DOWNLOAD PDF MULTISCALE MODELLING AND SIMULATION

Chapter 1 : Multiscale Modelling

Centered around multiscale phenomena, Multiscale Modeling and Simulation (MMS) is an interdisciplinary journal focusing on the fundamental modeling and computational principles underlying various multiscale methods.

Resources The first version of the workflow can be found in the Brain Simulation Platform. If you do not have an account to access the Brain Simulation Platform, please email bsp-support humanbrainproject. Front Neural Circuits, 12, 3. There are many possible levels of multiscale modelling relevant to brain simulation, for example: What makes multiscale models important? Multiscale models allow us to understand how changes occurring at one level of simulation can propagate to higher levels. What are the specific questions we want to address in the HBP? We aim to answer two types of questions: How can parameters be propagated across scales? How can simulations at multiple levels be run concurrently? In order to propagate parameters across scales, the equations used at one scale, must be compatible with those used at another. For example, if one examines the rate of spine head clearance of calcium, for a model in which this was done by kinetic models of calcium pumps and exchangers, one could measure a calcium clearance time constant and then use this in a model in which calcium decay is represented as an exponentially decaying function. In order to couple multiple simulations, information between simulators must be exchanged at periodic time intervals. It may be desirable to only model a small portion of the entire system at high resolution due to computational requirements. What is our specific take? Our initial multiscale models have focused on integrating intracellular signalling and electrophysiology. The flux of some ions through channels in the cell membrane does not only change the electrical properties of the membrane, e. These two functions of single ions are typically modelled using different types of models. The electrical properties are modelled in one type of model, while the intracellular changes are modelled using another. Thus, we have started out by simply adding more detail to simulations running at a coarser scale. When computational power becomes limiting we will explore other methods of multiscale simulation. Roadmap We are currently identifying what is needed and how it can be achieved. We are also looking into possible limitations. During the next phase of the HBP April March , we will further elaborate the portal and improve user interactivity. We will also expand the current intracellular cascade models to be more generalised. Since this work is in its initial phase, a small team is working to address these questions: Participate in community modelling: By participating you can expose your models to a wider community. We would be happy to hear from you if you would like to get involved and contribute to our community effort. You can also send a request on what type of models you think are needed.

Chapter 2 : Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal (MMS)

Figure above. Our Multiscale, Multiparadigm Simulation Strategy: Motivation and General Overview. Understanding natural phenomena from science or optimizing processes from engineering requires, by today's standard, synchronized contributions from theory, experiment and computation.

The National Science Foundation NSF Report on "Simulation-based Engineering Science" [1] showed the potential of using simulation technology and methods to revolutionize the engineering science. Among the reasons for the steadily increasing interest in simulation applications are the following: Using simulations is generally cheaper, safer and sometimes more ethical than conducting real-world experiments. For example, supercomputers are sometimes used to simulate the detonation of nuclear devices and their effects in order to support better preparedness in the event of a nuclear explosion. Hurricane Weather Research and Forecasting model Simulations can often be even more realistic than traditional experiments, as they allow the free configuration of environment parameters found in the operational application field of the final product. Examples are supporting deep water operation of the US Navy or the simulating the surface of neighbored planets in preparation of NASA missions. Simulations can often be conducted faster than real time. This allows using them for efficient if-then-else analyses of different alternatives, in particular when the necessary data to initialize the simulation can easily be obtained from operational data. This use of simulation adds decision support simulation systems to the tool box of traditional decision support systems. Simulations allow setting up a coherent synthetic environment that allows for integration of simulated systems in the early analysis phase via mixed virtual systems with first prototypical components to a virtual test environment for the final system. If managed correctly, the environment can be migrated from the development and test domain to the training and education domain in follow-on life cycle phases for the systems including the option to train and optimize a virtual twin of the real system under realistic constraints even before first components are being built. Other application domains, however, are currently catching up. Scientific modelling Modeling and simulation is important in research. Representing the real systems either via physical reproductions at smaller scale, or via mathematical models that allow representing the dynamics of the system via simulation, allows exploring system behavior in an articulated way which is often either not possible, or too risky in the real world. The diversity and application-oriented nature of this new discipline sometimes results in the challenge, that the supported application domains themselves already have vocabularies in place that are not necessarily aligned between disjunctive domains. Due to the broad variety of contributors, this process is still ongoing. The focus is general methods that can be applied in various problem domains. Models can be composed of different units models at finer granularity linked to achieve a specific goal; for this reason they can be also called modelling solutions. More generally, modeling and simulation is a key enabler for systems engineering activities as the system representation in a computer readable and possibly executable model enables engineers to reproduce the system or Systems of System behavior. A collection of applicative modeling and simulation method to support systems engineering activities in provided in. This rapid expansion has created a burden on existing clinical experimental sites. Simulation may not be utilized to supplant or replace the minimum expectation for time spent in actual pharmacy practice settings as set forth in the previously established policy. Several pharmacy colleges and schools have incorporated simulation as part of their core curricula. At the University of Pittsburgh School of Pharmacy, high-fidelity patient simulators are used to reinforce therapeutics. While the University of Rhode Island College of Pharmacy integrated their simulation program into their pharmacology and medicinal chemistry coursework; and was the first college of pharmacy to purchase a high-fidelity patient simulator. Some pharmacy colleges and schools host virtual reality and full environment simulation programs. Analyses Support is conducted in support of planning and experimentation. Very often, the search for an optimal solution that shall be implemented is driving these efforts. What-if analyses of alternatives fall into this category as well. This style of work is often accomplished by simulysts - those having skills in both simulation and as analysts. This blending of simulation and analyst is well noted in Kleijnen. This support can start in early phases and include topics like executable system

