Scientific HPC Applications in Cloud Computing Environment: A Trend of Containerization

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Abstract: Using cloud computing platform to support scientific researches is a flexible solution for universities and research centers. In term of providing computing services, virtualization was become the widely used technology which also supports HPC applications for reproducible researches. However, the computing resources and energy consumed by hypervisor and virtual machine are inevitable and considerably affect the performance of HPC applications. The trend of container-based virtualization recently emerged as a solution to reduce the overhead of existing technique while keeping the ability to easily and expeditiously reproduce researches' results, even when the scientific application requires a sophisticated system consists of various third-party libraries. In this paper, we shall discuss about the containerization in the context of supporting reproducible scientific HPC applications. We shall also analyze the performance of real applications (for hydrodynamics research) that were migrated to run on Docker - a newly emergent tool for containerization. With the considerable improvement in performance and portability, the result shows that container-based virtualization is a promising technique for future Cloud platform, especially in the context of supporting scientific HPC applications.

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