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Coupling of a continuum ice sheet model and a discrete element calving model using a scientific workflow system

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Scientific communities generate complex simulations through orchestration of semi-structured analysis pipelines which involves execution of large workflows on multiple, distributed and heterogeneous computing and data resources. Modeling ice dynamics of glaciers requires workflows consisting of many non-trivial, computationally expensive processing tasks which are coupled to each other. From this domain, we present an e-Science use case, a workflow, which requires the execution of a continuum ice flow model and a discrete element based calving model in an iterative manner. Apart from the execution, this workflow also contains data format conversion tasks that support the execution of ice flow and calving by means of transition through sequential, nested and iterative steps. Thus, the management and monitoring of all the processing tasks including data management and transfer of the workflow model becomes more complex. From the implementation perspective, this workflow model was initially developed on a set of scripts using static data input and output references. In the course of application usage when more scripts or modifications introduced as per user requirements, the debugging and validation of results were more cumbersome to achieve. To address these problems, we identified a need to have a high-level scientific workflow tool through which all the above mentioned processes can be achieved in an efficient and usable manner. We decided to make use of the e-Science middleware UNICORE (Uniform Interface to Computing Resources) that allows seamless and automated access to different heterogenous and distributed resources which is supported by a scientific workflow engine. Based on this, we developed a high-level scientific workflow model for coupling of massively parallel High-Performance Computing (HPC) jobs: a continuum ice sheet model (Elmer/Ice) and a discrete element calving and crevassing model (HiDEM). In our talk we present how the use of a high-level scientific workflow middleware enables reproducibility of results more convenient and also provides a reusable and portable workflow template that can be deployed across different computing infrastructures.

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