Thermonuclear Burn

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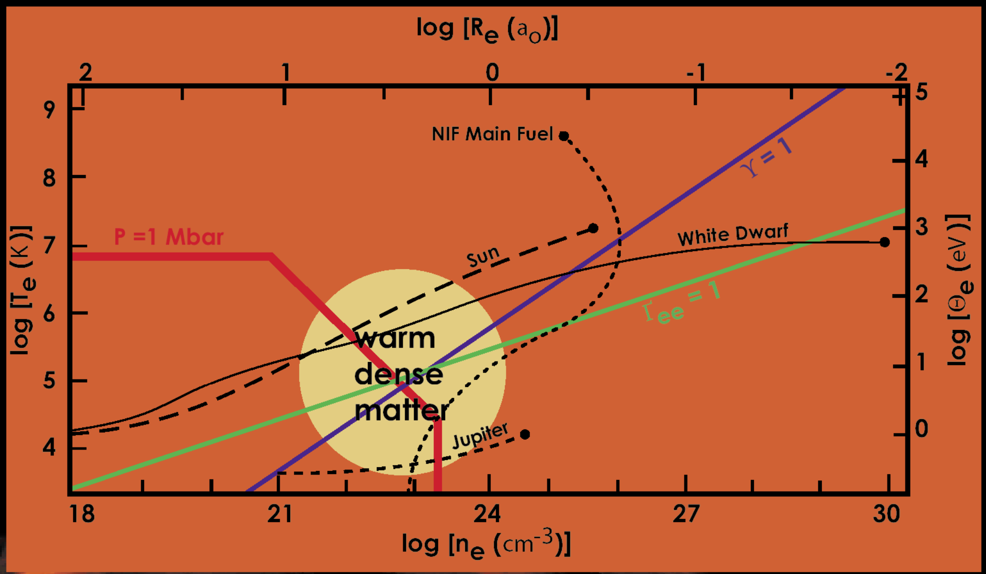
Michael S. Murillo, T-15

Thermonuclear burn is the process in which light elements fuse into heavier elements at high temperature with the release of energy. In stellar and inertial confinement fusion environments, burning occurs in a dense medium that complicates our ability to predict their behavior in detail. The effects of the dense medium are frequently quantified with the dimensionless parameters Υ and Γ. The parameter Υ is the ratio of the Fermi energy to the temperature and measures the degree of electron degeneracy, whereas Γ is the ratio of average potential to kinetic energy and measures the degree of Coulomb coupling. In the figure, where various physical regimes are shown versus temperature and density, the lines of constant $\Upsilon=1$ and $\Gamma=1$ are shown. The regimes of degeneracy and strong coupling are below the respective lines; note that at higher densities and lower temperatures plasmas tend to be degenerate and/or strongly coupled. When matter is both mildly degenerate and moderately coupled, we refer to it as "warm dense matter," which is shown as a circle in the figure.



The radial variation of temperature and density of the sun is shown as a dashed line in the figure. Note that the core of sun exceeds solid density but is hot enough that its plasma is weakly coupled and very mildly degenerate. This is typical of a burning plasma because very high temperatures are needed for the nuclear reactions to take place. If we consider inertial confinement fusion, however, we explore a wider range of conditions. Shown in the figure is the time-history of the main fuel of a NIF capsule. The capsule starts out cold and dense, deep in the warm dense matter regime, and is rapidly heated and compressed such that it remains nonideal until very late times when thermonuclear burn can occur in a fairly ideal plasma. To model such an implosion, we must describe a wide variety of processes through the entire time history, which requires physics models valid over orders of magnitude in temperature and density. This is the challenge of the thermonuclear burn project and other projects like it.

Although many processes are important to thermonuclear burn, a few contributions from X-1, T-1, T-4, T-15, and T-16 have been collected here. This topic of research remains a vibrant area of interdisciplinary, cross-divisional research.

Ionization State of Heavy Atom in Hydrogen Plasma by Molecular Dynamics

Ken LaGattuta, X-1

Fermion Molecular Dynamics (FMD) was applied to calculations of the net positive charge Z^* on a heavy atom embedded in a hydrogen plasma. Calculations were performed for a central atom with nuclear charge Z_0, where $18 \leq Z_0 \leq 92$, and for a range of hydrogen temperatures and densities, such that hydrogen was completely ionized. FMD results were compared with generally accepted values of Z^*, for plasmas formed from the pure elements. This work is intended to guide predictions of Z^* for atoms in mixtures of elements at high densities, obtained by less rigorous methods. Displayed here are FMD values of electron and proton density as a function of distance from a central krypton ion, when $kT_e = 20$ eV and $Z^* = 5$.

