1 UQ Algorithms and Software Development

In order to properly exercise a full validation cycle and accomplanying uncertainty quantification, we need software capable of assisting a modeler with the statistical inversion for parameters as well with the forward propogation. To this end, we implemented the state of the art Delayed Rejection Adaptive Metropolis (DRAM) Markov chain algorithm in C++ using the GNU Scientific Library (GSL). The code was then tested with two simple physical models: thermogravimetric analysis (TGA) and a Burgers equation turbulence model problem. The main objective was to learn by hands on experience and to disseminate UQ concepts among researchers in PECOS.

We then progressed to the more ambitious goal of implementing an initial C++ uniprocessor version of the Quantification of Uncertainty for Estimation, Simulation and Optimization (QUESO) toolkit. The QUESO toolkit contains classes for entities such as random variables, pdfs, cdfs, statistical inverse solvers (only DRAM at this moment) and statistical forward solvers (only Monte Carlo at this moment). All these classes are templated with respect to underlying vector and matrix classes, a feature that will save development time as we move from the current uniprocessor environment with wrapped GSL vectors and matrices to parallel environments using e.g. Trilinos and PETSc.

We successfully used QUESO to exercise the full validation cycle proposed by the PECOS Center again with our two simple model problems. These exercises enabled a collaborative understanding of many concepts present in the validation process: model parameters, scenario parameters, prior state of information, likelihood function, calibration experiments, validation experiments, posterior random variables, (surrogate) quantity of interest, assessment of confidence in the model and assessment of confidence in the system being modeled.

We are now extending the exercise of the full validation cycle to two more model problems: radiation and aero-thermo-chemistry. We also begun implementing the Stochastic Newton Markov chain algorithm in QUESO.

2 Model Development & Implementation

2.1 Turbulence Modeling

For the past six months, an effort has been made to properly formulate uncertainty quantification techniques for RANS turbulence models. In this context, a significant problem is the treatment of model form uncertainty. In particular, RANS turbulence models are known to be physically incorrect and, thus, incapable of exactly reproducing experimental results, even neglecting experimental error. This model uncertainty/inadequacy, which is present in many engineering models, not only turbulence models, must be quantitatively accounted for in both the statistical inverse and forward propagation problems.

However, the model uncertainty is typically not well known. Thus, uncertainty in the model uncertainty model must also be included in the complete uncertainty quantification. One way to accomplish this is to incorporate the model uncertainty model as part of the statistical inverse problem. Thus, the model uncertainty is calibrated and validated simultaneously with the model itself. This approach is being investigated in the context of a Burgers' equation model problem. In this model problem, Burgers' equation provides the "truth" dynamics, which are then modeled using the Reynolds-averaged Burgers' equation. Like RANS turbulence models, the Reynolds-averaged Burgulence model is incapable of reproducing the exact dynamics of the true system. The model inadequacy is modeled using a Gaussian process, the parameters of which are incorporated into the statistical inverse problems solved during the model calibration and validation phases. This approach has shown significant promise for treating the effects of model uncertainty. Future work will focus on extending the approach used in the model problem to the RANS equations.

Two sources of data are actively being pursued for the turbulence model calibration and validation problems. One important source of data is direct numerical simulation (DNS) of the Navier-Stokes equations. Over the past months, two DNS efforts have been pursued. The first effort uses an existing code that implements a high-order finite volume spatial discretization. This code is currently in the final stages of verification for compressible flows. The second DNS code will rely on a spectral discretization. This code is in the process of being refactored from a legacy implementation.

More recently, a concerted effort has begun to catalogue the experimental data available for turbulence model calibration as well as identify any gaps in the data available in the literature. Initially this effort has focused on turbulent, hypersonic flows over simple "building block" geometries. Furthermore, RANS simulations of the chosen experiments are being conducted using DPLR with standard turbulence models and model coefficients to prepare the cases—i.e. meshes and input files—for inclusion in the initial calibration effort.

