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HIGH-FIDELITY PLASMA CODES FOR BURN PHYSICS

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HIGH-FIDELITY PLASMA CODES FOR BURN PHYSICS

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Abstract: Accurate predictions of equation of state (EOS), ionic and electronic transport properties are of critical importance for high-energy-density plasma science. Transport coefficients inform radiation-hydrodynamic codes and impact diagnostic interpretation, which in turn impacts our understanding of the development of instabilities, the overall energy balance of burning plasmas, and the efficacy of self-heating from charged-particle stopping. Important processes include thermal and electrical conduction, electron-ion coupling, inter-diffusion, ion viscosity, and charged particle stopping. However, uncertainties in these coefficients are not well established. Fundamental plasma science codes, also called high-fidelity plasma codes are a relatively recent computational tool that augments both experimental data and theoretical foundations of transport coefficients. This paper addresses the current status of HFPC codes and their future development, and the potential impact they play in improving the predictive capability of the multi-physics hydrodynamic codes used in HED design.

1. Definition of HED and the role of integrated multi-physics codes and experiments

The National Academy of Science report [1] from 2003 called the frontiers in High Energy Density (HED) Physics the X-Games of contemporary science, and for good reason. Extreme states of matter in the high energy density (HED) regime are characterized by temperature and densities where total pressure is in excess of 1 Mbar. This definition spans a wide range of physical phenomena. HED includes the warm dense matter properties of the cores of the giant planets where matter is strongly coupled and degenerate [2]. HED also includes burning plasmas in an inertial confinement fusion capsule where plasmas are non-equilibrium, multiple species with varying ionization states, non-degenerate and weakly or strongly coupled, depending on the species type [3].

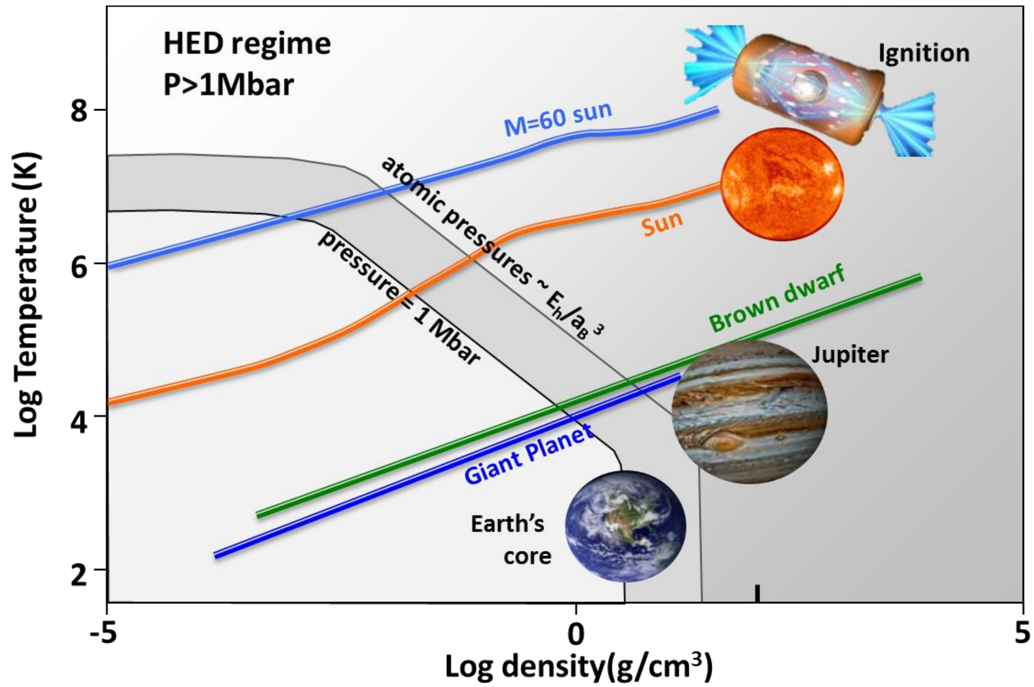

Figure 1: The high energy density regime defined on a temperature-density phase space diagram

The arrival of new high energy density (HED) physics facilities, such as the National Ignition Facility (NIF) [4], and next-generation light sources, such as the Linac Coherent Light Source (LCLS) [5], has enabled experiments on matter in the warm to hot dense regimes. The design and analysis of these experiments have necessarily motivated the development of complex, multi-physics hydrodynamic (MPH) codes [6].

