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An integrated framework for multi-scale materials simulation and design

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Abstract. In this paper, we describe initial results of an ongoing research activity involving materials scientists, computer scientists, mathematicians, and physicists from academia, industry and a national laboratory. The present work aims to develop a set of integrated computational tools to predict the relationships among chemistry, microstructure and mechanical properties of multicomponent materials systems. It contains a prototype grid-enabled package for multicomponent materials design with efficient information exchange between structure scales and effective algorithms and parallel computing schemes within individual simulation/modeling stages. As part of our multicomponent materials design framework, this paper reports the materials simulation segment in developing materials design knowledgebase, which involves four major computational steps: (1) Atomic-scale first-principles calculations to predict thermodynamic properties, lattice parameters, and kinetic data of unary, binary and ternary compounds and solutions phases; (2) CALPHAD data optimization approach to compute thermodynamic properties, lattice parameters, and kinetic data of multicomponent systems; (3) Multicomponent phase-field approach to predict the evolution of microstructures in one to three dimensions (1–3D); and (4) Finite element analysis to generate the mechanical response from the simulated microstructure. These four stages are to be integrated with advanced discretization and parallel algorithms and a software architecture for distributed computing systems.

Keywords: CALPHAD, finite element analysis, first-principles, grid computing, phase-field

1. Introduction

Traditionally, the field of materials science and engineering is predominantly focused on establishing the relationships among processing, microstructure, properties, and performance through large-scale experimental investigations. This traditional and often highly empirical approach is increasingly shifting towards the design of materials to achieve optimal functionality, driven largely by advances in information technology and computational materials science.

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From the viewpoint of engineering design, materials design is a process to determine optimal combinations of *controllable quantities* such as material chemistry, processing routes, and processing parameters to robustly meet specific performance requirements presented by *measurable quantities* such as mechanical properties. This process is iterative by nature due to the incompleteness of the design knowledgebase and the lack of one-to-one correspondence from measurable quantities to controllable quantities. This iterative process includes steps such as material concept, problem statement with non-material factors including cost and time constraints, information gather and brainstorm, design objectives, design selection, and prototype design and test, followed by final documentation. The bottleneck in terms of cost and time is the prototype design and test, which have been carried out predominantly by experimental investigations in the past. In this report, we present a framework that integrates first-principles calculations, multicomponent modeling, phase-field simulation, and finite element analysis to computationally test prototypes and contribute to development of materials design knowledgebase.

Recent advances in first-principles calculations have made it possible to routinely predict accurate thermodynamic properties, such as formation energies and enthalpies, of unary and binary alloys using only the atomic numbers and crystal structures as the input. Accurate calculations of entropic contributions, such as configurational or vibrational entropies, while more difficult, are also possible. However, it is not computationally tractable, for the foreseeable future, to use first-principles calculations alone to determine the total free energy directly for *multicomponent systems*, at least not with an accuracy comparable to experimental phase diagram measurements. On the other hand, semi-empirical methods based on the CALPHAD approach have been very successful in predicting the phase equilibria of multicomponent commercial alloys. The CALPHAD approach computes thermodynamic functions for multicomponent systems using thermodynamic data obtained in unary, binary and ternary systems. Therefore, an integration of first-principles calculations of simple low-order systems and the CALPHAD approach will allow one to develop thermodynamic databases for multicomponent systems from first-principles, as has been recently demonstrated [1]. A similar strategy can be adopted for developing kinetic databases and databases for lattice parameters [2], elastic constants and interfacial energies as a function of composition and temperature.

Another recent important development in computational materials science is the emergence of the powerful phase-field approach to simulate phase transformations and microstructure evolution. It has a number of advantages over other microstructure models, which make it uniquely suited to simulating microstructures in complex multicomponent alloy systems. First of all, the phase-field approach does not explicitly track the positions of interfaces, and hence the temporal evolution of arbitrary microstructures can be predicted without any *a priori* assumptions about their evolution path. Secondly, because the phase-field approach is based on the fundamental thermodynamic, kinetic, and crystallographic information, it can directly predict the microstructure evolution in complex systems by drawing on reliable thermodynamic and kinetic databases, thus contributing to the overall materials design approach. A recent coupling of first-principles thermodynamics with the phase-field approach has demonstrated how the combination of these approaches provides a pathway towards truly predictive modeling of microstructural evolution [3]. Finally, there is no

technical difficulty in extending from two-dimensional (2D) to three-dimensional (3D) simulations except a significant increase in computational time and memory requirements. Therefore, more efficient algorithms and high performance computer clusters are needed to predict realistic microstructure evolution in 3D.

The ultimate goal of many scientists and engineers in the materials design arena is to predict the mechanical behavior of materials as a function of chemistry, processing, and in-service conditions. Therefore, it is critical to link predicted microstructures to the properties of materials. One of the goals of our research is to extend the OOF program for object-oriented finite element analysis of material properties developed at NIST, and integrate it with the simulated microstructures from the above computational materials science approaches. The OOF program is designed to calculate macroscopic properties from images of microstructures and perform virtual experiments on realistic microstructures.

