Progress in the transferability of fusion workflows across HPC systems

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Understanding the behaviour of high-temperature plasmas is one of the main pillars in the development of fusion energy. It involves the development, validation, and use of several numerical models to describe complex physical processes and their interactions. Integrated modelling (IM) brings together multiple different numerical models connected with well-defined interfaces. Such IM workflows can be very complex to design, maintain and run efficiently on modern high-performance computers (HPC). To facilitate further progress, we present a scheme to tackle the execution of large fusion workflows on modern supercomputers using container technologies and a tool for their remote submission. To demonstrate the new capabilities, we focus on the packaging of a Docker [1] container image of the highly complex environment of the ITER IMAS [2] and running it on Marconi-Fusion, the European High-Performance Computer for fusion applications. This scheme provides a novel way to execute workflows remotely in a machine-independent manner. Our results demonstrate the feasibility of this solution for HPC codes in the field of fusion. We have tested the new capabilities with the electrostatic particle-in-cell (PIC) + Monte Carlo (MC) code BIT1 [3], the Monte Carlo code ASCOT [4] as well as the reference HPCG benchmark [5] with up to 3072 cores on Marconi-Fusion. Figure 1 shows an example of the good performance obtained. Applications are in progress on other supercomputers such as MareNostrum4, Eagle or the ITER cluster, addressing the needs of the fusion integrated modelling community including the European Transport Solver [6].
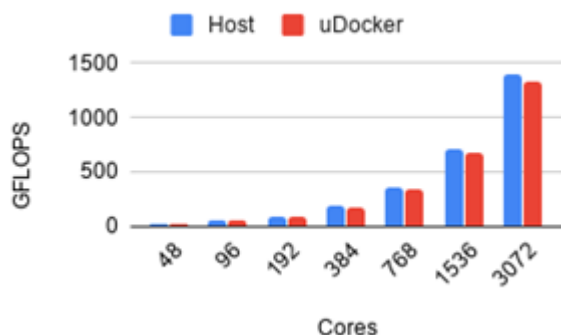

Figure 1. Execution time with and without containerization of the HPCG benchmark. The performance loss with the containerization is limited to low values of 3-7 %. Given the advantages provided by the container technologies (portability) and the remote submission capability (ease-of-use), such overhead is considered acceptable.

References
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