A Two-Dimensional Lagrangean Code for Laser-Produced Plasma Applications.
Pt. 1. Crater Formation in Plane Targets

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Abstract

A two-dimensional Lagrangean hydrodynamic code has been developed for laser-produced plasma applications. In testing the hydrodynamic part of the code the irradiation of thin foils with high-intensity laser beams was considered in a single-fluid single-temperature approximation. The computed shock velocities, compression ratios, velocity and pressure variations, etc. are in good agreement with estimates stemming from analytical solutions.
INTRODUCTION

The heating of solid, liquid, or gaseous targets by means of lasers is characterized by the presence of rather large spatial gradients in the substance interacting with the laser light. In the case of unshaped laser pulses the plasma parameters may vary by four or five orders of magnitude over distances not exceeding a few per cent of the characteristic length involved. Still larger are the spatial gradients if specially shaped laser pulses are used as, for example, in the case of compression by coalescing waves, etc. The use of Lagrangean hydrodynamic codes, which are particularly well suited to handling large gradients with one spatial dimension, is most common in such cases (see, for example, Kidder and Barnes [1], Clarke et al. [2], Christiansen et al. [3], Goldman [4], Lengyel [5], or the sources cited in the review paper of Mulser et al. [6]). The assumption of strict symmetry (slab, cylindrical, or spherical symmetry) is mandatory in calculations of this kind.

However, in the majority of cases that can be realized experimentally the boundary conditions are nonuniform and thus the application of more sophisticated numerical models becomes necessary. In some cases the existence of certain uniformity or symmetry properties allows the use of two-dimensional (2D) codes for modeling the problem. When plasma production by laser is considered, the assumption of axial symmetry may be a good approximation for numerous experimental situations (irradiation of plane surfaces or targets with rotational symmetry by a single cylindrically symmetric laser beam, double-sided coaxial irradiation of sheaths or rotationally symmetric targets, etc.). Note, however, that if a magnetic field is present, axial symmetry only exists if
the magnetic field is linear, rotationally symmetric and the target is irradiated along the magnetic field lines (beam axis coincides with the magnetic axis).

The question that may naturally arise is how well is a Lagrangean mass-cell system suited to handling truly two-dimensional problems, i.e. problems in which not only deviations from one-dimensional symmetry conditions are being considered. Most of the results published on 2D Lagrangean laser-induced fusion calculations are concerned with the destabilizing effects caused by deviations from 1D symmetry conditions (see, for example, [7]). Besides, no information at all has been available until recently on the details of 2D Lagrangean codes as applied to laser-produced plasma calculations (see, for example, [7],[8] or, more recently, [9]). Two-dimensional calculations have also been performed in Los Alamos [10] (a PIC code, the results are also described in [6]). A 2D ADI method based on a fixed-grid Eulerian system has been developed by Lindemuth [11]. It should be noted here that neither the particle-in-cell (PIC) method nor a fixed-grid Eulerian system seem to be particularly well suited to handling the extreme gradients inherent in laser-produced plasmas.

It was thus decided some time ago to develop a 2D Lagrangean hydrodynamic code [12] and test its applicability to axially-symmetric laser-produced plasma calculations with and without magnetic fields present. Some results obtained during the test runs and pertaining to the burn-through of deuterium ice layers irradiated from one side by single laser beams in the absence of magnetic fields are reported here.
MATHEMATICAL MODEL

An excellent treatise on 2D Lagrangean hydrodynamic calculations was written by Schulz [13]. Readers interested in details concerning the formulation of a generalized 2D Lagrangean coordinate system and the discretization of the conservation equations in the coordinate system thus defined are referred to [13]. Schulz also indicated some of the difficulties one may encounter while working with 2D Lagrangean codes (see the computational example provided by him). Since the computer code used in the present calculations closely follows the method presented in [13], we shall omit here the lengthy derivations and only outline the major modifications introduced in Schulz's original system (see also [14]).

