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## The OpenCalphad thermodynamic software interface

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Romain Le Tellier, Mauro Palumbo, Suzana G. Fries

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# Applications using the OpenCalphad thermodynamic software interface including parallelization.

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## Abstract

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Thermodynamic data are needed for all kind of simulations of materials processes. For kinetic models, for example, thermodynamic quantities, such as chemical potentials, driving forces for precipitation, thermodynamic factors for converting mobilities to diffusion coefficients, solubilities in different phases etc., are needed. It is very important that these data are consistent and accurate, also for predicting metastable states during phase transformations. Equally important is that the computation time must be reasonably short.

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Frequently thermodynamic data are pre-evaluated into “lookup tables” to speed up calculations. This creates additional uncertainties in the data as they must be interpolated or extrapolated and conditions may differ from those originally assumed for the creating the lookup table. It would be much better if a full local equilibrium calculation could be performed when

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*February 9, 2016*

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5 data are needed, e.g. for each grid-point during a finite element simulation.  
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7 Efficiency requires that the thermodynamic software is fully parallelized. The  
8  
9 OpenCalphad (OC) software is the first such software to do so.

10  
11 *Keywords:* Computational Thermodynamics, Phase Transformations,  
12 Simulations, Parallel Computing,  
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## 14 15 **1. Introduction**

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18 The background for the development of a free thermodynamic software  
19 for multicomponent calculations using the CALPHAD method (CALculation  
20 of PHase Diagrams) is described by Sundman et al. [1]. A very limited first  
21 version of the OpenCalphad (OC) software was released in 2013. In February  
22 2015 a second version capable also of multicomponent single equilibrium and  
23 some phase diagram calculations was released. During 2015 extensive new  
24 facilities were added and the software has become much more stable and both  
25 version 2 and 3 are available on [<http://www.opencalphad.org>]. Version 3 in-  
26 cludes parallel equilibrium calculations using the OpenMP [<http://www.openmp.org>]  
27 library, a rudimentary assessment module and an Application Software Inter-  
28 face, OCASI, callable from C++ as well as Fortran and other programming  
29 languages. OC is written in the new Fortran standard.  
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34 There is extensive literature describing the use of thermodynamic data  
35 for materials and process development. Although somewhat outdated, an  
36 excellent review can be found in the book by Miodownik and Saunders [3].  
37 Especially the development of phase field techniques [4, 5, 6] and other tech-  
38 niques, such as fluid dynamics [7] and finite element methods [8] for simulat-  
39 ing microstructure evolution has increased the demand for fast and reliable  
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5 calculations of chemical potentials, driving forces, mobilities etc. Within the  
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7 framework of Integrated Computational Materials Engineering (ICME) [9]  
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9 the necessary tools are coupled to accomplish the desired simulations and it  
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11 is the intention that the OC software becomes one of these tools.

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13 The OC software has been extensively tested on Windows and Linux sys-  
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15 tems and although there are limitations and occasional problems the overall  
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17 performance is comparable with commercial thermodynamics software for  
18  
19 materials science, such as FactSage [10], Pandat [11] or Thermo-Calc [12].  
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21 In addition, the OC software can perform many equilibrium calculations  
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23 in parallel, including calls to OCASI. The OCASI software is still under  
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25 development but has been used in some applications to demonstrate how  
26  
27 it can be integrated in simulations to utilize accurate and consistent ther-  
28  
29 modynamic data. Examples and full documentation of the source code as  
30  
31 well as macro files showing the interactive use of the software and the use  
32  
33 of OCASI are available on the OC web site [<http://www.opencalphad.org>].  
34  
35 A development version with some new features and bugfixes is available  
36  
37 at [<http://www.github.com>].

## 38 39 **2. Computational Thermodynamics**

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41 Computational thermodynamics consists of software and databases for  
42  
43 calculating phase diagrams and other kinds of thermodynamic data. The  
44  
45 databases are a collection of parameterized model descriptions of the phases  
46  
47 as function of constitution and state variables. The model descriptions are  
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49 obtained from the thermodynamic assessment (or optimization) of individual  
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51 systems. The basic techniques are described in the book by Lukas et al. [15].  
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5 An important advantage from using an assessed thermodynamic database is  
6 that all data calculated with such a database are consistent, including phase  
7 solubilities, melting temperatures, heat capacities, chemical potentials etc.  
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### 10 11 *2.1. State variables*

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13 A thermodynamic system is described by a set of state variables like  
14  $T, P, V$  for temperature, pressure and volume. The amounts of the compo-  
15 nents can be given in moles,  $N$ , mole fractions,  $x$ , or mass fractions,  $w$  and  
16 the equilibrium state is at a minimum of the appropriate state function like  
17 internal energy,  $U$ , Helmholtz energy,  $A$  or the Gibbs energy,  $G$ .  
18  
19

20  
21 Many properties can be derived from the state functions and some can  
22 also be used to control the system, such as chemical potentials,  $\mu$ , enthalpies,  
23  $H$  etc. All state variables and properties available in OC are listed in Ap-  
24 pendix 2.  
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### 31 32 *2.2. Thermodynamic models*

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34 In CALPHAD-type thermodynamic databases the Gibbs energy of each  
35 phase is described by a model reflecting its structure. Several different kinds  
36 of models are described by Lukas et al. [15]. The simplest model is that for  
37 an ideal gas:  
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$$41  
42 G_M^{\text{gas}} = \sum_i y_i \text{ }^\circ G_i + RT y_i \ln(y_i) + RT \ln(P) \quad (1)  
43  
44  
45$$

46 where  $^\circ G_i$  is the Gibbs energy of formation of the gas molecule  $i$  from the  
47 reference state of the elements,  $y_i$  is the constituent fraction of the molecule in  
48 the gas and  $P$  the pressure.  $R$  is the gas constant,  $T$  the absolute temperature  
49 and  $y_i \ln(y_i)$  is the random configurational entropy.  
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5 The Gibbs energy model is per mole formula unit of the gas as the number  
6 of atoms will vary with the species. The mole fractions of the elements,  $x_j$ ,  
7 are given by  
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$$10 \quad x_j = \frac{\sum_i b_{ji} y_i}{\sum_k \sum_i b_{ki} y_j} \quad (2)$$