MPH codes rely on a fluid description of the plasma. Given the length (micron) and time (nanosecond) scales, the fluid description is a practical and useful approach to solving complicated HED design problems. However, it is clear that MPH codes do not offer a complete description of HED matter in two significant ways. The first is that for certain ICF platforms, so-called kinetic effects exist. These are associated with long mean free paths of the particles of the plasma. The long mean free path means the hydrodynamic assumption has broken down. An example of these phenomena is barodiffusion where plasma phenomena associated with self-generated electric and magnetic fields can lead to the yield anomaly in direct-drive ICF implosions shot at the OMEGA facility [7].

The second reason for the incomplete description of HED matter by MPH is that they rely on a variety of equation of state (EOS) and transport model inputs. MPH codes solve a set of Euler or Navier-Stokes hydrodynamic equations. The Euler or Navier-Stokes hydrodynamic equations rely on theoretical or science code inputs, EOS information, transport coefficients and closure approximations. Examples of transport models include plasma viscosity, diffusivity, thermal and electrical conductivity, electron-ion relaxation rates, stopping power, etc. EOS models are typically calculated with high-fidelity plasma (HFP) codes like path-integral Monte Carlo (PIMC) [8] and quantum molecular dynamics (QMD) [9]. In addition, EOS data in HED relevant regimes is being obtained at the National Ignition Facility [10], the

Omega laser [11] and Z [12]. Although not in an ideal state, EOS models used in MPH codes tend to be better validated with a stronger theoretical basis than transport models. Transport models on the other hand have rarely been validated in the HED regime. Although experimental platforms have been developed for stopping power, for the most part, HED experimental platforms are sorely needed for validation of transport models. Recent design work on developing an experimental platform based on the polar direct drive exploding pusher capsule for electron-ion relaxation rates demonstrates the challenges involved. Isolating the specific physics in an HED platform is difficult which means identifying the other physical sources affecting the data and quantifying it are needed. In addition, transport models calculated with high-fidelity plasma (HFP) codes like QMD, molecular dynamics (MD) or kinetic equations (e.g. Vlasov Fokker-Planck) are relatively recent. A desired state for the MPH codes is to ensure the accuracy of the EOS and transport models through experimental validation and a firm theoretical basis through the use of HFP codes. This paper is about improving the predictive capability of MPH codes by using HFP codes to underwrite the EOS and transport models.

In section III we give a more complete description of the strengths and weaknesses of the various HFP codes in addition to their various levels of development.

2. Science drivers coming from the programs

Inertial confinement fusion experiments performed at NIF and Omega and pulse power experiments performed at Z rely on design calculations using MPH codes of highly non-linear integrated HED phenomena spanning the warm dense and hot dense matter regimes. A weak link in the MPH codes is the accuracy and ranges of validity of the EOS and transport models being used. Computational physicists and designers would like to know the following

- For pure materials, what is the accuracy of the transport and EOS models with quantified uncertainties?
- What is the accuracy with quantified uncertainties for transport and EOS models in the presence of mixtures?
- For both pure materials and mixtures, what are the bounds or ranges of validity of the models being used in the MPH codes?

Identifying the dominant processes and the largest uncertainties in an HED design calculation relies on sensitivity analysis methods [X]. The validity of the results coming from sensitivity analysis calculations relies on accurate uncertainty bounds placed on EOS and transport models. Unfortunately, the bounds just do not exist. HFP codes would play an important role in providing the quantitative uncertainties of EOS and transport models through HFP code comparison and comparison with data.

In October of 2016, the Plasma Transport Coefficient Comparison Workshop will be held. This workshop will focus on comparisons of transport coefficients such as viscosity and conductivity for C, H and CH (at a range of temperatures and densities) to help assess the current state of the art of HFP codes and to provide a forum for discussions of the detailed implementation and assumptions of the various codes. Specific goals will include:

- To quantify uncertainties in a variety of transport coefficients used in hydro codes
- To increase understanding of the strengths and weaknesses of various approaches
- To facilitate improved fits and tables for simulation and post-processing codes
- To identify research priorities for inertial confinement fusion and high energy density science in general

This workshop will be of great help in getting a better sense of the current assessment of the accuracy of transport coefficients and the HFP codes used to calculate them.