2.2 Radiation Modeling

Two different radiation models were implemented and coupled with NASA's DPLR code in order to solve the coupled hypersonic flow and radiative heat transfer. In the first, the radiative heat transfer equation is solved using the SP1-approximation while the other uses the discrete transfer method. Emitting absorbing properties of the high temperature air plasma are considered by applying a gray gas model at local-thermodynamic equilibrium. The gray gas absorption coefficient is a function of temperature and pressure and is computed using correlations fitted from line-by-line spectral data obtained with Specair, a program for modeling the absolute intensity spectral radiation emitted by gases and plasmas .

Comparisons between results obtained with the SP1-approximation, discrete transfer and Monte Carlo were conducted. Although the discrete transfer was computationally cheaper and somewhat more accurate than the SP1-approximation to the initial model, the SP1-approximation is considerable cheaper if it is necessary to increase the complexity of the model to account for scattering.

Calibration and validation cycles were applied to the initial gray gas model proposed, where the absorption coefficient was independent of chemical concentration, temperature, pressure and spectrum. Additionally, we investigated coupled radiation and hypersonic flow where the absorption coefficient is a function of temperature and pressure. In order to assist with the evaluation of the simple models, a code to compute radiation heat transfer by line-by-line integration was also developed.

2.3 Ablation Modeling

A detailed understanding of the ablation process is essential for the design of the thermal protection system (TPS) of an earth re-entry vehicle. The ablation process involves several chemical and physical sub-models that are strongly coupled. Furthermore, a number of simplified models exist for the different physical components. The use of simplified models allows the preliminary testing of various parameter estimation and uncertainty quantification (UQ) schemes that can later be used for more detailed models. The strongly coupled nature of the physical process (and governing equations) allows the testing of different physics-coupling strategies for integrated simulations of the multi-physics. This exercise can conceivably be extended to the complete re-entry vehicle problem in the future.

With these considerations in mind, we have adopted a two-pronged approach to ablation modelling within the project. One path has been to take simplified models and simple calibration experiments involving a small number of parameters. As an example, TGA experimental data was used to calibrate 2 parameters in a solid degragdation model. The QUESO toolkit was used to implement the Markov Chain Monte Carlo scheme for stochastic inversion analysis using the Bayesian approach.

The second path has been to develop a code that can handle the coupled non-linear system of equations governing the ablation process. Initially, we are following an approach similar to the one used in the Sandia code Chaleur. The solution method employs a loosely coupled solution of a system of equations describing the heat and mass transfer and solid decomposition. We have written and verified a code for a non-decomposing ablator with a straightforward verification problem. Ongoing work that will extend into year 2 will involve the implementation of gradient based methods such as adjoints and Hessians into the fully coupled set of equations. This exercise is expected to be a useful benchmark for the implementation of similar techniques for large-scale, strongly-coupled physical phenomena.

2.4 Aerothermochemistry Modeling

Understanding high-temperature chemistry is essential to make an accurate prediction of the heat-flux to the surface. However, there are many uncertainties associated with a detailed chemical modeling. At high-temperature, chemistry itself becomes rather difficult, involving a large number of chemical reactions. Therefore, a choice of reaction-set becomes a central research activity. Secondly, obtaining exact reaction rates of the chosen reactions is not fully accessible. Finally, a sufficient amount of experimental data for a range of high temperatures is often not obtainable.

As our initial exercise in UQ as it applies to aerothermochemistry modeling, we choose a cyano species mechanism that has been well investigated by past efforts in the combustion communities, and that has detailed experimental and chemical reaction data available. For our application, cyano species play an important role since carbon products from the surface react with the outflow, and the radiation of cyano species is experimentally observed. A simple zero-dimensional chemical model when exercised with QUESO gave promising result in identification of reaction rate. Our predicted reaction rate given by the probability density function (PDF) is in reasonable agreement with experimental values, however, due to the lack of experimental data with a range of temperature, the pdfs of each parameters in the Arrenius form have large uncertainties, and need to be calibrated against additional experimental data.

