Open Calphad - software and databases

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Calphad type databases and various application software have become a necessary tool for industrial development of new materials and alloys. In particular for applications in phase transformations and thus the simulation of microstructures and materials properties the thermodynamic and kinetic databases have now gained an established position. But this is also a field of intense research as new data and first principle techniques provide new ideas for models as well as thermodynamic data in composition ranges not accessible by experimental techniques. Thus there is a need for constant revision of databases and software to include these ideas and data. Unfortunately the companies providing the software and databases are too small to carry out heavy research projects. Since today all major thermodynamic software and databases are commercial this leaves very little opportunities for researchers to develop and test new ideas.

There are some minor open source software packages available for Calphad applications but the Sapiens project at ICAMS in Bochum, Germany, has taken the initiative to start developing open software with full modeling facilities and provide this to the scientific community [1]. It is called Open Calphad and it is still in the cradle but will be made available on the web, without cost, either as free or open software, making it possible to modify the source code and to implement it in any other software. This facility has already been utilized for evaluating new heat capacity models (see presentation by Mauro Palumbo).

This software, in part utilizing code that was developed by Leo Lukas [2], is written in Fortran 90 with a command driven user interface and a software interface based on the TQ definition [3]. We hope that several programmers will be interested to provide interfaces to other languages as well as a more advanced GUI.

[1] S.G. Fries, M. Palumbo, T. Hammerschmidt and B. Sundman, "The Sapiens project: A call for creating sustainable thermodynamic databases," CALPHAD XXXIX, Jeju, Korea, 2010.
[2] H.L. Lukas, J. Weiss and E.-Th. Henig, CALPHAD 6 (1982) 229.
[3] G. Eriksson, H. Sippola and B. Sundman, "Thermodynamic Calculation Interface (TQ)." Report to EC/Science Simulation Program "Computer Assisted Process Simulation" (1995).

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