3. High-fidelity plasma (HFP) codes-Current status

MPH codes solve a set of Euler or Navier-Stokes hydrodynamic equations. Models in the MPH codes rely on theoretical or science code inputs, EOS information, transport coefficients and closure approximations. The fundamental basis for the Euler or Navier-Stokes hydrodynamic equations is a many body description of the plasma electrons and ions based on the classical or quantum Liouville equation. Classical molecular dynamics (CMD) codes which use only the inter-particle potential and the Hamilton equations of motion are effectively solving the classical Liouville equation. Quantum molecular dynamics (QMD) codes such as VASP [X], use Born-Oppenheimer molecular dynamics computes an approximate solution to the many-body Schrödinger equation for the electrons, either within density functional theory (DFT), solving the Kohn-Sham equations, or within the Hartree-Fock approximation. The ions are treated with CMD. Electronic structure can also be solved from the many-body Schrodinger equation using Path Integral Monte Carlo (PIMC) [X] or Quantum Monte Carlo (QMC) [X] methods. For the lack of a better phrase we will refer to CMD, QMD, PIMC, and QMC codes as ab initio codes since they describe matter at a fundamental level. Because of their fundamental description of matter, ab initio codes treat the micro-physical aspects of HED matter on short length and time scales (Angstroms to hundredths of a micron and femto to pico seconds)

Velocity moments of the classical or quantum Liouville equation yield an infinite sequence of equations that describe the temporal and spatial evolution of 1-particle, 2-partcile, n-particle distribution functions. This sequence of equations is called the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy. By considering the first two equations of the BBGKY hierarchy and exploiting various properties of the physical system such as range of interaction, strength of interaction, density of particles, etc., the Vlasov, Landau (or Fokker-Planck), Boltzmann and Lenard-Balescu (LB) equations can be derived for both classical and quantum systems. We will refer to this class of codes as kinetic equation codes. Kinetic equation codes are intermediate between the ab initio codes and MPH codes. Given their underlying caveats, their numerical solution will automatically include non-hydrodynamic effects such as transport effects that MPH codes require as input.

The solution of the kinetic equation yields the 1-particle distribution function from which particle number, fluid velocity and energy can be determined. The length and time scales of kinetic equations tend to be similar to those seen in hydrodynamic simulations. Of particular interest to us will be the Vlasov, Landau and LB equations. These equations can only be used at density-temperature conditions appropriate for weakly coupled plasmas where the average kinetic energy is much larger than the average potential energy. Both mesh and particle based methods exist for solving these equations. The best known and mature particle based codes are Particle-in-Cell (PIC) which typically solve the Vlasov equation. PIC codes are the workhorse for many laser plasma interaction (LPI) and magnetic fusion energy (MFE) applications. Codes such as VPIC [X] rely on PIC coupled to the Landau collision operator to model collisional plasmas relevant to HED. Mesh based methods for solving Vlasov and Landau exist. The Eulerian-based kinetic code LOKI evolves the Vlasov-Poisson system in 2D+2V-dimensional phase space with collisional effects included. The new code iFP of Luis Chacon of LANL is an example of a mesh based 1D+2V Vlasov-Landau code that is targeted for ICF applications. Arguably, mesh based codes for Vlasov and Landau equations are not the equal to PIC codes as far as maturity and code production status. The classical or quantum LB equation has had very little algorithmic development work done until recently [X]. This is due to the complexity of the form of the equation.

HFP Code	Strengths	Weaknesses	Integrated code impact
Path integral and quantum Monte Carlo	Describes the N-body quantum problem. The Gold standard	Challenging at low-T. Application is equilibrium	EOS for high to moderate T mixtures
Quantum molecular dynamics	Gold standard at low-T. Gold standard for warm dense matter	Challenging at high-T. Electrons are in equilibrium. Electronic structure is usually calculated with density functional theory, MD for ions.	Transport properties of ions. EOS of mixtures
Classical molecular dynamics	Fast and large number of particles. Fully dynamic for ions and electrons	Relies on quantum statistical potential to describe quantum interactions. Short time scales and small length scales	Non-equilibrium phenomena such as equilibration, transport, stopping power. Dynamics of high-Z low-Z mixed plasmas
Kinetic Theory	Larger length and time scales. Interim between N-body codes and fluid descriptions of matter. Fully dynamical.	For weakly coupled plasmas. Numerical methods are either mesh based or Particle-in-Cell. Solution requires solving 6D or 12D phase space distribution functions.	Kinetic effects. Non-Maxwellian plasmas.
Fluids	*Large length and time scales. Of practical use for design calculations*	*Models rely on theoretical or science code inputs, EOS information and closure approximations.*	*These are the codes we target*

Table 1: Strengths and weaknesses of high fidelity plasma codes and their type

4. Addressing MPH needs through high-fidelity plasma (HFP) codes

For the purposes of establishing a timeline for HFP code development and their application, we list below near, mid and long term objectives. We have prioritized the set of tasks within each time element.

