1
Introduction

Georg J. Schmitz and Ulrich Prahl

1.1
Motivation

Integrated Computational Materials Engineering (ICME) – by its name and its nature – draws on the combination and the simultaneous or consecutive use of a variety of software and modeling tools. This simple phrase immediately raises a number of further questions:

How to combine tools?
How to select suitable tools?
How to decide on a specific tool?
And many more ....

Eventually, before answering these questions, some even more direct issues arise:

Which tools are available at all?
How to become aware about suitable tools?

Thus, there is obviously a need for something like the "yellow pages of software solutions for ICME" or a similar "one-stop shop" like institution. Such kind of yellow pages listing – even if being very comprehensive – would be quite boring to read (and also to write ...) and probably would even be outdated after a short time in view of new codes emerging and old codes being discontinued.

The ICMEg project partners [1] therefore decided to extend the scope of this book beyond the "yellow pages" and to include also a general introduction and overviews to the different fields, models, and software tools. The book content thus eventually evolved into an "overview" of overviews. All contributions are as generic as possible and references are mainly limited to "further reading" and refer to textbooks and tutorials for the different fields and review articles. The book also provides an "overview" of tutorials, reviews, and textbooks for the different fields.

Major scope, however, is to "name" phenomena, models, descriptors, and other terms and to arrange them in an overall context structure. Looking up the details

Handbook of Software Solutions for ICME, First Edition. Edited by Georg J. Schmitz and Ulrich Prahl.

Figure 1.1 A large variety of simulation tools is available around the globe. Not all codes in general have their own websites and logos. There is an even bigger number of particularly academic tools that are hidden and waiting to be exploited.

behind the different "names" is left to the reader and nowadays can often best be achieved by drawing on the Internet.

In summary, the ultimate motivation for the authors to write this book is that it could become a standard tutorial for future ICME engineers, which by nature of ICME need to have a holistic education, a general background, and a "bird's eye view" on things.

The motivation for this book is making the first steps toward providing a thematically structured directory of the huge and heterogeneous variety of state-of-the-art models (Figure 1.1). It is thus also particularly suited for young scientists and engineers seeking an overview of modern simulation tools in the area of Computational Materials Science and ICME.

1.2
What is ICME?

"Integrated computational materials engineering (ICME) as an emerging discipline aiming to integrate computational materials science tools into a holistic system will accelerate materials development, transform the engineering design optimization process, and unify design and manufacturing" [2].

Looking at the names, a definition of ICME has been attempted in a previous book [3] based on the analysis of the ingredients I, C, M, and E. An ambiguity has been identified with respect to the term “E” – engineering – which is applied to a product/component in Computational Engineering/Integrated Computational Engineering (CE/ICE) and to a specific material in Computational Materials/Computational Materials Engineering (CM/CME). This ambiguity can be resolved by putting the focus of ICME on:

> *Engineering the properties of a component as a function of the local properties of the material inside the component and along its entire production and service life cycle*

“I” in this context especially means integrating along the process chain (time, history), integrating across the scales (space, structures), integrating several models/tools, and integrating real and virtual worlds. “E” refers to engineering of technical alloy systems, engineering under industrial boundary conditions, and engineering of materials in components during manufacture and under operational load.

Technically, ICME is an approach for solving advanced engineering problems related to the design of new materials, processes, and products by combining individual materials and process models. Is ICME just a synonym for the coupling/linking of simulation tools by data exchange? From a systems point of view, the coupling of individual models and/or software codes across length scales and along material processing chains leads to highly complex metamodels.

ICME thus is more than just linking/coupling tools. The global optimum of a process chain might – and actually will – differ from a chain of individually optimized process steps (Figure 1.2).

ICME is also not only about exchange of some data between different simulation tools but further requires information contingency in view of subsequent processes downstream the value chain (Figure 1.3).

ICME currently is already known to combine, to address, and to exploit “processing–microstructure” relationships and “microstructure–property” relationships. An emerging area is the “microstructure–processing” relationship, which investigates how processing is affected by the initial microstructure or how the microstructure affects the robustness of a process – in other words, how the history of a component affects its response to processing and how it defines its properties for operation.

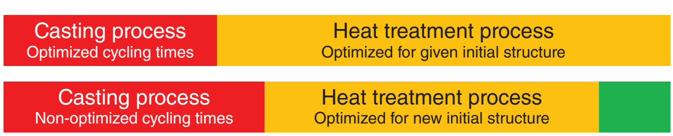

Figure 1.2 Example for a global optimum. Slightly suboptimal casting cycles with samples remaining at higher temperature for some more time may allow for shorter heat treatment times and thus result in an overall shorter production cycle.