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14 where  $j$  and  $k$  denote elements and  $i$  the molecules.  $b_{ji}$  is the stoichiometric  
15 factor of element  $j$  in molecule  $i$ .  
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18 More complex phase models with sublattices for interstitials, chemical  
19 ordering or defects, including ionic constituents are implemented in OC. The  
20 interactions between the constituents on a sublattices can be described by  
21 excess parameters and a model to describe the contribution of magnetic or-  
22 dering depending on the Curie or Néel temperature and the Bohr magneton  
23 number to the heat capacity is available. All these models are special cases of  
24 Compound Energy Formalism (CEF) [16] and are implemented in OC as well  
25 as the partially ionic 2-sublattice liquid model [17] for short range ordering  
26 (SRO) in the liquid phase. More models will be implemented with time and  
27 since the source code of OC is available skilled users can implement their  
28 own models.  
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### 40 *2.3. Equilibrium calculations*

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42 The equilibrium algorithm used in OC was proposed by Hillert [18] and  
43 implemented by Jansson [19] in the POLY module of Thermo-Calc software  
44 and in the PMLFKT software by Lukas [20]. The implementation of this  
45 algorithm in OC is described in [21]. In this context it is sufficient to mention  
46 that the data structure, described in [21], is designed to allow calculation of  
47 several equilibria in parallel and it has an additional grid minimizer to ensure  
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5 that the calculated equilibrium is a global and not a local one. It can also  
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7 detect miscibility gaps.

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9 A special feature of Hillerts algorithm [18] is the possibility to prescribe  
10 that a phase should be stable. This feature is essential for the ability to  
11 calculate phase diagrams and the direct calculation of a transition, such as  
12 the melting temperature of an alloy.  
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#### 17 *2.4. Parallel calculations*

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19 Calculation of multiple equilibria in parallel is not only useful for simula-  
20 tions but also for assessments of model parameters. Such assessments usually  
21 include a large number of experimental data, each representing a value deter-  
22 mined at equilibrium. The assessment procedure calculates these equilibria  
23 many times varying the selected model parameters in order to find the best  
24 fit. Traditionally the equilibria are calculated sequentially but with the OC  
25 software it is possible to calculate them in parallel.  
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33 When tested on a PC with 4 CPU, each with 2 threads, the gain in speed  
34 for a calculation with 400 experimental equilibria in parallel was almost a  
35 factor of 4, i.e. no significant overhead.  
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38 The occurrence of a miscibility gap in a phase requires special treatment  
39 for parallel processing. A miscibility gap means that the phase is stable with  
40 two different compositions which requires that an extra composition set must  
41 be created in OC, see section 3.7. This must be done at the same time in  
42 all equilibria otherwise the data structure would become inconsistent. Thus  
43 the threads must be stopped while the extra composition set is created.  
44 Normally this is not a problem during an assessments as miscibility gaps  
45 should be known from the experimental data and the user can manually  
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5 create a sufficient number of composition sets before starting the parallel  
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7 session. However, miscibility gaps or order/disorder transformations can  
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9 create problems when encountered during simulations.

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11 *2.5. Additional data depending on  $T, P$  and phase composition*  
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14 Thermodynamic data are important but not sufficient to simulate a phase  
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16 transformation. For example, to consider the diffusion of elements their  
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18 mobilities together with the thermodynamic factor need to be described to  
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20 obtain the diffusion coefficient. In addition, there are also interface energies,  
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22 interface mobilities, elastic constants and other phase based properties that  
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24 may be of interest [22].

25  
26 In the OC software such property descriptions can be stored together with  
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28 the thermodynamic data for each phase as functions of  $T, P$  and constitution  
29  
30 of the phase. The values of these properties are calculated together with the  
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32 thermodynamic properties during the equilibrium calculation and can be  
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34 accessed by the application software.

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36 For example, the natural logarithm of the mobility of Fe in the face  
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38 centered cubic (FCC) phase of the binary Fe-Ni system, in OC denoted  
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40  $MQ\&Fe(FCC)$ , can be described by a linear function:

41  
42 
$$MQ\&Fe(FCC) = x_{Fe}^{FCC} MQ\&Fe(FCC, Fe) + x_{Ni}^{FCC} MQ\&Fe(FCC, Ni) \quad (3)$$

43  
44 where  $x_{Fe}^{FCC}$  and  $x_{Ni}^{FCC}$  are the mole fractions of Fe and Ni in FCC, re-  
45  
46 spectively,  $MQ\&Fe(FCC, Fe)$  is the mobility of Fe in pure FCC Fe and  
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48  $MQ\&Fe(FCC, Ni)$  is the mobility of a single Fe atom in pure FCC Ni, both  
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50 of which may depend on  $T$  as:

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$$MQ\&Fe(FCC, Ni) = \frac{Q_{Fe}}{RT} \ln(\nu_{Fe}) \quad (4)$$



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5 where  $Q_{\text{Fe}}$  is the activation energy and  $\nu_{\text{Fe}}$  the pre-exponential factor. As  
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7 mobilities can vary several orders of magnitude it is a better approximation  
8  
9 to describe the composition dependence by a linear relation of its logarithm.  
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11 If sufficient experimental or theoretical data are available, non-linear terms  
12  
13 can be added to eq. 3.

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15 Together with the thermodynamic factor the mobility can be transformed  
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17 to a diffusion coefficient needed for the simulation of microstructure evolution  
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19 in diffusion controlled processes.  
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### 21 **3. The OCASI application software interface**

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24 Software interfaces for coupling thermodynamic calculations with appli-  
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26 cation software following a proposed standard [23] implemented in slightly  
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28 different ways in ChemApp [24] and Thermo-Calc TQ [25]. The idea behind  
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30 this proposed standard is to overcome the differences between the different  
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32 thermodynamic software packages which can make the implementation into  
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34 application software difficult. The methodology with many separate sub-  
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36 routines and functions performing specific tasks makes the implementation  
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38 straightforward and used also for OCASI.

