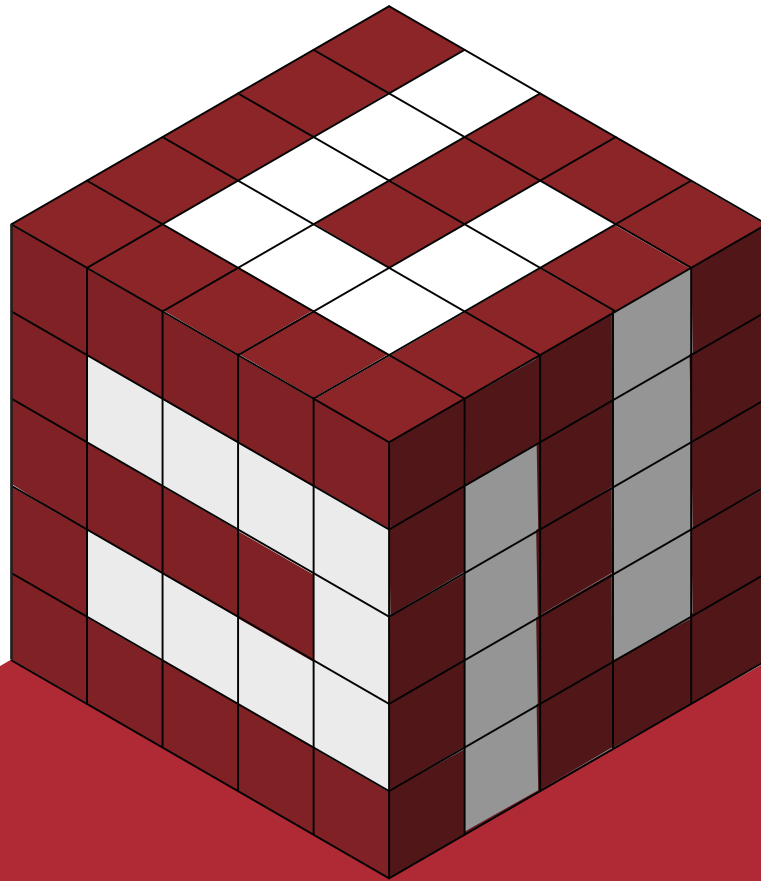


GENESIS

Overview and Demo at SC17



01

14th Nov. AM11:00-11:10

General introduction of GENESIS

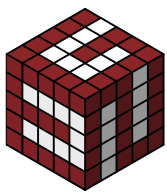
Chigusa Kobayashi (RIKEN, AICS)

02

14th Nov. AM11:10-11:20

High performance scheme in GENESIS

Jaewoon Jung (RIKEN, AICS)



GENESIS

Generalized-ensemble simulation system



K computer
Computer simulations
create the future

Molecular dynamics (MD) software for biomolecular systems.

Open source software distributed under the GPLv2 license.

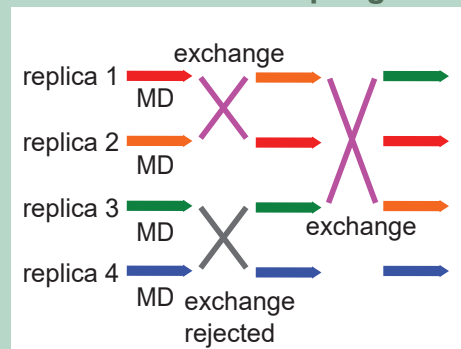


Please check 'GENESIS' website
URL: <http://www.aics.riken.jp/labs/cbrt/>

Feature

1. High performance schemes using hybrid parallelization (MPI+OpenMP) and/or GPGPU
2. Enhanced sampling algorithm for free-energy calculation
3. Multi-scale MD (All atom, Coarse-Grained, QM/MM)
4. Data assimilation

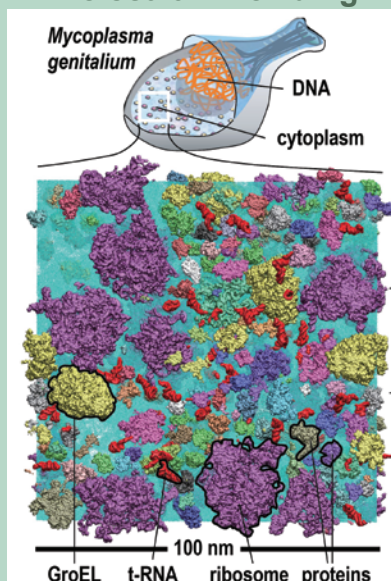
Enhanced sampling



Target Application

1. Molecular crowding
2. Structure/Dynamics of biomolecules
3. Data driven simulations

Molecular Crowding



eLife 5, e19274 (2016)

Performance of GENESIS on K computer