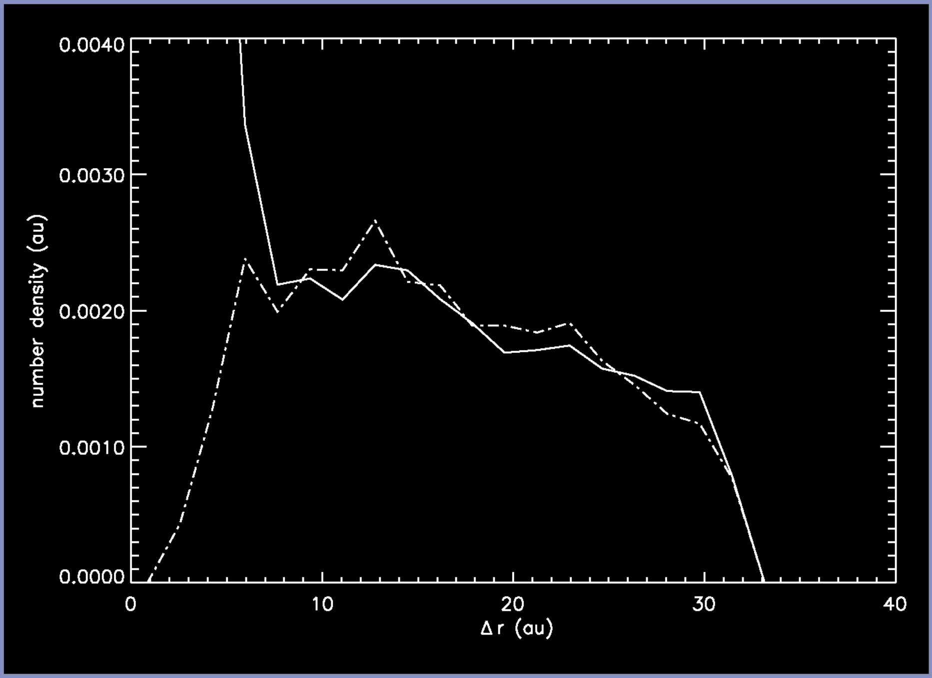
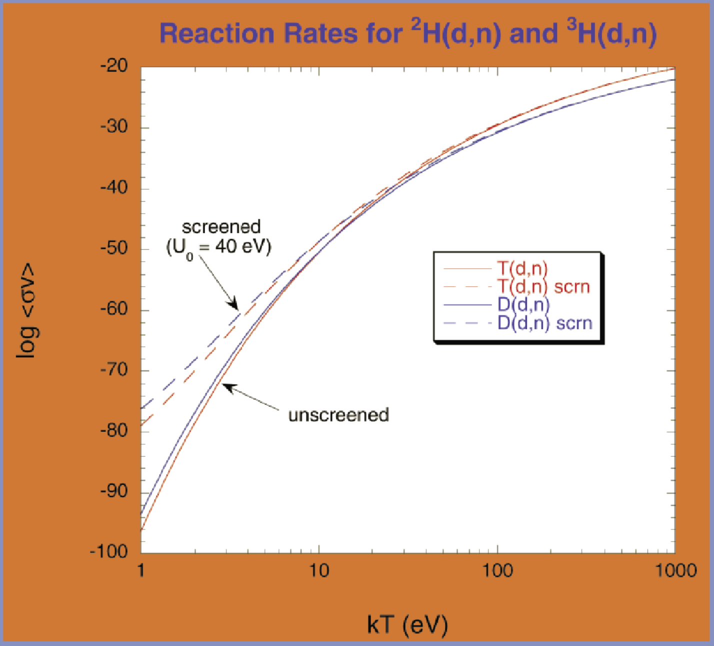


Figure: *$n_e(\Delta r)$ (solid line); $n_p(\Delta r)$ (chaindot line) vs. Δr.*

Screened Rates for Thermonuclear Reactions of Hydrogen Isotopes

Gerry Hale, T-16

The screening of thermalized nuclear reaction rates can be quite sizeable at low temperatures, even considering only the electrons surrounding the isotopes of hydrogen. We calculated the screening of d+d and d+t reactions at low temperatures, using a value of screening potential constant, $U_0 = 40$ eV, obtained in some regions of electron density and temperature from a combination of Density-Functional Schrödinger and Hypernetted Chain theories. These are shown in the figure to the right. The first interesting thing to note is that the unscreened rate for the d+d reaction (solid blue line) becomes larger than that for d+t (solid red line) at temperatures below about 10 eV. The screened rates (dashed lines) begin to deviate from the unscreened ones below about 100 eV and became as much as 20 orders of magnitude larger at 1-eV temperature.



