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A PRIMER ON HIGH ENERGY DENSITY SYSTEM SIMULATIONS AND TYPICAL RESULTS

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TABLE OF CONTENTS

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Abstract

High energy density physics involves experimental, theoretical and computational research in high pressure equation of state of matter, opacity of materials in the plasma state, neutral and charged particle cross-section libraries, database for high explosives, shock wave propagation, radiation and explosive driven hydrodynamics, particle transport theory, and modelling of complex experimental systems. These fields are intimately related to inertial confinement fusion as well as nuclear weapons research. This report provides a primer on simulations and some typical results.

1. *Introduction*

High energy density (HED) physics deals with behaviour of matter under extreme conditions of pressure and temperature. Several fields of research involve HED - astrophysics, geophysics, inertial confinement fusion (ICF), explosive and impact loading of materials, nuclear warhead physics, Z-pinch devices, etc. All of these fields involve a common feature: i.e., concentration of high power energy from intense sources in a small region. This leads to hydrodynamic phenomena involving rapid motion of materials due to large pressure gradients generated inside the system. Nuclear detonations produce a very large energy and no laboratory tool can deliver more than a small fraction of the nuclear yield. New facilities, such as the National Ignition Facility in USA, will potentially reach regimes of material temperature ~ 10 keV and pressure ~ 10^9 bars in the laboratory.

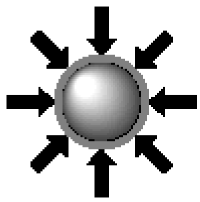


Fig.1a: ICF Capsule

Some of the physics issues involved in laser driven thermonuclear micro-explosions and nuclear explosions are the same; but the underlying details are quite different. The relevance of laser driven ICF to nuclear weapons science is that the states of matter produced, and the physical processes involved, are similar.

2. *Inertial confinement fusion (ICF)*

Two basic approaches to micro fission/fusion are currently being pursued in inertial confinement fusion (ICF): (i) the directly driven approach (Fig.1a) and (ii) the indirectly driven approach (Fig.1b). In the direct approach, several laser beams impinge on a target and generate an ablating plasma, which implodes the fuel to conditions appropriate for the initiation of fusion reactions. In indirect approach, laser or particle beams generate a thermal bath of x-rays in a radiation confining case called hohlraum, which implodes the fuel capsule, again by ablation process. In all stages of the different processes involved - that is, generation and re-distribution of x-rays, heating of target, ablation of plasma, implosion of fuel, initiation of fusion and subsequent burn - matter is heated to high temperature, and so energy transport via radiation is an essential feature.

Fig.1b: Hohlraum

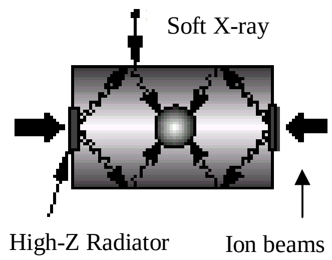
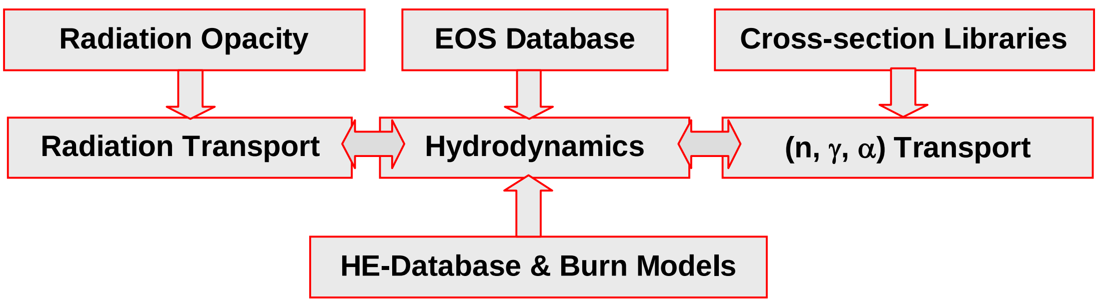