Another activity in aerothermochemistry modeling is the development of a one-dimensional compressible flow solver specifically designed for shock-tube validation. The Euler equations are solved using an upwind-central difference finite volume scheme. The upwind scheme approximates the solution to the Riemann problem using a Harten, Lax, and van Leer (HLL) scheme. The Monotone Upstream-Centered Scheme for Conservation Laws (MUSCL) method is used with the monotized-central (MC) slope limiter in order to maintain second-order spatial accuracy. Second-order accurate explicit time-integration is employed with the implementation of the MacCormack scheme. At this moment, the code is still designed for non-reacting thermally perfect gas. However, we are planning to couple it with our oxygen molecule dissociation mechanism, and also implement more realistic boundary condition to take care of any pressure wave reflection from the subsonic outflow exit.

3 Coupling Efforts

The coupling of the many physical phenomena for the reentry problem is a complex problem involving personnel in the modeling effort as well as groups studying inverse analysis and uncertainty quantification. The focus for the first year regarding multiphysics coupling has been a strong effort to provide a basic platform for coupled hypersonic, shock layer radiation, and ablation modeling using existing code frameworks. In this case, the NASA code DPLR was used for studying hypersonic flow physics, including some turbulence modeling and aerothermochemistry. The radiation modeling group developed a code implementing a simple one-dimensional radiation model, while the ablation group implemented a one-dimensional ablation model.

The initial effort in simulating shock layer radiative heat transfer is the specification of the radiative heat flux source term that is supplied to the energy equation. That is, the radiation code, given the properties of the fluid flow, computes the radiative heat flux in the flow. This is a ”loose” coupling strategy in that the flow solver is converged to some degree and the solution is used as input for the radiation solver, which feeds back to the flow solver. This process is iterated until convergence. Several results have been obtained on two-dimensional, high Mach number flows.

The ablation model couples through the catalytic boundary condition in the flow. That is, there is an existing infrastructure within the DPLR code to model chemistry taking place on the surface of the object in the flow. The existing catalytic models are replaced with the ablation model. First, the ablation model is homogeneous on the surface - that is, the entire surface is treated as one ablator. Then, we study how the behavior of the ablating surface as we allow more and more cells on the surface to be independent ablators.

4 Experimental Validation Efforts

The V&V/ UQ framework requires experimental data to calibrate the physics models being developed at PECOS and to validate predictions of multi-physics phenomena made using simulations that couple those models. PECOS is close to finalizing an agreement with the National Aeronautics and Space Administration (NASA) that will allow us access to all past, present, and future experimental data acquired by the NASA. Of particular interest to PECOS are contemporary experiments being conducted by the NASA Crew ExplorationVehicle (CEV) Aerosciences Project team (CAP team) in support of agency efforts to develop the next generation space capsule. To better understand the data coming out of this test program, members of the PECOS working group have regularly attended pertinent NASA CAP technical meetings and interact with the NASA CAP program on an almost weekly basis by participating in their experimental teleconferences.

Recently, Faculty and Postdoctoral Fellows attended the NASA Thermal Protection System Advanced Development Project (TPS ADP) quarterly workshop (28-30 October 2008, the NASA Ames Research Park, Mountain View, CA). Among other topics, the meeting discussed arc jet tests conducted in the NASA Ames Interactive Heating Test (IHT) and Advanced Heating Test (AHT) facilities. NASA is using these facilities to certify the CEV thermal protection system (TPS) material. The recession rate data measured during arc jet testing will benefit validation of the recession rate predictions PECOS is working toward. The trip also afforded our faculty and staff an opportunity to visit the NASA Ames Electric Arc Shock Tube (EAST) during a modernization of the facility that includes new instrumentation, new calibration sources and procedures, and a new test section. The EAST facility can duplicate the radiative environment corresponding to peak heating during atmospheric reentry from the moon and provides the NASA CAP team with its primary source of data to validate radiative heat flux predictions. In the short term, PECOS intends to use EAST data to validate shock tube radiation predictions made using a simulation that couples radiation and chemistry models to a 1-D inviscid, compressible flow solver.