Near Term

Mature HFP codes and their application

There exist a fairly mature set of computational tools which should be exercised to compute the transport properties of HED matter at a variety of density and temperature conditions. Through significant programmatic and LDRD investment, these computational tools include PIC, QMD, MD and kinetic equation solvers. The Plasma Transport Coefficient Comparison Workshop will be an excellent opportunity to compare the computational results of a single transport model coming from different HFP codes. A study should be carried out that prioritizes kinetic problems of interest, leading to a white paper endorsed by the broad kinetic community. The current situation is not focused on solving the larger physics problems of interest to the HED community using the suite of HFP codes available. Instead, the computational HED community has evolved into a collection of code efforts without a larger strategic vision.

Recommendations:

- Detailed code comparisons should be made. (Murillo has designed one such test problem for the transport coefficients workshop in October 2016). Validation of the different collision modes across species, temperature and density for physics accuracy is needed. MD has a ground truth can be used in lieu of experimental data.
- Use relevant HFP codes to compute the transport properties (viscosity, diffusivity, conductivity) for HED relevant materials and low-Z and high-Z mixtures at warm dense matter conditions and compare with theory. Assess impact on ICF calculations.
- Use relevant HFP codes to compute the transport properties (stopping power, diffusivity, conductivity, viscosity) for HED relevant materials and mixtures at hot dense matter conditions and compare with theory. Assess impact on ICF calculations.

BGK

This effort solves a new multispecies extension of the Vlasov-BGK kinetic model. The Bhatnagar-Gross-Krook (BGK) collision operator replaces the integral form of the Boltzmann collision operator with a nonlinear relaxation operator that drives the distribution function to equilibrium. By removing the integral operators, this drastically reduces the amount of computation required to calculate the effect of collisions. Further savings are realized because each species can trivially have separate velocity space grids, which removes the resolution requirements needed when using integral operators for problems with large mass ratios between species. The Vlasov-BGK model for single gas species is very mature and has been widely used in the aerospace community, however multispecies extensions have not been explored in a rigorous fashion. Several implementations, including one given in the Naval Research Laboratory Plasma Formulary, do not conserve momentum or energy in general, and others do not satisfy an entropy inequality, a key feature of kinetic theory.

Jeff Haack, Cory Hauck, and Michael Murillo have developed a new multispecies BGK approach that is both conservative and entropic, in contrast to previous multispecies BGK attempts. In addition, this model directly incorporates the molecular-dynamics verified cross sections for dense plasmas developed by Stanton and Murillo. An ionic transport model has been derived for this system and a 1D+3V code is under development.

Recommendations

- Develop a full electron-ion plasma transport model based on this BGK model. This could give improvement on the Lee-More model for electron and thermal conductivities in dense plasmas.
- Use this 1D-3V model to study interface diffusion and mixing in ICF-relevant problems.
- Development of a multi-scale code that directly connects the relaxation rates to a molecular dynamics code in the Heterogeneous Multiscale Method (HMM) framework.

High dimension kinetic theory

This effort strives to solve the kinetic equations of the Vlasov-Landau, Vlasov-LB or hybrid approaches. The 1-particle distribution function f(r,v) is in general a function of three space and three velocity directions. This is a daunting computational problem. In the past, researchers have focused on developing Landau equation solvers for homogeneous and isotropic plasmas where the 1-partilce distribution function has only one dimension, speed. Even in the 0D+1V case, mesh based methods are non-trivial since not all numerical methods preserve conservation of particle number or energy. Hybrid approaches discussed above.

Because there is need for very accurate kinetic solvers for a wide variety of applications, new approaches are desired. The usual "solution" to this "curse of dimensionality" (COD) is to use particle-based methods rather than grid-based methods, which in turn poorly treat collisions and are subject to noise. Recently, mesh based methods for Vlasov-Landau are being pursued in 1D+2V dimensions. LLNL has the LOKI code which solves the Vlasov-Landau equation UCLA under the leadership of Warren Mori have the OSHUN code that is a relativistic 2D+3V Vlasov-Landau (C++) code that incorporates a spherical harmonic expansion of the distribution function, where the number of terms is an input parameter that determines the angular resolution in momentum-space. Luis Chacon is developing a 1D+2V Vlasov-Landau code for ICF applications. .