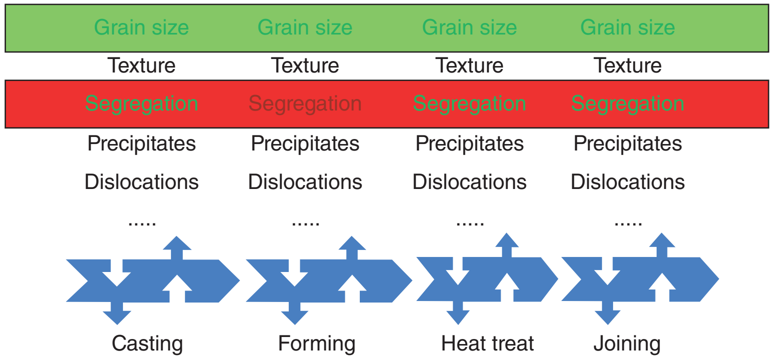

Figure 1.3 The importance of information contingency for the example of a process chain. While, for example, the grain size is simulated in all tools, the segregation of alloy elements is not modeled in the "forming" step. Segregation however becomes important again in subsequent processes.

In summary, ICME is an emerging discipline spanning various disciplines from materials technology, mechanical engineering, chemical and physical science, information technology, and numerical and mathematical science, for which a generic structural framework has to be elaborated, established, and maintained.

1.3 Industrial Needs for ICME

When discussing the industrial needs for ICME, two perspectives have to be differentiated. On the one hand, there are the commercial software providers trying to provide their software solutions to as many customers as possible. On the other hand, any industrial user of software tools is interested in exploiting software solutions to design new materials and production processes for components with tailored performance. The interests and needs of these two communities have to be discussed independently.

The interests of commercial software providers in ICME essentially relate to providing software solutions, to continuously developing new functionalities, to providing data along with their models, to making models faster and/or more robust, to making reliable/predictive models, and eventually to earning money by selling their software solutions and/or their simulation-based consulting competence.

Commercial software industry needs to identify, meet, and anticipate the needs of industrial users of their models and codes. This especially includes anticipating the potential needs not even yet being identified by these users themselves. The situation somehow corresponds to a fire brigade, which in general is not needed but anybody is happy to have it in case of a fire. The better the software provider meets the industrial user's needs for specific application tasks, the higher the user's motivation will be to further use (and thus to pay for …) the provider's software solution.

Even before any type of simulation was available, people were already able to construct airplanes. Nowadays – using simulations – they can do it faster, cheaper, better, and also with less ecologic impact. Currently, however, materials data entering respective finite element method (FEM) simulations are still often estimates based on similar materials, being isotropic and often revealing no temperature dependency. Large safety margins thus have still to be considered making the airplane heavier than needed. Better understanding and knowledge of materials and their processing will open pathways to new designs and even lighter airplanes.

From the application point of view, the industrial user of ICME is interested in solutions to his actual, real problems in ongoing production processes. He aims at optimizing current production sequences and the value of his products or at obtaining an improved understanding and control of materials and processes along the production chain. He aims at improving his products and processes in terms of cost and time and to increase the planning quality toward predictability of process chains to decrease waste and recycling material. Additionally he will develop new materials, new processes, and new products and will exploit emerging new options and applications. Eventually, simulation shall support a faster time to market of new material and process solutions by minimizing risks. This especially holds for "first-time-right" products where a classical trial-and-error approach bears unacceptable financial risks. Additional benefit of ICME can be generated for industrial users by using simulation results originating from their suppliers to improve their own processes or by providing a simulation history as an added value of products to their customers.

Industrial users of ICME are interested in designing their product as efficient as possible. ICME will be applied to reduce the design effort for new products/processes/materials in terms of costs and time. A specific requirement during modern simulation tasks within industrial design process concerns the configurable combination of different tools from different providers instead of monolithic solutions. A "plug-and-play"-type combination of tools in workflows and open simulation platforms is the key vision of future ICME. A future standardized data exchange will drastically decrease the efforts of software providers with respect to providing and maintaining a large number of import and export functionalities for their tools.

Though the benefits of using advanced material simulations are widely accepted, the application of the ICME approach within industrial settings still is a challenge in terms of complexity, capacity, and specific knowledge needed. Analyzing the needs of industry for ICME the following general conclusions can be drawn:

Conclusion 1

Cheap, fast, readily available, and reliable solutions are needed to tackle complex topics of technical interest.