To integrate these multiscale materials modeling and simulations, we developed a four-stage system approach as shown in Figure 1, in which the four stages are connected through materials databases and managed through an asynchronous, distributed software architecture (see Figure 2). This approach includes the following components:

- Databases of fundamental materials properties constructed from first-principles atomistic calculations to enable more robust CALPHAD modeling of multicomponent materials systems through efficient information exchange;

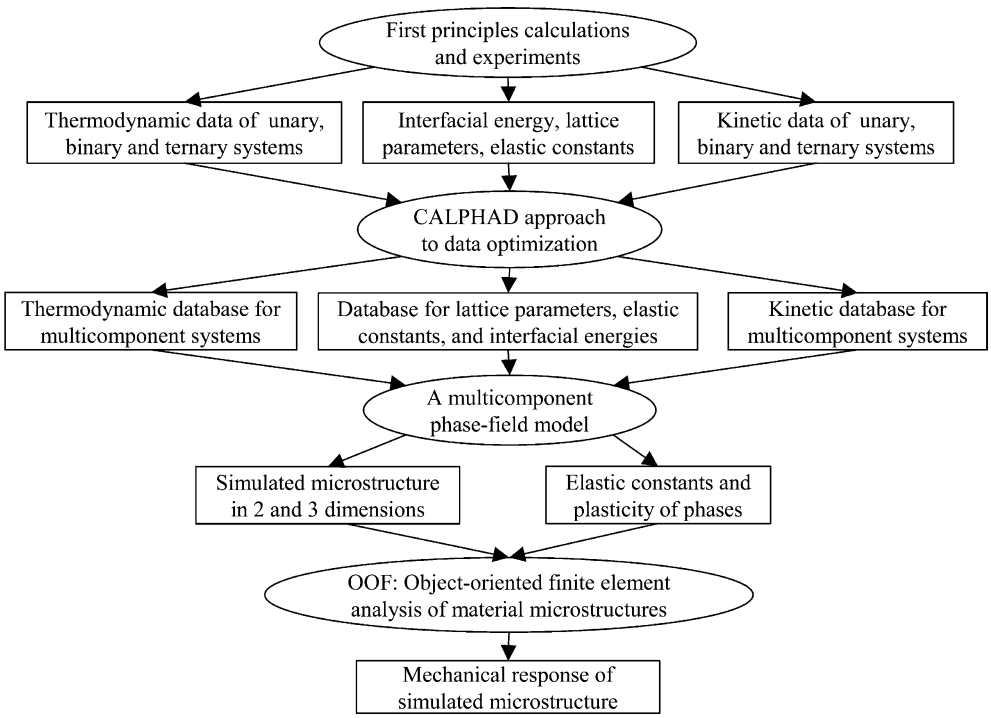

Figure 1. An integrated four-stage multiscale approach for multicomponent materials modeling, simulation and design.

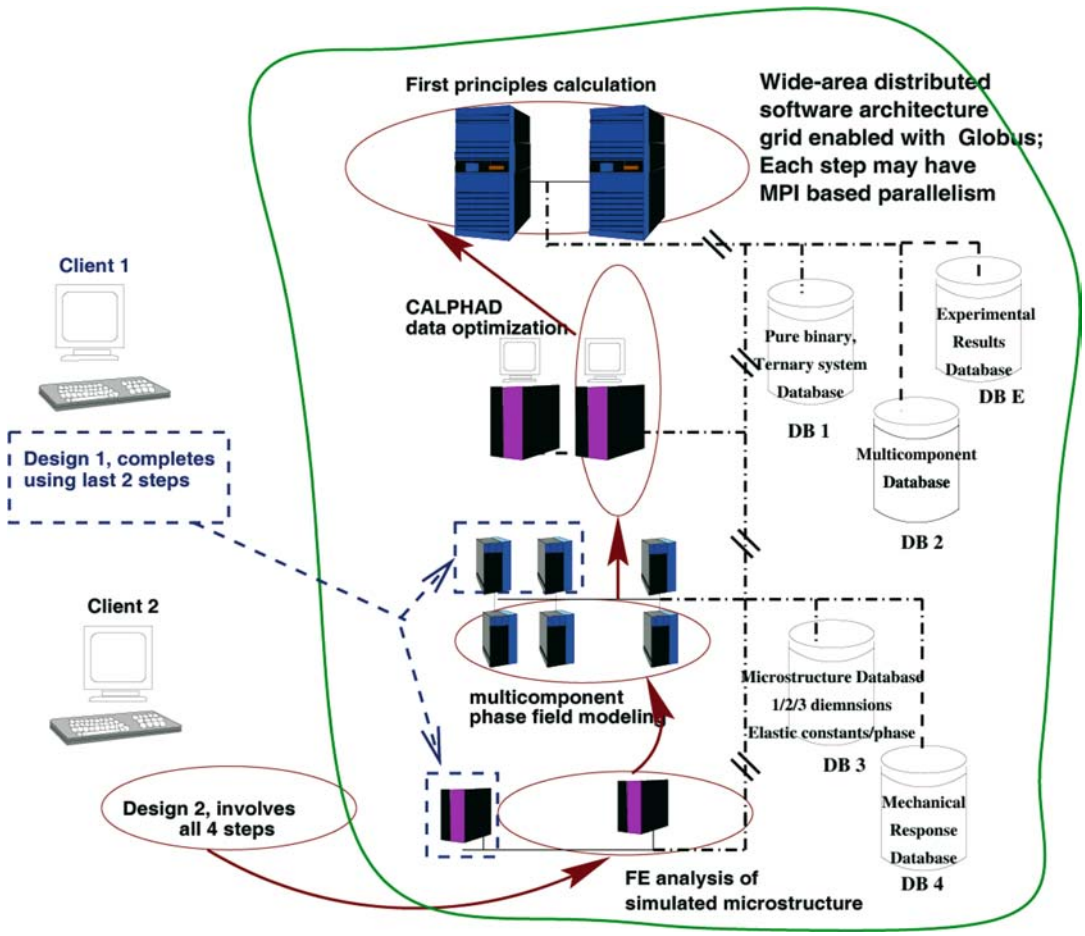

Figure 2. A schematic chart of software architecture for distributed materials design.

- A phase-field model for materials microstructure simulation in complex multicomponent systemts through advanced algorithms and parallel computing schemes;
- Object-oriented programming for finite element analysis of mechanical response of simulated microstructures;
- An asynchronous, distributed software architecture (and its implementation) for end-to-end materials simulation and design suitable for wide area distributed grid-computing.