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40 A full documentation of OCASI is under preparation but a preliminary  
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42 version is available at the websites mentioned above. Again, as the source  
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44 code is available any user can directly access the source code and also data  
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46 which are not primarily available. However, any such access should be done  
47  
48 with caution as the data structure and source code may change in a later  
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50 update whereas the OCASI interface should remain stable. A summary of  
51  
52 the available subroutines is given in Appendix 1.  
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### 3.1. Fortran and C++ data structure compatibility

Using the ISO C standard it is possible to access data structures defined in the OC software written in Fortran from C++ and other languages. For example, the data for a composition set of a phase in OC are described by:

```
TYPE gtp_phase_varres
! Data here are for a composition set of a phase in an equilibrium
! There can be several equilibria for assessments or parallel calculations
! phlink: is index of phase record for this phase_varres record
! status2: has phase status bits like
! phstate: indicate state: fix/stable/entered/unknown/dormant/suspended
! phtupx: phase tuple index
    integer nextfree,phlink,status2,phstate,phtupx
! abnorm(1): amount moles of atoms for a formula unit of the composition set
! abnorm(2): mass/formula unit (both set by call to set_constitution)
! prefix and suffix are added to the name for composition sets 2 and higher
    double precision, dimension(2) :: abnorm
    character*4 prefix,suffix
! constat: array with status word for each constituent
! yfr: the constituent fraction array
! mmyfr: min/max fractions, negative is a minimum
! sites: site ratios (which can vary for ionic liquids)
    integer, dimension(:), allocatable :: constat
    double precision, dimension(:), allocatable :: yfr
    real, dimension(:), allocatable :: mmyfr
    double precision, dimension(:), allocatable :: sites
! for ionic liquid derivatives of sites wrt fractions (it is the charge),
    double precision, dimension(:), allocatable :: dpqdy
    double precision, dimension(:), allocatable :: d2pqdvay
! disfra: a structure describing the disordered fraction set (if any)
    type(gtp_fraction_set) :: disfra
! arrays for storing calculated results for each phase (composition set)
! amfu: is amount formula units of the composition set (calculated result)
! netcharge: is net charge of phase (must be zero for stable phases)
! dgm: driving force
    double precision amfu,netcharge,dgm
! nprop: the number of different properties (set in allocate)
! listprop(1): is number of calculated properties
! listprop(2:listprop(1)): identifies the property stored in gval(1,ipy) etc
! 1=G, 2=TC, 3=EMAG. Properties defined in the gtp_propid record
    integer nprop
    integer, dimension(:), allocatable :: listprop
! gval etc are for all composition dependent properties, gval(*,1) for G
! gval(*,1): is G, G.T, G.P, G.T.T, G.T.P and G.P.P
! dgval(1,j,1): is first derivatives of G wrt fractions j
! dgval(2,j,1): is second derivatives of G wrt fractions j and T
! dgval(3,j,1): is second derivatives of G wrt fractions j and P
! d2gval(ixsym(i,j),1): is second derivatives of G wrt fractions i and j
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5     double precision, dimension(:,,:), allocatable :: gval
6     double precision, dimension(:,,:), allocatable :: dgval
7     double precision, dimension(:,,:), allocatable :: d2gval
8 ! added for strain/stress, current values of lattice parameters
9     double precision, dimension(3,3) :: curlat
10    END TYPE gtp_phase_varres
11 ! an array of these records is created inside each equilibrium record
12

```

This can be summarized for C++ software by the ISO C interface as:

```

15 typedef struct {
16     int nextfree, phlink, status2, phstate;
17     double abnorm[2];
18     char prefix[4], suffix[4];
19     int *constat;
20     double *yfr;
21     double *mmyfr;
22     double *sites;
23     double *dpqdy;
24     double *d2pqdvay;
25     //struct gtp_fraction_set disfra;
26     double amfu, netcharge, dgm, amcom, damount;
27     int nprop, ncc;
28     int *listprop;
29     double **gval;
30     double ***dgval;
31     double **d2gval;
32     double curlat[3][3];
33 } gtp_phase_varres;

```

### 3.2. Interfacing with Java

Based on Fortran and C(++) compatibility, it is also possible to interface OC functionalities in the Java language thanks to the Java Native Interface (JNI) [26]. For the PROCOR software [27], such an interfacing has been developed for C. Cardon Ph.D. thesis regarding the development of a Cahn-Hilliard based multicomponent multiphase diffusion model [28]. This application is briefly described in section 4.4. In addition to the Cahn-Hilliard model requirements, equilibrium calculation functionalities have been interfaced for the coupling of other physical models to evaluate some physical parameters using the phase compositions obtained from OC equilibrium calculations.

### 3.3. Reading the database

The thermodynamic data for a system will normally be read from a database. The OC software supports the TDB format [29] proposed originally by SGTE [30] and is used by several other software, most notably by Thermo-Calc and DICTRA [12]. The application software allows to select the elements for which data that should be extracted from the database and then to suspend phases that are not of interest for the application.

The application software must initiate the OC memory structure by a special subroutine call. This returns a pointer to an equilibrium record in the dynamic memory structure which contains information about the constitution and calculated results for all the phases as described in section 3.1. Only after this initialization other subroutines, such as reading the database, can be called. The database has data like the models of phases and their thermodynamic model parameters and these data are stored in the static part of the OC memory structure since they are independent of the external conditions. The external conditions, the constitution of the phases and the calculated results are in the dynamic data memory. A schematic representation of both static and dynamic memory is shown in Fig. 1.

