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

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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. Especially, 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).

Statement of need

`ultrasphere` and `ultrasphere-harmonics` are Python packages for hyperspherical coordinates and hyperspherical harmonics techniques. Our packages is that they support any type of Vilenkin–Kuznetsov–Smorodinsky polyspherical coordinate systems (Vilenkin & Klimyk, 1993). This allows to write codes that work in any type of polyspherical coordinates and thus in any number of dimensions. To demonstrate this, we implemented acoustic scattering from a single sphere for any type of polyspherical coordinates, which could be verified by command-line interface.

Our api is compatible with the array API standard (Meurer et al., 2023). This 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 for high performance computing.

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