CODE_BRIGHT
v9

QUALITY ASSURANCE DOCUMENT

https://deca.upc.edu/en/projects/code_bright

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1 SCOPE

CODE_BRIGHT (COupled DEformation BRIne, Gas and Heat Transport) is a program that allows for thermo-hydro-mechanical (THM) analysis in geological media. Its consists of a Finite Element program developed at the Department of the Geotechnical Engineering and Geosciences of the Technical University of Catalonia (UPC) merged into the pre/post-processor GiD developed by the International Center for Numerical Methods in Engineering (CIMNE).

Research and development of the code is supported by the UPC and CIMNE. A consortium of International companies contributes financially to these developments and checks the efficiency and quality of the resulting software. The consortium also provides a valuable link with geoenvironmental and geotechnical engineering practice. Future developments are discussed within the consortium and feedback is provided after new releases of the code. Appendix A contains a list of members of the consortium.

This Quality assurance document describes the requirements of development, verification, validation, interactions and use of Code_Bright. This document is divided in different sections. A general description of the code is given in section 2. Criterions to design, developments and interactions are presented in section 3. Section 4 contains requirements of configuration and installation. Validation and verification of code functionality is given in section 5. Finally, in section 6, responsibilities for the use of Code_Bright are given.

2 GENERAL DESCRIPTION OF CODE_BRIGHT

CODE_BRIGHT is a tool designed to handle coupled THM problems in geological media. The code is able to solve non-saturated multiphase flow under non-isothermal conditions. The equations that govern the THM problem are categorized into four main groups, namely, balance equations, constitutive equations, equilibrium restrictions and definition constraints. Equations for mass balance were established following the compositional approach (Olivella et al., 1994). That is, mass balance is performed for water, air and mineral species instead of using solid, liquid and gas phases. Equation for balance of energy is established for the medium as a whole. The equation of momentum balance for the porous medium is reduced to that of stress equilibrium (Olivella et al., 1996).

The constitutive equations establish the link between the independent variables (or unknowns) and the dependent variables. There are several categories of dependent variables depending on the complexity with which they are related to the unknowns. Basic constitutive laws are divided in thermal, hydraulic and mechanical. The governing equations are finally written in terms of the unknowns when the constitutive equations are substituted into the balance equations. The unknowns are obtained by solving the system of PDE’s (Partial Differential Equations) numerically in a coupled way. From state variables, dependent variables are calculated using the constitutive equations or the equilibrium restrictions.

For the numerical treatment of the different terms of the balance equations, the first step is the approximation of the material derivate with respect to the solid as an eulerian derivate, owing to the assumption of small strain rate. Details related to the discretization of the problem and the numerical technique used can be found in CODE_BRIGHT User’s Manual (2009). In summary, it can be mentioned that the numerical approach can be viewed as divided into two parts: spatial and temporal discretization. Galerkin finite element method is used for the spatial discretization while finite differences are used for the temporal discretization. The discretization in time is linear and an implicit scheme is used. Finally, since the problem presented here is non-linear, the Newton-Raphson method was adopted as iterative scheme.

As a main feature of the numerical approach, it can be mentioned that it can use a wide library of elements with segments, triangles, quadrilaterals, tetrahedrons, triangular prisms and quadrilateral prisms. Linear interpolation functions and quadratic interpolation functions for some elements are also available. Analytical integration is used for segments, triangles and tetrahedrons. Numerical integration is used for quadrilateral, triangular prisms (6 points) and quadrilateral prisms (8 points). For the mechanical problem, selective integration is used for quadrilateral and quadrilateral prisms (this means that the volumetric part is integrated with a reduced quadrature of 1 point). Finally, for all elements the flow equations are solved using element-wise and cell-wise approximations.

As commented before, finite differences and an implicit scheme are used for time integration. The program has an automatic discretization of time. Reduction of time increment may be caused by excessive variation of unknowns per iteration or to excessive number of iterations to reach convergence or if the correction is larger than in the previous iteration (more details in CODE_BRIGHT User's Manual). CODE_BRIGHT is a FORTRAN code.

Regarding the boundary conditions of the mechanical problem, forces and displacement rate can be enforced in any spatial direction and at any node. In the hydraulic problem, mass flow rate of water and dry gas can be prescribed at any node, and liquid/gas pressure can be also enforced at any node. Finally, regarding the thermal problem, heat flow and temperature can be prescribed at any node of the mesh (CODE_BRIGHT User's Manual).