### 3.4. Setting conditions

The conditions are set individually by a call to a subroutine. In the simplest case these represent the temperature,  $T$ , pressure,  $P$ , and amount of the components,  $N_i$ . The number of conditions needed to calculate the equilibrium is given by Gibbs phase rule

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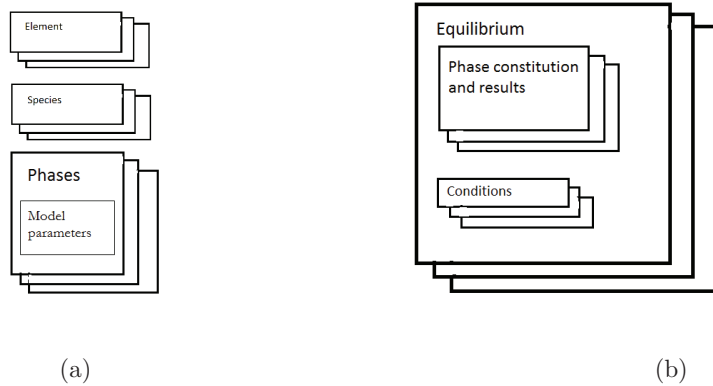


Figure 1: The static (a) and dynamic (b) parts of the OC memory. Each equilibrium record in (b) is independent and can be calculated in parallel.

where  $f$  is the degrees of freedom,  $n$  the number of components and  $p$  is the number of stable phases. Normally the number of stable phases is the result of the equilibrium calculation but OC allows that one or more phases are prescribed to be stable. If there are no prescribed stable phases, a system with a single component,  $n = 1$ , must have 3 conditions, for example  $T, P$  and  $N$  where  $N$  is the size of the system. For a binary system 4 conditions must be set and so on.

The amount of a component  $i$  can be given in moles,  $N_i$ , or mass and if there is a major component they are often given in mole or mass fractions or per cent and the total size of the system is given as  $N$ . Chemical potentials or activities of the components can also be used instead of amounts.. It is also possible to specify the volume or the enthalpy of the system, or as already mentioned, specify that a phase has to be stable. It is important that all conditions are independent of one another. However, this does not mean that it is not possible to set irrational conditions, i.e. those that do

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5 not represent a possible equilibrium state. A full list of state variables in OC  
6 is given in Appendix 2.  
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### 9 10 *3.5. Creating additional equilibria*

11 Additional equilibrium records can be created to represent local equilibria  
12 in a simulation or assessment. These may be calculated sequentially or in  
13 parallel as they have independent sets of conditions and related data. Each  
14 equilibrium record has a pointer to its own dynamic data structure and this  
15 pointer must be supplied in the calls to most of the OCASI routines to  
16 indicate which equilibrium should be used.  
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### 24 *3.6. Calculations*

25 When the degree of freedom according to eq. 5 is zero the equilibrium  
26 can be calculated by calling a subroutine. The calculation procedure in OC  
27 is described in detail in [21]. In the call it is possible to specify whether the  
28 global minimizer should be used or the calculation should start from the last  
29 calculated set of stable phases and constitutions.  
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### 37 *3.7. Composition sets and phase tuples*

38 The number of phases in the system when reading from the database  
39 is equal to the number of phases with unique names and structures in the  
40 database. However, as phases can have miscibility gaps or several types of  
41 ordering transformations some of the phases may become stable with two  
42 or more unique compositions. In some software the user must specify this  
43 in advance but in OC the global grid-minimizer will detect miscibility gaps  
44 automatically. A phase may thus have several independent composition sets  
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5 and each of these is called a phase tuple. The composition set index of a  
6 phase is specified after the phase name by the character "#" followed by a  
7 digit, for example LIQUID#2.  
8  
9

10  
11 In some cases, for example phases with order/disorder transitions, it is  
12 important to know the state of ordering of a particular phase tuple. For  
13 such cases composition sets can be created explicitly and they can be given  
14 a unique name and default composition that can be used to identify the  
15 ordered state.  
16  
17

18  
19 The first composition set created when the phase is read from the database  
20 has no explicit set indication. A composition set created automatically by  
21 the grid-minimizer will have a suffix "\_AUTO" added to its name (before the  
22 # sign).  
23  
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27  
28 In OCASI there is an array of phase tuples where each index represents  
29 the combination of a phase and composition set. Thus the number of phase  
30 tuples may change whenever the grid-minimizer is called.  
31  
32

### 33 34 *3.8. Extracting results* 35

36  
37 The normal way to obtain calculated results is to call a subroutine using  
38 state variable symbols from the list in Appendix 2. The values of properties  
39 that are modeled separately, like the Curie temperature, mobilities etc. and  
40 that have been read from the database can be obtained in the same way.  
41  
42  
43

44  
45 Using the pointer to the equilibrium data structure provided when read-  
46 ing the database it is possible to extract individual calculated results of an  
47 equilibrium. For example, if the equilibrium record pointer is called "ceq"  
48 and as the array of records for each phase is called "phase\_varres", the value  
49 of the Gibbs energy per mole formula unit of the phase after an equilibrium  
50  
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5 calculation can be obtained as  
6

7 `gfu = ceq%phase_varres(lokcs)%gval(1,1)`  
8  
9

10 where the % sign is used in the new Fortran standard to indicate items  
11 in a record. The lokcs variable is the index of the composition set of the  
12 phase and this is stored in the phase tuple record and thus provides an easy  
13 link between the phase tuple index and the phase data. For example, if the  
14 calculated mobility of component 1 of the same phase is stored in the location  
15 “ipy”, see section 3.1, its value is obtained by  
16  
17  
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21

22 `mob(1) = ceq%phase_varres(lokcs)%gval(1,ipy)`  
23  
24

25 Great care must be taken that the relevant data is extracted. The application  
26 program must not change the OC data structure.  
27  
28

## 29 30 **4. Examples of application software** 31 32

33 Several simple examples of how to use the OC software interface are  
34 provided with the source code. Some of the examples presented here may  
35 require the use of proprietary software components.  
36  
37  
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39