A Postdoctoral Fellow also attended a meeting between members of the NASA CAP team and engineers at the Calspan University of Buffalo Research Center (16 December 2008, CUBRC, Buffalo, NY). CUBRC runs one of the premier hypersonic facilities in the country, the Large Energy National Shock Tunnel (LENS) facility, and is finishing construction of a shock-expansion tunnel (LENS XX) that will provide the NASA CAP with additional radiation data. The meeting discussed the results of an experiment conducted by CUBRC to study convective heating augmentation due to surface roughness as well as the specifics of two upcoming tests, one to measure laminar and turbulent convective heating levels in and about compression pad cavities on the forebody of a CEV model and one to measure heating on a high-fidelity CEV model. The high-fidelity model will include fore body and aft body cavities and protrusions as well as reaction control system (RCS) jets. A quantity of interest to PECOS is the heating experienced at the intersection of the RCS jets and the boundary layer/shear layer flow on the aft body of the CEV. The high fidelity tests at CUBRC could benefit validation of the PECOS heating prediction assuming raw data from the test series is provided to the NASA CAP. (Apparently, CUBRC only provides the NASA CAP with reduced data and not the raw traces).

Though the NASA CAP experimental program offers PECOS a unique source of validation data, members of the PECOS working group are constantly researching alternative sources of calibration and/or validation data. These alternative sources are reviewed, uploaded to a network repository, and summarized to the group at weekly staff meetings. When a data set appropriate for calibration and/or validation of a particular PECOS prediction is found, potential sources of error and uncertainty in the data are investigated and the results are summarized on the repository. In addition to outside sources of validation data, an effort is currently under way to generate validation data at the J. J. Pickle Research Center High-Speed Wind Tunnel at the University of Texas at Austin. In particular, the design of an experiment to study turbulent convective heating augmentation due to surface roughness is currently being considered. The experiment will likely measure heat-flux with techniques employed at low-enthalpy hypersonic facilities utilized by the NASA CAP (e.g. the Arnold Engineering Development Center Tunnel 9 and the Langley Research Center 20-inch M=6 wind tunnel) and will likely utilize advanced optical diagnostic techniques as well; e.g. particle imaging velocimetry (PIV). These tests could benefit calibration of the RANS models being developed at PECOS, will complement tests already conducted by the NASA CAP to determine the effect of surface roughness on convective heating levels, and will help PECOS to better understand the measurement techniques employed at AEDC T9, LaRC, and other low-enthalpy blow down wind tunnel facilities.

5 Hypersonic Code Research

The PECOS hypersonics flow team has evaluated several flow software packages this year. NASA's parallel line relaxation finite volume code DPLR has been selected and is being used for the current PECOS multiphysics experiments, a decision based primarily on the wide availability of advanced physics models already integrated, as well as the well-structured nature of the code which has proven easy to extend via loose coupling. We have successfully used DPLR to obtain converged flow results for verification benchmark problems, 2D reentry flow problems, and 3D flow on an axisymmetric capsule mesh provided by the CEV program.

For future work, the stabilized finite element hypersonic flow code FINS, originally by NASA researcher Ben Kirk and currently being extended by PECOS staff, has been selected as a primary development target. Although FINS currently lacks the sophisticated chemistry modeling that is necessary for correctly solving orbital reentry problems, FINS does provide mathematical and numerical capabilities that our staff have determined to be impossible or impractical to quickly add to DPLR, including adaptive mesh refinement, extraction of sparse Jacobian data, and interfaces with modern linear algebra libraries. For proper discretization error control, features like adaptivity and adjoint-based error estimation from consistent Jacobians are essential; these features are either already complete or in development with FINS. Stabilized finite element formulations are still an open research topic in hypersonic flows, and we are collaborating with NASA and Sandia Labs in their efforts to explore their potential. So far FINS has been successfully used by PECOS for forward uncertainty propagation studies, perfect gas flow comparison runs against DPLR, and shock tube verification problems. Current work is aimed at adding chemistry model support, exact analytic Jacobians, and adjoint solves. The libMesh finite element library, a popular open source toolkit used by FEM researchers worldwide, has also seen new development this year to further PECOS goals, including the addition of Trilinos and the improvement of PETSc linear algebra interfaces, and improved support for fully coupled multiphysics problems.