Future markets will not relate to *products* and their *properties* but rather to *functionalities* and *performance*. An airplane manufacturer – or the airline as its final customer – is not really interested in the turbine but in procuring and having "a propulsion *functionality*" performing best for an estimated operational scenario. Best *performance* could, for example, be a long operational period with a minimum of interrupts in operation or a low price with a minimum of operational costs (fuel), meeting environmental constraints and laws and many other conditions.

Topics and materials of interest are exemplarily depicted for processing and properties of bulk materials/components essentially being made from metallic alloys. Typical customers for metallic alloys are the aerospace industry (superalloys, light materials), the steel industry (steel), power utilities and respective industry (superalloys, steels, etc.), automotive industry (steels, Al alloys, and Mg alloys), electronics industry (solders, semiconductors, solar silicon), biomedical devices (Ti alloys), and other industrial branches. The alloys of interest, in general, comprise a large number of alloy elements each of them purposely added in a well-defined amount to fulfill a specific functionality (Figure 1.4). The specification of the exact amounts of alloy elements by now is a long-lasting and expensive – in terms of both time and money – task. The development and qualification of new materials and their processing in the past took years to decades. These development cycles will be drastically shortened by future ICME-type approaches.

In other areas, the relevance of treating numerous chemical elements results from the small size of components being at the scale of the diffusion length such as in electronic solder configuration, where the composition of the solder joint is determined by both the solder composition comprising, for example, some melting point depressants, and the coatings on the components to be joined (Figure 1.5):

Conclusion 2

Models and tools are needed for complex multicomponent and multiphase materials and their processing.

Fe	C	Mn	Si	P	Cr	Ni
Bulk material, defines temperature stability range	Workability, hardness, wear	Binds sulphur, hardness, cold workability, machinability	Electromagnetic properties, surface properties, hardness, and so on	Hardness, hot workability	Corrosion resistance, wear/heat resistance	Toughness, formability, thermal expansion matching
Bulk	0.003–2.1%	0.02–27%	0.01–6%	0.01–0.6%	0.01–13%	0.01–12%

Figure 1.4 The technical metallic alloy steel consists of numerous alloying elements with very different amounts and specific contribution to the overall performance and processing of the material.

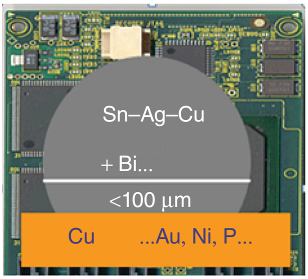

Figure 1.5 Steadily increasing miniaturization requires consideration of the effects of boundaries dissolving their chemical elements, for example, into a solder ball. A ternary Sn–Ag–Cu solder ball thus rapidly turns into a complex multicomponent, multiphase alloy system.

Advanced technical materials are not only a composition of various ingredients (alloy composition) but also consist of various phases of different crystallographic nature and/or local chemical composition. In steels and also in aluminum alloys, hard and brittle precipitates and inclusions are embedded in a more ductile matrix controlling the dislocation mobility. For example, steel may consist of two or more crystalline phases (e.g., ferrite, martensite, and austenite in parallel) being present in specific size, shape, and orientation. Recent developments aim at decreasing the structural length of single components (nanosized microstructures) and at exploiting metastable phases revealing complex deformation mechanisms during loading (e.g., transformation-induced phase transformation or inhomogeneous dislocation gliding) (Figure 1.6).

The costs of components are determined by the raw material, the production costs, and the costs arising during service life including repair and recycling. It is not only about the alloy composition. The *processing history* plays a decisive role in achieving the desired properties. During production, the material undergoes various process steps like casting and solidification, hot or cold forming, annealing, machining, joining, and coating. Each process during the entire production

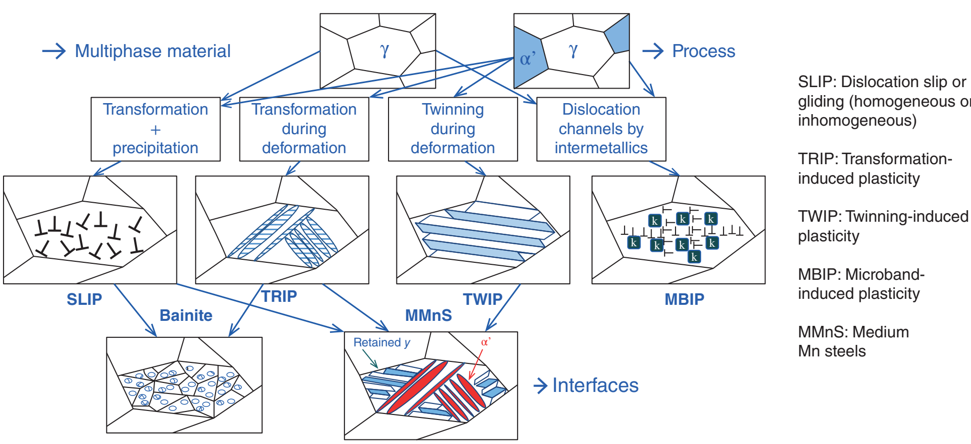

Figure 1.6 Modern steel development aims at tailored properties by adjusting a multiphase microstructure by applying deformation mechanisms based on metastable phases and by decreasing the structural length scale of microstructural components.

