Description

A NAMD user has emailed the NAMD mailing list with the following:

So you can take pure NAMD/Charm++, build it with GCC8 compilers and try to run - you'll receive the same hang behavior (at least on our computers which are employs the same environment it's true).

Plumed team is already maintains NAMD-2.12 and 2.13 version, but once again - seems like the problem is related to the newest GCC compilers, not Plumed

One important note: when hang occurs all dedicated CPUs (i. e., via namd2 +pN) are fully busy.

Thus, it seems like there may be some issue with gcc 8 or other new versions of the compiler in NAMD or in Charm++.