3 DESIGN AND DEVELOPMENT

The design and development of CODE_BRIGHT is responsibility of the software developers (i.e., Technical University of Catalonia). UPC decides what to be implemented into the new versions of the official code. Criterion to upgrade the current version to a new one is 1) the incorporation of new models which have been proved to be general and robust and/or 2) improvements of numerical algorithms or environment of the program in GID.

The users of the consortium may come with suggestions for developments. Discussions on development of the code can be prepared for and discussed at the steering committee meeting and feedback is provided after new releases of the code.

New versions of the Code_Bright and documentation will be updated in the webpage of the Department: https://deca.upc.edu/en/projects/code_bright. Current documentation of the code is listed in Appendix B. Some files and documents are available in the web site but others are restricted to the consortium members. Restricted documents as the updating of the code source will be sent by e-mail to the members of committee and their delegates (see Appendix A).

The internet site https://deca.upc.edu/en/projects/code_bright contains general information about CODE_BRIGHT. Download files of CODE_BRIGHT and GiD and the instructions for installation of these programs is given. User's guide, tutorials and some examples also will be downloading from web site. A brief description of CODE_BRIGHT User's guide chapters can be found in Appendix C.

Information on activities, courses and workshops will be updated in the web site. Courses dealing with both theoretical and practical aspects of computer modelling in geoenvironmental and geotechnical engineering are given. Courses will be held by UPC. This should be self financed, and not restricted to consortium members. Workshops will be indented to show the current applications and capabilities of the code to modelling a variety of engineering problems. Contributions to the workshops are open to all users of Code_Bright.

Technical support is provided by e-mail through: code.bright@upc.edu. A professional helpdesk is available for users who wish to obtain prompt and extensive technical and scientific support.

4 CONFIGURATION AND INSTALLATION

CODE_BRIGHT uses GiD system for preprocessing and post-processing. GiD is developed by CIMNE. GiD is an interactive graphical user interface that is used for the definition, preparation and visualization of all the data related to numerical simulations. This data includes the definition of the geometry, materials, conditions, solution information and other parameters. Detailed information will be found in CODE_BRIGHT User's guide in chapters CODE_BRIGHT Preprocess and Postprocess.

Installation of CODE_BRIGHT requires installation of GiD pre-post processor. For the installation of GiD, user should consult the website http://www.gidhome.com/ for conditions of download and use of GiD software. Last version of GiD for which the proper performance of CODE_BRIGHT has been verified is the v13. It is recommended to download the GiD User Manual and GiD Tutorials trough website, for detailed information of the pre/ post-processing options.

After installation of GiD, CODE_BRIGHT may be installed. CODE_BRIGHT works under Windows operative system. The latest version can be downloaded from the website: https://deca.upc.edu/en/projects/code_bright. After unzipping, the user should copy the folder Code_bright_v**n**.gid into the folder /PROBLEMTYPES within the main folder of GiD. This subdirectory is by default in C:\Program Files\GiD\GiDversion**n**\problemtypes for Windows English version and GiD version**n** except if another destination folder was specified for GiD program during its installation.

For version 9, parallel versions of CODE_BRIGHT have been compiled. Versions are available for two (2), four (4) and six (6) processors or cores. Versions can be prepared for other values, but it has to be taken into account that these are versions to be used in a workstation windows environment.

Parallel versions are based on Fortran OpenMP, which is a programing/compiling technique. Parallelization of CODE_BRIGHT focusses on the iterative solution of the linear system of equations. Iterative methods are easy to parallelize as matrix-vector products and vector-vector products are carried during the solution algorithm. Therefore, parallel computing is only possible for relatively large problems that use the iterative solver available in CODE_BRIGHT. It is a conjugate gradient method. An additional advantage of the iterative method is that facilitates the sparse storage of the system matrix. This is a fully optimized method to store the coefficients of the matrix. This minimizes de required RAM memory. In contrast, direct methods (LU decomposition and back-substitution) show more difficulties to use sparse storage and, usually, are based on band or skyline storage.

In computer architecture, Amdahl's law is a formula, which gives the theoretical speedup in latency of the execution of a task at fixed workload that can be expected of a system whose resources are improved. The law is named after computer scientist Gene Amdahl, and was presented at the AFIPS Spring Joint Computer Conference in 1967.

Amdahl's law in parallel computing is applied to predict the theoretical speed-up when using multiple processors. For example, consider a model that needs 10 hours using a single processor core. A particular part of the model that cannot be parallelize takes one hour to execute and the remaining 9 hours (p = 0.9) of execution time can be parallelized. Then regardless of how many processors are devoted to a parallelized execution of this program, the minimum execution time cannot be less than that critical one hour. Hence, the theoretical speedup is limited to at most 10 times (speed-up = $1/(1 - p) = 10$). For this reason, parallel computing with many processors is useful only for very parallelizable programs.

