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Profiling and application of the multi-scale universal interface code-coupling library

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Computational simulations have become a useful tool in the modelling of many systems. Such systems are almost uniquely governed by the mathematical models of several scientific disciplines – they are 'multi-physics'. When simulating multi-physics problems in a High Performance Computing (HPC) environment, care must be taken to ensure the scalability of the method. Specifically, by adopting an operator-splitting strategy, one can decompose a complex multi-physics system into a series of interlinked subproblems, which can then be tackled individually using specialised numerical algorithms and/or optimised codes.

This paper will provide a brief review of current state-of-the-art coupling libraries, with the specific emphasis of their use in large-scale HPC simulations. We will demonstrate the use of an MPI MPMD point-to-point based, light-weight extensible library known as the Multi-scale Universal Interface (MUI) [1] at scale by passing $\mathcal{O}(10^8)$ data points (representative of a large-scale volumetric coupling), and providing detailed profiling of the MPI communication overhead on standard x86, IBM Power8 and Intel Knights Landing architectures. In the full paper, we will also discuss the ongoing development of a GPU enabled extension to the MUI library that will allow offloading of the compute-intensive interpolation aspect of the coupling.

Finally, we demonstrate the use of the MUI library in coupling an open-source Monte-Carlo neutronics code (OpenMC) to a highly scalable CFD solver (Code Saturne). We discuss the scalability of the resulting software combination up to $\mathcal{O}(10^4)$ MPI tasks (within the linear scalability of each individual software) in order to assess any bottlenecks introduced by the coupling.

In neutronics coupling, thermal energy released by fission events is transferred to the moderator via cladding material. Additional physics due to the conjugate heat transfer through the cladding must therefore also be accounted for. The resulting change in the fluid properties induced by this thermal heating alters the flow dynamics, which in turn alters the reactivity of the neutronics by the temperature feedback. This strongly coupled physical problem is particularly challenging due to its volumetric nature, as well as the need for both tight and conservative coupling algorithms. In the full presentation we will present conjugate heat transfer calculations of a Pressurised Water Reactor fuel assembly.

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