Comparing Different Procedures for Generating Equations of State of Mixtures and Compounds

Eric D. Chisolm, T-1

The equation of state (EOS) program at Los Alamos uses a variety of methods for constructing EOS for mixtures and compounds, some of which involve combining EOS from constituent substances to get the EOS of the compound. Each method incorporates different physics and is appropriate to different situations. We have been studying the differences between these methods to see if experiments in the foreseeable future could differentiate between them, thus providing more reliable EOS of these materials for Laboratory computer simulations.

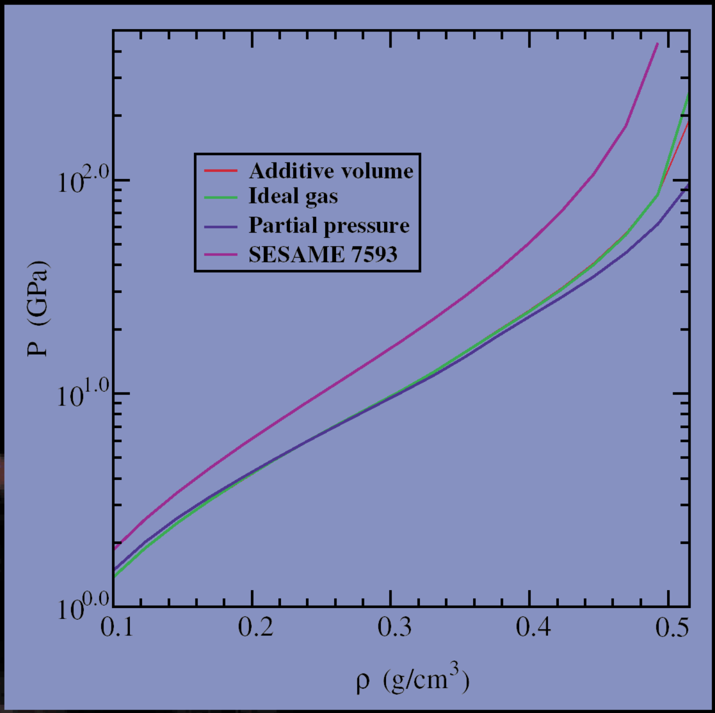
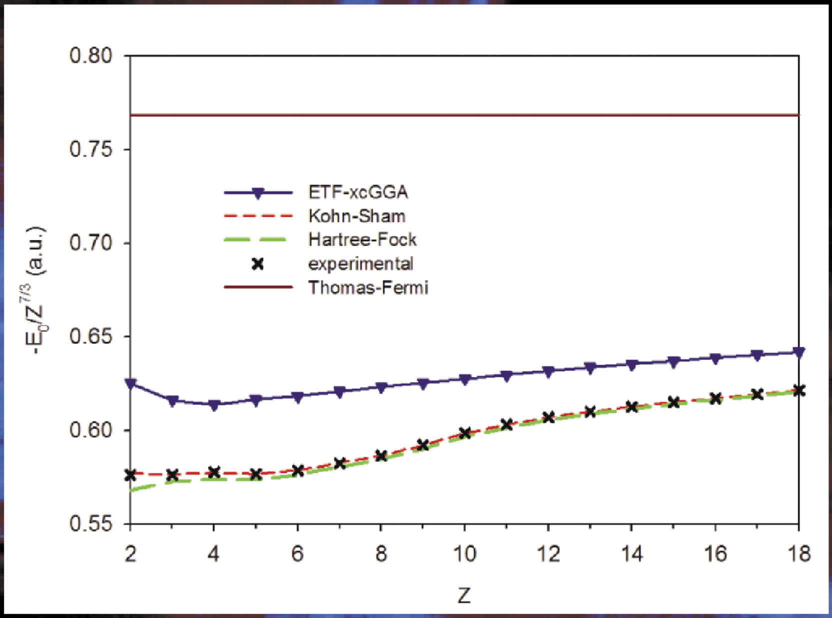


Figure: The density-pressure Hugoniots for four EOS for CH shocked from an initial density of 0.1 g/cc and an initial temperature of 1 eV. The first three EOS (bottom curves) were generated from carbon and hydrogen EOS using the indicated mixing procedures, while the fourth (top curve) was generated using experimental measurements of properties of the compound.

