

Preamble

In recent years, numerical methods and computational simulations provide a new way to deal with many geoscience problems, for which the traditionally-used theoretical and experimental methods may not be valid as a result of the large time and length scales of the problems themselves. This enables many hitherto unsolvable geoscience problems to be solved using numerical methods and computational simulations. In particular, through wide application of computational science to geoscience problems, a new discipline, namely computational geoscience, has been established. However, because of the extremely large length and time scales, the numerical simulation of a real geological world also provides many challenging problems for researchers involved in the field of computational science. For this reason, multidisciplinary knowledge and expertise from mathematicians, physicists, chemists, computational scientists and geoscientists are required in the process of establishing the research methodology of computational geoscience.

Since computational geoscience is an amalgamation of geoscience and computational science, theoretical analysis and computational simulation are two of its core members. On the theoretical analysis front, we need: (1) to measure and gather data and information through traditional geoscience observations and measurements such as those widely used in geology, geophysics, geochemistry and many other scientific and engineering fields; (2) to conduct research to find the key factors and processes that control the geoscience problem under consideration; (3) to establish the theoretical foundations of the geoscience problem through formulating a set of partial differential equations on the basis of fundamental scientific principles; (4) to investigate the solution characteristics of these partial differential equations using rigorous mathematical treatments. On the computational simulation front, we need: (1) to develop advanced numerical methods, procedures and algorithms for simulating multi-scale and multi-process aspects of the geoscience problem on the basis of contemporary computational science knowledge and expertise; (2) to verify computational codes established on the basis of these advanced numerical methods, procedures and algorithms through comparing numerical solutions with benchmark solutions; (3) to produce and validate numerical solutions of real geoscience problems.

Owing to the broad nature of geoscience problems, computational geoscience is at a developing stage. Nevertheless, under the stimulus of ever-increasing demand

for natural mineral resources, computational geoscience has achieved much in the past decade, driven from the need to understand controlling mechanisms behind ore body formation and mineralization in hydrothermal systems within the upper crust of the Earth. In order to disseminate widely the existing knowledge of computational geoscience, to promote extensively and fastly further development of the computational geoscience, and to facilitate efficiently the broad applications of computational geoscience, it is high time to publish a monograph to report the current knowledge in a systematic manner. This monograph aims to provide state-of-the-art numerical methods, procedures and algorithms in the field of computational geoscience, based on the authors' own work during the last decade. For this purpose, although some theoretical results are provided to verify numerical ones, the main focus of this monograph is on computational simulation aspects of this newly-developed computational geoscience discipline. The advanced numerical methods, procedures and algorithms contained in this monograph are also applicable to a wide range of problems of other length-scales such as engineering length-scales. To broaden the readership of this monograph, common mathematical notations are used to describe the theoretical aspects of geoscience problems. This enables this monograph to be used either as a useful textbook for postgraduate students or as an indispensable reference book for computational geoscientists, mathematicians, engineers and geoscientists. In addition, each chapter is written independently of the remainder of the monograph so that readers may read the chapter of interest separately.

In this monograph we use the finite element method, the finite difference method and the particle simulation method as basic numerical methods for dealing with geoscience problems. Not only have these three methods been well developed in the field of computational science, but also they have been successfully applied to a wide range of small-scale scientific and engineering problems. Based on these three methods, we have developed advanced numerical procedures and algorithms to tackle the large-scale aspects of geoscience problems. The specific geoscience problem under consideration is the ore body formation and mineralization problem in hydrothermal systems within the upper crust of the Earth. Towards this end, we present the advanced procedures and algorithms in this monograph as follows: (1) Due to the important role that convective pore-fluid flow plays in the controlling processes of ore body formation and mineralization, a progressive asymptotic approach procedure is proposed to solve steady-state convective pore-fluid flow problems within the upper crust of the Earth. (2) To consider both the thermoelastic effect and the double diffusion effect, a consistent point-searching interpolation algorithm is proposed to develop a general interface between two commercial computer codes, Fluid Dynamics Analysis Package (FIDAP) and Fast Lagrangian Analysis of Continua (FLAC). This general interface allows a combination use of the two commercial codes for solving coupled problems between medium deformation, pore-fluid flow, heat transfer and reactive mass transport processes that can occur simultaneously in hydrothermal systems. (3) To simulate mineral dissolution/precipitation and metamorphic processes, a term splitting algorithm is developed for dealing with fluid-rock interaction problems in fluid-saturated hy-

drothermal/sedimentary basins of subcritical Zhao numbers, in which the chemical dissolution fronts are stable during their propagation. Note that the Zhao number is a dimensionless number that can be used to represent the geometrical, hydrodynamic, thermodynamic and chemical kinetic characteristics of a reactive transport system in a comprehensive manner. The condition, under which a chemical dissolution front in the fluid-saturated porous medium becomes unstable, can be expressed by the critical value of this dimensionless number. (4) For a geochemical system of critical and supercritical Zhao numbers, a segregated algorithm is proposed for solving chemical-dissolution front instability problems in fluid-saturated porous rocks. Thus, the morphological evolution of chemical dissolution fronts in fluid-saturated porous media can be appropriately simulated. (5) To investigate the effects of non-equilibrium redox chemical reactions on the mineralization patterns in hydrothermal systems, a decoupling procedure is proposed for simulating fluids mixing, heat transfer and non-equilibrium redox chemical reactions in fluid-saturated porous rocks. (6) When thermal and chemical effects of intruded magma are taken into account, an equivalent source algorithm is presented for simulating thermal and chemical effects of intruded magma solidification problems. This algorithm enables the moving boundary problem associated with magma solidification to be effectively and efficiently solved using the fixed finite element meshes. (7) To simulate spontaneous crack generation in brittle rocks within the upper crust of the Earth, the particle simulation method is extended to solve spontaneous crack generation problems associated with faulting and folding in large length-scale geological systems. The resulting cracks may be connected to form flow channels, which can control ore body formation and mineralization patterns within the upper crust of the Earth.

August 12, 2008

*Chongbin Zhao
Bruce E. Hobbs
Alison Ord*



<http://www.springer.com/978-3-540-89742-2>

Fundamentals of Computational Geoscience

Numerical Methods and Algorithms

Zhao, C.; Hobbs, B.E.; Ord, A.

2009, XVI, 241 p., Hardcover

ISBN: 978-3-540-89742-2