architectures, and it can support testing by providing a virtual environment in which tests are conducted. This style of work is often accomplished by engineers and architects. Training and Education Support provides simulators, virtual training environments, and serious games to train and educate people. This style of work is often accomplished by trainers working in concert with computer scientists. A special use of Analyses Support is applied to ongoing business operations. Traditionally, decision support systems provide this functionality. Simulation systems improve their functionality by adding the dynamic element and allow to compute estimates and predictions, including optimization and what-if analyses. Modeling is understood as the purposeful abstraction of reality, resulting in the formal specification of a conceptualization and underlying assumptions and constraints. The execution of a model over time is understood as the simulation. While modeling targets the conceptualization , simulation challenges mainly focus on implementation , in other words, modeling resides on the abstraction level, whereas simulation resides on the implementation level. Conceptualization and implementation â€" modeling and simulation â€" are two activities that are mutually dependent, but can nonetheless be conducted by separate individuals. Management and engineering knowledge and guidelines are needed to ensure that they are well connected. Like an engineering management professional in systems engineering needs to make sure that the systems design captured in a systems architecture is aligned with the systems development, this task needs to be conducted with the same level of professionalism for the model that has to be implemented as well. As the role of big data and analytics continues to grow, the role of combined simulation of analysis is the realm of yet another professional called a simulyst â€" in order to blend algorithmic and analytic techniques through visualizations available directly to decision makers. A study designed for the Bureau of Labor and Statistics [13] by Lee et al. Academic programs[edit] Modeling and simulation has only recently become an academic discipline of its own. Formerly, those working in the field usually had a background in engineering. The following institutions offer degrees in Modeling and Simulation:

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In engineering, mathematics, physics, chemistry, bioinformatics, computational biology, meteorology and computer science, multiscale modeling or multiscale mathematics is the field of solving problems which have important features at multiple scales of time and/or space.