5 VALIDATION AND VERIFICATION

CODE_BRIGHT has been extensively verified and validated in international benchmark exercises and has been applied to the analysis of different geoenvironmental schemes, waste disposal designs and geotechnical problems involving saturated/ unsaturated soil behaviour.

Verifications of the accuracy of the code functionality have been developed and some examples are included in a new document label *Verification document*. Appendix B contains a list with all documents related with Code_Bright. *Verification document* will be used for assuring the authorities of the quality of the code. Verifications included comparisons of solutions of problems using Code Bright with analytical solutions.

Also, examples and cases of validations of the implemented models are included in a new document called *Validation document*. This document contains a summary of the most relevant research projects and publications in which Code_Bright has been used. Validations examples included comparisons of the solutions when using different models incorporated in the code and experimental data.

6 USE OF CODE_BRIGHT

The CODE_BRIGHT code and its constitutive models have been developed with great care. Although a lot of testing and validation have been performed, it cannot be guaranteed that the CODE_BRIGHT is free of errors. Moreover, the simulation of geoenvironmental and geotechnical problems by means of the finite element method implicitly involves some inevitable numerical and modelling errors. The accuracy at which reality is approximated depends highly on the expertise of the user regarding the modelling of the problem, the understanding of the constitutive models and their limitations, the selection of model parameters, and the ability to judge the reliability of the computational results. Hence, CODE_BRIGHT may only be used by professionals that possess the aforementioned expertise. The user must be aware of his/her responsibility when he/she uses the computational results for geoenvironmental or geotechnical design purposes. The CODE_BRIGHT organisation cannot be held responsible or liable for design errors that are based on the output of CODE_BRIGHT calculations.

Questions related to the code features, executions, deficiencies and errors should be directed to the software developers (i.e. UPC) through his technical support service.

7 PRESENCE IN SOCIAL NETWORKS

Pages of CODE_BRIGHT in Facebook, YouTube and Twitter are available.

Videos (8) have been prepared based on the tutorials and have been published in the YouTube channel. These videos have hundreds of views and are a good complement for the tutorial document.

Facebook page and Twitter account are intended for promotion of CODE_BRIGHT activities.

REFERENCES

CODE_BRIGHT User's Guide. Geotechnical Engineering Department, Technical University of Catalunya, Spain (digital format available at http://www.etcg.upc.edu/recerca/webs/code_bright).

Olivella, S., Carrera J., Gens, A. & Alonso, E.E. (1994). "Non-isothermal multiphase flow of brine and gas through saline media". Transport in porous media, 15, pp. 271-293.

Olivella, S., Gens, A., Carrera, J. & Alonso, E.E. (1996). "Numerical formulation for a simulator (CODE_BRIGHT) for the coupled analysis of saline media". Engineering Computations, 13, 7, pp. 87-112.

APPENDIX A

List of member of the CODE_BRIGHT Consortium:

Organization	Delegates	e-mail
SKB	Anders Sjöland, Chairman Mattias Åkesson Ola Kristensson Lennart Börgesson	anders.sjoland@skb.se ma@claytech.se osk@claytech.se
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APPENDIX B

DOCUMENTATION OF CODE_BRIGHT v9

A series of documentation related with Code_Bright has been developed. Some files and documents may be downloaded through the website: https://deca.upc.edu/en/projects/code_bright; others will be restricted to the consortium members. These are:

Documentation	**Access**
User's Guide v9	web site
Tutorials	web site
Executable file of Code_Bright v9	web site
Fortran Code sources v9	consortium members
Quality Assurance Document (this document)	consortium members
Validation Document	consortium members
Verification Document	consortium members

APPENDIX C

CODE_BRIGHT v9 User's Guide

The User Manual has been split into several chapters as:

CODE_BRIGHT. *Foreword*

CODE_BRIGHT. *Pre-process, problem data.* It is described how to enter the data of the problem, i. e. general data, constitutive laws, boundary conditions, initial conditions and interval data

CODE_BRIGHT. *Process*. It is related to the calculation process. This part also contains the description of input files.

CODE_BRIGHT. *Post-process*. Contain the details on post-processing information using GiD software.

CODE_BRIGHT. *Theoretical aspects*. Contain the theoretical basis of CODE_BRIGHT, and the numerical solution.

CODE_BRIGHT. *Constitutive laws*. Contains the different constitutive laws available which has been divided in thermal, hydraulic, mechanical and phase properties. Parameters required by each law and history variables for elasto-plastic models are described.

CODE_BRIGHT. *References*.