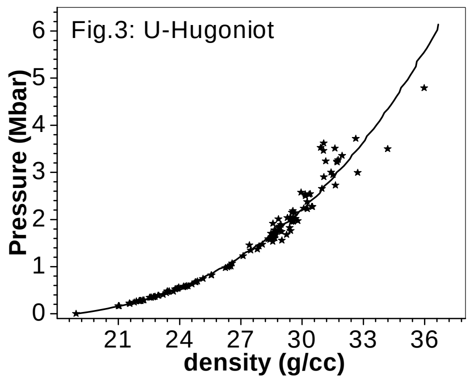
Fig.2: Computational Modules



In indirectly driven ICF, modelling transport of x-rays in the hohlraum generated by laser and radiation-driven implosion of the fuel capsule is a complex problem. While the EOS, opacity and nuclear data for low-Z fusion materials are often freely available, these data for high-Z materials used in the hohlraum and capsule are classified. So the databases need to be developed and verified against appropriate experiments for evolving any meaningful simulation programme. Similarly, the computer programs for modelling shock and explosive driven waves, radiation driven hydrodynamics, particle (neutron, gamma and alpha) transport are also not freely available, In fact, some commercially codes can generate totally meaningless results as they are not meant for simulations in the regimes of relevant pressures and temperatures. The Block Diagram in Fig.2 displays important areas of computational research, and their interdependence in HED Physics.

3. *EOS database and Hydrodynamics*

On heating a medium, the atoms or molecules acquire random kinetic energy which generates large pressure gradients. This induces macroscopic motion of the medium and changes in its density, which, in turn, affects the pressure distribution in the medium in a self-consistent manner. The resulting hydrodynamic process, characterized by four variables - macroscopic velocity, density, pressure and internal energy - is described by three conservation equations of mass, momentum and energy, and an EOS formally expressing pressure as a function of energy and density: $p=f(\rho,e)$. In detailed material models, which are needed in the lower pressure regimes (say, below 100 kilobar) the complete stress-strain tensors are also used.



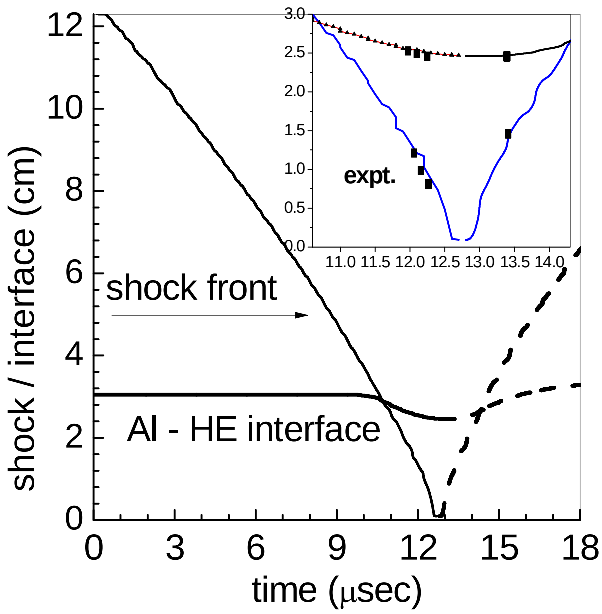
For ICF as well as weapon configurations, EOS databases are needed, over density ranges from 10^{-4} to 10^{4} gm/cc and temperature up about 10^{10} K, for various elements, compounds, and alloys. Fig.3 shows a comparison of theoretical and experimental Hugoniot for uranium.

Hydrodynamic codes generally use Euler and Lagrange numerical schemes. EOS data for high explosive (HE) materials are also required for interpreting the explosively driven experiments. A burn model simulates the detonation of the high explosive. Such a model, when used in numerical hydrodynamic calculations, must reproduce the important features like detonation speed, pressure behind the detonation wave etc.