2. Four-stage approaches to materials design

Materials design is an integration of materials science and system engineering design [4–6] through tools such as computational thermodynamics, kinetic simulations, property modeling, and prototype evaluation. From the engineering design point of view, hierarchically structured materials can be considered as a system consisting of three subsystems, i.e. performance/property, structure, and processing with functional requirements, design parameters and processing variables as the counterparts in the scheme of system design [7]. Understanding and predicting the complex behavior

of materials from the atomistic scale to the macroscopic scale in a multicomponent environment can be aided by advances in information and computational technology. Expanding computational power and the numerical implementation of materials science are the principal agents shifting the traditional balance between theory and empiricism. In the following, the numerical implementation of materials science in first-principles calculations, CALPHAD development of materials databases, mesoscale microstructure simulation and macroscopic materials behavior modeling are briefly presented.

First-principles calculations, based on density functional theory, require only knowledge of the atomic species and crystal structure, and hence are predictive in nature. The first-principles methods to be used here include the full-potential linearized augmented plane wave (FLAPW) method (the 'benchmark' for accuracy in density-functional-based methods), and the highly efficient Vienna *ab-initio* Simulation Package (VASP). These methods yield quantities related to the electronic structure and total energy of a given system, and can be used to accurately predict phase stabilities of compounds at 0 K. By combining first-principles techniques with statistical mechanics methods such as the cluster expansion/Monte Carlo approach [8, 9], one can explore, without any fitting parameters, thermodynamic phenomena such as phase transformation temperatures, phase diagrams, and short-range order. Coupling with frozen phonon or linear response techniques opens the possibility for exploring finite-temperature vibrational effects. Furthermore, these approaches are applicable to any phases of a given alloy system, not only the equilibrium ones. Hence, first-principles techniques can provide a method to obtain properties of metastable phases, which are often crucial to mechanical properties (e.g., strengthening precipitates) but can be difficult to isolate and study experimentally. In addition to thermodynamic properties, first-principles calculations can also provide lattice parameters and interfacial energies.

CALPHAD uses a wealth of thermodynamic information, some taken from first-principles calculations, to model multicomponent systems [10, 11]. In the CALPHAD approach, a large number of thermochemical and phase equilibrium data are used to extract parameters describing the alloy energetics, which are then used in calculations of thermodynamic properties, phase equilibria, phase diagrams, and phase transformations through the minimization of free energy and calculation of thermodynamic driving forces. The approach produces reliable phase diagrams and stability maps for complicated multicomponent commercial alloys. CALPHAD modeling begins with the evaluation of descriptions of unary and binary systems. By combining the constitutive binary systems and ternary experimental data, ternary interactions and Gibbs energy of ternary phases are obtained. Materials databases thus developed cover the whole composition and temperature ranges, including experimentally uninvestigated regions. In this approach, properties of individual phases are modeled, and the model parameters are collected in databases. The modeling of the Gibbs energy of individual phases and the coupling of phase diagram and thermochemistry are the keys to developing unambiguous thermodynamic descriptions of multi-component materials with sound fundamentals and predictive power because these two sets of data are deduced from the Gibbs energy of individual phases under given constraints. Similar approaches will be used to construct databases for diffusional mobility of species in

individual phases, lattice parameters, elastic constants and interfacial energies based on existing experimental data and first-principles calculations [2].

Phase-field models describe a microstructure by using a set of field variables [12, 13]. The most familiar example is the composition field that characterizes the compositional distribution in a microstructure. The composition fields completely specify the local composition of all the species in a microstructure, whereas the long-range order parameter field distinguishes the structural difference between precipitates and matrix. Within the phase-field description, the total free energy, including the elastic strain energy and interfacial energy, of a microstructure can be written in terms of field variables. The temporal evolution of these field variables is then described by time-dependent kinetic field equations – namely, the Cahn-Hilliard equations [14] for the composition fields and the time-dependent Allen-Cahn [15] (Ginzburg-Landau) equations for the long-range order parameter fields. The phase-field approach has been extensively applied to modeling microstructure evolution in a wide variety of important materials. One of the main advantages of the approach is that any arbitrary morphology can be described easily by choosing appropriate field variables. There is no *a priori* assumption on transient and non-equilibrium morphologies along an evolution path. Despite the remarkable success of phase-field simulations in providing fundamental understanding of the underlying thermodynamic and kinetic mechanisms leading to various morphological evolution, existing phase-field simulation results are largely qualitative. Integrating phase-field simulations with thermodynamic and kinetic databases is thus the key to *quantitatively* predicting microstructural evolutions during materials processing.

The ultimate goal of materials simulations is to predict the behavior of materials. Therefore, it is critical to link predicted microstructures to properties. One approach is to reduce the representation of a microstructure to a small number of physical parameters (such as grain size or porosity) and develop a mechanical property model that depends on them. However, when mechanical properties depend on microstructural details (such as the spatial correlation of crystallite orientation, the shapes and dispersion of second phases, extremes of statistical distributions, or local anisotropies) such data reduction is often difficult or pointless. In our project, the object-oriented finite element analysis of material properties based on the OOF program developed at NIST [16] is integrated with the simulated microstructure. The OOF program takes a non-reductionist, brute force approach, but in a user-friendly way. The user starts with a digitized microstructure and builds a data structure on top of it. All the data in the image plus any that can be inferred by the user is used. For OOF, the microstructure is a data structure composed of image and property data. In our case, the image data would be the output from a phase field calculation, and the property data would come from a first principles or CALPHAD calculation. The OOF package constructs a finite element mesh from the image data and allows the user to assign material properties and perform virtual experiments on the mesh. The first version of OOF handled only linear elasticity and thermal conductivity. The second version of OFF, OOF2, being developed in conjunction with this project, will be easily extendable to a wide range of linear and non-linear physics, including (for example) plasticity and piezoelectricity.

