Summary of the

1st Workshop on Multi-Paradigm Multi-Multi-Scale Modeling in the Computational Materials Design Facility (CMDF)

Caltech, Aug. 23/24 2005

Review and impact

The CMDF workshop provided an inspiring overview over the activities in the field of code integration and application as well as development of multi-scale modeling techniques within the CMDF framework. The technical talks were concluded by an interdisciplinary panel discussion led by Paul von Allmen (JPL), Ioana Cozmuta (Eloret, NASA Ames Research Center), Valeria Molinero (Caltech and ASU), as well as Markus Buehler (Caltech). One of the important results of this workshop was that we have received critical feedback to our work from outside participants in the workshop, and that we have learned about areas of high demand for future funding and collaboration and further development of CMDF.

In addition to scientific talks covering those various aspects of multi-paradigm multi-scale modeling, the training sessions on the second day were quite successful and well received. A group of about 10 scientists obtained a copy of CMDF and played with several example calculations demonstrating the powerful tools and packages. The example involved 6 of the (currently) more than 35 computational packages in CMDF and outlined how CMDF enables to couple various computational paradigms to easily build complicated multi-scale materials simulations. A focus area of the training session was further addressing practical computer science aspects related to CMDF, including methods such as SWIG, PYFORT and F2PY to enable code development. We emphasized on the procedure of integrating new codes into CMDF. Paired with the coupling to existing web portal technology like WIGLAF (JPL) as platform independent and remote interface to CMDF this provides fertile ground for future developments and to cover new grounds.

We have observed significant interest in the workshop with very good attendance even until the evening discussion sessions and the panel discussion. We had over 70 registered participants at the workshop. The attendees are affiliated with various universities and institutes from all over the country. Also, we appreciated to have an audience including people who have been involved in the early day developments of CMDF (including Rick

Muller from Sandia National Labs and Peter Meulbroek now at Yahoo!) who were involved in the first CMDF related research proposals funded by DARPA and DoE. We have also reached out to other multi-scale groups within Caltech (e.g. the CIMMS center), which will hopefully lead to fruitful collaboration and exchange of ideas in the future.

The talks and discussions at the CMDF workshop addressed many scales and issues, including scale coupling, computational science, and error bar analysis to understand sensitivity of macroscopic variables with respect to fine scale accuracy of computational methods.

A general consensus of the workshop was that our new CMDF methods are now at a stage where they become applicable to real problems and that the CMDF approach may set examples or the basis of further developments in other labs. In addition to providing intellectual stimulation, we have initiated several concrete projects and application areas. This will lead to close collaboration with groups at Sandia National Labs, NASA Ames Research Labs and the Army Research Labs. Several specific additional areas of applications were mentioned by the audience, including polymers, explosives, catalysis and biological systems. This workshop has laid the ground for establishing relationships outside the Caltech-JPL PROM team, which will significantly increase the impact of our results and CMDF developments in a wider community.

This success clearly demonstrates the usefulness of our method and approach. Future funding will help to complete the remaining tasks and make CMDF a generally useful tool in the materials science and chemistry community.

We have set up a TWiki website (see http://twiki.wag.caltech.edu/twiki/bin/view/; for your first login use: username: MscFriend and the password: gwiki) to exchange ideas within the team of researchers formed within the scope of this meeting. This straightforward means of communicating through internet Wiki sites will hopefully further stimulate collaboration.

Outlook and immediate plans

We expect that many new applications and collaborations will develop as a consequence of the CMDF workshop. The development and research team at Caltech, JPL and Rutgers has received valuable stimulus for immediate improvements of the methods.

One of the possible focuses is to explore ways for improving coupling of different force fields in hybrid atomistic simulations by the use of the higher-order approximation formulas for matching Hamiltonians and its derivatives within the transition layer between areas with different potentials. Another focus is a development of the CMDF library of analysis tools such as calculations of local flows and distributions (e.g. mass and heat transport, temperature and strain-stress maps), vibrational spectra, phonon density of states, electronic band structure, etc. It could require both incorporation into the CMDF of the analysis subroutines already present in simulation codes and the development of more general purpose (or data structure) algorithms within the CMDF.

It has become apparent that seamless integration at continuum level is lacking in the CMDF method. Therefore, we will work closely with Alberto Cuitino. This will help to integrate his continuum scale methods into CMDF, this adding another new flavor. In addition to the development of hybrid continuum-atomistic simulations within the CMDF framework, it could be also important to explore new approaches for integration of atomistic simulations with mesoparticle dynamics which is currently under development both at Caltech group (Valeria Molinero) and at LANL (Alejandro Strachan, now at Purdue Univ.). This might not only provide a smoother transition between different scales in the CMDF, but also allow for the incorporation of quantum effects into energy exchange between translational motion of such mesoparticles and their internal degrees of freedom. Preliminary studies performed in CMDF already within the scope of Valeria Molinero's bead models of glucose and Tod Pascal's meso-DNA theory are a first step toward that goal.

Further, we discussed the applicability of our method for use by engineers and non-experts. Although initial progress has been made, we still see further need for developments, in particular in further advancing our visual builders and analysis tools (GUIs). The purpose here is to enhance the CMDF not only to hybrid simulations, but also to the combination of different analysis and building tools in such a way that they could be easily called during or after the simulation by using a few commands in the script. Here we will provide assistance to users and non-experts in incorporation of their analysis algorithms and favorite codes into the CMDF, as well as develop necessary infrastructure within the CMDF (e.g. for inclusion GUIs tools, etc).

Further, we have made concrete plans to integrate a parallelized version of ReaxFF developed at Sandia National Labs (SNL) as part of the GRASP package. We will form a team of scientists from Caltech, JPL and SNL to reach this goal within the PROM project. The GRASP package is currently used at Sandia, Los Alamos and elsewhere to perform large parallel molecular dynamics simulations with advanced force fields, including ReaxFF. Integration of GRASP into CMDF will make it easier for team members to add functionality to the parallel implementation of ReaxFF. It will also make it easier for GRASP users to get up and running quickly. This will allow users to perform large-scale hybrid simulations within the CMDF using both reactive and non-reactive force fields, such as cracking of the oxidation layer of an aluminum nanoparticle which is important for study of burning of solid composite propellants (e.g. Al_2O_3/Al-nanoparticles embedded into RDX matrix). CMDF will also be installed at Sandia National Labs in the coming weeks. During the workshop we have had numerous discussions with Aidan Thompson (chief GRASP developer, SNL), which identified a range of research topics for which the GRASP/CMDF-framework can make a direct impact.

We will also intensify our efforts in automating procedures of error detection and sensitivity analysis. This effort will be led by Paul von Allmen (JPL) with close interaction with the Goddard group at Caltech. The on-going coupling within CMDF of first principles tools existing at Caltech with parametrized tight-binding approaches that were developed at JPL has revealed the importance of a consistent analysis of the

uncertainty propagation from one modeling tool to another. Since the tight-binding approach allows for the computation of macroscopic quantities such as electrical and thermal transport properties of structures in the tens of nanometer scale range, this effort also addresses the impact of uncertainties of atomic level calculations on directly measurable “device-level” quantities. Recent work at JPL in collaboration with MSC has demonstrated the stiffness of the mapping between the tight-binding parameter space and first principles data. Error bars inherent to the optimization process yielding the tight-binding parameters were shown to prevent the numerical evaluation of a stable sensitivity correlation matrix. One of the focuses in making progress in this area could be to include into the CMDF tools and algorithms for solution of ill-posed inverse problems (e.g. for noisy data or ill-conditioned linear systems) such as the Tikhonov regularization and filtering.