4. ***Explosive driven sphere***

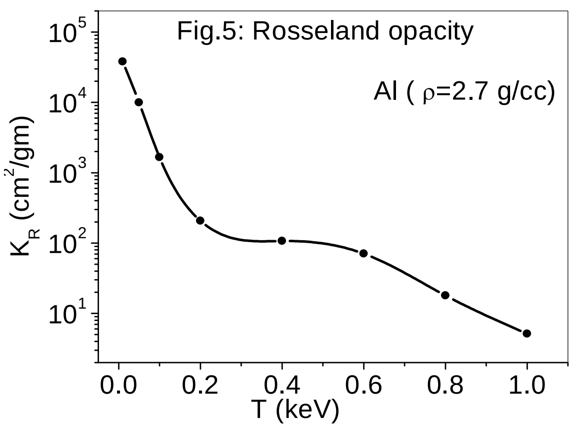
For evaluating the detonation models of HE, several experimental benchmarks are available as the PHERMEX facility reports. In one of them, a sphere of the HE called PBX-9404, of 12.319 cm in outer radius, implodes an aluminium sphere of 3.048 cm radius. The HE is initiated with a lens system so as to generate a spherical detonation wave at its surface. Fig.4 shows the calculated and experimental positions of the shock waves and the Al-HE interface. Experimental data are also shown in the inset.

Fig.4 Aluminum Sphere



5. *Radiation Opacity*

Absorption and emission characteristics of radiation -usually called opacities- of many important materials are of great significance in modelling HED systems. These properties are needed as a function of several physical parameters: (i) material density, (ii) temperature of the plasma, and (iii) frequency of radiation, etc. Calculation of radiation opacities is performed by different methods, which are of varying degrees of complexity. An important aspect of all the methods is the choice of an 'appropriate' atom model, which accurately describes the energy levels and wave functions of bound as well as free electrons. The screened hydrogen model (SHM) of

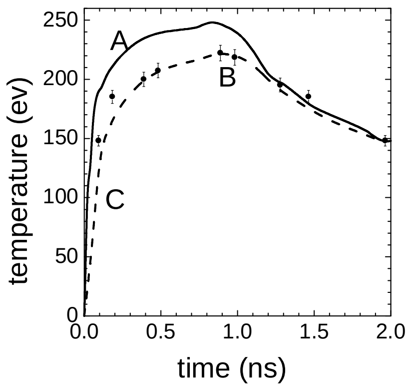


an average atom and its improved versions form the simplest of all the atom models. Local thermodynamic equilibrium (LTE) is one of the simplifying approximations used for calculating radiation opacities. Matter and radiation are characterized in terms of a single temperature in LTE approximation. Then, the Fermi-Dirac distribution specifies the energy distribution of electrons, while Planck's distribution describes the energy (or frequency) distribution of radiation. Both these distributions are crucial to characterize the opacities of materials. A typical plot of the Rosseland opacity for aluminium is shown in Fig.5.

6. *Radiation Transport*

For the design of ICF hohlraum, or a thermonuclear warhead, it is essential to have a method to model production of x-rays, its time dependent transport, absorption and re-emission from the walls. This problem is somewhat involved as absorption of thermal x-rays leads to blow-off of wall material and subsequent hydrodynamic motion of the wall. In fact, the radiation diffusing into the cold wall material heats and ablates it, and develops into a heat wave.

Fig.6 Holrum Temperature



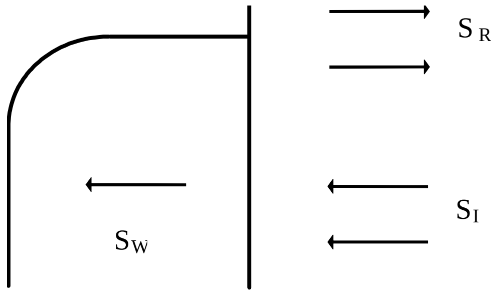
Drive and Wall Temperatures for Nova Hohlraum. (A) Drive Temperature. (B) Experimental Wall Temperature. C) Wall Temperature from Numerical Simulation (Au).

The ICF capsule is spherical in shape and the hohlraum is usually a cylindrical cavity. Therefore, it is necessary to have a general mesh of quadrilateral shape to represent the spherical capsule. 2D transport codes, using quadrilateral meshes in cylindrical R-Z geometry, are essential for determining the time dependent x-ray distribution in the hohlraum. The re-emitted radiation fluxes from wall elements can be incorporated as boundary sources in these discrete ordinate transport theory codes. Fig.6 shows the temperature-time profile in a hohlraum driven by laser beams, and its comparison with experimental data.

