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Multiscale Hub: An Open-Source Framework for Practical Atomistic-To-Continuum Coupling

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Abstract : Despite vast amount of existing theoretical knowledge, the implementation of a universal multiscale modeling, analysis, and simulation software framework remains challenging. Existing multiscale software and solutions are often domain-specific, closed-source and mandate a high-level of experience and skills in both multiscale analysis and programming. Furthermore, tools currently existing for Atomistic-to-Continuum (AtC) multiscaling are developed with the assumptions such as accessibility of high-performance computing facilities to the users. These issues mentioned plus many other challenges have reduced the adoption of multiscale in academia and especially industry. In the current work, we introduce Multiscale Hub (MsHub), an effort towards making AtC more accessible through cloud services. As a joint effort between academia and industry, MsHub provides a universal web-enabled framework for practical multiscaling. Developed on top of universally acclaimed scientific programming language Python, the package currently provides an open-source, comprehensive, easy-to-use framework for AtC coupling. MsHub offers an easy to use interface to prominent molecular dynamics and multiphysics continuum mechanics packages such as LAMMPS and MFEM (a free, lightweight, scalable C++ library for finite element methods). In this work, we first report on the design philosophy of MsHub, challenges identified and issues faced regarding its implementation. MsHub takes the advantage of a comprehensive set of tools and algorithms developed for AtC that can be used for a variety of governing physics. We then briefly report key AtC algorithms implemented in MsHub. Finally, we conclude with a few examples illustrating the capabilities of the package and its future directions.

Keywords : atomistic, continuum, coupling, multiscale
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