### 40 *4.1. The beginnings of a reactor module* 41

42 A process can sometimes be simulated by dividing it into sections, each  
43 of which represent a local equilibrium, and a transport of matter between  
44 these by diffusion or other means. The equilibrium calculation can be done  
45 by OC in a function “localequil” with the following arguments:  
46  
47  
48  
49

```
50 integer function localequil(todo,nse1,sele1,tp,nmz,outspec,outval)  
51 !  
52 ! This routine calculates an equilibrium and return values  
53
```



```

1
2
3
4
5      ! todo character variable          with "commands" to be executed
6      ! nsel integer                    number of components
7      ! selel character*2 array         element names
8      ! tp double precision array(2)   with values of T and P
9      ! nmz double precision array(nsel) with molar content for elements
10     ! outspec character variable      with information which data to extract
11     ! outval double precision array(*) with extracted values
12     ! if there is no error the function value returned is zero

```

13 The `todo` argument passes a number of instructions to `localequil`, `nsel`
14 gives the number of elements specified in argument `selel`, `tp` provides the
15 values of  $T$  and  $P$  and `nmz` the element amounts. The argument `outspec`
16 specifies which state variable values will be returned in `outval`. A call of this
17 function to calculate a local equilibrium for the system Si-O-C at 1800 K and
18 1 bar with a specified amount of moles of the elements can be:

```

25     nsel=3
26     selel(1)='C '; selel(2)='O '; selel(3)='Si'
27     tp(1)=1.80D2; tp(2)=1.0D5;
28     nmz(si)=1.0D0; nmz(2)=2.0D0; nmz(3)=1.8D0
29     todo='verbose open cosi.tdb '
30     outspec='n(gas,*) mu(*) h h(gas) '
31     ierr=localequil(todo,nsel,selel,tp,nmz,outspec,outval)

```

32 Here the `todo` argument specifies `VERBOSE` to generate extra output,
33 then to open the database file `cosi.tdb` and read the data for the system
34 with the elements in the argument `selel` and calculate the equilibrium at
35 the specified values of  $T$ ,  $P$  and amounts of the elements. After a successful
36 calculation the amounts of all elements in the gas,  $n(\text{gas},*)$ , their chemical
37 potentials,  $\mu(*)$ , the total enthalpy,  $h$ , and the enthalpy of the gas,  $h(\text{gas})$ ,
38 will be provided in the `outval` array argument. The state variables that can
39 be used are listed in Appendix 2. If there is an error the function will return
40 a non-zero number.

41 The `localequil` function will remember whether it has already read a
42 database and if no database is specified in a subsequent call the routine will

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5 use the static data that it has already stored. In the application software the  
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7 amounts of elements in the gas and the other phases may be redistributed  
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9 between different local equilibria to simulate a process. The range of options  
10  
11 in the localequil function can easily be extended. One of the intentions of  
12  
13 this function is to provide an application programmer a simple access of the  
14  
15 OCASI interface.  
16

#### 17 *4.2. Simulation of homogenization of an alloy AA7449*

18

19 The OpenCalphad Software has been recently coupled to the Constellium  
20  
21 thermodynamic package, ProPhase, using OCASI in order to use the faster  
22  
23 equilibrium routine included in OC as well as the new parallelization recently  
24  
25 implemented. ProPhase includes a long range diffusion subroutine which is  
26  
27 used when simulating a solidification path with back diffusion or a homog-  
28  
29 enizing treatment of an as cast structure. The long-range diffusion within  
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31 the FCC aluminum solid solution is simulated using an explicit finite differ-  
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33 ence scheme, assuming local equilibrium in each volume element, calculating  
34  
35 the solute concentration in solid solution, and using Fick's diffusion equation  
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37 in the solid solution to compute solute exchange between adjacent volume  
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39 elements. For each time step, this routine performs many independent equi-  
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41 librium calculations, one for each volume element, and is very well suited  
42  
43 for parallelization. The simulation of a laboratory heat treatment at 472 °C  
44  
45 of a multicomponent aerospace 7449 alloy (an Al-Mg-Zn-Cu-Fe-Si alloy, see  
46  
47 Table 1) after casting has been used to measure the gain in speed provided  
48  
49 by OpenCalphad in comparison with the previous software. The cast was  
50  
51 performed in the laboratory using the Aluminum Association TP-1 grain  
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53 refiner test crucible. The corresponding cast structure, as shown in Fig. 2  
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was simulated by a modified Scheil calculation with back diffusion. For this particular case, a two dimensional cylindrical geometry was chosen with a 61  $\mu\text{m}$  secondary dendrite arm spacing. Care must be taken to mesh the dendritic cylinder with sufficiently small enough radius increments especially towards the end of solidification where the concentration gradients may be very steep.

Table 1: Composition range of AA7449 according to the Aluminum Association

	Si	Fe	Cu	Mn	Mg	Zn	Ti+Zr	rest
min	0	0	1.4	0	1.8	7.5	0	Al
max	0.12	0.15	2.1	0.2	2.7	8.7	0.25	Al

The evolution of composition gradients has been studied for a heat treatment consisting in a linear heating of 40  $^{\circ}\text{C}/\text{h}$  up to 472  $^{\circ}\text{C}$  followed by holding at 472  $^{\circ}\text{C}$  for 10 h. The corresponding predicted and measured incipient melting temperatures and integrated enthalpies for the DSC first melting peak are compared in Fig. 3. Overall, good agreement is obtained indicating that the proposed physical description of the phenomena occurring during solidification and homogenizing is acceptable. With our previous software such a calculation took 3.5 days on one processor. By using the parallel OpenCalphad routine the total computation time was reduced to 3.5 hours on 12 processors.