3. Towards a grid enabled system

Our software architecture seeks to utilize high performance parallel computing to reduce application turnaround time while providing a flexible client–server interface to the user. Clients can initiate particular designs and the server satisfies the design requirements by ultimately scheduling appropriate tasks on underlying computational resources. This basic client–server architecture is enhanced in several ways to allow the design of a web-portal, which can cater to concurrent exploration of the materials design space by potentially dozens of clients.

Several steps for our four step multicomponent materials design scheme are compute-intensive. Consequently, these steps should be executed on either high-performance 'shared memory' multiprocessors or local-memory multiprocessors that can execute codes using the 'single program multiple data' (SPMD) model. Such SPMD codes are currently being developed for phase-field simulations. Even though the computation in these steps is substantial, the results generated are sufficiently compact to make the linkage of successive steps through intermediate databases natural. In this model, each step could execute on disjoint sets of processors of suitable size. The coupling between steps should satisfy precedence requirements but it need not be direct nor synchronous. Processors for a given step proceed with the computation after asynchronously accessing the database updated by an earlier step.

The implementation of our software architecture would not be feasible without appropriate utilization of emerging infrastructure in the form of 'grid computing.' Grid tools are in the form of a software environment to which our server can be linked. The grid environment provides the functionality to set-up and execute tasks on hardware resources like SMPs (Shared memory multiprocessor) and NOWs (Network of Workstations). It also provides mechanisms for monitoring the status of tasks, signaling completion and providing access for multiple tasks to shared databases while maintaining data-integrity. These mechanisms will be used as a 'back-end' in our server to manage a pool of tasks that are the consequence of client requests for design space exploration.

In our client–server design, each client instance is associated with a request handler on the server side. The design of the request handler is quite complicated because there are several sets of requirements that must be satisfied to allow effective design space exploration.

The request handler should meet the requirements of the materials science community while allowing a portable and extensible system that can utilize a set of networked high-performance computing resources that are potentially geographically distributed, i.e., utilize a 'computational grid.' The design requirements come from three different sources. First, there is a clear need to interact with the user to set up simulation parameters and modify them as the computations proceed. Second, a design investigation will need coupling of tasks corresponding to one or more of the four main steps. The computational demands imposed by application codes for each of the four stages are varied. Furthermore, there can be multiple implementations of the same step with different costs and limitations and interface descriptions. Third, the current state-of-the art in the materials science community provides only a partial set of rules and heuristics for determining meaningful explorations of the multicomponent materials design space. These rules will clearly influence both the interaction with the user and the specifics of the tasks to be used for a given design instance.

We define our overall request handler in functional terms with a simple pattern of interaction and control flow between its main components. We view the system as providing three sets of services.

- The interaction service, which allows an initial problem specification and further interaction to define constraints, refine model, and present and evaluate results.
- The simulation service, which is responsible for remote execution of tasks, their interaction and data management.
- The analysis service, which converts the initial problem specification using rules and heuristics from the materials science community into an instance of the four-stage simulation process. It continues to control the design status and specifies the actions of the simulation and interaction handlers.

Each of these sets of services is executed by a corresponding component; we refer to these as interaction and simulation handlers, and the analyzer. The analyzer will interface with both the interaction and simulation handlers as shown in Figure 3. Our first goal is the development of a fully functional simulation handler with a grid-enabled 'back-end' using Globus-2.4 [17, 18] with somewhat rudimentary forms of the other two components. Our next goal is to develop a full-featured interaction handler

