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THC-MP: High performance numerical simulation of reactive transport and multiphase flow in porous media

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ABSTRACT

The numerical simulation of multiphase flow and reactive transport in the porous media on complex subsurface problem is a computationally intensive application. To meet the increasingly computational requirements, this paper presents a parallel computing method and architecture. Derived from TOUGHREACT that is a well-established code for simulating subsurface multi-phase flow and reactive transport problems, we developed a high performance computing THC-MP based on massive parallel computer, which extends greatly on the computational capability for the original code. The domain decomposition method was applied to the coupled numerical computing procedure in the THC-MP. We designed the distributed data structure, implemented the data initialization and exchange between the computing nodes and the core solving module using the hybrid parallel iterative and direct solver. Numerical accuracy of the THC-MP was verified through a CO_2 injection-induced reactive transport problem by comparing the results obtained from the parallel computing and sequential computing (original code). Execution efficiency and code scalability were examined through field scale carbon sequestration applications on the multicore cluster. The results demonstrate successfully the enhanced performance using the THC-MP on parallel computing facilities.

1. Introduction

Subsurface multiphase flow coupled with solute transport and chemical reactions is a crucial topic on modeling and analyzing complex geologic and environmental problems (Steefel et al., 2005), which is applied to a number of problems related to coupling different physical processes, such as carbon geological sequestration, geothermal systems, and nuclear waste geological disposal.

All above problems tend to require detailed simulating model involving multiphase fluids and numerous chemical components, while the domain scales over orders of magnitude. This scientific computing issue on natural system needs enhanced algorithms and software packages to describe complex processes involved in large scale with high spatial resolution.

With respect to reactive transport research, the numerical simulation of coupled processes is made continuously and actively within many research institutions. Numerous simulators can be used in the underground geochemical survey, such as PHREEQC/PHAST (Parkhurst et al., 2005), CrunchFlow (Steefel, 2009), Hydrogeochem (Yeh et al., 2010), and Geochemist's Workbench (Bethke, 2002). The coupled processes like THC, thermal–hydrologic–mechanical (THM) (Rutqvist et al., 2002), and thermal–hydrologic–chemical–mechanical (THCM) (Tsang, 2009) improve the understanding in highly dynamic kinds of behavior of subsurface coupled processes. With the complexity of increasing subsurface geological processes, the numerical analysis is becoming a time consuming work that requires a high performance capability to reduce the computing burden.

In recent years, there are some new developed codes for the subsurface environmental simulation. GPRS (Cao, 2002; Fan, 2010), an object-oriented programming code initially developed for reservoir simulation, has been extended to include chemical reaction modeling. A coupled flow-reaction-transport process formulation and applications to CO_2 geological sequestration simulation are presented in Fan et al. (2012). PLOTRAN (Hammond et al., 2012) is a massive parallel computing code for simulating multiphase flow and multicomponent reactive transport. It leverages parallel data structures and solvers provided by PETSc (Balay et al., 1997). OpenGeoSys (Kolditz et al., 2012) is designed as a platform for simulation of coupled processes in porous and fractured media based on an object-oriented FEM concept. There are some other

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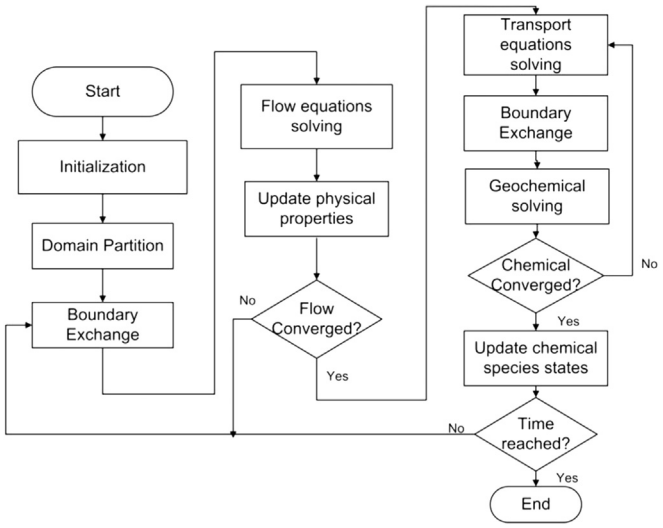

Fig. 1. Simplified flow chart of THC-MP.

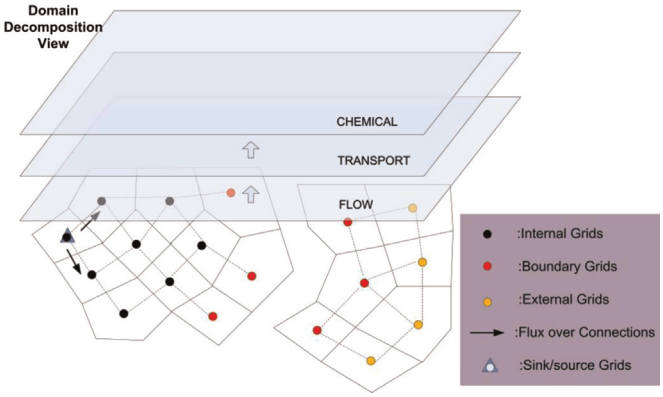

Fig. 2. The coupled process based on local mesh from domain decomposition.