#### 4.3. Phase-field models and OCASI

Many modern thermodynamic consistent phase-field models [31, 32, 33, 34] rely on thermodynamic and kinetic properties that can be obtained or ap-

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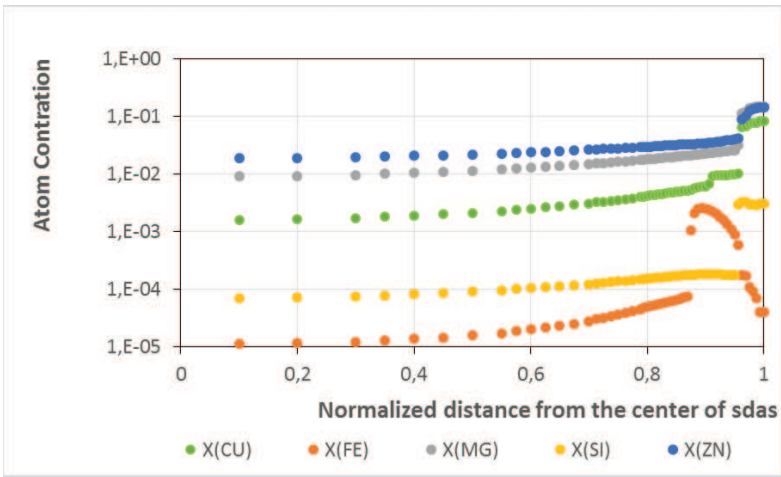


Figure 2: Simulated concentration gradients after solidification of aerospace alloy AA7449

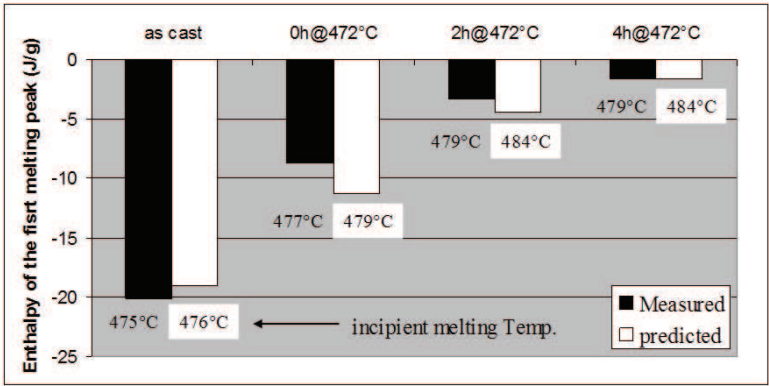


Figure 3: Simulated and measured incipient melting temperatures and enthalpies of the first melting peak during calorimetric heat up at a rate of 20 °C/min.

proximated from CALPHAD calculations. OpenCalphad [<http://www.opencalphad.org>] as an open source tool is perfectly suited for this purpose. The speed of the OCASI software with additional parallelization allows for an efficient way to compute separate phase-properties in the diffuse interfaces with equilibrium calculations or with separate phase-compositions as in-

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5 put parameters. Coupled to the phase-field software framework of Open-  
6 Phase [<http://www.openphase.de>], OCASI has been proven to be an efficient  
7 tool for meso-scale microstructure simulations. As extensive phase data can  
8 be shared via this interface too, a user friendly simulation setup can be ar-  
9 ranged.  
10

11  
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14 To be able to compute the equations governing phase-transformation and  
15 diffusion in the phase-field model with finite interface dissipation [34], Gibbs  
16 energies of the phases,  $G_m^\alpha$ , their derivatives  $\partial G_m^\alpha / \partial y_i^{\alpha,(s)}$  and the atomic  
17 mobilities  $M_i^\alpha$  can be calculated with an input consisting of the temperature  
18  $T$ , pressure  $P$  and compositions  $y_i^{\alpha,(s)}$  through the OCASI interface.  
19  
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24 This does not only speed up the simulations and increases the accuracy  
25 of the results, it also allows for a quick simulation setup of multi-component  
26 multi-phase simulations, as no analytical implementation of the Gibbs en-  
27 ergies or parallelization of phase equilibria calculations, has to be carried  
28 out.  
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33  
34 This is demonstrated here for a small microstructure simulation example  
35 with two austenitic steel samples with different alloy composition in contact.  
36 The two samples containing iron, manganese, silicon and carbon are chosen to  
37 represent the experiments on uphill diffusion by Darken [36]. Apart from the  
38 chosen thermodynamic and kinetic databases [37] under the Open Database  
39 License, only the temperature, the time step and the grid spacing had to be  
40 specified as in Tab. 2  
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47 The results of the quaternary simulation are shown in Fig. 4 for an exper-  
48 iment with a duration of 10 days at constant 1323 K and are compared with  
49 the results of a DICTRA sharp-interface simulation as well as measurements  
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Table 2: Simulation parameters

Box size	50x10x10
Grid spacing	0.001 m
Time step	1000 s
Temperature T	1323 K
Thermodynamic database	MatCalc mc_fe_v2.057.tdb [37]
Mobility database	MatCalc mc_fe_v2.008.ddb [37]

from Darke, [36]. The results obtained with only openly available tools and data show excellent agreement with the results from the commercial DIC-TRA software.

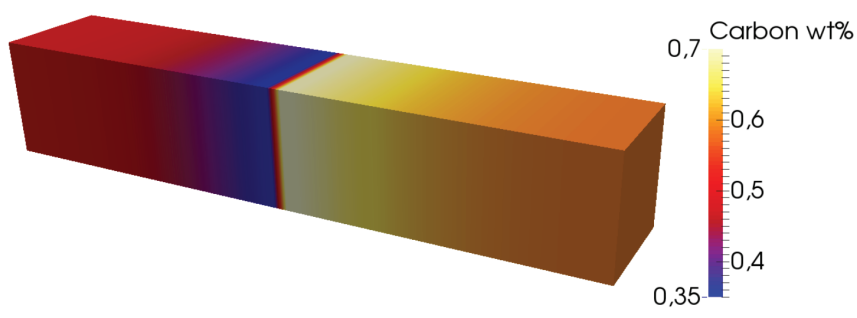
Beyond that, the coupling of OpenCalphad and phase-field software like OpenPhase has been proven to be an efficient, accurate and easy to use tool for meso-scopic microstructure simulations.

