Advances in the Development of OpenCalphad Software and Databases

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Extended Abstract

Thermodynamics is at the core of materials science. The CALPHAD (Calculation of Phase Diagrams) method, a powerful tool for materials design and engineering applications, has been shown to be an excellent platform for linking results from experiments and density functional theory calculations as well as empirical relations. It is currently the only method available for efficient calculation of the properties of multicomponent, multiphase systems with the accuracy that is required for commercial applications. It has been long recognized that coupling CALPHAD thermodynamics with other physical models for kinetic simulations is useful for better understanding and improvement of many materials processes. Most of today's databases and software are proprietary restricting expansion and development of new models and their integration into software tools for materials simulations. The goal of OpenCalphad (OC) is to develop free high quality software for thermodynamic calculations and databases with parametric physical models of the pure elements as basis for multicomponent databases as well as conventional CALPHAD databases. OC provides a highly structured tool that can be used, together with kinetic models, in microstructure and continuum simulations.

The essential elements of CALPHAD type software are model descriptions of the thermodynamics, the Gibbs energy minimization and a programming interface. The thermodynamic parameters are stored relative to the model selected for each phase. A variety of models have been implemented in OC, from a simple stoichiometric model with no variation in composition to multisublattice models for complex crystalline phases and liquids with short range order to a gas phase with more than 100 species. The most frequently used models are variants of the Compound Energy Formalism (CEF) [1]. This formalism describes the gas phase, regular solutions, intermetallics, ordered phases and liquids with short range order. An efficient and flexible data structure [2] is used to store composition dependencies in the program memory as binary trees. The elements, species and model parameters are 'static' as they do not change with external conditions while the calculated results are 'dynamic' and are stored as separate records. This strategy is the basis for enabling the possibility of parallel execution of the code.

A two-step Lagrange method [3] is used for the Gibbs energy minimization. External conditions and internal constraints are taken into account using Lagrange multipliers. Lagrange multipliers are also used to replace the Gibbs energy with the appropriate

function considering external conditions on the volume, chemical potentials or prescribed stable phases. This two step approach can efficiently handle changes in the set of phases that may occur during the iterations. To ensure that the global equilibrium is found a grid minimizer has been implemented. The grid points from the grid minimizer provide an initial guess of the stable phases and the resulting values are then used as start constitutions for the iterative algorithm to find the global minimum.

The programming interface implemented in OC, OC-TQ, is written in the new Fortran standard and is extended with a C interface making the routines callable from C, C++ and other object-oriented programming languages, thus enabling seamless integration into other tools used within computational materials science and engineering.

The thermodynamic descriptions needed by OC for the equilibrium calculations are read from thermodynamic database (TDB) files [4]. This format has developed into a *de-facto* standard and is supported by most of the commercial software. However, the OC code will not be able to read proprietary, encrypted database files. Files with descriptions of individual systems or databases for multicomponent systems can be found as supplemental material of journal articles or in file repositories [5].

Since the release of version 1 [6] a number of new features were implemented such as a method for the analytical calculation of state variable derivatives, a model for describing ionic liquids, selection of a subsystem from a TDB file, permutations for a simplified description of the order/disorder model for the cubic and hexagonal close-packed phases, an alternate description for phases exhibiting only long range order to name just a few. The robustness of the procedures for stepping and mapping has been improved although more work is needed. The OC-TQ interface has been expanded but the data transfer to C/C++ code needs refinement. The code is in the process of constantly being expanded and improved. The most recent version of the OC software can be found at http://www.opencalphad.org and https://github.com/sundmanbo/opencalphad.

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