Orbital-Free Models for Electronic Structure Calculations

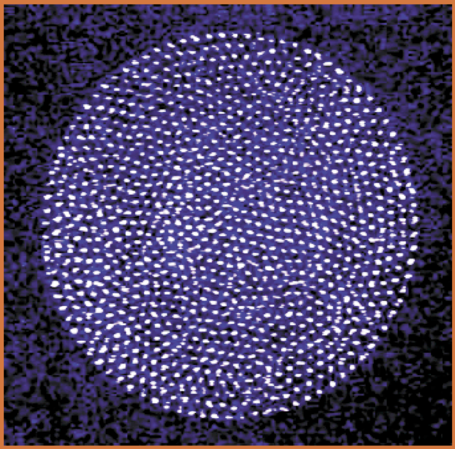
George Csanak, T-4
Jérôme Daligault and Michael Murillo, T-15

The Hohenberg-Kohn theorems guarantee that the ground state energy can be written as a functional of the density; that is, orbitals are not needed. Indeed, the thermal-electronic portion of EOS tables employs Thomas-Fermi-Dirac (TFD), which depends only upon the density. We wish to extend TFD to allow for a more accurate treatment at moderate temperatures and densities. In the figure we show the (scaled) ground state energies of various low-Z elements, as computed with various Thomas-Fermi-like models. The top line is the basic Thomas-Fermi result, and the crosses are the experimental values. The blue curve is one of our extended Thomas-Fermi results, which compares favorably with the experimental result and the Hartree-Fock (green) and Kohn-Sham (red) results, which are considerably more difficult calculations.



Dusty Plasmas

Dan Winske, X-1



The introduction of small, micron-size particulates into a plasma can change its properties significantly, and the resultant system is commonly referred to as a “dusty plasma.” The particulates become electrically charged by their contact with the plasma species and change the ionization balance of the plasma, i.e., how charge is redistributed between the ions, electrons, neutrals, and the particulates. The charge on the particulates also affects how they interact with themselves—the grains can charge up so much that they can behave as a strongly coupled Coulomb liquid or solid (see figure), how they are transported through the plasma, how they affect transport in the plasma through the excitation of new collective modes, and how they interact with walls and surfaces. In this project we assess dusty plasma phenomena for regimes of interest and compare to typical laboratory conditions, where numerous experiments have been conducted and used to validate theoretical models.

Figure: Micron-size grains in an rf discharge plasma that have become charged and aligned themselves into a Coulomb solid (photo courtesy of Lin I).

Scattering and Reaction Cross Sections

Charles M. Snell, X-1

We are generating elastic scattering and reaction cross sections for 363 fission products, Z = 30 to 64, on neutrons and light ions, Z = 1 to 3. The fission isotopes chosen were those with yields $>10^{-6}$, based on W. Wilson’s comprehensive yield tables. The calculations utilize the best currently available optical model parameters provided by P. Young and others. The total scattering and reaction cross sections and a typical angular distribution are displayed in left figure (^{77}Zn on p). For charged-particle collisions, it was found essential to use variable fine angular binning to capture the steep increase at small angles. A Rutherford-based interpolation scheme was devised to achieve accurate interpolation, right figure. The goals of this research are (1) to simulate in full detail the fission fragment/light-ion cascade for cases of interest; (2) to determine the effect of the cascade upon energy coupling and subsequent light-ion TN reactions; and (3) if these effects are deemed significant, to devise a simplified treatment or a reduced model that will accurately reproduce the increased ranges and enchanced reactions from the knock-on cascade.

Left figure: Cross sections versus energy, ^{77}Zn on proton: total scattering (red), reaction (blue). Right figure: Angular interpolation errors, ^{77}Zn on proton, E = 1 MeV: linear and log without correction (red and blue); linear and log with correction (orange and green).