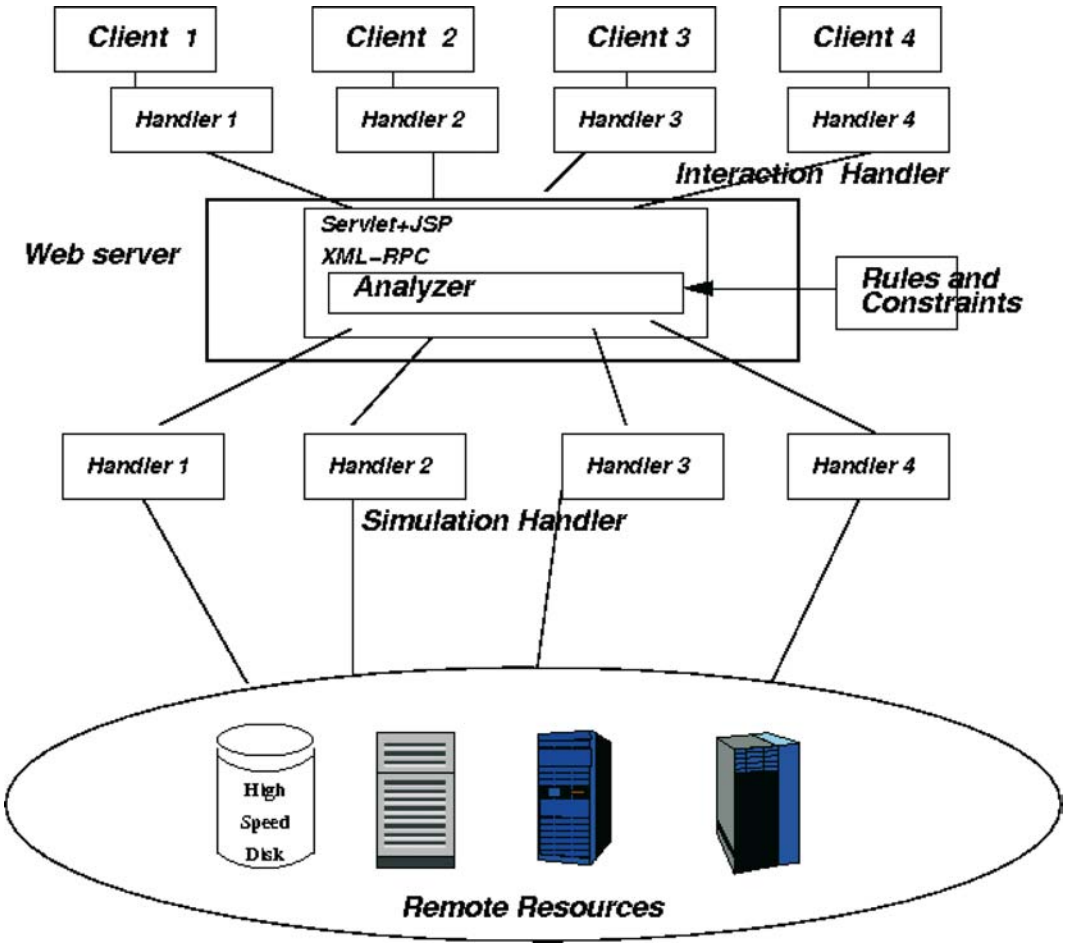

Figure 3. The three main functional components of our grid-enabled simulation server.

using JSP [19], Java servlet [20], DOM [21] enabled Java-XML parsing etc. XML allows the storage of information as a relational database with keywords and notations and hierarchies that can be extended to meet the requirements of our materials science application. The resulting artifact is an XML file containing the database. This database must be accessed and modified to enable simulations for the four steps and to incorporate the results of such simulations. Such access and modifications are possible only by executing a program through our software system. Such a program can be in one of several programming languages such as C++, Java etc. Java is used because programs in Java are particularly suitable for deployment through our web-based client-server system; such Java programs are at the core of our interaction service with the client to set up design requirements, report on intermediate calculations etc. We anticipate that the development of the analyzer will probably be the most challenging part as many of the rules for design space exploration need to be developed [22].

The Al–Cu system used in the present work provides useful feedback on the design of our software architecture. A benefit of our scheme is that licensing and usage issues related to the software for each of the four steps are no longer issues; the software runs on our systems and the clients (who are typically materials scientists at remote sites) have automated access to them through our interaction service. We found that Globus provides useful functionality to enable our simulation service component that schedules simulation tasks on hardware resources. It should be mentioned that even in the automation of the simple Al–Cu example, there are gaps in available parameters, scopes of simulation software etc. that must be resolved through interaction. The latter must be 'dynamic', i.e., get the client response, check the databases to verify/validate requirements, and report back to the client with any limitations, to iteratively obtain a full specification that can be translated into computations. The implementation of our software architecture involves several software packages in different languages, support for parallelism through message-passing, support for wide-area deployment and the managing of databases that can be updates by many different simulations. It is conceivable, that based on our experiences, we may be able to automate the generation of such systems for our application domain and related domains through a process of compilation, i.e., by developing a language for specifying the components of the system and then compiling it to produce an implementation of the system.

4. Advanced discretization and parallel algorithms

Efficient, reliable and scalable numerical algorithms that conduct simulations of the material properties are the backbone of our software infrastructure for multicomponent multiscale computational material design and simulation tools. Currently, algorithms development is underway on several fronts that range from CALPHAD computations of phase diagrams, scalable solvers for phase field simulation of microstructure evolutions, to the OOF programs for computing mechanical properties. The most notable progress, however, since the inception of our collaborative project, has been associated with the CALPHAD computation and the phase field simulations.

Computationally, the equilibrium analysis of a n-component system with K-phases leads to a nonlinear minimization problem with $K(n+2)$ non-negative unknowns

and $n+2$ equality constraints. For the ranges of n and K that are of interest to us, it is desirable to make minimization procedures more robust and to automatically determine the existence of any miscibility gaps. Combining a domain decomposition/subdivision and local quadratic fitting approach, we developed an approximation method that solves the minimization problem and conducts stability and co-planarity checks with a linear complexity in terms of the number of subdivisions. The new method works competitively in our preliminary testing, in comparison with the existing methods in ThermoCalc [23, 24] and Pandat [25, 26]. More complicated examples are now being worked out with an adaptive subdivision strategy [43].

In recent years, efficient and accurate numerical algorithms for the phase-field models based on spectral spatial discretization and semi-implicit in time schemes have been demonstrated to be orders of magnitude more efficient and accurate than the conventional difference method [13, 27]. Continuing in the spirits of the semi-implicit time discretization, we have studied high order exponential differencing schemes for the phase-field models, which have better stability and higher accuracy than the 1-st and 2-nd order semi-implicit methods and are compatible with the high spatial resolution offered by the spectral approximation. We also investigated the operator splitting and adaptive and variable time step techniques for improving the efficiency of time dependent approximations.

To accurately capture the microstructure evolution, phase-field models have incorporated many features such as the elastic effect on precipitate morphology in coherent systems with a significant elastic inhomogeneity. An efficient iterative algorithm developed by Hu and Chen [28] can provide accurate simulation results that are consistent with the perturbation method developed by Khachaturyan et al. [29]. Our recent analysis provided further insight as well as mathematical justifications to the performance of the algorithm. We found a method to eliminate a slowly convergent mode to improve the convergence speed of the iterative scheme. Another feature to be incorporated into the phase-field modeling is the adoption of an anisotropic mobility. It is both a modeling and a computational challenge to define the anisotropic mobility function on the whole simulation domain while the interfacial normal can only be meaningfully determined on the interface. We have recently proposed a variational approach to construct a smoothed mobility function that mimics the prescribed anisotropic mobility on the interface and extends smoothly to the whole simulation domain (see Figure 4). The smooth property allows one to take the full advantage of high-resolution features of the spatial spectral discretization.

Making the spectral codes spatially adaptive and introducing scalable solution strategies based on domain decompositions (of the physical domain, or the variable and frequency domains) into the computational tasks are some of the on-going algorithmic research which fits nicely with the software environment under development and the grid enabled computing platform.