Whereas the Landau equation contains Coulomb logarithms to regularize infinities in the Coulomb collision integral, the quantum LB equation has no such terms. The quantum LB equation is finite and needs no cutoff terms to keep it finite. Therefore, there is a tremendous advantage from a predictive capability standpoint to invest the appropriate resources and develop the numerical methods for the quantum LB equation. Current research efforts have focused on spectral methods applied to the quantum LB equation in 0D+1V. The spectral method ensures conservation of particle number and energy automatically. This research avenue is offering promising results but more work needs to be done in the area of extending the method to anisotropic plasmas.

The kinetic equations Vlasov, Landau, LB are an approximation to the first two coupled equations of the BBGKY hierarchy. Another approach is to obtain the 2-particle distribution function in another fashion outside of the usual kinetic equation solver paradigm. This idea is cutting edge from a research point of view but it should be pursued. The first equation of the BBGKY hierarchy contains a source term which is a function of the 2-particle distribution function. MD can be used to obtain the 2-particle distribution function, and then this result could act as a source term for the kinetic equation for the 1-particle distribution function. Various assumptions underlying kinetic theory could be tested including the Bogolyubov hypothesis [X] and the underlying assumptions of the Landau and LB equations.

Recommendations

- Exercise kinetic equation codes (e.g. OSHUN, LOKI and iFP) on 1D ICF implosions and compare to MPH simulations. Investigate the effects of electromagnetic field on complex flows. Add needed physics as required. This could include radiation transport, thermonuclear burn,etc.
- Extend the spectral method technique to anisotropic and inhomogeneous plasmas. Develop a 1D+2V Vlasov-quantum LB code for ICF implosions.
- Reduce the BY2 equation into something manageable through a 12D Grad expansion. This idea has been explored by Lebowitz, Frisch and Helfand (LFH) (Phys. Fluids 3, 325 (1960)). However, while the idea is there, nothing was done with it computationally. The idea is to develop Section 4 of LFH into a computational approach, explore algorithms, and validate with MD.
- Develop the required technology to extract 2-particle distribution functions from MD codes. Test the Bogolyubov hypothesis. Longer term, develop a BY1 code with on the fly input from 2-particle distribution function information coming from MD codes.

Mid Term

Multi-temperature equations of state

The state of thermodynamic equilibrium is very special. In this state there are many very powerful and simple things we can say about a system. Conversely, in a state of non-equilibrium, there is almost nothing we can say; there are an infinity of possibilities and each needs to be treated as a special case. Even the seemingly innocuous case of two temperatures (2T) is nearly impossible to treat, and this is the case for all plasmas of interest. This can be seen in the following way: to say a species S has a temperature is to say that the one-body distribution function is Maxwellian (classically) with temperature T. And, we can also say that this temperature varies in space, so that in reality, the 1-particle distribution function describes T(x). But, there are two serious problems:

We specify the temperature in terms of the one-body distribution function, for which there are an infinite number of consistent two-body functions. Saying a system is multi-temperature does not provide enough information.

If the system is 2T, kinetic theory may give an undesired result. For example, the Boltzmann collision integral vanishes in equilibrium and yields the Maxwellian; thus, if you have a 2T system, the collision terms vanish and the system cannot equilibrate further. There is always an δf in a 2T system that we generally don't know.

Recommendations:

- Much of this is very easy for the case of an ideal gas - 2T EOS for the ideal is trivial. The issues arise when there are important interactions, so an approach at least at the Vlasov-BGK level is needed.
- Some work has been done with the full BBGKY and that should be examined and extended.
- An experiment could be designed to test 2T EOS concepts, and LCLS looks best since it can span the region of WDM to HDM where correlations can be well controlled in a simpler experimental geometry that capitalizes on the XFEL/slab geometry/etc.

Hybrid approaches for solving kinetic equations

In the previous discussions of HFP codes, we have made a distinction between MD type codes, kinetic equation solvers and MPH. A different approach is to take advantage of the relative strengths of each approach and combine them for increased effectiveness. This idea has recently been explored using quantum kinetic theory for electrons and classical MD ions in a formulation called kinetic theory molecular dynamics. This approach could be useful for addressing transport properties of hot dense matter.

A similar hybrid method is being explored for warm dense matter where the electrons exhibit quantum degeneracy and strong coupling. In an idea proposed by Michael Murillo and Liam Stanton, Using quantum hydrodynamics (QHD) to treat the electrons and classical MD for the ions, David Michta of LLNL has developed a massively parallel 3D QHD-MD code for simulating stopping power in warm dense matter.

