ParRichy: Parallel Simulation of Bioreactive Multicomponent Transport Processes in Porous Media

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Abstract. Numerical simulations have become an important tool to predict the evolution of groundwater and subsurface contamination by organic compounds. Due to the observation of sharp interfaces on which biochemical degradation of the contaminants takes place, a reliable and accurate prognosis requires high spatial resolution of the considered subsurface domain and/or the application of higher order discretization methods. A successful realization of these simulations can only be provided by parallel computer systems with high computing power and memory availability. In this article, our concepts and simulation results of “real world” scenarios of organic contamination are presented.

1 Introduction

Groundwater contamination by organic compounds has become a serious and widespread environmental problem in industrialized countries. Major organic contaminants include petroleum fuels (gasoline, diesel), petroleum byproducts (coal tar, creosote), and chlorinated solvents. In many cases, groundwater contains a variety of organic contaminants, either due to the complex mixture in many non-aqueous phase liquids (NAPLs) or due to co-disposal/co-spillage (e.g., landfill leachates). The degradation of these contaminants is controlled to a large extent by the biological and geochemical conditions in the groundwater. Fortunately, biodegradation tends to attenuate at least some organics during groundwater transport. The question of whether costly active remediation is required, or whether natural processes of attenuation will be sufficient is a critical issue in “real world” situations.

Numerical models can be used to help to answer this question and to predict the long-term behaviour of the contaminant plume. However, the decision-making capability of numerical simulations requires that the mathematical model includes the full range of the controlling processes. These processes are often nonlinear, and the large number of (bio-)chemical species and reactions requires large computational power provided by parallel computers. Recently it was observed that biodegradation
processes typically occur on small interfaces where the reactants (e.g., the contaminant and oxygen) are mixing ([BaK04] and references therein). Such processes require a high spatial resolution of the computational domain (which usually covers several square kilometers) as well as advanced numerical techniques (e.g., higher order numerical approximation schemes to avoid artificial diffusion).

2 The project

The authors of this article participated in the interdisciplinary network project “Sustainable remediation involving natural attenuation” (Bayerisches Verbundvorhaben “Nachhaltige Altlastenbewältigung unter Einbeziehung des natürlichen Reinigungsvermögens”) funded by the BaySMLU under coordination of the Gesellschaft zur Altlastensanierung in Bayern (GAB). In cooperation with environmental scientists who investigated several contaminated sites in Bavaria, the authors’ research group was responsible for the mathematical modelling of the identified processes, the development and implementation of numerical schemes and numerical studies. While the intention of the GAB-project was to develop codes running on PCs and workstations (e.g., in engineers’ offices or at local authorities), the support by KONWIHR enabled the implementation and adaption of the codes on parallel computer systems. This gain of cpu power and memory enabled the use of a higher resolution as well as more detailed biogeochemical models, which are crucial factors for prognoses.

In this article we consider two “real world” scenarios: The first one is the study of the long-term behaviour of a BTEX (Benzene Toluene Ethylbenzene Xylene) plume in the earth’s subsurface at a site in southern Bavaria (cf. Sections 3,4) investigated in the GAB project. The second one deals with the reactions and biodegradation in the groundwater and in sediments of the metal complexant Ethylene Diamine Tetraacetic Acid (EDTA) which can be found in groundwater systems near military sites (cf. Sect. 5). The main aspect of the first problem was the implementation and comparison of two different numerical approximation schemes (lowest order mixed finite elements vs. second order conforming elements) and different programming platforms: UG/DDD (“unstructured grids”, “Dynamic Distributed Data”) vs. M++ (“Meshes, Multigrid and More”, [Wie04]). The second problem involves 14 (bio)chemical species and 10 reactions and demonstrates the performance of the developed software for larger reaction networks. M++ was designed to have more transparent structures and to enable an easier handling. In contrast to UG/DDD, M++ references all geometric objects by their barycentric coordinates (‘distributed point objects’) which are stored in hash-tables. Communication and load balancing concepts are similar to those of UG/DDD.

Both programming models are implemented on the Linux cluster of the Institute of Applied Mathematics at the University of Erlangen-Nuremberg. The cluster consists of 18 nodes with 1GB RAM and two 2.4-GHz-Xeon-processors each.