chain affects the microstructure and thus the properties of the material. Also, the process itself is affected by the properties being controlled by the microstructure. Thus, there is a strong dependence between processing and properties during the production and also during the final operation of the component. It should be mentioned that the macroscopic properties of the component in general are determined by mechanisms occurring at the length scale of nanometers or even below.

Damascus steel can be considered as a thousand-year-old nanomaterial although nobody really knew about "nano" at that time. Knowledge about the process parameters for the repeated and well-defined application of numerous individual forming and heat-treatment steps eventually leading to the superior properties of Damascus steel took generations to evolve on the basis of trial-and-error approaches.

Conclusion 3

Models are needed to track the evolution of materials and components along their entire production and service life cycle.

Modern simulation techniques will drastically shorten the development times for new materials and their processing. Respective developments will become much more targeted. However, the vision of "materials design out of the computer" by now is still only in reach for few examples. Nevertheless, it is widely accepted that simulating processes and materials evolution during processes significantly supports the design process. Some modern materials and components can only be produced using quantitative simulations of their microstructure, their processing, and their performance.

Eventually, simulation results have to be validated against measurements, existing data, and real – sometimes even financial – arguments increasing the confidence into the model, in its predictive capabilities and in its commercial value. Such validation can be based on data provided and shared by companies and academia alike. This validation includes information about the quality of calculated results including the uncertainty to be expected due to the use of nonexact input parameters and also due to the limits of the models. In particular, any user has to be aware of such uncertainties and limitations if he is applying models for situations or questions that are not within the – hopefully well-defined – input parameter space.

Conclusion 4

Validation is needed requiring improved interaction between virtual and real worlds.

Validation does not only include proving that models are able to predict materials properties correctly in a quantitative manner. The modeling-based design approach itself has to be validated respectively has to be evaluated against a traditional design approach based on trial and error combined with tailored experiments. Thus, it is mandatory to know the quantitative predictability of models and to balance the benefit against the simulation costs. Only if modeling costs and efforts can be turned into an added value, for example, by improved production results, industry will continue to invest into simulations. To decrease simulation costs, it will be necessary to integrate all modeling components into a single work flow in a way that all tools are independent, but mutually connected.

This financial validation is a major industrial requirement. All industrial applications of ICME will focus on the delivery of the outcome. The following four key questions have to be discussed: (i) What is the outcome and the contribution of simulated results to the design or optimization process? (ii) How much does a specific tool and its application cost? (iii) How much does a specific calculation cost? (iv) What is the risk associated with feeding the virtual simulation results into real production?

Quantifying the "risk" becomes a priority, especially for SME use. A desirable output would be a predictive tool running hypothetical scenarios, which include both the technical and the market inputs into a holistic decision-making process by optimizing component performance and cost efficiency in parallel.

Conclusion 5

Multicriteria optimization of the workflow is needed to balance all business.

Improving the knowledge about processes and materials is not the final aim of an industrial ICME user. Eventually, simulations shall support the industrial user in making his business decisions and in optimizing his products. Simulations are an investment for a company in terms of software tools, IT infrastructure, and a highly skilled work force.

In terms of business decisions, the optimal solution from a technical point of view may not be the most effective solution from an economic point of view. The same holds for simulations during the design process. The perfect, quantitative, and predictive simulation approach is not always needed. Often simpler approaches offering a sufficient depth of understanding in a shorter response time are more appropriate to meet a specific design objective. This implies the need for nonmonolithic software solutions and for an effective adaptation of various software tools into a single simulation workflow. Different types of software solutions have to be available to tackle the same topic with different degrees of accuracy. These may reach from fast solutions providing quick estimates for decision making up to highly precise approaches requiring substantial simulation times for complex trouble shooting.

