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CHALLENGES IN EFFICIENT PARALLEL SIMULATIONS OF SPATIALLY RESOLVED PACKED-BED CHROMATOGRAPHY.

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Packed bed liquid chromatography is an essential unit operation for separating compounds in the pharmaceutical and chemical industry. Current trends aim at saving costly material by evaluating processes for new products in micro-columns. However, transfer of the results to production-scale columns is not straightforward due to different flow regimes. Hence, spatially resolved simulations in random sphere packings [1] are performed for analyzing specific inhomogeneities in micro-scale columns.

We present an efficient parallel finite element method for 3D simulations of both fluid flow and mass transfer processes in packed beds of up to 10K spherical porous particles, see also [2]. For an accurate approximation, such systems require a discretization into several hundred million elements. Scalability on massively parallel computers is hence essential to solve these problems in acceptable time.

The main focus of the talk lies in the algorithmic changes of the used finite element solver XNS as well as adaption of pre- and post-processing tools towards huge problem sizes. Meshes with up to 600 million elements were generated to develop and analyze the complete simulation workflow. We will present some of the changes to the solver, which were needed to run test simulations with up to 65536 MPI-processes efficiently. In addition to that, we will show the extended-dual approach for mesh decomposition and some hardware specific issues which have to be considered when running these large-scale simulations.

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