Recommendations

- Develop a 1D+2V kinetic equation solver for the quantum 1-particle kinetic equation. Integrate the solver with an MD code for ions. Use the code to address transport model issues and ICF implosions.
- Further develop the QHD-MD code to address transport issues and hydrodynamic instabilities in warm dense matter.

Multi-species hydrodynamics of dense plasmas

Modeling transport in HED experiments is challenging because of material mixing processes that are typically not included in lowest-order hydrodynamics models (e.g., Euler). It is imperative that we model these processes accurately as they impact mixture physics (e.g., opacities and equations of state) that drive the material evolution, nuclear reactivities and radiative losses.

Modeling of diffusive mixing is complicated by the fact that hydrodynamic models rarely explicitly model large numbers of species. For example, in a (plastic) ablator-fuel region, there are five species: H, D, T, C, O (and other impurities and fusion products). For this reason, it is common to retain the single momentum equation but generalize the continuity equation to N-species non-linear diffusion equations. However, due to couplings among all species through total momentum and energy conservation, the resulting diffusion equations are difficult to obtain in closed form, usually involving a matrix inversion to obtain the species fluxes. While some excellent work appears in the astrophysics literature (based on the work of Burgers), a {\it complete} set of equations for wide-ranging HED applications that is experimentally or computationally validated (using high fidelity physics codes) has never been developed.

Recommendations:

- Sustained theoretical effort to develop models from { exact} hierarchy equations for mixtures. Develop new closures, and understand each approximation across material properties. Reduce carefully to practical reduced-order-models, but don't leave holes.
- Develop fast algorithms for solving many-species non-linear diffusion equations.
- Understand in detail how to treat the electric field, and the implications of the common use of the electron pressure (and how that is connected to EOS data bases) in its place.
- Once each approximation from the above is detailed, perform large-scale molecular dynamics to validate the assumptions.
- Develop data for the transport model in the form of transport coefficients. (This overlaps with other areas.)

Long Term

Next generation multi-scale: On the fly data

Modern MPH code methods extract out the microscale data into static tables which are read and interpolated on to provide EOS and opacity points to the ICF codes. Modern exascale systems will struggle managing the scale of data in memory in the not too distant future. To address this issue one possibility is to use the fact that floating point operations are effectively free on these systems to calculate the EOS and opacity properties dynamically. This solution would allow for the treatment of mixtures to be more accurate and account for the possibility that the individual ion species and the electrons may not be in equilibrium, a situation that would be impossible to track for a table based method.

Adaptive Method of Refinement

AMR is a method in which the right method is used for the right situation. It should be considered as the "optimal" approach to a problem in the sense that the best expansion is used for a given situation. The usual example is: when the collisionality is high, use hydro; when it is not, use Vlasov kinetic theory.

Viewed this way, there are a number of issues we should begin to explore. How we do treat the "transition region" between hydrodynamics and Vlasov kinetic theory? We need a method that bridges hydrodynamics to Vlasov kinetic theory; this is an outstanding problem in science, not just HED science. How do we stitch together at the boundaries? Suppose a metric tells us to switch from Vlasov kinetic theory to hydrodynamics, how is this done, given that there is very different information content?

Recommendations

- Consider a 1D set of problems, such as shocks, laser-driven plasma, etc. Develop two codes (hydrodynamics and Vlasov kinetic theory), develop metrics for transitioning in each direction and code transitioning capabilities. What issues emerge?
- How sensitive is the result to choices (e.g., transition metric, level of hydro, level of KT, etc.). Are there problems in which the codes should run side by side (e.g., hydro away from the shock, KT near the shock)?

5. Summary

The maturity of leadership-class experimental and computational facilities is ushering in qualitative changes in our approach to understanding, modeling and exploiting high energy-density physics environments. In particular, exascale computing will advance our current capabilities in terms of accuracy and fidelity, allowing us to achieve an unprecedented predictive capability. Moreover, exascale computing will also allow paradigm shifts in which we approach computational modeling through qualitatively new methods, algorithms and models. This document discusses a broad spectrum of novel approaches for purposes of discussion, improvement and prioritization.

Significant investments have already been made in HFP codes and continued advances are being made in algorithms and methods. The time is ripe to integrate these approaches and provide a clear development path based on a single goal which is to improve the predictive capability of the HED design codes. The HFP codes provide the microphysical detail lost in MPH codes. Since MPH codes require EOS and transport models as input, and experimental validation data of these models is scarce, HFP provide an important role in supplying the MPH codes with the best models possible.

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