History[edit] Horstemeyer , [13] [14] presented a historical review of the different disciplines solid mechanics, [15] numerical methods, [16] mathematics, physics, and materials science for solid materials related to multiscale materials modeling. The recent surge of multiscale modeling from the smallest scale atoms to full system level e. Since the US Department of Energy DOE national labs started to reduce nuclear underground tests in the mid s, with the last one in , the idea of simulation-based design and analysis concepts were birthed. Multiscale modeling was a key in garnering more precise and accurate predictive tools. In essence, the number of large scale systems level tests that were previously used to validate a design was reduced to nothing, thus warranting the increase in simulation results of the complex systems for design verification and validation purposes. Within ASCI, the basic recognized premise was to provide more accurate and precise simulation-based design and analysis tools. Because of the requirements for greater complexity in the simulations, parallel computing and multiscale modeling became the major challenges that needed to be addressed. With this perspective, the idea of experiments shifted from the large scale complex tests to multiscale experiments that provided material models with validation at different length scales. If the modeling and simulations were physically based and less empirical, then a predictive capability could be realized for other conditions. As such, various multiscale modeling methodologies were independently being created at the DOE national labs: In addition, personnel from these national labs encouraged, funded, and managed academic research related to multiscale modeling. Hence, the creation of different methodologies and computational algorithms for parallel environments gave rise to different emphases regarding multiscale modeling and the associated multiscale experiments. The advent of parallel computing also contributed to the development of multiscale modeling. Since more degrees of freedom could be resolved by parallel computing environments, more accurate and precise algorithmic formulations could be admitted. This thought also drove the political leaders to encourage the simulation-based design concepts. Each had different programs that tried to unify computational efforts, materials science information, and applied mechanics algorithms with different levels of success. Multiple scientific articles were written, and the multiscale activities took different lives of their own. At SNL, the multiscale modeling effort was an engineering top-down approach starting from continuum mechanics perspective, which was already rich with a computational paradigm. SNL tried to merge the materials science community into the continuum mechanics community to address the lower length scale issues that could help solve engineering problems in practice. Once this management infrastructure and associated funding was in place at the various DOE institutions, different academic research projects started, initiating various satellite networks of multiscale modeling research. Technological transfer also arose into other labs within the Department of Defense and industrial research communities. The growth of multiscale modeling in the industrial sector was primarily due to financial motivations. From the DOE national labs perspective, the shift from large scale systems experiments mentality occurred because of the Nuclear Ban Treaty. Once industry realized that the notions of multiscale modeling and simulation based design were invariant to the type of product and that effective multiscale simulations could in fact lead to design optimization, a paradigm shift began to occur, in various measures within different industries, as cost savings and accuracy in product warranty estimates were rationalized. The aforementioned DOE multiscale modeling efforts were hierarchical in nature. The first concurrent multiscale model occurred when Michael Ortiz Caltech took the molecular dynamics code, Dynamo, developed by Mike Baskes at Sandia National Labs and with his students embedded it into a finite element code for the first time. On each level particular approaches are used for description of a system. The following levels are usually distinguished: Each level addresses a phenomenon over a specific window of length and time. Multiscale modeling is particularly important in integrated computational materials engineering since it allows the prediction of material properties or system

behavior based on knowledge of the process-structure-property relationships. In operations research , multiscale modeling addresses challenges for decision makers which come from multiscale phenomena across organizational, temporal and spatial scales. This theory fuses decision theory and multiscale mathematics and is referred to as multiscale decision-making. Multiscale decision-making draws upon the analogies between physical systems and complex man-made systems. In meteorology, multiscale modeling is the modeling of interaction between weather systems of different spatial and temporal scales that produces the weather that we experience. The most challenging task is to model the way through which the weather systems interact as models cannot see beyond the limit of the model grid size. So we need to come to a balance point so that the model becomes computationally feasible and at the same time we do not lose much information, with the help of making some rational guesses, a process called Parametrization. Besides the many specific applications, one area of research is methods for the accurate and efficient solution of multiscale modeling problems. The primary areas of mathematical and algorithmic development include:

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Through this workshop we aim to provide a forum for multiscale application modellers, framework developers and experts from the distributed infrastructure 1 This space is reserved for the Procedia header, do not use it Multiscale Modelling and Simulation, 14th International Workshop Derek Groen1, Bartosz Bosak2, Valeria Krzhizhanovskaya3,4.