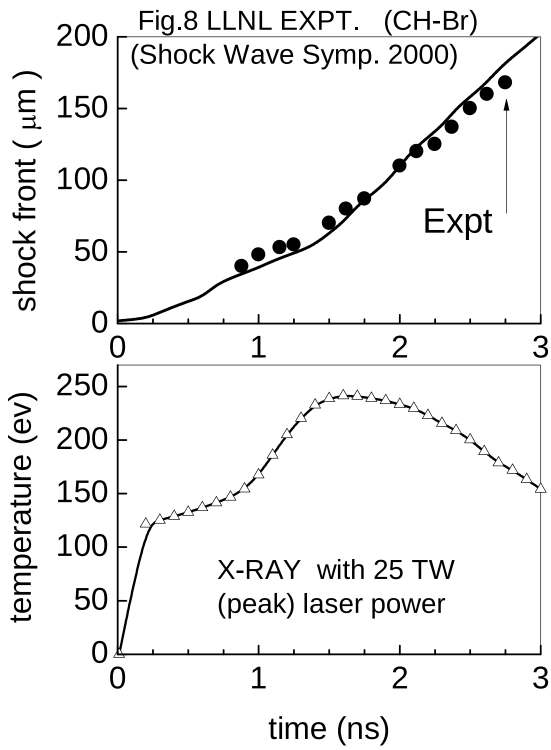
7. *Radiation Hydrodynamics*

Hohlraum wall is always made of materials with high atomic number (high-Z) such as gold or uranium. A dense-plasma medium is formed when thermal x-rays fall on the high-Z materials. Even with x-rays of 1-keV energy, the plasma is opaque because of the high number density of ions and atomic number. The radiation energy, which diffuses into the material through the plasma, develops into an ablative heat wave. The absorbed energy first appears as internal energy and pressure, which is partially converted into kinetic energy of the ablating plasma. This leads to ablation of the plasma, which in turn launches a shock wave into the medium. The shock, which is supersonic, overtakes the heat wave and propagates inwards. Radiation is emitted back by the optically thick ablating plasma. The incident flux S_I, re-emitted flux S_R, x-ray flux into the wall S_W and spatial profile of material temperature, in an ablative heat wave, are shown in Fig.7

Fig.7: Heat wave in to the wall



Somewhat similar processes occur when the radiation falls onto a spherical fusion capsule placed at the centre of the hohlraum. The compression and central heating of the capsule is also achieved with the radiation driven shock wave. The complete simulation of this process is done with radiation hydrodynamic methods. In Lagrange formulation of hydrodynamics, the mass of each cell remains constant, thereby automatically incorporating mass conservation. This approach is invariably used for compressible fluid flow problems with



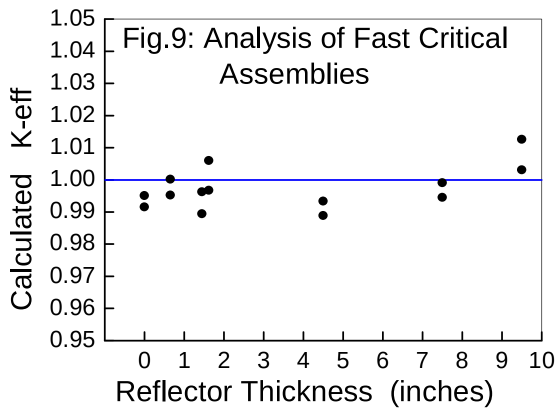
multi-material interfaces.

In Eulerian scheme, the spatial meshes are fixed in space, and material moves through the meshes. Then, time dependent radiation transport equation is solved over these meshes. Temperature of each mesh, determined from hydrodynamics, provides the radiation source, while the energy transported by radiation is fed back into hydrodynamics.

Several sets of experimental data on radiation driven shocks can be compared against the simulation data to ascertain the accuracy of the method. The comparison shown in Fig.8 is for shock wave propagation in CH-Br medium which is used as ablator material around the fusion capsule.