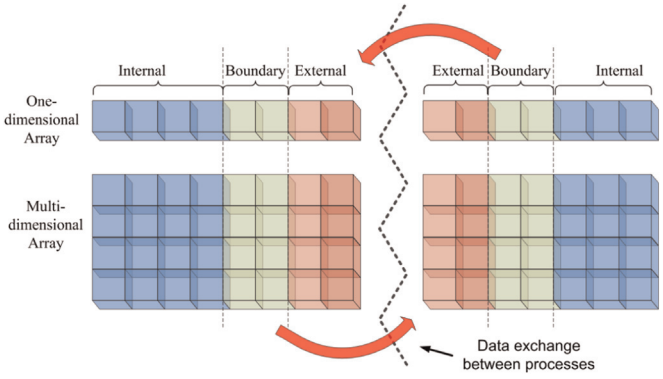

Fig. 3. Data arrangement and data exchange among subdomains.

commercial simulation programs, such as COMSOL Multiphysics.

TOUGH2 (Pruess, 2004) is a multiphase flow simulator developed in Lawrence Berkeley National Laboratory for years with an advantage of handling irregular discrete grids. To meet the need of large scale simulation, a domain decomposition method is applied to construct a parallel scheme for TOUGH2 code (Elmroth et al., 2001). TOUGH2-MP (Zhang et al., 2003b) is a code that implements more modules and optimizes the efficiency in massive parallel large problems based on the parallel scheme. This simulator has been applied to three-dimensioned field-scale model simulation of Yucca Mountain site (Wu et al., 2002; Zhang et al., 2003a).

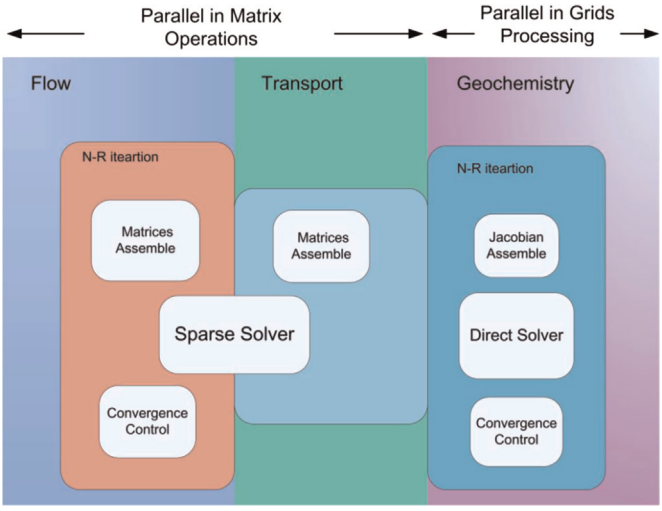

Fig. 4. Hybrid parallel computing architecture.

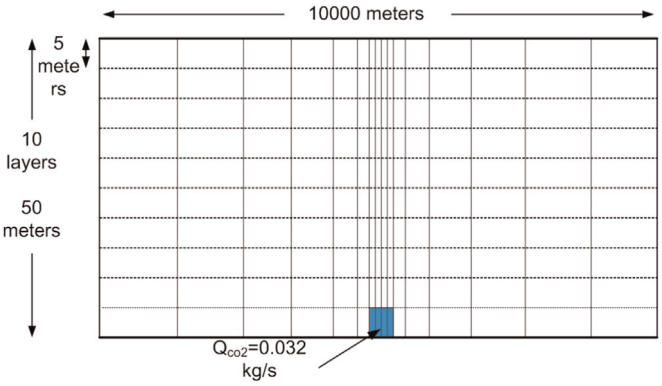

Fig. 5. Conceptual model of verification case.

As one family code of TOUGH, TOUGHREACT (Xu et al., 2011) is developed by introducing reactive transport into the existing TOUGH2 simulator. Comprehensive geochemical modeling capabilities are constantly incorporated into TOUGHREACT. It has been widely used internationally for studies in CO_2 geological sequestration, nuclear waste isolation, geothermal energy development, environmental remediation, and increasingly for petroleum applications. More coupled simulation processes with high spatial resolution lead to increasing computation burdens, and parallel computing technique is a possible solution to this challenge.

A number of parallel simulation codes, such as HBGC123D (Gwo et al., 2001), RT3D (McLaughlin, 2008), MODFLOW (Dong and Li, 2009), Hydrogeochem (Tang et al., 2010), utilize OpenMP to achieve parallel processing. MPI is commonly accepted owing to its extreme scalability potential. For instance, PFLOTRAN is a typical code developed with MPI from inception, and its scalability has been further enhanced (Mills et al., 2007). Other implementations using MPI include MODFLOW/RT3D (Huang et al., 2008). However, to build a parallel software based on MPI is still a challenging work, especially for retaining legacy code capabilities developed for decades.

This paper presents a parallel computing design and implementation of TOUGHREACT using MPI, which is efficient in simulating the coupled thermal–hydrologic–chemical processes. Note that the TOUGHREACT license can be obtained from U.S. Lawrence Berkeley National Laboratory's Technology Transfer Department (*website*: http://esd.lbl.gov/research/projects/tough/licensing/toughreact.html). The parallel version THC-MP inherits all the modeling features of TOUGHREACT that can be applied to one-