Methods for Multiscale Models Coupling

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Abstract

Nature is observed on an abundance of scales. Scientists are now using multiscale modeling to connect models and data from different scales in a wholistic approach to understand and control nature. Multiscale applications require more and more often the coupling of many sub-models, usually originating form different fields of science. Therefore, it is increasingly important to propose an effective description language that can help scientists with different background to co-develop a multiscale application. From a computational point of view, every submodel of a multiscale model may have different, even contradictory, hardware and software requirements. The models on these different scales may require significant but also heterogeneous computational resources, creating the need for distributed multiscale computing. A particularly demanding type of multiscale models, tightly coupled, brings with it a number of theoretical and practical issues.

In this paper, the usability of a *Multiscale Modeling Language (MML)* [1], i.e. a description language aiming at specifying the architecture of a multiscale simulation program, will be discussed. This language is based on a graphical representation or XML language. In particular, it allows the scientists to specify the list of submodels, their coupling, the relation between the computational domains and scales, the type of coupling, input and output data, etc. MML is bridging the gap between multiscale modelers and execution environments. It introduces a well-defined multiscale modeling terminology that can be used to describe, verify, analyze, and execute a multiscale model.

First, multiscale modelers decompose a multiscale phenomenon in multiple single scale phenomena. These phenomena form the basis for single scale models or submodels, while their interactions are grounds for couplings between submodels. Combined, these constitute a multiscale model. This step is aided by making a *Scale Separation Map (SSM)*, showing the scales and interactions of the phenomena involved.

The next step is to analyze the coupling topology of the multiscale model. A coupling topology describes how a multiscale model is coupled by explicitly creating a directed graph with submodel instances as nodes, coupling as edges, and number of times that the coupling is invoked as edge weights.

MML specifies submodels and submodels instances but also their scale, computational requirements, and implementation details. Coupling are made explicit using the concept of conduits that bind the specific ports od submodels. Submodels should not be aware of other submodels, rather, data

messages between submodels are manipulated by applying user-defined conduit filters to conduits. For distributing or collecting messages fan-in and fan-out mappers are used.

Once a multiscale model is implemented and fully described with MML, it is possible for software to verify, analyze, and execute it.

References

[1] Joris Borgdorff, Carles Bona-Casas, Mariusz Mamonski, Krzysztof Kurowski, Tomasz Piontek, Bartosz Bosak, Katarzyna Rycerz, Eryk Ciepiela, Tomasz Gubala, Daniel Harezlak, Marian Bubak, Eric Lorenz, and Alfons G. Hoekstra. A distributed multiscale computation of a tightly coupled model using the Multiscale Modeling Language. In *Procedia Computer Science*, volume 9, pages 596–605, 2012.