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Uncertainty Quantification

Feature Extraction Metrics for Quantitative Comparison Between Simulations and Experimental Results
MJ Grosskopf, RP Drake, J Holloway, P Poon, CC Kuranz, B Fryxell, EM Rutter, N Andronova, DBingham

In order to perform quantitative predictive analysis on simulations results of the radiative shock system, output metrics must be devised which can be meaningfully compared between the model and the experiment. For the radiographic data, we have explored output metrics related to the amount and distribution of dense xenon, including the shock location as defined by a breakpoint in a piecewise constant fit to data integrated radially over a fixed window and the total area and axial centroid of xenon which absorbs more than a set threshold of backlighter x-ray emission. Examples and results of the metrics are reported and discussed.

UQ Run Set 10: October 2008 Experimental Design Using the CRASH Laser Package
MJ Grosskopf, RP Drake, JP Holloway, DBingham, B van der Holst, EM Rutter, BFryxell, E Myra, G Toth

The development of the CRASH Laser physics module allows for simulation of high-energy-density laboratory astrophysics experiments fully within CRASH. Previous 2D models of radiative shock experiments used in uncertainty quantification studies the CRASH program have been carried out using the coupled H2D-CRASH codes. Due to the improvement in model fidelity that has been demonstrated, carrying out UQ run sets with the laser package has been considered a critical task. Run Set 10 is the first such set, designed to model the original circular tube design varying 3 modeling parameters and 4 experimental parameters. Preliminary results of those runs are reported and discussed.

Uncertainty Quantification Run Sets
E.M.Rutter, M.J.Grosskopf, J.P. Holloway, R.P. Drake

The uncertainty quantification (UQ) aspects of CRASH are used to assess the predictive capability of the code. To prepare for predicting the Year 5 experiments, uncertainties in code and in experiments need to be estimated and understood. This poster examines the input, running of, and results of several of the UQ run sets that have been performed in the last year, ranging from 1D-3D and focused on code parameters, convergence, and experimental parameters.
Radiative transfer is one of the physics used to model high energy density physics such as the CRASH problem. Opacities are the parameters that describe how electromagnetic radiation propagates through the material. These opacities are generally in tabular form which comprise thousands of points; so, it would be infeasible to try to gain any uncertainty information from this. We have developed methods which apply uncertainty quantification for the first principles models used to calculate the opacities. One of the physics that is used to calculate opacities is statistical mechanics which rely on the ionization potentials of the different elements. It is these ionization potentials that we have defined uncertainty bounds, which are based on open literature data compiled in the SPECTR-w3 database. We have performed 1000's of radiative transfer calculations to determine bounds on quantities of interest which are useful and relevant to the CRASH problem. We show results of this work.

Response surfaces provide a nonintrusive framework for quantifying the effects of uncertainties in the inputs on resulting computational outputs. Using gradient information can in turn provide substantially improved representations of the response surface, which may enable significant computational savings. Here we assess various ways that gradient information based on discrete adjoints can be used to obtain such computational efficiencies within the context of a radiation hydrodynamics simulation. These include piecewise as well as global interpolation schemes. Additionally, we examine effects of the discretization level used in representing the response surface.
Radiation hydrodynamics and radiative shock are of fundamental interest in high-energy-density physics research due to their importance in understanding astrophysical phenomena such as supernovae. The shock waves of similar feature can also be reproduced in a controlled laboratory experiment. However, the cost and time constraints of the experiment necessitates use of an algorithm to generate reasonable number of outputs for making valid inference. We focus on modeling emulators that can efficiently assimilate these two sources of information accounting for their intrinsic differences. The goal is to learn about how to predict the breakout time of the shock given the information on associated parameters such as pressure and energy. Under the framework of Kennedy-O’Hagan model, we introduced an emulator based on adaptive splines. Depending on the preference of having an interpolator for the computer code output or a computationally fast model, a couple of different variants were proposed. Those choices are shown to perform better than the conventional Gaussian process based emulator. For the shock experiment dataset, a number of features related to computer model validation such as using interpolator, necessity of discrepancy function or accounting for experimental heterogeneity were discussed, implemented and validated for the current dataset. In addition to the typical Gaussian measurement error for real data, we considered alternative specifications suitable to incorporate noninformativeness in error distributions, more in agreement with the current experiment. Comparative diagnostics, to highlight the effect of measurement error model on predictive uncertainty, were also presented.
We explore various metrics that indicate the degree to which diffusion does or does not agree with transport in radiative-transfer problems that are relevant to CRASH. One set of metrics involves the "Eddington" tensor, which in a highly diffusive region becomes $1/3$ times the identity tensor. A great deal of information about radiation flow can be extracted from the Eddington tensor. Another set of metrics involves the difference between the divergence of the transport net flux, integrated over each cell, and the divergence of the diffusion approximation to this net flux, also integrated over each cell. This difference can be viewed as the (artificial) source term that would have to be added to the diffusion equation to force it to give the correct solution. Both sets of metrics can be calculated from within a transport code. We use PDT for this.
Simulation Studies