1.4
Present ICME

A major target of ICME is a holistic simulation approach comprising entire process chains for engineering components. ICME addresses not only the macroscopic component and the process scale, but also the local material properties of individual components on the microscopic scale. ICME not only encompasses

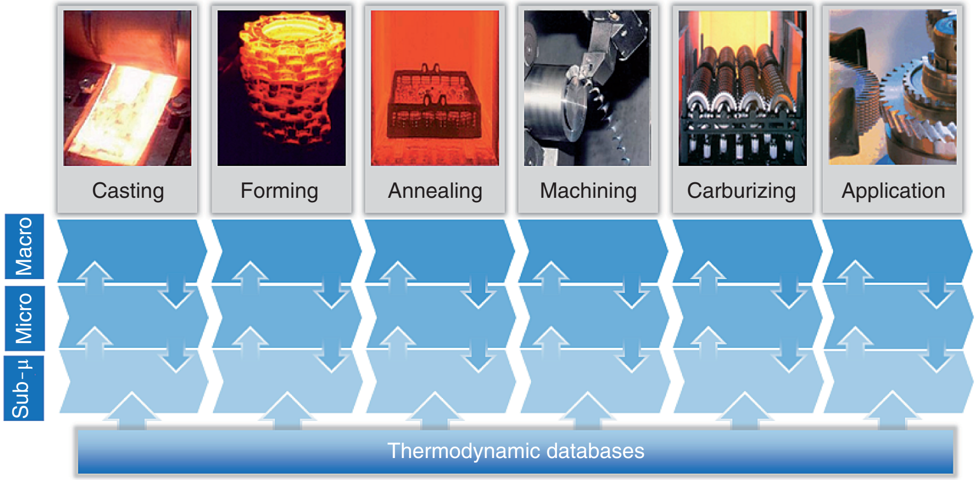

Figure 1.7 ICME aims to combine multiscale and through-process simulation toward a thorough description of all mechanisms being relevant for the production and performance of technical materials.

the material state for a given time at various length scales, but it also integrates the evolution of local material properties along the entire manufacturing process and eventually during service life (Figure 1.7). This concept promises better predictions and control of performance and service time of individual components or component assemblies. In this context, material microstructures and their evolution represent central issues in ICME as the microstructure is the carrier of the material properties.

Currently, numerous software solutions have reached a level allowing for valuable contributions to modern engineering tasks within knowledge-driven production models.

Simulations on the macroscopic scale of the manufacturing processes already are widely accepted and successfully used in industry on a Technology Readiness Level (TRL, according to the European Commission definition) of 8–9. Microstructure evolution codes and even more detailed electronic, atomistic, and mesoscopic models by now have reached a TRL of approximately 4–5 or even less. Respective approaches thus essentially are used in very specialized laboratories. However, the benefits of respective simulation tools and especially the needs for their mutual coupling and linking are widely accepted. The need for describing and simulating materials in more detail and at higher resolution is clearly formulated from an industrial perspective.

A major gap has especially been identified between continuum mesoscale models and world of discrete models (electronic/atomistic/mesoscopic). The usability, compatibility, and interoperability between these two model worlds have been formulated to be one of the major challenges for future ICME.

In spite of ICME currently emerging as a new and powerful discipline, coupling of different software tools is, however, still in its infancy and represents an issue consuming significant effort in terms of time and workforce if a coupling is realized at all. The combination of models by now is mainly achieved by manual transformation of the output of a simulation to form the input to a subsequent one. This subsequent simulation is either performed at a different length scale or constitutes a subsequent step along the process chain. Concerning the return of investment, the industry still complains on the significant amount of engineering efforts spent in data conversion and result management at the interfaces between different heterogeneous software tools. And indeed, there are several serious hindering factors: the missing of general standards for data format and platforms (in particular, the user friendliness of lower scale models is limited in most cases), the limited simulation knowledge at user side, expensive IT capacities, and no license schemes for short term but challenging calculation projects have to be mentioned.

1.5 Scope of this Book

The book covers essentially process chain for metals and alloys and to some extent also plastics, composites, and bulk components for structural applications (including coatings). These specific process chains could be composed based on the experience of the contributing authors. The developed concepts and descriptions, however, are all meant to be generic and may in future be extended to other fields actually not yet being covered, for example, pharmaceuticals, smart or functional materials, electronic or optical materials, textiles, and human tissue.

The book does not address (at least not explicitly):

- Hardware requirements
- Processing of nanoparticles, powder, molecules, and so on
- Subsystems of ICME like ICE not comprising materials as a central ingredient
- ICME politics

Scopes of this book are to:

1) *Serve as a tutorial for ICME engineers and scientists*
   Currently, there are only few educational schemes of “ICME engineers and scientists”. ICME by now, in general, is performed by “self-learning” by people who recognized the importance of combining models and tools to achieve better performance of their materials, processes/products, and software tools. There is a need to at least basically acquaint engineers and scientists in a specific field with the basic concepts, problems, and solutions of all other field downstream or upstream the production chain. This handbook shall allow skilled engineers and scientists to get such an overview of adjacent fields. It shall create awareness about the possibilities and the needs/requirements of the other fields and possible limitations.