#### 4.4. Mesoscopic modelling of a liquid miscibility gap

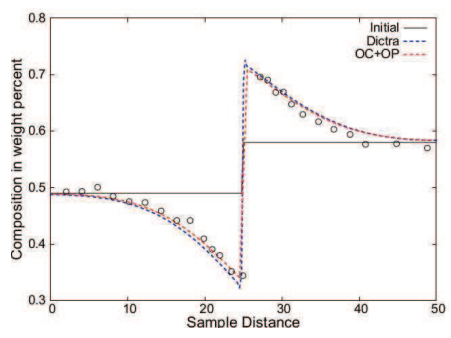
For the study of severe accidents in light water nuclear reactors (LWR), the OpenCalphad software has been used in the development of a Cahn-Hilliard based diffusion model for treating the liquid-liquid miscibility gap associated with the corium (oxidic and metallic liquid materials present during a reactor core meltdown) in a reactor vessel lower head.

In-vessel corium is a complex thermodynamic system because of the phases that are present. In addition to partially oxidized cladding and fuel materials ( $\text{UO}_2$ ,  $\text{ZrO}_2$  and Zr), the corium contains stainless steel elements

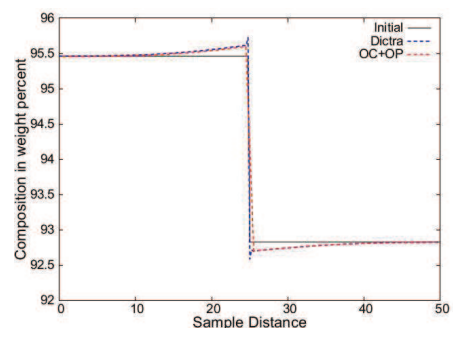
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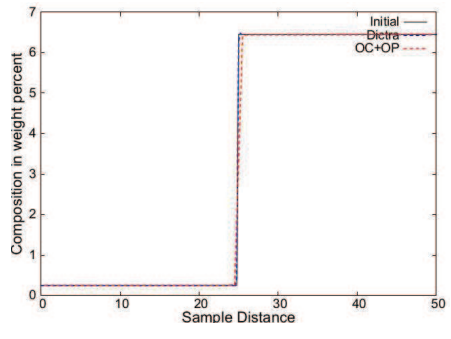
(a) Carbon composition over the whole simulation sample



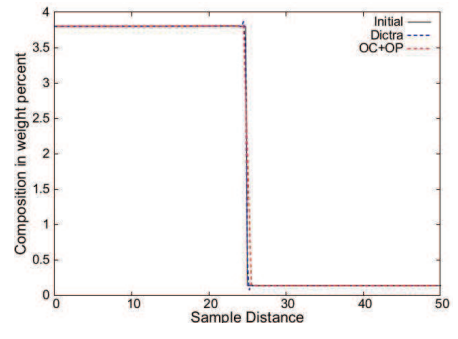
(b) Carbon composition



(c) Iron composition



(d) Manganese composition



(e) Silicon composition

Figure 4: Simulated composition profiles after 10 days of tempering at 1050 °C, with experimental measurements by Darken [36] as circles.

(Fe, Ni, Cr) from the reactor’s internal structures. In particular, the U-O-Zr-Fe system exhibits a liquid-liquid miscibility gap responsible for a liquid phases stratification of tremendous importance on the corium propagation [38].

This stratification phenomenon results from the combination of multi-component multiphase species diffusion and gravitational material movement due to buoyancy effects initiated by Rayleigh-Taylor instabilities. The natural convection in a corium pool can be simulated by Computational Fluid Dynamics (CFD) and a Cahn-Hilliard based mesoscopic modeling of the species diffusion appears to be a promising way to account for the stratification phenomenon in detailed simulations. This R&D effort regarding a detailed modeling of the thermohydraulic/thermochemical behavior of in-vessel corium has been undertaken at CEA Cadarache in support of integral models development in the context of the PROCOR software platform for sensitivity/uncertainty studies regarding corium propagation.

A Cahn-Hilliard based diffusion model was first developed for the U-O binary case [28] and is under development for U-O-Zr and U-O-Zr-Fe. Under the assumption of constant molar volume, the model for a n-component system is based on Cahn-Hilliard evolution equations for molar fractions of n-1 components with diffusion potentials,  $\tilde{\mu}_i$ , expressed as:

$$\tilde{\mu}_i = a \left( \frac{\partial \tilde{g}}{\partial x_i} \right)_{x_j \neq i} - \sum_j \kappa_{i,j} \nabla^2 x_j \quad (6)$$

where  $a$  and  $\kappa_{i,j}$  are parameters of the model related to the interface thickness (a “numerical” parameter in this mesoscopic modeling) and interface tension while  $\tilde{g}$  is the free energy density (in  $\text{Jm}^{-3}$ ) of the homogeneous system.



In the binary U-O case, the  $\left(\frac{d\bar{g}}{dx_O}\right)$  term was calculated applying the chain rule to the liquid Gibbs energy  $G_m^{liq}$  and its derivatives  $\partial G_m^{liq} / \partial y_i^{liq}$  obtained from the OCASI interface [28].

For the ternary and quaternary systems, the additional hypothesis that local equilibrium of the redox chemical reactions is instantaneously reached is made. Therefore,  $\left(\frac{\partial \bar{g}}{\partial x_i}\right)_{x_{j \neq i}}$  can be related to the chemical potentials obtained from “local” equilibrium calculations performed using the OCASI interface where the phase separation associated with the miscibility gap is not taken into account (*i.e.* the grid minimizer is turned off, *cf.* Section 2.3).

In order to illustrate this modeling, a 1D calculation for the U-O binary case is presented here; the domain length is  $L = 10.0$  cm and the temperature and pressure conditions are  $T = 3200$  K and  $p = 1$  bar. Fig. 5 schematically depicts the initial configuration and the steady-state of the system. The interface thickness has been set to 1 cm.