PDT Performance and Scaling
Daryl Hawkins, Marvin Adams, Timmie Smith, Nicolas Castet, Nathan Thomas, Nancy Amato, Lawrence Rauchwerger, Silvius Rus (Quanetcast), Gabriel Tanase (IBM)

To solve problems of interest to the CRASH project, it is critical that PDT perform well on large numbers of processor cores. We report improvements in PDT's parallel efficiency and solve time per unknown. We also present a model for determining the efficiency of parallel transport sweeps on orthogonal grids. Using this model, we have implemented an algorithm in PDT to determine the optimal processor layout and aggregation factors that minimize run time for a given problem.

Preliminary Modeling of Collisionless Shock Experiments With the CRASH Code

The CRASH radiation-hydrodynamics code is designed to model laser-driven high-energy-density experiments. CRASH has been used to simulate collisionless shock experiments performed on the OMEGA laser, with the intent to provide meaningful analysis of the ablative corona of a laser-irradiated plastic foil. Characterization of this ablated plasma will allow for improved experimental design and analysis of existing data. Previous results utilizing H2D as the CRASH preprocessor will be reported, along with the early stages of modeling this experimental design with the CRASH laser package.

Effects of Opacity Uncertainties on Simulations of Radiative Shock Experiments
Bruce Fryxell, Eric Myra

It is straightforward to generate radiative shocks in the laboratory using high-energy lasers. In one such experiment, a thin Be disk is attached to a shock tube filled with Xe gas. The laser pulse accelerates the Be disk, which acts like a piston, driving a strong shock into the Xe. Radiation produced in the hot, post-shock Xe, heats the tube walls ahead of the shock. Material then ablates from the tube walls, and a "wall shock" is driven inward toward the center of the shock tube. This results in a complex shock structure in which the primary shock and the wall shock intersect at a triple point. To date, attempts to simulate this morphology have produced shock structures far more complex than what has been seen in the experiments. One possible explanation for this discrepancy is uncertainty in the opacities of Xe and polyimide, which is used for the shock tube walls. A series of simulations is discussed in which these opacities are varied in order to see what effects they have on the flow morphology. The goal is to determine what opacity values produce results that are the most consistent with the experimental data.
A comparison of discrete-ordinates and flux-limited-diffusion methods for modeling radiation transport in radiative shock tubes
Eric S. Myra and Wm. Daryl Hawkins

The Center for Radiative Shock Hydrodynamics (CRASH) seeks to improve the predictive capability for models of Omega laser experiments of radiative shock waves. The laser is used to shock, ionize, and accelerate a beryllium plate into a xenon-filled shock tube. These shocks, when driven above a threshold velocity of about 60 km/s, become strongly radiative and convert most of the incoming energy flux into radiation.

Radiative shocks have properties that are significantly different from purely hydrodynamic shocks and, in modeling this phenomenon numerically, it is important to compute radiative effects accurately. In this presentation, we examine approaches to modeling radiation transport by comparing two methods: (i) a computationally efficient approximation (multigroup flux-limited diffusion), currently in use in the CRASH code, with (ii) a more accurate discrete-ordinates treatment that is offered by the code PDT. We present a selection of results from a suite of comparison tests, showing both idealized problems and those that are representative of conditions found in the CRASH experiment.

