

Pre-exascale HPC approaches for molecular dynamics simulations. Covid-19 research: A use case

URL: <https://onlinelibrary.wiley.com/doi/10.1002/wcms.1622>

Authors: [Wieczór, Miłosz](#) / [Genna, Vito](#) / [Aranda, Juan](#) / [Badia, Rosa](#) / [Gelpí, Josep](#) / [Gapsys, Vytautas](#) / [de Groot, Bert](#) / [Lindahl, Erik](#) / [Municoy, Martí](#) / [Hospital, Adam](#) / [Orozco, Modesto](#)

Research Lines: [Computational infrastructures for biomolecular research](#) / [HPC Workflows](#) / [New approaches to the prediction of protein structure and interactions](#)

Publication: WIREs Computational Molecular Science

Volume:

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 25 abr 2024 - 02:14): <https://www.bsc.es/ca/research-and-development/publications/wiley-interdisciplinary-reviews-computational-molecular>