

Exabiosim: Establishing the Accessible Computational Regimes for Biomolecular Simulations at Exascale

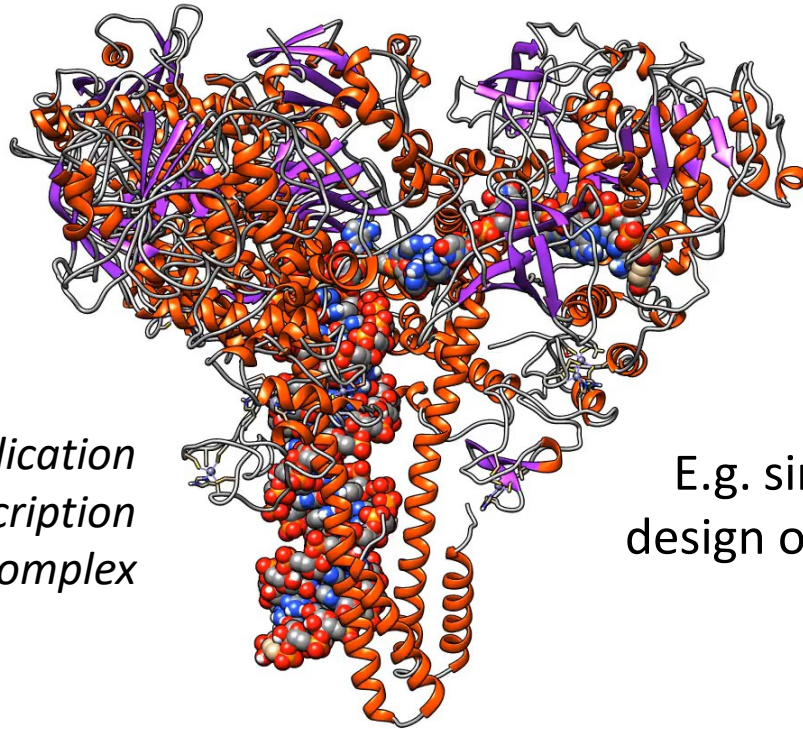
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Why biomolecular simulation?



*SARS-CoV-2 replication
and transcription
complex*

Computer simulations provide key dynamical information on biomacromolecules relevant to human health and disease

E.g. simulations of spike proteins,
design of small molecule therapeutics

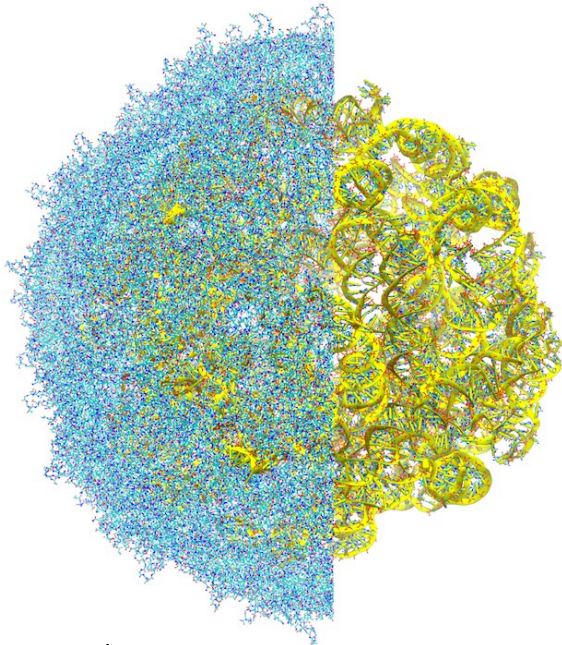


But biology is heterogeneous, multiscale (length and time), is driven by small free energy changes, and is challenging to compare with experiment

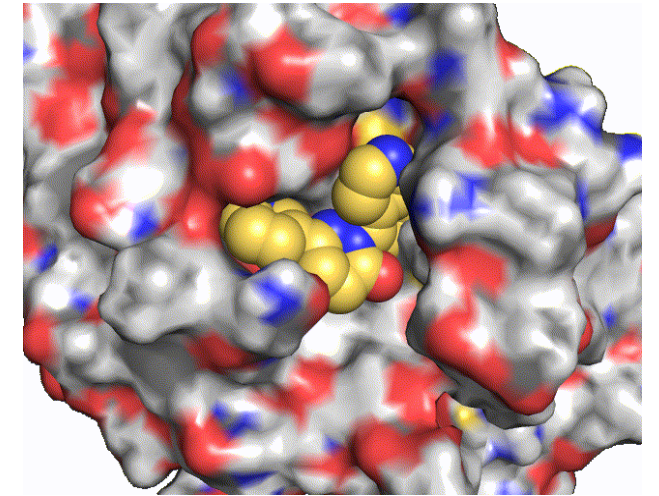
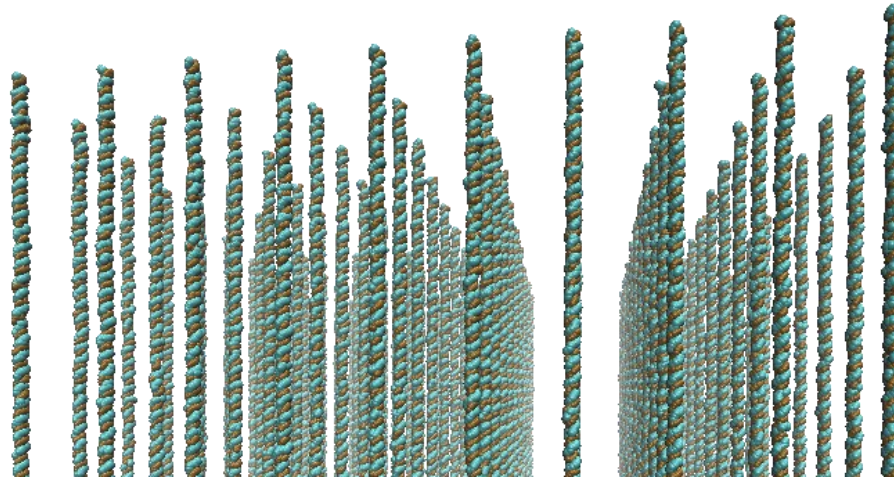


Opportunities at Exascale

1000x
Ensemble
Ensemble
Ensemble
Ensemble
Ensemble
Ensemble
Ensemble
LARGE
multiscale



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Massive systems & integrating with experimental data will help us explore the limits of current parallel programming

Multiscale DNA modeling at the atomistic and coarse-grained level, up to the scale of chromatin and entire chromosomes

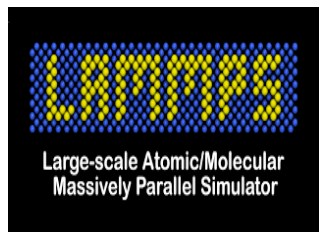
Ensemble computing for drug discovery requires huge numbers of lightly coupled compute resources

Our Community



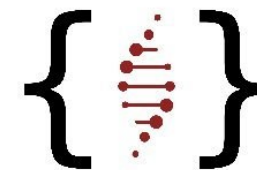
NAMD

Scalable Molecular Dynamics



FAST. FLEXIBLE. FREE.

GROMACS



CCP BioSim



Software landscape: few, but widely-used and well-maintained codes

We are generating toy and showcase application benchmarks to test performance on Excalibur testbeds

Community development:

- Open community workshops
- Training the next generation of biomolecular simulators
- WHPC@Exascale workshop



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