Simulation of Jacobs Richtmyer-Meshkov Instability Experiment with CRASH
Jason Chou, Paul Drake, Bruce Fryxell, Guy Malamud, Pooya Movahed

As part of the CRASH hydrodynamic validation effort, we replicated Collins and Jacobs' Richtmyer-Meshkov instability experiment with CRASH and compared the result with the experimental measurement and visualization, along with results given by other code packages. We achieved good agreement before the re-shock but not afterward, since none of the code packages adequately models the subsequent turbulence and energy cascade.

The Effects of Transport Discretization on the Plastic Wall Energy Absorption Model
Hayes Stripling, Marvin Adams, Daryl Hawkins

Streaming radiation ahead of the shock in the CRASH problem is absorbed in and ablates the tube's plastic wall. The result is a series of secondary radial shocks which strongly interact with and affect the main shock evolution. We present the results of a CRASH-like test problem run-set using the PDT radiative transfer code; each run varies in its energy group structure, angular quadrature, and spatial discretization in the plastic wall. The goal is to determine the level of resolution in energy, angle, and space required to accurately model energy absorption in the plastic wall "downstream" from the main shock.
Radiative Reverse Shock Simulations with the CRASH Laser
R. Sweeney, C. Krauland, M. Grosskopf, E. Rutter, R. P. Drake

Simulations of laboratory scale astrophysics experiments are being implemented using the CRASH code. These experiments are designed to probe properties of Cataclysmic Binary Star systems, also known as Cataclysmic Variables (CV’s), using a laser irradiated shock-tube-target to produce radiative shocks and plasma flows characteristic of CV systems. Experimental data is difficult to collect due to availability of laser facilities and diagnostic limitations and therefore simulations provide a complimentary tool for understanding the evolution of the system. CRASH simulations using the new laser package are being employed to recreate these shock-tube experiments where a tin shock propagates in vacuum down an acrylic tube and produces a reflected, radiative shock when impeded by a fixed aluminum wall. The first results of these simulations have been produced and are shown here. Comparisons to experiment and previous H2D-initialized CRASH simulations are discussed and the future direction for these simulations is presented.

A Data-Model Comparison Using a Novel X-Ray Thomson Scattering Diagnostic
M.R. Trantham, E.J. Gamboa, R.P. Drake

We have developed a novel X-ray Thomson scattering diagnostic capable of creating high-resolution spatially resolved one-dimensional profiles while spectrally resolving the scattered radiation (see poster by Gamboa, et al). This instrument will collect spatially-resolved data profiling the temperature, density, and ionization state of a radiation-driven wave in low-density carbon foam. This data set will be compared to results from CRASH, a numerical model for radiation-hydrodynamics. We expect this study to be very important in analyzing the overall model performance, but also potentially important in refining equation of state and opacity information.

Radiative Properties of Mixtures in and out of LTE
M.Klapisch & M.Busquet

We compare 4 models for the effective densities of components of mixtures. These models, applied to polystyrene (CH ) and polyimide ( C_{22}H_{10}O_{5}N_{2} ) in LTE, yield very different opacities. Two of these models are not thermodynamically consistent. These are the "partial density mix model" (M1), formerly in use, and (M2)-a tentative correction of it. The other two models minimize the free energy. M3 uses equality of chemical potential ; M4 uses commonality of free electron density. These give essentially identical results in LTE. M4 is easily generalized to non-LTE conditions. The non-LTE effects are shown by the variation of Planck mean opacity of the mixtures with temperature and density. Some non LTE results are also shown for Xenon. We conclude that non-LTE effects are important. The non-LTE M4 model is general and could be applied to other mixtures (doped foam, tracers in gases, etc…)
Algorithms and Code Development

Multi-level Preconditioning in CRASH
Gabor Toth, Rob Falgout, Ken Powell, Paul Drake

The Code for Radiative Shock Hydrodynamics (CRASH) solves the flux-limited multigroup diffusion radiation transport and the electron heat transport with a semi-implicit time-stepping scheme. We can solve either for all variables together, or solve one-by-one. While the computational speed and scaling of the two approaches is comparable, we find that the accuracy of the solution is much improved when the equations are solved separately, and it also requires much less memory.