5. Application to the prototype Al-Cu system

The present project uses aluminum-based alloys as model materials with a particular emphasis on the Al–Cu–Mg–Si quaternary system. In the Al–Cu–Mg–Si quaternary system, many of the metastable precipitate phases (e.g., GP zones in Al–Cu and Al–Mg–Si, θ' in Al–Cu, β' in Al–Mg–Si) are currently not included in any

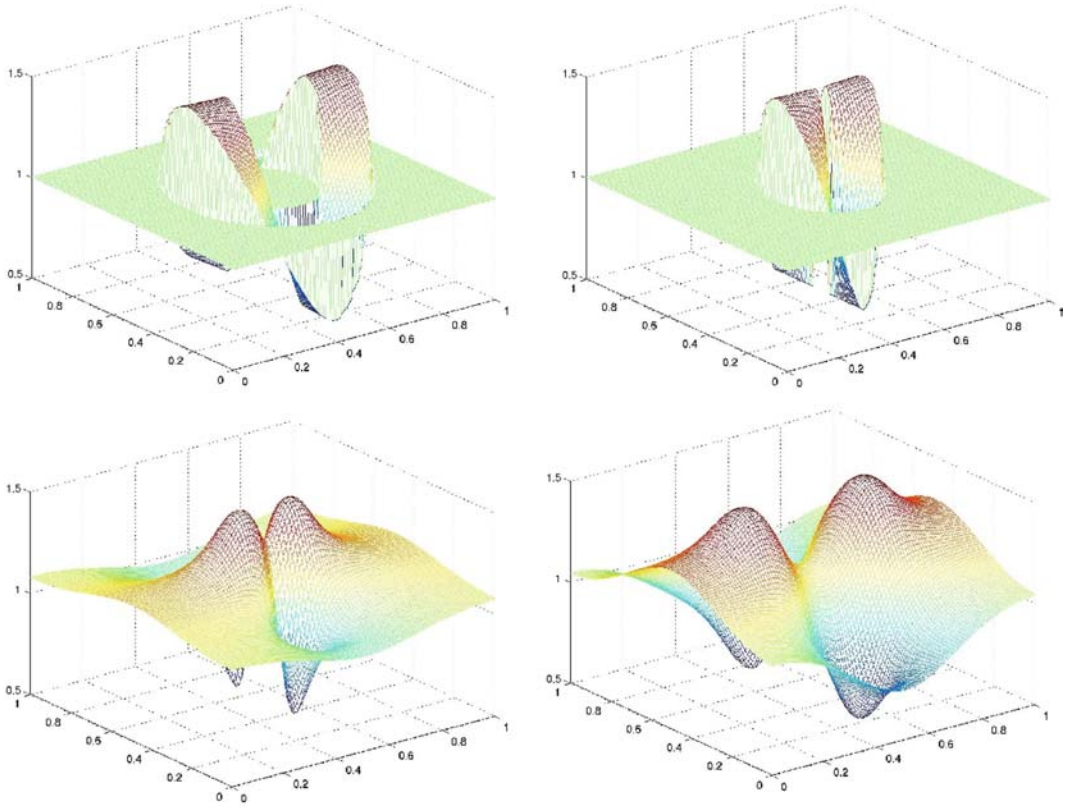

Figure 4. The cutoff mobility (top) vs. the smoothed mobility (bottom).

thermodynamic databases, due to the difficulty in obtaining the thermodynamic functions of these phases. Our initial effort has been on the Al–Cu binary system. The existing thermodynamic databases of the Al–Cu binary system do not include all known metastable and stable phases.

5.1. First-principles calculations of stable and metstable phases

First-principles calculations play a significant role in building thermodynamic databases for complex alloys. Figure 5 collects some of the recent calculation results compared with available data in the literature [30]. Initial promising efforts have even been made in incorporating first-principles-calculated free energies of θ' into CALPHAD databases resulting in a previously unsuspected change in the binary Al–Cu phase diagram [1].

In addition to the metastable GP and θ' phases, there is little thermodynamic information on stable compounds at intermediate compositions of the Al–Cu binary system. Therefore, we systematically carried out first-principles calculations to determine the enthalpies of formation of both stable and metastable phases. Furthermore, the vibrational entropy of θ' and θ were available in the literature [31], and an estimate for that of GP zones was calculated in the present work [C. Ravi et al., Personal Communication]. In addition to phases with stoichiometric compositions,

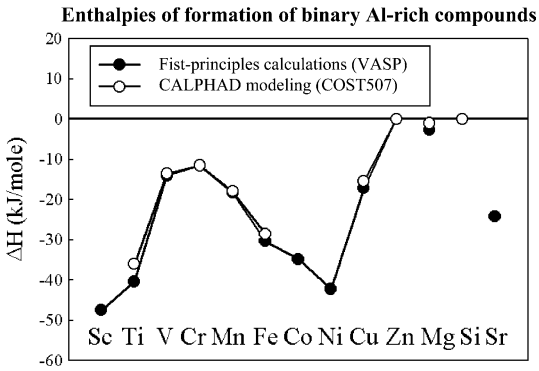

Figure 5. First-principles vs. COST507 for enthalpies of formation of ordered Al-rich intermetallics.

the enthalpy of mixing in fcc was calculated by Muller et al. [32] using the mixed space cluster expansion, and the enthalpy of mixing in bcc was calculated in the present work using both cluster expansion and Special Quasirandom Structure (SQS) approach [33, 34]. In addition to thermodynamic properties, first-principles calculations can also provide lattice parameters and interfacial energies. Figure 6 shows the two interfaces between the θ' plate and Al matrix, in which the interfacial energies can be obtained from VASP calculations [35, 36].