This overview shall further encompass the phenomena, models, and tools across all length scales relevant for the production process and for the properties of the materials and eventually the final product.

2) *Provide an introduction to different processes along the production chain including the lifetime of components*
   For each of the process steps along the value chain like casting, forming, heat treatment, coating, joining, machining, corrosion, and recycling, an introduction is given even substructuring the particular field (e.g., casting: continuous casting, die casting, investment casting, etc.) and highlighting the relevant phenomena for each of these process steps. For each of these fields, current trends and actual developments are also shortly highlighted.
3) *Provide a general overview about concepts, methods, models, and tools across all scales*
   The book addresses different concepts and methodologies like numerical methods, pre- and postprocessing of simulation results, thermodynamics, electronics, atomistics, mesoscopic, and discrete models as well as continuum models for both microstructure and processing scales.
4) *Provide references for further reading*
   For each field, a number of references like review articles are provided for further reading, which themselves may be considered as "standard handbooks" or tutorials, reviews, or key publications for the field.
5) *Provide a structured directory of some prominent software tools in the different fields*
   This book provides a directory of globally available software tools in the area of ICME. However, it does not simply draw on an alphabetic list-type directory. In contrast, it provides a structured compilation of these tools. The structure in this context is provided by the processes along the value chain during the production of a component.
6) *Discuss the origin of different data, initial conditions, and boundary conditions necessary to run the tools*
   This discussion allows the identification of possible interactions between different models, for example, by providing data by one model for another model at the same or at a different scale. A similar strategy is applied for data on initial and boundary conditions. Further needs for new models to create required data may emerge from this discussion. Another topic under this discussion is the harmonization of information exchange between real and virtual worlds.
7) *Discuss current concepts to combine simulation tools in platform-type approaches*
   The identified simulation tools are further discussed with respect to their integration into simulation platforms and ICME types of operation. This discussion especially focuses on interfaces and data formats being provided for import/export of information and also covers aspects of workflow management.

8) *Identify missing tools and functionalities and formulate suggestion for further development*
   In view of covering an entire life cycle of a component by simulations, also "missing tools" and "missing functionalities" are identified and suggestions for their development are outlined.

1.6 Structure of the Book

The structure of this book is "top-down" instead of "bottom-up" and thus follows the philosophy of "starting from the outcome." This outcome may be a certain consumer-desirable property of a specific product or of a specific component. Based on the respective requirements the physical, processing, and additional requirements allowing meeting the objective and tools for their simulation can be identified. Based on the identified requirements at each length scale, models at smaller scales eventually are either needed or allow for refining "down to the atoms" wherever this seems necessary or beneficial. This strategy is based on the conclusion that processing and properties cannot be treated independently but are strongly correlated. Materials cannot be tailored without considering their processing, and processes can only be optimized if materials behavior during processing is well understood in a quantitative manner.

A future strategy in ICME may be to investigate and consider only those scales contributing relevant information for understanding the given problem – a strategy of scale hopping instead of multiscale modeling. Even at a specific length scale, a fast and robust model providing estimates might be given preference over a sophisticated and very detailed model. This choice eventually will depend on the risks associated with the given task and the time and capacity being available to tackle it.

This chapter provides an introduction to the field and the motivation for future readers. Following an overview on "Integrated Computational Materials Engineering (ICME)," the potential benefits to industrial users are shortly highlighted. A section on industrial needs for ICME is followed by a short review of the current status on ICME. The introduction concludes with an outline of the book.

Chapter 2 details the variety of processes, simulations, models, tools, and phenomena occurring at the scale of component and being relevant to its production and its use. Following a short overview over a typical process chain, this chapter starts from primary shaping processes, for example, by solidification of a melt and then follows the entire manufacturing cycle, comprising the fundamental processes of forming, heat treatment, joining, coating, and machining. Eventually, this chapter also addresses the service life cycle in terms of corrosion, fatigue, and recycling.

Understanding of component behavior during processing or operation often requires understanding the microstructures of the materials building up the component. The evolution of microstructures is not only affected by the process conditions but by phenomena at all length scales.

Chapter 3 summarizes different models and tools to describe the evolution of microstructures. Following an overview and a specification of the term microstructure, a categorization is provided to describe microstructures at different levels of detail. Subsequent to the identification of the major phenomena affecting microstructure evolution, an overview of the different modeling approaches is provided. A section on nucleation modeling is followed by sections on models/methods describing diffusion/reaction processes and precipitation phenomena. Models and methods for the description of the spatiotemporal evolution of microstructures based on cell, lattice, or field representations are outlined. These include cellular automata and Potts Hamiltonian lattice models solved by Monte Carlo methods, as well as phase-field and multiphase-field models, phase-field crystal models, and crystal plasticity models. The chapter concludes with a structured list of software tools, specifically comprising tools for the analysis of 3D digital experimental microstructures.