Develop multiscale material models using forward homogenization and inverse optimization technologies Built-in parametric unit cells for unidirectional, woven, chopped, and particulate fiber composites Simulate nonlinear material behavior including ultimate failure at the micro-scale Obtain virtual material allowables supported by test and perform fatigue analysis Efficient plugins to commercial FEA codes OptiStruct, RADIOSS, LS-DYNA, and Abaqus Benefits While a number of multiscale modeling frameworks exist, Multiscale Designer provides unmatched combination of practicality, mathematical rigor, validation, and versatility. Practicality Multiscale Designer is equipped with a systematic model reduction technology that reduces complex unit cells, having hundreds of thousands of finite elements, to a manageable number of deformation modes and state variables. The optimal kinematics modes and state variables are automatically selected to provide the desired level of accuracy for quantities of interest. Multiscale Designer is equipped with an extensible parametric library of unit cell models generated automatically using built-in CAD and meshing tools that permit optimization and stochastic simulations. The current parametric library of unit cell models includes; continuous fiber, woven fabrics, short and long chopped fiber, ordered particles, and random particle microstructures. This eliminates the overhead of generating complex unit cell models and their linkage to macroscale FEA solvers. Mathematical Rigor Multiscale Designer is free of scale separation and provides mesh insensitive results inherent to competing multiscale products. The characteristic material length scale is automatically identified by Multiscale Designer based on user-specified experimental data at the coupon-level. Multiscale Designer is equipped with stochastic multiscale capabilities that translate geometrical and material uncertainties into macro-level component uncertainties. Versatility Advanced Multiscale Designer features include; generation of A- and B-basis allowable material properties with minimum testing without compromising on accuracy, microstructural optimization, multiscale fatigue, and multiscale multiphysics. Capabilities Multiscale Designer â€" Mechanical Multiscale Designer - Mechanical is based on a micromechanical approach that possesses a minimal number of internal variables representing inelastic deformation of the microphases and their interfaces. It resolves microscale fields at a computational cost comparable to that of macroscale modeling. Multiscale Designer - Mechanical precomputes a material database, such as transformation influence functions, in the preprocessing stage prior to nonlinear analysis, which is subsequently reused in the nonlinear analysis. Multiscale Designer - Mechanical has been validated against more than 50 benchmark problems at the coupon and component levels with various composite product forms. Multiscale Designer - Stochastics Multiscale Designer - Stochastics provides forward and inverse stochastic simulation capabilities. The forward stochastic simulation process computes a probability distribution function for macroscale quantities of interest given the variability of the microscale geometry and constitutive properties. The inverse stochastic simulation process reverse engineers the probability distribution function of the microscale constitutive properties based on the variability of the experimental data at a macroscale coupon level. Multiscale Designer â€" Stochastics provides the data for the calculation of A- and B-basis allowables via a virtual allowables supported by test methodology. Multiscale Designer â€" Fatigue Multiscale Designer - Fatigue is based on the two-scale asymptotic homogenization approach in time, and reduced order homogenization in space, that can be effectively applied to any material architecture and any constitutive equations of microphases. Multiscale Designer â€" Multiphysics Multiscale Designer - Multiphysics is based on the unified coupled multiscale mechano-diffusion-reaction model of environmental degradation of polymer and ceramic matrix composites. The salient feature of Multiscale Designer - Multiphysics is its computational efficiency accomplished through model reduction for multiple physical processes. Complementary Solutions OptiStruct Industry proven, modern structural analysis solver for linear and non-linear structural problems under static and dynamic loadings. The market-leading solution for

structural design and optimization. Overview Video Learn More HyperMesh High-performance finite element pre-processor to prepare largest models, starting from import of CAD geometry to exporting an analysis run for various disciplines. Overview Video Learn More Loading Subscribe to join our Newsletter Learn about product training, news, events and more.

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Multiscale models are models that expand and link beyond the domain of single-level models. There are many possible levels of multiscale modelling relevant to brain simulation, for example: systems models, point-neuron models, morphologically-detailed models, different-equation subcellular models and molecular dynamics models.

