

The University of Chicago hereby disclaims all copyright interest in “RAPTOR” and “FitRMD”, which are software packages used for multi-scale reactive molecular dynamics simulations and developed by the research laboratory of Professor Gregory A. Voth, the “Developer”.

Copyright © 2012-2023, The University of Chicago and Authors. All rights reserved.

RAPTOR and FitRMD are open-source software packages. All parts in both packages, which including computer source codes, installation and tools scripts, runtime configurations and parameters computer files, any related printed, electronic, and online documents, and any other files that may accompany the product, are hereby granted to any person, free of charge, permissions of modification and redistribution with all purposes, under the terms of the GNU Public License Version 2 (GPLv2).

The above copyright notice and this permission notice shall be included in all copies or substantial portions of the software: The legal text of the GPL as it applies to the original and all derived distributions of RAPTOR and FitRMD. A copy of the GNU General Public License along with this program shall be found in the accompanying file GPL.txt. If not, see <<https://www.gnu.org/licenses/>>.

Any publications or public reports that use results or benchmarks from the software packages shall cite *at least* the two references listed in the footnote* and acknowledge the Developer in the acknowledgements of the publication.

RAPTOR and FitRMD come with no warranty that use of them will be uninterrupted or error-free. The developers do not guarantee timely responses to questions or responses to requests for assistance.

* (1) T. Yamashita, Y. Peng, C. Knight, and G. A. Voth, “Computationally Efficient Multiconfigurational Reactive Molecular Dynamics”, *J. Chem. Theory Comp.* **8**, 4863–4875 (2012). PMID: PMC412084.. (2) Y. Peng, C. Knight, P. Blood, L. Crosby, and G. A. Voth, “Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations”, *XSEDE’12: Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the Campus and Beyond*, Article No. 37 (ACM, New York, 2012)..