The CEMRACS project HPC-IlBioS : scientific background, motivation and overview

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Many models describe the emission of greenhouse gases, including CO_2 and N_2O. Global models like RothC, Century or Ceres need improvements to release more accurate predictions. The stated models ignore the high level of heterogeneity at the microbial habitat- and pore scale, caused by soil structure which can lead to a spatial disconnection between soil carbon and nitrogen, energy sources, oxygen, and microorganisms, which are the decomposers. Micro-scale processes that occur within the soil pore system affect phenomena at much larger spatial and temporal scales. New inputs and parameters are needed for the global "circulation" models used by climatologists to predict future climate patterns. The ANR project "Soil µ3D-- Emergent properties of soil microbial functions: upscaling from 3D modelling and spatial descriptors of pore scale heterogeneity" tackles this lack of knowledge developing a 3D pore scale model and using it to improve models at a larger scale of description, the soil profile, more amenable to further upscale to larger geographic scales. The 3D pore scale modelling approach used by the ANR Soil µ3D project combines a lattice-Boltzmann model to simulate the fluid dynamic in the complex porous media, and an individual-based model (aka, agent-based approach in other disciplines) of the soil bacteria taking into account the biological part of the system. Due to the particularities of these two modelling approaches, HPC techniques involving both CPU and GPU programming are required to allow simulations in a reasonable time. A thorough investigation of the best HPC computing approach involving both CPU and GPU programming is performed in the CEMRACS project "HPC-IlBioS". An overview of the ANR project Soil µ3D and of the IlBioS modelling approach, uncovering the critical model algorithms complicating code parallelization, will be provided by the proposed talk.