Major requirements for any type of microstructure simulation are thermodynamic data and kinetic data as well as other parameters/properties of the phases present in the microstructure. Also the properties of the interfaces play a significant role. Respective data can be obtained from thermodynamic/kinetic databases and calculations as depicted in Chapter 4 or from electronic/atomistic/mesoscopic models as described in Chapter 5.

Chapter 4 provides an overview and an introduction to thermodynamics and thermodynamic modeling. Following a discussion on the role of thermodynamic modeling in ICME, the CALPHAD approach is explained. Based on its history and the minimization of the Gibbs energy as theoretical basis, the crystallography and models of phases, the development of CALPHAD databases, their formats, and future extensions are highlighted. The chapter concludes with sections on "use of thermodynamics at larger scales" and on "deriving thermodynamics/materials properties from small scale models." This section addresses the future of determination of effective properties in ICME where first principles' DFT methods are used to predict, for example, thermoelastic properties of materials.

Chapter 5 focuses on mesoscopic, atomistic, and electronic models following the overall "top-down" structure of the book. Following an overview on discrete and semidiscrete mesoscopic models in materials science, the specification of some definitions and an introduction to atomistic simulations like kinetic Monte Carlo and molecular dynamics is provided. A section on electronic structure methods addresses Hartree–Fock theory and post-Hartree–Fock methods and density functional theory (DFT) in its different approximations (local density approximation, "LDA," generalized gradient approach, GGA). Further sections address actual developments like meta-GGA methods, hybrid DFT–Hartree–Fock approaches, and van der Waals-corrected DFT. In addition to providing a structured overview of approximately 80 different simulation tools in the area of electronic, atomistic, and mesoscopic simulations, the chapter further provides a number of links to online sources for potentials, force fields, and effective cluster interactions.

Chapter 6 goes back to larger scales and is devoted to the determination of effective properties and provides an overview of different approaches like finite-element-based homogenization methods, mean-field homogenization methods, and virtual testing approaches. Finite-element-based homogenization methods apply the method of homogenization on the continuum description of the microstructure of the material – resulting, for example, from phase-field models – being discretized into a finite element description. Details of this approach such as sensitivity of the obtained properties to the underlying microstructure and to numerical influences, for example, size of representative volume elements (RVEs), mesh density, and element type are highlighted and discussed on the basis of examples. Mean-field homogenization methods are explained based on example(s) for fiber-reinforced materials and address especially nonlinear and evolving material properties. A section on screening and virtual testing of material properties highlights the potential of usage of computationally derived effective properties to obtain tailor-made materials from the virtual stage and is presented for an application to a polycrystalline material and cover the subsequent usage for different microstructures.

Chapter 7 deals with numerical methods for the computational simulation of a wide range of multiphysics and multiscale problems within an ICME framework. Following an overview on preprocess and space discretization methods, a large section provides an overview of different kinematic descriptions, solution methods for coupled problems, and numerical methods for the solution of a wide variety of engineering problems such as the finite difference method (FDM), FEM, boundary element method (BEM), discrete element method (DEM), mesh-free methods (MFMs), particle finite element method (PFEM), extended finite element method (XFEM), isogeometric analysis (IGA) method, and model order reduction (MOR) methods. This overview is followed by a description of numerical methods for contact problems, such as Lagrange multipliers, penalty and augmented Lagrangian, direct elimination, mortar, and IGA methods. Further sections address postprocessing and visualization methods, and numerical methods for mapping and data transfer in the FEM simulation of multiphysics/multiscale problems using either Lagrangian or arbitrary Lagrangian–Eulerian (ALE) formalisms. Data transfer algorithms are discussed for the numerical simulation of a single process using Lagrangian or ALE formalisms and requiring remeshing operations. Sections on reduced-order models and on different issues related to high-performance computing (HPC) and parallelization precede a list of software tools for pre- and postprocessing.

Chapter 8 addresses "software platforms" and "software integration," which in industry currently essentially correspond to integrating continuum models. Respective developments are dominated by structural mechanics or computational fluid dynamics tools based on finite elements or finite volume numerical schemes as part of product life management or computer-aided engineering (PLM/CAE) environments. However, advances in nanotechnology require descriptions of processes occurring on the smaller scales, which can be provided by electronic, atomistic, and mesoscopic models and continuum models applied to the mesoscale. This demand requires extending the tools and approaches of ICME to include tools on the smaller scales as well and to make this variety of tools "interoperable." Following an overview of different integration approaches (object-oriented, component-based, service-oriented, data-centric, model-based, and ontology-based approaches), existing standards for integration and different available approaches to coupling and linking are briefly highlighted.