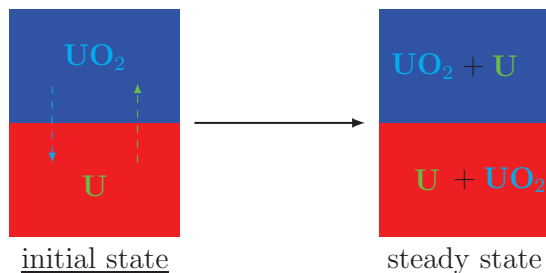
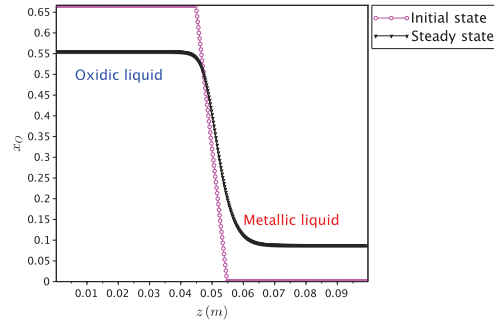


Figure 5: U-O system initial configuration and steady state

The initial configuration corresponds to an oxidic phase (uranium dioxide  $UO_2$ ) above a metallic phase (in this case metallic uranium U). The diffusion process leads to a steady state configuration with two suboxidized phases.

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5 Fig. 6 shows the profile of oxygen molar fraction  $x_O$  in the initial state and  
6 at steady state where it is verified that, far from the interface, the oxygen  
7 molar fraction is equal to the values given by an equilibrium calculation.  
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25 Figure 6: Profile of molar oxygen fraction  $x_O$  versus position  $z$   
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## 28 5. Summary

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31 Thermodynamic data needed in simulations, such as melting temper-  
32 atures, solubilities, heat capacities etc., are often collected from different  
33 sources. In most cases little or no efforts are made to verify that these data  
34 are consistent. Data from calculations using thermodynamic databases have  
35 the advantage of being consistent but the fact that the equilibrium calcu-  
36 lations are usually quite slow poses a severe problem. The possibility to  
37 calculate local equilibria at each point in space in parallel is a major im-  
38 provement. Still, it may not be possible to completely avoid the use of inter-  
39 polation methods in very large simulations with several thousand grid-points.  
40 In this case the availability of parallel processing offers the opportunity to  
41 update the results in real time during the simulation avoiding the need for  
42 look-up tables created in advance thus allowing more accurate input for the  
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5 simulation. The examples selected are from very different fields showing the  
6 flexibility of the OC software.  
7

## 8 9 10 **6. Acknowledgement**

11  
12 One author (BS) is grateful for a senior research grant from the Humboldt  
13 Foundation. Two authors (SGF, MP) acknowledge the Deutsche Forschungs-  
14 gemeinschaft (DFG) through Project C6 of SFB/TR 103. The work reported  
15 in Section 4.4 has been carried out within the framework of the PROCOR  
16 platform development funded by CEA, EDF and AREVA. Commercial prod-  
17 ucts are identified for reference purposes this does not imply an endorsement  
18 by the National Institute of Standards and Technology.  
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# Appendix 1

Summary of current subroutines included in OCASI.

tqcceq	Create and copy equilibrium
tqce	Calculate equilibrium
tqcph1	Calculate phase tuple properties
tqdceq	Delete equilibrium
tqgcef	Get stoichiometry of component
tqgcom	Get the component names
tqgetv	Get state variable value
tqgnp	Get number of phase tuples
tqgnpc	Get number of constituents in phase
tqgpci	Get index of phase constituent using name
tqgpcn2	Get phase constituent index using name
tqgpcs	Get stoichiometry of constituent
tqgphc1	Get phase constitution
tqgpi	Get phase tuple index using phase name
tqgpn	Get phase name using phase tuple index
tqini	Initiate OC and the OCASI interface
tqphtupsts	Set phase tuple status
tqrpfil	Read data for selected elements from a database
tqselceq	Select equilibrium
tqsetc	Set condition
tqsphc1	Set constitution of phase tuple



## Appendix 2

The available state variables and their notation in OC. All of them can be used to extract calculated values and many also to set conditions.

In this notation  $N$  is the total amount of moles,  $N(O)$  is the total amount of oxygen in moles,  $N(\text{GAS},O)$  is the amount of moles of O in the gas phase.  $NM(O)$  or  $X(O)$  is the overall mole fraction of O. The total number of moles of components in the gas phase is  $NP(\text{GAS})$ .

The heat capacity is not included in this list since it can be calculated as a “dot derivative, H.T” , as explained in [21].

Symbol	Index		Normalizing	Meaning
	1	2	suffix (z)	
Intensive properties				
T	-	-	-	Temperature
P	-	-	-	Pressure
MU	component	-/phase	-	Chemical potential
AC	component	-/phase	-	Activity
LNAC	component	-/phase	-	LN(activity)
Extensive and normalized properties				
U	-/phase#set	-	-	Internal energy for system
UM	-/phase#set	-	M	Internal energy per mole
UW	-/phase#set	-	W	Internal energy per mass
UV	-/phase#set	-	V	Internal energy per m <sup>3</sup>
UF	phase#set	-	F	Internal energy/mole formula unit
Sz	-/phase#set	-	-/M/W/V/F	Entropy
Vz	-/phase#set	-	-/M/W/V/F	Volume
Hz	-/phase#set	-	-/M/W/V/F	Enthalpy
Az	-/phase#set	-	-/M/W/V/F	Helmholtz energy
Gz	-/phase#set	-	-/M/W/V/F	Gibbs energy
NPz	phase#set	-	-/M/W/V/F	Moles of phase
BPz	phase#set	-	-/M/W/V/F	Mass of phase
Qz	phase#set	-	-/M/W/V/F	Stability of phase
DGz	phase#set	-	-/M/W/V/F	Driving force of phase
Nz	-/phase#set/comp	-/comp	-/M/W/V/F	Moles of component
X	phase#set/comp	-/comp	-%	Mole fraction/per cent
Bz	-/phase#set/comp	-/comp	-/M/W/V/F	Mass of component
W	phase#set/comp	-/comp	-%	Mass fraction/per cent
Y	phase#set	const#subl	-	Constituent fraction
Some model parameter identifiers				
TC	phase#set	-	-	Curie temperature
BMAG	phase#set	-	-	Aver. Bohr magneton number
MQ&X	phase#set	constituent	-	Mobility of X
THET	phase#set	-	-	Debye temperature