High-Performance Fluid Flow Simulation through Porous Media: Coupling micro- and macro- scale on geometrically complex domains

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ABSTRACT

In order to perform any kind of a fluid flow simulation on a geometrically complex large physical domain, a generation of a homologous sufficiently refined numerical domain is considered to be the first, logical and conditional step. Assuming no later limitations, with this procedure huge data set for a rather small physical area is introduced, giving a possibility to analyse the computational results on a ,up to several billions of computational unknowns, resolved domain. Bearing in mind that the simulation of fluid flow through porous media, in order to be relevant, should be studied on the large physical domains, and therefore a hundred thousand times larger numerical domain, in this work we present an alternative approach based on the coupling of two different scale models, micro- and macro-, in order to obtain both quantitative analyses on the fine level as well as a qualitative information on the coarse level of the structure.

Beside the coupling techniques, here will be presented a comparative study about the drawbacks and benefits while applying adaptive and uniform mesh generation approach within the discretization for this specific case of porous media, then the tool for an interactive exploration and visualisation of data and in the end some general scaling results, which our developed code has shown, while being executed on the large MUC super-computer infrastructure.

The idea of coupling of two different scales, in such a way that the macro-scale model represents a homogeneous field on which the qualitative analyses can be performed, whereas a micro-scale model is treated as a heterogeneous field and it is directly extracted from the macro-scale model at an arbitrary number of points of interests, where the quantitative analyses can be performed, is applicable to the variety of types of porous media (such as sand filters, water reservoirs, agricultural earth layers etc.) and can contribute with such information, as permeability, porosity, pressure or velocity depending on the purpose of particular research.

In order to create a representative porous media sample, two different codes were employed, both however on the basis of a real geotechnical information about the composition of the soil layers, represented through the granulometric distribution curve. With this data on disposal and additional definition of the domain boundaries within which several thousand intersection tests were performed in order to achieve a good physical representation of the domain, different samples were created. Numerical treatment of such artificially created samples involves the generation of space-tree

structure of Cartesian non-overlapping grids distributed into predefined number of levels of refinement. Such complex structure, which contains up to several tens of millions of computational grids on the deepest level is firstly used for the implementation of different communication patterns and necessary parallelisation techniques, in order to support massive high-performance computing, but it is also efficiently used for the interactive exploration of the data, enabling a user to communicate with the computation processes in real time as well as for the multiple data analyses across the different scales.

In the most general case, all relevant parameters in the process of generation of space-tree structure can be set to one particular value, which would lead to the uniform distribution of grids across all levels and in all three dimensions. In order to show an efficiency achieved with introduction of an adaptive over a uniform mesh generation approach, a sensitivity analysis with respect to the type of the discretisation for a specific case will be presented with discrepancy of barely 2% of measured values, whereas the obtained speed-up goes up to several times, depending on the particular geometry file.

Having had the numerical domain generated, two different mathematical models, namely Navier-Stokes equations' based model and pore-scale model were discretized according to the finite-volume scheme, and solved accomplishing the conservation and momentum equilibrium laws. For the execution of a calculation across numerous processes that work in parallel, a message passing interface (MPI) approach was used for the communication and transfer of the data in three different directions, whereas the load balancing was implemented using Morten space filling curves. Furthermore, different post-processing actions were applied over such calculated and moreover well-structured data set, as to obtain a set of scaled values that can be used for some further macro-scale analyses.

To provide a better insight into first calculated results, a tool for the interactive exploration of the data is integrated into the code, giving a possibility to visualize an intermediate calculated results, already during the runtime of the calculation without disturbance of employed calculation processes. With this visualisation tool it can be easily and interactively controlled, which data results should be depicted, as well as their density, location and the type, supporting a customer in the decision-making process.

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