Chapter 9 discusses the needs for future developments required toward the objective of covering an entire life cycle of a component by simulations. In view of covering an entire life cycle of a component by simulations, also "missing tools" and "missing functionalities" and needs for interoperability are identified and some suggestions for future developments into these directions are outlined.

This book eventually provides a *directory of globally available software tools* in the area of ICME. However, it does not simply draw on an alphabetic list-type directory. In contrast, it provides a structured compilation of relevant models and tools. The structure in this context is provided by the processes along the value chain during the production of a component from a given material as depicted in the individual chapters. Almost all chapters identify the most relevant simulation tools and discuss them with respect to their underlying models, the origin of the required data, the necessary initial and boundary conditions, and eventually with respect to their integration into simulation platforms and ICME types of interoperation. A structured table of software solutions for each field marks the end of each chapter.

These tables are based on and compiled from a survey of modeling tools in a number of resources:

- Precompiled lists of software codes, for example, the TMS [4], or a recent Japanese activity [5]
- A list of software tools being used in research project funded by the European Commission with a focus on electronic/atomistic/mesoscopic models [6]
- Software repositories such as GitHub [7], nanoHub [8], or SourceForge [9]
- Software identified during the 1st International Workshop on Software Solutions for ICME
- Software companies in different fields being compiled on the basis of personal acquaintance and by Internet search
- A private homepage [10] providing a survey of public domain and commercial mesh generators
- The NIST Materials Data Digital Library [11]
- Two TMS studies on ICME [12, 13].

The resulting list – eventually comprising approximately 350 different software tools – was then further complemented by the knowledge of the authors of the individual chapters. Each of the almost 70 authors from at least 12 countries in 3 continents is a renowned scientist or engineer in his/her field making their comments on the different tools a highly valuable piece of information and advice.

The focus of the book definitely is on structural mechanics applications. In other areas, for example, electronic design automation, the Technology CAD (Technology computer-aided design or TCAD) is an ICME-type approach of modeling semiconductor fabrication and semiconductor device operation. The modeling of the fabrication is termed Process TCAD, while the modeling of the device operation is termed Device TCAD. The software tools available in this field are widely documented in [14]. Some thematic overlap between structural and electronic materials processing already occurs in the domains of crystal growth and thin-film deposition.

In the end, the book has actually become what it was originally intended to be: "the yellow pages for software solutions for ICME." But the book has evolved even further into something the editors and authors would like it to become: "a tutorial for young students in the emerging field of ICME" and a handbook for scientists and engineer wanting to get a quick but sound impression on adjacent fields of expertise.

References

1. ICMEg (2013) Integrated Computational Materials Engineering expert group – a Coordination and Support action of the European Commission, www.icmeg.eu (accessed 25 April 2016).
2. National Research Council (2008) *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*, National Academic Press, Washington, DC. ISBN: 0-309-12000-4
3. Schmitz, G.J. and Prahl, U. (eds) (2012) *Integrative Computational Materials Engineering – Concepts and Applications of a Modular Simulation Platform*, Wiley-VCH Verlag GmbH, Weinheim. ISBN: 978-3-527-33081-2
4. TMS http://www.tms.org/cyberportal/showData.aspx?tooltype=properties#grid (accessed 25 April 2016).
5. MateriApps http://ma.cms-initiative.jp/en (accessed 25 April 2016)
6. European Commission Review of Materials Modelling being Performed in European Projects, http://ec.europa.eu/research/industrial_technologies/e-library.cfm (accessed 25 April 2016).
7. GitHub, Inc. https://github.com/ (accessed 25 April 2016).
8. NanoHUB https://nanohub.org/resources/tools (accessed 25 April 2016).
9. Sourceforge http://sourceforge.net/ (accessed 25 April 2016).
10. www.robertschneiders.de/meshgeneration (accessed 25 April 2016).
11. NIST MATDL www.MatDl.org (accessed 25 April 2016).
12. TMS (2013) Implementing ICME in the Aerospace, Automotive, and Maritime Industries, http://www.tms.org/ICMEstudy/ (accessed 25 April 2016).
13. TMS (2015) Modeling Across Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales, http://www.tms.org/multiscalestudy/ (accessed 25 April 2016).
14. TCAD Central http://www.tcadcentral.com/index.php/CommercialTCAD (accessed 25 April 2016).