The implicit scheme uses a preconditioned Krylov solver (GMRES, BiCGSTAB, PCG). Our original preconditioner is based on the Incomplete Lower Upper (ILU) decomposition with no fill-in. Since CRASH uses a block-adaptive grid, we opted for a Schwarz type preconditioning performed on a block-by-block basis. While the ILU preconditioner gives satisfactory results on small to medium size problems, the number of iteration grows to several 100s on large problems.

As an alternative to the ILU preconditioner, we have implemented an Algebraic Multi-Grid (AMG) preconditioner into CRASH using the BoomerAMG solver from the HYPRE library. Using AMG drastically reduces the number of Krylov iterations, however, the multi-grid solves are more expensive than the ILU preconditioned Krylov iterations. The setup time for AMG is also considerable.

We compare the efficiency and scaling of the ILU and AMG preconditioners for several CRASH problems.

A non-LTE model for the CRASH code, the RADIOM model
M.Busquet & M.Klapisch

We show when and why non-LTE atomic physics is important for hydrodynamic simulations. The foundations of and justifications for the RADIOM model will be discussed. The basis of the implementation will be presented, as well as a road map for full implementation. In addition, we are modifying the HULLAC code in order to solve time dependent non-LTE rate equations. The purpose of this is to evaluate relaxation times of the plasma following changes in temperature, density, and/or incoming radiation.
Grey Diffusion Acceleration for Discontinuous Finite Element Radiative Transport Problems
Anthony Barbu, Marvin Adams

We analyze and test the effectiveness of a new grey-diffusion preconditioner for accelerating the iterative convergence of multi-frequency radiation transport problems. The grey diffusion equation is the diffusion approximation of Larsen's grey transport acceleration (GTA) equation, and it makes use of the frequency-averaged opacities that are consistent with his definitions. The spatial discretization of the diffusion equation was inspired by the work of Wareing, et al. It finds the global solution of a continuous finite element method (CFEM) diffusion equation, then uses this CFEM solution to decouple the cells in a Discontinuous FEM (DFEM) cell-by-cell solution. The result is a DFEM additive correction to the absorption-rate density, which drives the multi-frequency transport problem. We analyze the behavior of this method for a multi-frequency homogeneous problem using Fourier analysis, and test the behavior for CRASH-relevant test problems.

We also show a simple temperature iteration verification problem for PDT. This problem shows agreement between the solution of a non-linear temperature solution, a linearized solution, and PDT's solution.

Low-dissipation hybrid schemes for simulations of compressible multicomponent flows
Pooya Movahed, Sreenivas Varadan, Eric Johnsen

Type Ia supernovae are thought to be the standard candles of the Universe. Numerical simulations have shown that the fusion front in this phenomenon produces a series of expanding bubbles that exhibit Rayleigh-Taylor (RT) and Richtmyer-Meshkov (RM) instabilities and transition to turbulence. These also occur in Inertial Confinement Fusion (ICF), where uneven compression of the target surface leads to premature mixing, thereby reducing the heating efficacy. Thus, an understanding of RT and RM is important in explaining carbon detonation in Type Ia supernovae as well as preventing premature mixing in ICF. In the present work an efficient hybrid scheme is proposed for numerical simulations of compressible multicomponent flows. The algorithm is based on a high-order accurate weighted essentially non-oscillatory (WENO) scheme for shock capturing and a non-dissipative central scheme in the split form for smooth regions. The central-difference method results in a reasonable speed up and exhibits better resolution properties for turbulence. The shock capturing is handled using the AUSM+up Riemann solver with a WENO reconstruction of the primitive variables. A new sensor based on the first norm of the difference of WENO weights from the ideal weights is used at the beginning of each Runge-Kutta step for a smooth transition between the central and WENO fluxes at interfaces. The scheme is shown to prevent spurious pressure oscillations at interfaces. The performance of the method is presented for a set of problems including the Sod shock tube problem, the Shu-Osher problem, the planar Richtmyer-Meshkov instability, the three-dimensional Rayleigh-Taylor instability and the three-dimensional isotropic turbulence problem inside a box.
Investigation of Mixed Cell Treatment via the Support Operator Method
N Patterson, K Thornton