Macroscale models require constitutive relations which are almost always obtained empirically, by guessing. Making the right guess often requires and represents far-reaching physical insight, as we see from the work of Newton and Landau, for example. It also means that for complex systems , the guessing game can be quite hard and less productive, as we have learned from our experience with modeling complex fluids. The other extreme is to work with a microscale model, such as the first principle of quantum mechanics. As was declared by Dirac back in Dirac, , the right physical principle for most of what we are interested in is already provided by the principles of quantum mechanics, there is no need to look further. There are no empirical parameters in the quantum many-body problem. We simply have to input the atomic numbers of all the participating atoms, then we have a complete model which is sufficient for chemistry, much of physics, material science, biology, etc. Dirac also recognized the daunting mathematical difficulties with such an approach -- after all, we are dealing with a quantum many-body problem. With each additional particle, the dimensionality of the problem is increased by three. For this reason, direct applications of the first principle are limited to rather simple systems without much happening at the macroscale. Take for example, the incompressible fluids. The fundamental laws are simply that of the conservation of mass and momentum, which, after introducing the notion of stress, can be expressed as follows: To close this system of equations, we need an expression for the stress tensor in terms of the velocity field. Here is where the guessing game begins. The standard approach is to ask: Even though the reasoning that went into the derivation of the Navier-Stokes equation is exceedingly simple, the model itself has proven to be extremely successful in describing virtually all phenomena that we encounter for simple fluids, i. Partly for this reason, the same approach has been followed in modeling complex fluids, such as polymeric fluids. Unfortunately the success there is quite limited. The first problem is that simplicity is largely lost. In order to model the complex rheological properties of polymer fluids, one is forced to make more complicated constitutive assumptions with more and more parameters. The second difficulty is that accuracy is not guaranteed. For polymer fluids we are often interested in understanding how the conformation of the polymer interacts with the flow. This kind of information is missing in the kind of empirical approach described above. A more rigorous approach is to derive the constitutive relation from microscopic models, such as atomistic models, by taking the hydrodynamic limit. This is an example of the multiscale analysis approach. But for complex fluids, this would result in rather different kinds of models. This is one of the starting points of multiscale modeling. Multiscale modeling In the multiscale approach, one uses a variety of models at different levels of resolution and complexity to study one system. The different models are linked together either analytically or numerically. For example, one may study the mechanical behavior of solids using both the atomistic and continuum models at the same time, with the constitutive relations needed in the continuum model computed from the atomistic model. The hope is that by using such a multi-scale and multi-physics approach, one might be able to strike a balance between accuracy which favors using more detailed and microscopic models and feasibility which favors using less detailed, more macroscopic models. Illustration of the multi-physics hierarchy. It should be noted that this diagram is slightly misleading: Quantum mechanics is valid not just at the microscale, it also applies at the macroscale -- only that much simpler models are already quite sufficient at the macroscale. Sequential multiscale modeling In sequential multiscale modeling, one has a macroscale model in which some details of the constitutive relations are precomputed using microscale models. For example, if the macroscale model is the gas dynamics equation, then an equation of state is needed. This equation of state can be precomputed using kinetic theory. When performing molecular dynamics simulation using empirical potentials, one assumes a functional form of the empirical potential, the parameters in the potential are precomputed using quantum mechanics. Sequential multiscale modeling is mostly limited to the

case when only a few parameters are passed between the macro and microscale models. For this reason, it is also called parameter passing. This does not have to be the case though: It has been demonstrated that constitutive relations which are functions of up to 6 variables can be effectively precomputed if sparse representations are used Bungartz and Griebel, ; Garcia-Cervera, Ren, Lu and E, Concurrent multiscale modeling In concurrent multiscale modeling, the quantities needed in the macroscale model are computed on-the-fly from the microscale models as the computation proceeds. In this setup, the macro- and micro-scale models are used concurrently. Take again the example of molecular dynamics. If one wants to compute the inter-atomic forces from the first principle instead of modeling them empirically, then it is much more efficient to do this on-the-fly. Precomputing the inter-atomic forces as functions of the positions of all the atoms in the system is not practical since there are too many independent variables. On the other hand, in a typical simulation, one only probes an extremely small portion of the potential energy surface. Concurrent coupling allows one to evaluate these forces at the locations where they are needed. The two types of multiscale problems The first type are problems where some interesting events, such as chemical reactions, singularities or defects, are happening locally. In this situation, we need to use a microscale model to resolve the local behavior of these events, and we can use macroscale models elsewhere. The second type are problems for which some constitutive information is missing in the macroscale model, and coupling with the microscale model is required in order to supply this missing information. We refer to the first type as type A problems and the second type as type B problems. Examples of multiscale methods Car-Parrinello molecular dynamics To model the classical dynamics of the atoms or nuclei, we need the inter-atomic forces, which arise from the Coulomb interaction between the nuclei and the electrons. This is a type B problem. Knowing the position of the atoms, we should in principle be able to evaluate the electronic structure and determine the inter-atomic forces. However, precomputing such functions is unfeasible due to the large number of degrees of freedom in the problem. The Car-Parrinello molecular dynamics Car and Parrinello, , or CPMD, is a way of performing molecular dynamics with inter-atomic forces evaluated on-the-fly using electronic structure models such as the ones from density functional theory. There are two technical aspects that are worth mentioning. The first is that the implementation of CPMD is based on an extended Lagrangian framework by considering the wavefunctions for electrons in the same setting as the positions of the nuclei. In this extended phase space , one can write down a Lagrangian which incorporates both the Hamiltonian for the nuclei and the wavefunctions. The second is the choice of the mass parameter for the wavefunctions. Perhaps the most natural choice should be the mass of an electron. This makes the system stiff since the time scales of the electrons and the nuclei are quite disparate. However, since we are only interested in the dynamics of the nuclei, not the electrons, we can choose a value which is much larger than the electron mass, so long as it still gives us satisfactory accuracy for the nuclear dynamics. Quantum mechanics - molecular mechanics QM-MM methods When studying chemical reactions involving large molecules, it often happens that the active areas of the molecules involved in the reaction are rather small. The rest of the molecules just serves to provide the environment for the reaction. In this case, it is natural to only treat the reaction zone quantum mechanically, and treat the rest using classical description. This is a type A problem. The most important ingredient in such a method is the Hamiltonian which should consist of the quantum mechanical Hamiltonian for the active region, the classical Hamiltonian for the rest as well as the part that represents the interaction between the two regions. Another important ingredient is how one terminates the quantum mechanical region, in particular, the covalent bonds. Many ideas have been proposed, among which we mention the linked atom methods, hybrid orbitals, and the pseudo-bond approach. Quasicontinuum QC method Quasicontinuum method Tadmor, Ortiz and Phillips, ; Knap and Ortiz, is a finite element type of method for analyzing the mechanical behavior of crystalline solids based on atomistic models. A triangulation of the physical domain is formed using a subset of the atoms, the representative atoms or rep-atoms. The rep-atoms are selected using an adaptive mesh refinement strategy. In regions where the deformation is smooth, few atoms are selected. In regions where the deformation gradient is large, more atoms are selected. Typically, near defects such as dislocations, all the atoms are selected. The next ingredient in the quasicontinuum method is a simplified way of computing the energy of a trial configuration. This is done based on the following principle: In the smooth region, one uses