5.2. CALPHAD modeling of the Al-Cu system

The thermodynamic modeling of the Al–Cu system was previously carried out by Kaufman and Nesor [37], Murray [38, 39] and Saunders in the COST507 project [40]. Murray considered three stoichiometric compounds, improved Kaufman and Nesor's modeling of liquid, fcc, and bcc solution phases, and also discussed the extension to the GP zones, while Saunders studied the intermetallic compounds in

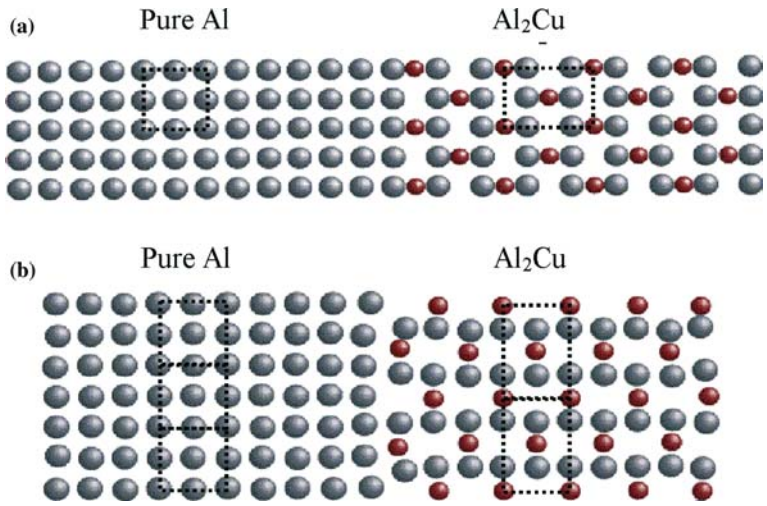

Figure 6. Relaxed supercells used to calculate $Al_2Cu(\theta\prime)$/Al interfacial energies for both the (a) coherent (100) and (b) "semi-coherent" (001) interfaces.

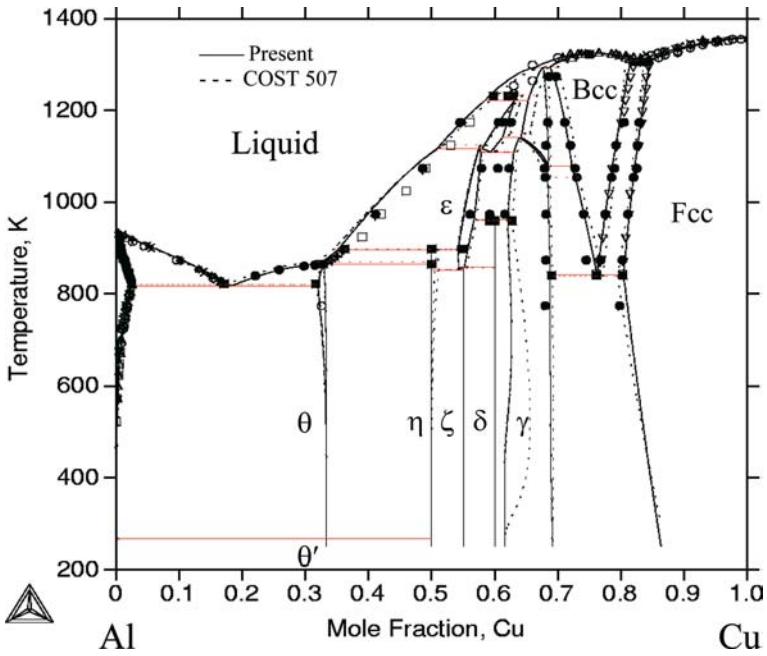

Figure 7. Calculated equilibrium phase diagram of the Al–Cu binary system.

more detail and modeled all stable phases in the system with homogeneity ranges for most intermetalic compounds. However, they did not include metastable phases in their modeling. The phase diagram calculated using the COST507 database is shown in Figure 7.

In the present work, thermodynamic modeling of the Al–Cu system was carried out including metastable GP and θ' phases and all known stable phases. The enthalpies of formation of all stable and metastable solid compounds were obtained from the first-principles calculations using VASP [35, 36]. The enthalpy of mixing in fcc was taken from the literature [32] and that of bcc was calculated using the Alloy-Theoretic Automated Toolkit (ATAT) [41]. A complete thermodynamic database of the Al–Cu binary system was obtained by integrating the first-principles calculations and vibrational entropies of GP, θ', and θ with experimental phase equilibrium and thermochemical data from the literature by means of the ThermoCalc package [24]. The calculated phase diagram is showed in Figure 7 in comparison with the phase diagram calculated from the COST507 database [40] and experimental phase boundary data. Both calculations represent the experimental phase boundaries well, but the present thermodynamic database has a better defined set of thermochemical data from first-principles calculations for both stable and metastable phases. The calculated solvus boundaries of GP, θ', and θ phases are shown in Figure 8.

5.3. Phase-field simulation of the θ' precipitate microstructure evolution

In this information technology project, we are developing a phase-field approach for predicting the growth and coarsening of various precipitates in Al alloys. Our preliminary work has been focused on the metastable θ' (Al_2Cu) phase in Al–Cu

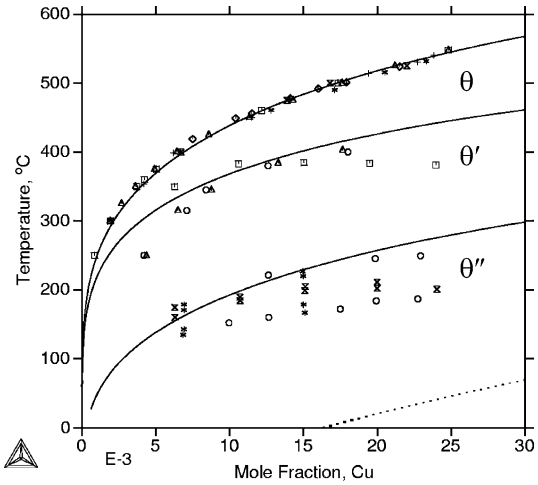

Figure 8. Calculated solvus of GP/θ'', θ' and θ phases in the fcc solution in comparison with experimental data in the literature.

