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Towards Multi-Scale Transport Simulation in complex geometries with advanced Lattice Boltzmann methods on CPUs and GPGPUs

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The quantification of soil evaporation and of soil water content dynamics near the soil surface are critical in the physics of land-surface processes on many scales and are dominated by multi-component and multi-phase mass and energy fluxes between the ground and the atmosphere. Although it is widely recognized that both liquid and gaseous water movement are fundamental factors in the quantification of soil heat flux and surface evaporation, their computation has only started to be taken into account using simplified macroscopic models.
As the flow field over the soil can be safely considered as turbulent, it would be natural to study the detailed transient flow dynamics by means of Large Eddy Simulation (LES [1]) where the three-dimensional flow field is resolved down to the laminar sub-layer. Yet this requires very fine resolved meshes allowing a grid resolution of at least one order of magnitude below the typical grain diameter of the soil under consideration. In order to gain reliable turbulence statistics, up to several hundred eddy turnover times have to be simulated which adds up to several seconds of real time. Yet, the time scale of the receding saturated water front dynamics in the soil is on the order of hours. Thus we are faced with the task of solving a transient turbulent flow problem including the advection-diffusion of water vapour over the soil-atmospheric interface represented by a realistic tomographic reconstruction of a real porous medium taken from laboratory probes (see Fig. 1).

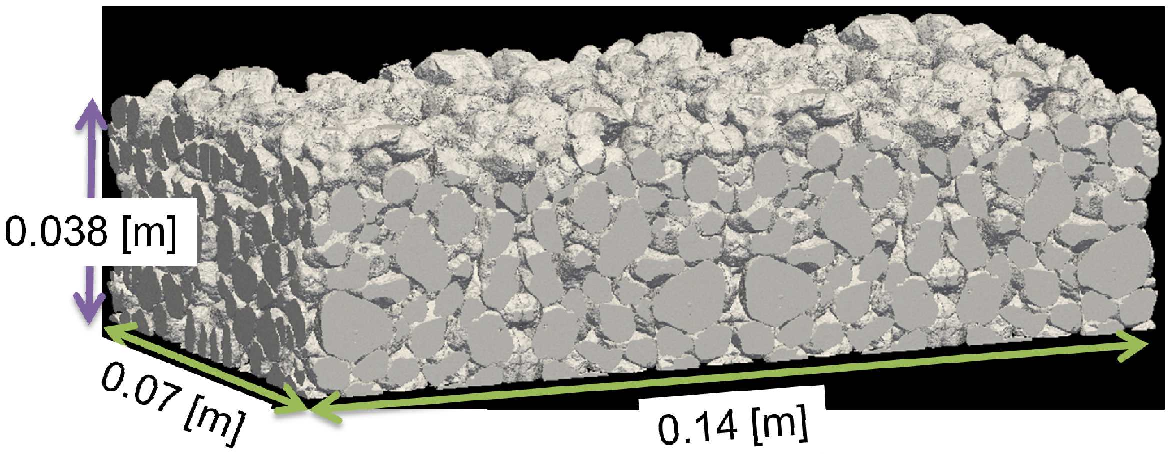

Figure 1: Tomographic reconstruction of the porous medium at the pore scale
(courtesy of Dr. P. Lehmann, ETH Zurich)

Our flow solver is based on the Lattice Boltzmann method (LBM) [2] which has been extended by a Cumulant approach similar to the one described in [3,4] to minimize the spurious coupling between the degrees of freedom in previous LBM approaches and can be used as an implicit LES turbulence model due to its low numerical dissipation and increased stability at high Reynolds numbers. A preliminary impression of the turbulent flow field over a porous medium is depicted in Fig. 2. The kernel has been integrated into the research code *Virtualfluids* [5] and delivers up to 30% of the peak performance of modern General Purpose Graphics Processing Units (GPGPU, [6]) allowing the simulation of several minutes real-time for an LES LBM model.

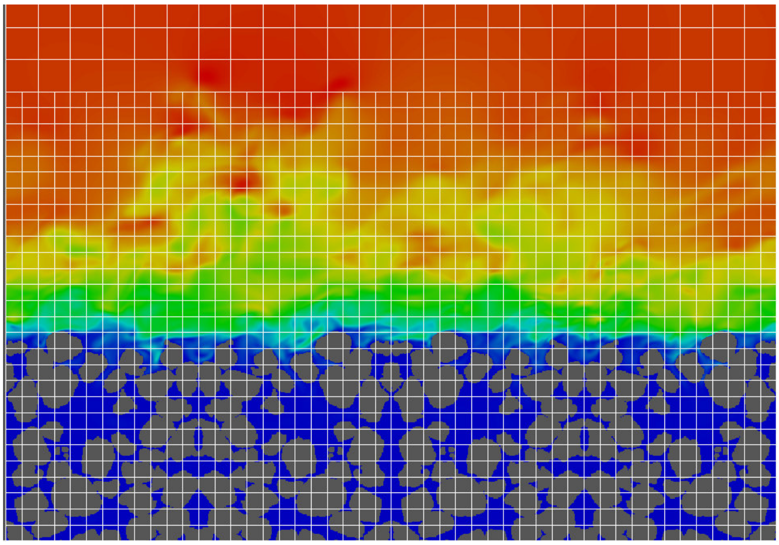

Figure 2: Snapshot of the turbulent flow field simulated by the Cumulant LBM. Each square (i.e. cube) represents 16^3 grid cells resulting in a mesh with app. 4×10^9 DOF.

In our final contribution we will present detailed profiles of the velocity distribution for different surface roughnesses, describe our multi-scale approach for the advection diffusion and estimate water vapour fluxes from transient simulations of the coupled problem.

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