A support operator method (SOM) discretization of the diffusion equation is used to examine treatment of mixed cells. The diffusion equation is used to simulate radiation transport in optically thick system. Multiple fluids or species can be simulated by assigning distinct diffusivities to different regions of the computational domain. A mixed cell occurs when the boundaries of the fluids do not align with the boundary of the mesh cells. The SOM discretizes the diffusion equation into a symmetric and positive-definite matrix system, which allows for more efficient solvers. The SOM is spatially second-order accurate for isotropic, anisotropic, continuous, or discontinuous diffusion coefficients. The use of anisotropic diffusion tensor is explored as a means of simulating the material interface in a mixed cell by rotating a diagonal diffusion tensor. The results are compared with more typical mixed cell treatments, such as global or local grid refinement, or setting the diffusivity equal to that of the fluid occupying the largest volume of the cell.

Resolution in Time for Multiphysics Systems: Operator Splitting and Radiation-Hydrodynamics
David Starinshak and Smadar Karni

Multiphysics models are oftentimes complicated by competing physical processes which act over differing spatial and temporal scales. Numerical analysis is challenging: a naive but efficient discretization risks failing to resolve significant physical processes over time. Likewise, multiphysical timescales may be too restrictive to achieve accurate temporal resolution in any reasonable amount of CPU time. We explore this issue using a multiphysics model for radiation-hydrodynamics. Three examples of temporal inaccuracy are highlighted, arising from using an operator-split methodology to discretize the system. A numerical test relevant to the CRASH problem--1D wall ablation--illustrates our findings.

Multimaterial Radiative Shock Hydrodynamics Using Level Sets
David Starinshak and Smadar Karni

We are actively developing a numerical framework based on level sets to simulate radiative hydrodynamic systems which contain multiple fluid components. We present a summary of our model equations, their discretization in space and time, as well as strategies for discretizing material-dependent quantities. Topics include (i) the removal of spurious pressure oscillations across material interfaces, (ii) the implementation of multiple level set functions to model three or more fluid components, and (iii) the related issues of species mass conservation and spurious evaporation.
A Higher-Order Face Finite Element Radiation Diffusion Method for Unstructured Curvilinear Meshes
Andrew Till, Thomas Brunner, Teresa Bailey

We implement a novel mixed-finite-element method for the radiation diffusion system. The tight material-to-radiation-field coupling requires consistency. Standard continuous finite element methods yield node-centered diffusion discretizations flux that are inconsistent with hydrodynamic zone-centered discretizations for the material temperature; diffusion discretizations that are zone-centered are generally limited to orthogonal or non-curved meshes and first-order accuracy. We overcome this difficulty by solving for the pointwise current in the Raviart-Thomas space of arbitrary order and then by taking a discrete divergence to obtain the flux that is now zone-centered and piecewise-polynomial-discontinuous. The MFEM code system provides the necessary basis functions, matrix assembly tools, and linear solvers. We find that the mixed-finite-element method converges at expected rates even on highly distorted and twisted meshes. The system appears to conserve energy; research is on-going.

Shock Capturing Anomalies and the Jump Conditions in One Dimension
Daniel W. Zaide, Philip L. Roe

In this work we examine how the nonlinearity of the Rankine-Hugoniot jump conditions dictates the behavior of shock capturing methods, particularly of Godunov-type schemes. Here we present four related one-dimensional examples of the artifacts caused by this: sub-cell shock position in the stationary shock, the slowly moving shock, the wall heating problem, and the carbuncle phenomenon. Each one of these well known problems is shown to be directly related to the nonlinearity of the Hugoniot and numerical experiments are performed to verify the connection. Lastly, a system with a straight Hugoniot is described and shown not to suffer from any of these phenomena.
Experiments

Radiative shock experiments at the Omega Laser Facility
CC Kuranz, CM Huntington, CM Krauland, FW Doss, SR Klein, PJ Susalla, R Gillespie, RP Drake and the CRASH team

An overview of several CRASH experiments regarding radiative shocks will be presented. We have performed experiments on the Omega Laser that irradiate a 20µm thick Be disk with ~4 kJ of laser energy. This shocks and accelerates the disk into a Xe gas at 1.1 atm. These radiative shocks can reach up to 130 km/s. Several diagnostic techniques have been used to acquire data from shock breakout time up to 30 ns. These techniques include area x-ray radiography, ungated pinhole x-ray radiography, streaked radiography, interferometry and optical pyrometer. We have recently explored the effects of tube geometry on shock evolution, including wider shock tubes, cylindrical nozzle targets and elliptical nozzle targets.

