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Amber 2023 David A. Case,H. Metin Aktulga,Kellon Belfon,Ido Y. Ben-Shalom,Joshua T. Berryman,Scott R. Brozell,David S. Cerutti,Thomas E. Cheatham III,G. Andrés Cisneros,Vinícius Wilian D. Cruzeiro,Tom A. Darden,Negin Forouzesh,George Giambasu,Timothy Giese,Michael K. Gilson,Holger Gohlke,Andreas W. Goetz,Julie Harris,Saeed Izadi,Sergei A. Izmailov,Koushik Kasavajhala,Mehmet C. Kaymak,Edward King,Andriy Kovalenko,Tom Kurtzman,Taisung Lee,Pengfei Li,Charles Lin,Jian Liu,Tyler Luchko,Ray Luo,Matias Machado,Viet Man,Madushanka Manathunga,Kenneth M. Merz,Yinglong Miao,Oleg Mikhailovskii,Gérald Monard,Hai Nguyen,Kurt A. O’Hearn,Alexey Onufriev,Feng Pan,Sergio Pantano,Ruxi Qi,Ali Rahnamoun,Daniel R. Roe,Adrian Roitberg,Celeste Sagui,Stephan Schott-Verdugo,Akhil Shajan,Jana Shen,Carlos L. Simmerling,Nikolai R. Skrynnikov,Jamie Smith,Jason Swails,Ross C. Walker,Jinan Wang,Junmei Wang,Haixin Wei,Xiongwu Wu,Yeyue Xiong,Yi Xue,Darrin M. York,Shiji Zhao,Qiang Zhu,Peter A. Kollman,2023-04-30 Amber is the collective name for a suite of programs that allow users to carry out molecular dynamics simulations, particularly on biomolecules. None of the individual programs carries this name, but the various parts work reasonably well together, and provide a powerful framework for many common calculations.[1, 2] The term Amber is also used to refer to the empirical force fields that are implemented here.[3, 4] It should be recognized, however, that the code and force field are separate: several other computer packages have implemented the Amber force fields, and other force fields can be implemented with the Amber programs. Further, the force fields are in the public domain, whereas the codes are distributed under a license agreement. The Amber software suite is divided into two parts: AmberTools23, a collection of freely available programs mostly under the GPL license, and Amber22, which is centered around the pmemd simulation program, and which continues to be licensed as before, under a more restrictive license. Amber22 represents a significant change from the most recent previous version, Amber20. (We have moved to numbering Amber releases by the last two digits of the calendar year, so there are no odd-numbered versions.) Please see <https://ambermd.org> for an overview of the most important changes. AmberTools is a set of programs for biomolecular simulation and analysis. They are designed to work well with each other, and with the “regular” Amber suite of programs. You can perform many simulation tasks with AmberTools, and you can do more extensive simulations with the combination of AmberTools and Amber itself. Most components of AmberTools are released under the GNU General Public License (GPL). A few components are in the public domain or have other open-source licenses. See the README file for more information.

Household Divisions of Labour E. Birch,A. Le,P. W. Miller,2009-11-18 This book investigates the extent of gender inequality in the division of labour in the modern household. Through comparisons of the time allocations of single couple families without children, couple families with children and lone parents, a comprehensive account of the evolution of gender inequality over a typical lifecourse is presented.

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