6 Software Architecture

In the context of software architecture, a number of initiatives were undertaken during this reporting period. The first was a global initiative, focused on developing a software management framework for tracking the various development initiatives being undertaken. Source code management is straightforward and has been accomplished using the subversion package since the inception of the project. However, a higher-level framework was also required to define project milestones and interdependency relationships between current physical model developments (e.g. ablation and radiation models) and their coupling implementation with flow models and subsequent UQ analysis. To that end, we evaluated a new project management web application named Redmine that has seen a lot of recent development activity. Note that Redmine has overlapping functionality with a more well-known software project system (trac) but also includes an abstraction for project/subproject relationships which maps well to the PECOS Center efforts. After an initial evaluation phase, we found this package provided a sufficiently rich feature set to track our internal software development projects and we transitioned to its use for our normal production operation. Note that while this is the central repository for development efforts to define milestones, delegate work, track bugs and feature requests, it is also serves as our technical document repository and general collaboration location for all faculty, staff, and students contributing to the project.

A second initiative begun during this reporting period was to begin initial development on a High Performance Computing Toolkit (HPCT) to provide commonly used support functions for the modeling efforts. Given the multi-physics and multi-scale required to adequately resolve vehicle re-entry, we are faced with doing development work in a multi-language environment (C/C++ and Fortran) but still have some common functionality requirements among individual physics modules. The HPCT library was thus envisioned as a simple aggregating mechanism to standardize these needs and avoid duplicating effort. By necessity, the HPCT library must support both Fortran and C and the initial version accommodates this in the usual fashion by defining a Fortran API which wraps internal C++ functions.

The initial HPCT version has functionality to support two common modeling needs: ascii input file parsing and performance timing. Input parsing is a must for any numerical model and the HPCT library leverages an existing C++ mechanism for arbitrary order file parsing (GetPot). This approach allows for flexible and organized input files to be used which can also include a hierarchical designation. For example, a user can define a main solver section along with a subsection named solve/turbulence. This flexibility allows for non-unique input variable names as long as the variables are not defined within the same input section. The performance timing functionality is currently based on a timeofday type mechanism for maximum portability and to avoid SMP issues that can arise with cycle-based timers. The implementation is based on having application programmers define an outermost area of performance interest (for example, a global time-stepping loop) and then any arbitrary number of subregions via a unique name identifier. Typically, these subregions represent specific functions or subroutines in order to quantify the runtime performance of the routine of interest.

7 Deliverables

Expected deliverables for 04/16/2009 - 04/15/2010:

1. Model Development, Implementation & Code Verification
    (a) Ablation Modeling
        i. Implementation and evaluation of existing thermo-mechanical TPS constitutive model
        ii. Collection of relevant validation and calibration data
    (b) Aerothermochemistry
        i. Evaluation of turbulence reaction model in DPLR
        ii. Implementation of standard aerothermochemistry models for shock tube validation
        iii. Implementation of enhanced turbulent reaction and ablation product chemistry models
    (c) Hypersonic Flow code (HyFlow)
        i. Continuation of rigorous code verification of DPLR
        ii. Integration of Hyflow with updated physics models
    (d) Radiation
        i. Implementation and integration of models of air radiative properties for reentry conditions
        ii. Verification of simplified radiation models against higher fidelity models
        iii. Implementation of spectral radiation emission modeling of shock tube experiments
    (e) Turbulence
        i. Continuation of implementation and verification of high speed boundary layer DNS code
        ii. Continuation of DNS simulations
        iii. Implementation of standard RANS and hybrid RANS/LES models
2. UQ Algorithm Development and Implementation
    (a) Development of large-scale variants of Stochastic Newton method
    (b) Exploration of adjoint-enhanced forward propagation of uncertainty
    (c) Development of adjoint-enabled ablation code
3. Validation Exercises
    (a) Calibration and Validation of CMA-type ablation model using relevant data
    (b) Initial calibration of coupled radiation and aerothermochemistry models using shock tube data
4. Full System Simulations
    Completion of coupled system simulations of reentry capsule using new coupling interface and uncertainty propagation. This first quantification of uncertainty in heat fluxes and ablation rates will use available estimates of input uncertainties.