NAMD CAAR Project - First Results

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We present first results on the NAMD CAAR project. The goal of the project is to have NAMD molecular dynamics engine running at scale on the upcoming Summit system. Essential to this goal is to have most of the computation running on the GPUs. In this poster we will give a brief introduction to NAMD, show modifications that were made to improve non-bonded force CUDA kernel performance, and discuss plans for further work.