the Cauchy-Born rule which is a way of evaluating the continuum stored energy density using the atomistic model. Near defects, one uses the atomistic model. Some hybrid of these two approaches are used in between. In the language used below, the quasicontinuum method can be thought of as an example of domain decomposition methods. Macro-micro formulations for polymer fluids One way of overcoming the difficulties associated with the empirical constitutive relations for modeling polymer fluids is as follows Bird, Armstrong and Hassager, ; Oettinger, One can model the microscale dynamics of the constituent polymers within the flow, and then evaluate the polymer stress using the microscopic configurations of the polymers. This is referred to as a macro-micro model since the macroscale fluid dynamics affect the dynamics of the polymers by providing the background in which the polymers move, and the microscale polymer configurations affect the flow by supplying the polymer contribution of the stress. Typically the microscale polymer dynamics is modeled using some coarse-grained empirical models such as the dumbbell model, the bead-and-spring model or the rigid rod model. The polymers obey Brownian dynamics: Even though the polymer model is still empirical, such an approach usually provides a better physical picture than models based on empirical constitutive laws. Other examples including large eddy simulation of turbulent flows, solvers for stiff ordinary differential equations, techniques such as super-parametrization in climate modeling, the generalized finite element method that enriches the finite element space with multiscale trial and test functions, etc. Examples of classical multiscale algorithms Multiscale ideas have also been used extensively in contexts where no multi-physics models are involved. Multi-grid method Brandt, Classically this is a way of solving the system of algebraic equations that arise from discretizing differential equations by simultaneously using different levels of grids. In this way, one can more efficiently eliminate the errors on different scales using different grids. In particular, it is typically much more efficient to eliminate large scale or smooth component of the errors using coarse grids. Fast multipole method Greengard and Rokhlin, This is a way of summing up long range interaction potentials for a large set of particles. The contribution to the interaction potential is decomposed into components with different scales and these different contributions are evaluated at different levels in a hierarchy of grids.

Chapter 6 : Multiscale Modeling and Simulation

The Vanderbilt Multiscale Modeling and Simulation (MuMS) interdisciplinary research facility houses faculty and researchers from the School of Engineering, specifically: Chemical and Biomolecular Engineering Civil Engineering, and Mechanical Engineering.

Chapter 7 : MMM@HPC - Home - Welcome to the MMM@HPC project!

The simulation methods used include mean-field model,, combined model of DFT and self-consistent field (SCF), and molecular dynamic model,. Table 1 presents a brief description of the theoretical studies on the thermodynamics of polymer nanocomposites.

Chapter 8 : Design & Analysis of Engineered Components | Altair Multiscale Designer

This is where multiscale modeling comes in. By considering simultaneously models at dïˆ€erent scales, we hope to arrive at an approach that shares the eï¬ƒciency of the macro-.

Chapter 9 : ZARM: Fluid Dynamics

Multiscale Material Modelling on High Performance Computer Architectures. With the accelerating materials development cycles, the development of simulation approaches for predictive, de-novo characterization and optimization of materials and device properties emerges as a grand challenge to European R&D.