano-Casado, M., Fan, T. J., Reddy,
83 T., Passos, A., Kwon, H., Oliphant, T., & Standards, C. for P. D. A. (2023). Python
84 array API standard: Toward array interoperability in the scientific python ecosystem. *Scipy*.
85 <https://doi.org/10.25080/gerudo-f2bc6f59-001>

- 86 Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z.,
87 Gimelshein, N., Antiga, L., Desmaison, A., Köpf, A., Yang, E., DeVito, Z., Raison, M.,
88 Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., ... Chintala, S. (2019). PyTorch:
89 An imperative style, high-performance deep learning library. In *Proceedings of the 33rd*
90 *international conference on neural information processing systems* (pp. 8026–8037). Curran
91 Associates Inc.
- 92 Szwajcowski, A. (2023). Continuous head-related transfer function representation based on
93 hyperspherical harmonics. *Archives of Acoustics*, 48(1), 127–139. <https://doi.org/10.24425/aoa.2023.144267>
94
- 95 Vilenkin, N. Ja., & Klimyk, A. U. (1993). *Representation of lie groups and special functions*
96 (Vol. 74). Springer Netherlands. <https://doi.org/10.1007/978-94-017-2883-6>
- 97 Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D.,
98 Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson,
99 J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., ... SciPy
100 1.0 Contributors. (2020). SciPy 1.0: Fundamental Algorithms for Scientific Computing in
101 Python. *Nature Methods*, 17, 261–272. <https://doi.org/10.1038/s41592-019-0686-2>

DRAFT