Preform MM/PBSA on Fugaku

Introduction

PROFESSEUR: M.DA ROS

It is not recommanded to perform MM/PBSA on the Fugaku compute node. Although each compute node has 48 cores, the RAM for each compute node is only 32G. However, performing MM/PBSA parallelly needs a large amount of RAM. So when the system is large, it is impossible to used all the cores in one node. It is a kind of waste.

So please be careful!

In this tutorial, we will try to perform MM/PBSA on the fugaku. First, we will install software for perform MM/PBSA, then we will perform MM/PBSA on the compute node.

Currently, we only performed MM/PBSA analysis, so if there are other errors, we will try to correct it when we find it. You can also report it to us.