Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Multiscale Simulations of Mass Transport in Physically Reconstructed Porous Media

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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
MPI

Institute
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University
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Introduction

The goal of this preparation project was porting and scalability analysis of the in-house parallel codes developed for multiscale simulations of advective–diffusive transport of solutes through macro–mesoporous materials with functionalized surfaces, e.g., in a chromatographic bed in a chromatography particle-packed column equilibrated with a water–organic solvent mobile phase. The central parameter in chromatography characterizing separation efficiency is the plate height (*H*), defined as the slope of the dependence of the variance of an analyte band on its migration distance along the column. The separation efficiency of a particle-packed chromatographic column is inversely proportional to *H*, which is mainly a function of (i) the average mobile-phase velocity (*u*) through the column, (ii) the molecular-level interfacial dynamics (generally characterized by the retention factor, k), and (iii) the morphology of the bed. While a number of theoretical models were developed to analyze the *H-u* dependence, the quantification of the effects of the bed morphology and the retention on *H* is still a challenging task. One of the challenges is widely different time and length scales of mass transport processes inside mesoporous particles (with the typical mean pore size of ~10 nm) of the chromatographic column and in the interparticle void space (with the mean particle size of several microns). To address this problem, we developed a bottom-up multiscale simulation methodology to model fluid and analyte dynamics in hierarchical porosity – from diffusion inside mesoporous particle (the characteristic length is $\sim 10^{-8}$ m) up to advective–diffusive transport in a representative macroscopic section of the chromatographic column ($\sim 10^{-4}$ m). Physical 3D reconstructions of the mesoporous domain (with the resolution of 0.64 nm) and macroporous domain (with the resolution of 41.5 nm) are employed as geometrical models. The main objective of this preparation project was an estimation of the computational time required for a planned research (normal) project. The retention factor (and resulting *H)* depends on the physiochemical properties of the analyte and the mobile phase composition. A single simulation (one analyte, one mobile phase composition, one flow velocity) required ≈20 hours x 104 cores (one MPI-section node) ≈ 2000 core-h. A generation of one *H-u* curve required about 25 points corresponding to different flow velocities (50000 core-h). We are going to perform simulations for 16 different mobile phase compositions used in chromatographic practice and 6 analytes with different physiochemical properties. Thus, the total required computational time can be estimated as about 5 Mio. core-h.

Methods

Effective mesopore diffusion is addressed by Brownian dynamics (BD) simulations, while the advection–diffusion problem in the macropore space is resolved by the lattice-Bolzmann method (LBM) for fluid flow combined with the random-walk particle-tracking (RWPT) approach. The hallmark of the developed simulation approach are efficient linker schemes that guarantee the integration of the detailed, molecular-level, interfacial dynamics information into complex hierarchical porosity and

multiscale transport models.

Results

During the course of the project, the in-house parallel codes were compile at Lichtenberg cluster. A number of the test simulations was performed to analyze the stability as well as scalability of the codes. With the use of two nodes (208 cores) the wall-time of a single simulation reduced with the factor very close to 2 as compared to the wall-time at one node (104 cores).

Discussion

Already the test simulations demonstrated a complex behavior of the plate height as a function of the retention. To our knowledge, results of systematic investigations in this field never were reported.

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