Spike morphology in supernova-relevant hydrodynamics experiments

This presentation describes experiments performed on the Omega and Omega EP lasers exploring the 3D Rayleigh-Taylor instability at a blast-wave-driven interface. These experiments are well-scaled to the He-H interface during the explosion phase of SN1987A. Laser energy is used to create a planar blast wave in a plastic disk, which then crosses the interface between the disk and a lower-density foam, inducing the RT instability. The plastic disk has an intentional pattern machined at this interface. This seed perturbation is three-dimensional with a basic structure of two orthogonal sine waves with a wavelength of 71 µm and amplitude of 2.5 µm. Interface structure has been detected under these conditions using dual, orthogonal radiography, and some of the resulting data will be shown. Current experiments are further examining the features of the unstable interface using proton radiography.

Imaging X-Ray Thomson Scattering Spectroscopy for Characterizing Extreme Matter States

In many laboratory astrophysics experiments, intense laser irradiation creates novel material conditions with large, one-dimensional gradients in the temperature, density, and ionization state. X-ray Thomson scattering (XRTS) is a powerful technique for measuring these plasma parameters. However, the scattered signal is typically measured with little or no spatial resolution, which limits the ability to diagnose these inhomogeneous plasmas.

We report on an experiment at the Omega laser to diagnose a radiation-driven heat wave in a low density carbon foam. The temperature profile is resolved spatially using a new imaging x-ray Thomson scattering diagnostic. Diffraction of scattered x-rays from a toroidally curved crystal creates high-resolution images that are spatially resolved along a one-dimensional profile in the target while simultaneously spectrally resolving the scattered radiation.
Same Shot x-ray Thomson Scattering and Streaked Imaging of Xenon Radiative Shock Experiments.

These experiments seek to measure the plasma parameters of the CRASH xenon radiative shock system with high accuracy, employing streaked x-ray radiography and x-ray Thomson scattering diagnostics on each shot. We detail how this diagnostic combination allows for precise interrogation of the different regions of the shock, including the radiation-heated upstream precursor, the radiatively collapsed cooling layer, and the downstream material. Spatially and temporally correlated data from the x-ray streak camera and gated spectrometer is shown, and plans for future iterations of radiative shock experiments are also discussed.

Reverse Radiative Shock Experiments Relevant to Accreting Stream-Disk Impact in Interacting Binaries
C.M. Krauland, R.P. Drake, C.C. Kuranz, C.M. Huntington, S. Klein, R. Young, R. Sweeney, B. Loupias, E. Falize, T. Plewa

In many Cataclysmic Binary systems, mass onto an accretion disk produces a ‘hot spot’ where the infalling flow obliquely strikes the rotating accretion disk. It has been argued (Armitage & Livio, ApJ 493, 898) that the shocked region may be optically thin, thick, or intermediate, which has the potential to significantly alter its structure and emissions. We report two experimental attempts to produce this type of radiative reverse shock in a colliding plasma stream. In the laboratory this requires producing a sufficiently fast flow (>100 km/s) within a material whose opacity is large enough to produce energetically significant emission from experimentally achievable layers. The experiments have been performed at the Omega-60 laser facility. We will discuss the astrophysical context, our experimental design, and the available data.

Target Fabrication for OMEGA Campaigns at the University of Michigan
S. R. Klein, D. C. Marion, R P. Drake, C. C. Kuranz, C. M. Huntington, C. Di Stefano, C. M. Krauland

The University of Michigan has been fabricating targets for OMEGA campaigns since 2003. These experiments explore supernova-relevant high-energy-density physics. Using an automated system of stages and through the ever innovated designs of University of Michigan graduate students, our targets have become increasingly sophisticated. Our systematic approach has earned us repeatability that is reflected in our successful data. A large portion of our target fabrication is accomplished by our undergrads, whose involvement has proven to be invaluable. We present improvements in our capability techniques and their results from recent campaigns.