8. *Neutron Gamma libraries*

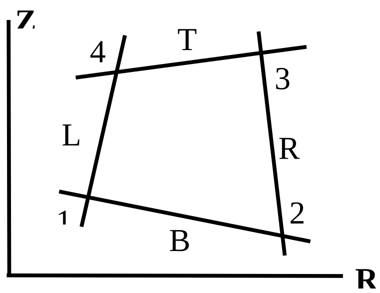
Coupled neutron-gamma cross-section libraries are generated using ENDF (neutron) and EPDL (photon) files of nuclides published by IAEA nuclear data centre and their processing codes. Accuracy and consistency of these cross-section sets can be checked by analysing criticality (neutron) and source (coupled neutron-gamma) benchmarks published by IAEA. Fig.9 shows computed values of neutron multiplication factor, K_{EFF} and comparison with experimental data for several clean plutonium critical assemblies.



Bare & reflected spheres of Pu with & without dilution metals

9. *Neutron / radiation transport Codes*

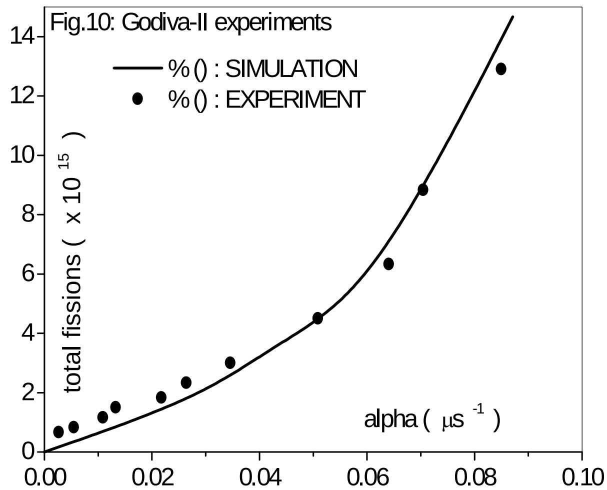
Neutron and radiation transport processes form important energy production and transport mechanisms in HED systems. The geometrical arrangement of a spherical fuel capsule in a cylindrical hohlraum or a thermonuclear primary in a radiation case needs at least 2D transport codes with general quadrilateral meshes for



their representation. Thus the transport equation is to be discretized on non-orthogonal quadrilateral meshes. The discrete ordinates numerical schemes for solving the transport equation are well developed with ample literature. However, such 2D codes with quadrilateral meshes are not freely distributed and have to be evolved for carrying out any meaningful simulations.

10. Coupled neutronics-hydrodynamics

Controlled burst reactors can be simulated to check coupled neutronics-hydrodynamics calculations. These involve equations governing hydrodynamics, neutron transport and radiation transport phenomena. An increase in reactivity increases fissions, which generate heat and pressure causing material to expand and reduce the reactivity. If the material temperature is high, then radiation transport also plays an important role in energy transfer. At very low energy yields, the computational method consists of solving the coupled neutron transport and hydrodynamic equations. For ensuring mass conservation, equations are written in Lagrangian coordinates.



A fission system is fully specified at initial time with spatial profiles of material composition, density, internal energy and material velocity. Initial spatial profiles of neutron density and energy are also given. The subsequent behaviour of the system is determined by solving the coupled neutron transport and hydrodynamics equations.

In Godiva-II experiments published in the literature, reactivity is suddenly increased in a 93.5% enriched uranium sphere, by means of adjustable uranium rods, thereby causing a power excursion. This is terminated due to increase in temperature which causes fuel expansion and consequent decrease in density. A comparison with experimental data is shown in Fig.10.

11. Conclusions

Methods outlined above are the bare minimum for simulations of high energy density systems. There are a number of topics where accuracy has be assertained: (i) Improvements in details of physics packages for EOS, radiation opacity and particle interaction cross-sections, (ii) New methods like smooth particle hydrodynamics (SPH) for 3D simulations, (iii) Integrated radiation hydrodynamics of hohlraums, (iv) Monte Carlo methods for radiation transport in 3D hohlraums, (v) Hydrodynamic instabilities, (vi) Z-pinch driven ICF experiments for verifications, etc.

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