Prediction of conformational dynamics of proteins on the surface of SARS-Cov-2 using Fugaku

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Research contents:

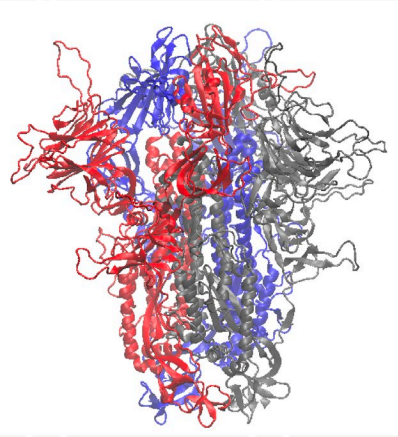
On the surface of the coronavirus, there are many spike proteins that interact with virial receptor ACE2 on the host cell surface. To block the interaction between the spike protein and the receptor is an important research subject to develop a drug for COVID-19.

Recently, atomic structures of the spike protein were determined using cryo-electron microscopy (cryo-EM). We perform atomistic molecular dynamics (MD) simulations of the spike protein in solution to predict experimentally undetectable dynamic structures. We use GENESIS MD software, which allows us about 125 times faster MD simulations on Fugaku compared to K computer. Furthermore, we enhance motions of a part of the spike protein using a multicopy simulation method to predict a large-scale conformational dynamics of the spike proteins.

Expected results:

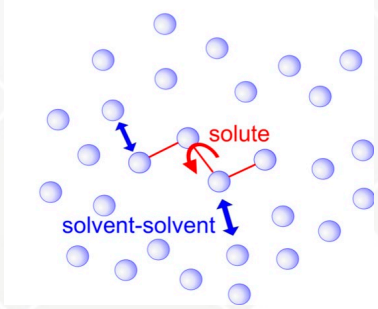
Large-scale conformational dynamics of spike proteins will be obtained, which is hardly attainable using the conventional MD simulations and experimental measurements.

Predicted dynamic structures of the spike protein will be used to develop drugs for inhibiting the interaction between the spike protein and the receptor on the host cell.



S-protein on the surface of SARS-Cov-2

GENESIS
Generalized-ensemble simulation system



gREST can enhance motions of the solute region