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NuclearToolkit.jl: A Julia package for nuclear structure calculations

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Software

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Summary

One of the ultimate goals in nuclear physics is to understand and predict various properties of nuclei from a fundamental interaction among nucleons, the nuclear force. Owing to recent developments in the community, especially in describing the nuclear force and in nuclear many-body methods, it is becoming possible to make quantitative discussions and predictions on various properties with first-principles calculations. On the other hand, it is a common situation that different degrees of freedom can be important (e.g., nucleons, alpha-cluster) to describe one nucleus or one state of a target nucleus, so nuclear models are becoming more and more diverse. It can therefore be difficult to familiarize oneself with the technical details of all those methods. `NuclearToolkit.jl` was designed to circumvent the situation and to be helpful for both students and researchers to tackle nuclear many-body problems.

Statement of need

`NuclearToolkit.jl` provides self-contained codes for nuclear physics covering from nuclear forces to various nuclear many-body methods. Users can generate nucleon-nucleon (NN) potentials based on chiral effective field theory (Epelbaum et al., 2009, 2020; R. Machleidt & Entem, 2011; R. Machleidt & Sammarruca, 2016) and use them in many-body methods such as Hartree-Fock many-body perturbation theory (which is well known as Møller–Plesset method in the community of chemistry) (Shavitt & Bartlett, 2009), in-medium similarity renormalization group (IM-SRG) (S. Ragnar Stroberg et al., 2019), and valence shell model (configuration interaction method) (B. A. Brown, 2001; Caurier et al., 2005; Otsuka et al., 2020).

In the nuclear physics community, many public codes are already available. Although it may not be possible to list them all, representative examples are ANTOINE (Caurier & Nowacki, 1999), NuShellX (B. A. Brown & Rae, 2014), BIGSTICK (Johnson et al., 2013, 2018), and KSHELL (Shimizu, 2013; Shimizu et al., 2019) for valence shell-model and imsrg (S. R. Stroberg, n.d.) for IM-SRG. People are using those various codes, which are typically written in Fortran, C++, etc., and call them in their homemade shell or Python scripts. `NuclearToolkit.jl`, which is not a wrapper of those existing codes, provides a new interface that combines these various methods into one and works on a variety of environments, including Linux, Mac, and Windows. This is achieved thanks to the high readability and portability of the Julia programming language (Bezanson et al., 2012).

This code has been used in previous works (Yoshida, 2022; Yoshida & Shimizu, 2022).

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