alloys as θ' is one of the primary strengthening precipitates in Al–Cu alloys. Experimental results demonstrate that θ' precipitates have a tetragonal structure with an orientation relationship $(100)_{\theta'}//(100)_{\alpha}$ between the precipitate and matrix. θ' precipitates in the matrix tend to be disc/plate like. The broad face of the θ' precipitate is coherent and thus has low interface energy while the interface around the edge is semi-coherent and has high interface energy. The orientation relationship, where the *c*-axis of tetragonal structure (precipitate) aligns along the coordinate axes of the cubic structure (matrix) implies three possible orientation variants. Therefore, θ' precipitation is controlled by a number of factors such as anisotropic interface energy, anisotropic interface mobility, and elastic energy associated with the lattice mismatch between precipitates and matrix. Our recent work using phase-field simulations showed that both interfacial energy anisotropy and elastic interactions are important in determining the equilibrium morphology of θ' precipitates [3]. Figure 9 displays typical morphologies obtained from a two-dimensional phase-field simulation of θ' precipitation in an Al-Cu alloy with thermodynamic and kinetic parameters from databases [42]. Corresponding three-dimensional simulations are possible although the computation is much more intensive. The matrix + θ' two-phase microstructures from phase-field simulations can then be used in the OOF software for determining the mechanical properties.

5.4. Deformation of the fcc and θ' mixture

As an example of the application of OOF2 to the Al–Cu system, the matrix + θ' two-phase microstructure was obtained from the current phase-field simulation. The first step in using OOF2 is to assign material properties to the pixels in the image by the different sheds. Both the particles and the matrix have a cubic elastic modulus $C_{11} = 108\,\text{GPa}$, $C_{12} = 62\,\text{GPa}$, and $C_{44} = 28.3\,\text{GPa}$ with the crystal axes aligned with the edges of the image. The particles have a stress-free strain given by $\varepsilon_{11} = 0.0076$, $\varepsilon_{22} = -0.051$, and $\varepsilon_{33} = 0.0076$, where the crystalline direction is perpendicular

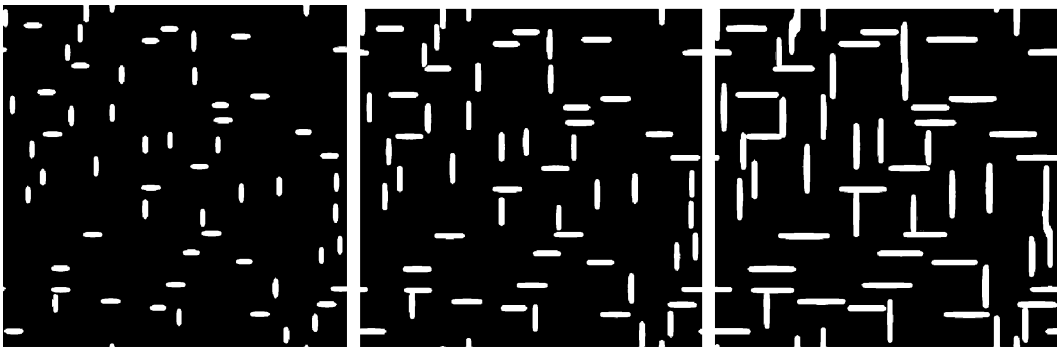

Figure 9. Evolution of θ' precipitates (white) obtained from a two-dimensional phase-field simulation with thermodynamic and kinetic parameters from their corresponding databases and interfacial energy from first-principles calculations [3]. Conditions: systems size – $1.028\mu m \times 1.028\mu m$, overall composition – Al-5 at%Cu, and temperature -500 K.

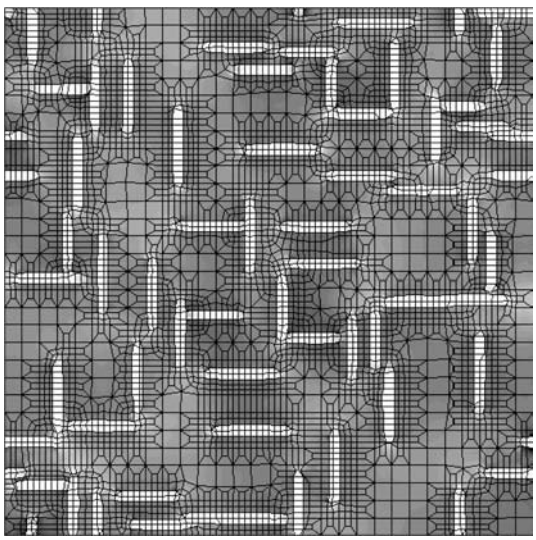

Figure 10. Trace of the elastic strain tensor of the matrix $+\theta'$ two-phase mixture with the bounds being -3 MPa (black) to 6 MPa (white).

to each particle's long axis. Finite element meshes shown in Figure 10 are adapted to match the interior material boundaries. Figure 10 also shows a result of the finite element calculation. In this case, the plot shows the trace of the stress generated by the stress-free strain of the particles, with zero-displacement boundary conditions.

6. Summary

In this paper, we present our strategy in building up the four-stage simulation approach, i.e. first-principles calculations, CALPHAD modeling, phase-field simulation, and finite element analysis, through databases. The concept of a grid-enabled system was introduced, and advanced discretization and parallel algorithms were

discussed. Initial results are shown, illustrating how the four simulation stages may be linked in an application to the prototype Al–Cu binary system.

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