The conservation equations are written in a one-temperature ideal gas approximation:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad , \]  
\[ \rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = - \nabla \vec{P} \quad , \]  
\[ \rho \left( \frac{\partial e}{\partial t} + \vec{u} \cdot \nabla e \right) = - \nabla \cdot \vec{\phi} - \vec{P} \cdot \nabla \vec{u} \quad , \]  

where \( \vec{P} = \rho + \gamma \) and

\[ e = \frac{1}{\gamma - 1} \frac{\rho}{\gamma} \quad , \]

The symbols \( \gamma \) and \( \vec{\phi} \) represent artificial viscosity and laser flux intensity, respectively. Introducing a pair of generalized curvilinear coordinates \( a, b \) and defining a vector \( \vec{\xi} \) by a clock-wise rotation of the radius vector \( \vec{r} \) over an angle of \( \pi/2 \), the transformation formulae from the old cylindrical coordinate system \((r, z)\) to the new curvilinear one \((a, b)\) may be written as follows:
\[ \nabla \cdot f = \frac{1}{J} \left( \frac{\partial}{\partial b} \frac{\partial}{\partial a} - \frac{\partial}{\partial a} \frac{\partial}{\partial b} \right) f = \frac{1}{J} \left[ \frac{\partial}{\partial b} \left( \frac{\partial}{\partial a} - \frac{\partial}{\partial a} \frac{\partial}{\partial b} \right) - \frac{\partial}{\partial a} \left( \frac{\partial}{\partial b} - \frac{\partial}{\partial b} \frac{\partial}{\partial a} \right) \right] f \] (1.5)

\[ \text{div} \, \vec{f} = \frac{1}{J} \left( \frac{\partial}{\partial b} \vec{f} - \frac{\partial}{\partial a} \vec{f} \cdot \vec{a} \right) = \frac{1}{J} \left( \frac{\partial}{\partial b} \vec{f} - \frac{\partial}{\partial a} \vec{f} \cdot \vec{a} \right) \cdot \vec{a} \] (1.6)

where \( J = \gamma(\alpha, \beta) / \gamma(\beta, \alpha) = \frac{\partial}{\partial a} \frac{\partial}{\partial b} - \frac{\partial}{\partial b} \frac{\partial}{\partial a} \) \( (1.7) \)

and \( \vec{a} = (\vec{a}_1, \vec{a}_2), \quad \vec{f} = (-\vec{f}_1, \vec{f}_2) \). \( (1.8) \)

Applying the transformation to the conservation equations we obtain the following set of Lagrangean equations:

\[ \rho + J = \text{const} = \rho \] (1.9)

\[ \frac{\partial \vec{v}}{\partial t} = -\frac{f}{\rho} \left( \lambda_b \frac{\partial \rho}{\partial a} - \lambda_a \frac{\partial \rho}{\partial b} + \lambda_b \frac{\partial}{\partial a} \left( \frac{\partial}{\partial b} \vec{v} \right) - \lambda_a \frac{\partial}{\partial b} \left( \frac{\partial}{\partial a} \vec{v} \right) \right) \] (1.10)

\[ \frac{\partial \vec{v}}{\partial t} = \vec{u} \] (1.11)

\[ \vec{V} = \frac{1}{\rho} \] (1.12)

\[ \frac{\partial \phi}{\partial t} = -\nabla \cdot \vec{V} - \frac{\rho}{\rho} \left( \frac{\partial}{\partial a} \left( \frac{\partial}{\partial a} \vec{V} \right) + \frac{\partial}{\partial b} \left( \frac{\partial}{\partial b} \vec{V} \right) \right) \] (1.13)

The rate of change of the total energy per unit mass is given by

\[ \frac{\partial}{\partial t} \left( \frac{\rho}{\rho} + e \right) = -\nabla \cdot \vec{V} - \frac{\rho}{\rho} \left( \frac{\partial}{\partial a} \left( \frac{\partial}{\partial a} \vec{V} \right) + \frac{\partial}{\partial b} \left( \frac{\partial}{\partial b} \vec{V} \right) \right) + \frac{1}{\rho} \left( \frac{\partial}{\partial a} \left( \frac{\partial}{\partial a} \vec{V} \right) + \frac{\partial}{\partial b} \left( \frac{\partial}{\partial b} \vec{V} \right) \right) \] (1.14)

In the above expressions, the subscripts of \( \phi \) denote derivatives with respect to the coordinates indicated.

As one may notice, the scalar artificial viscosity \( q \)
appearing in eqs. (1.2) and (1.3) has been replaced by a tensor artificial viscosity \( \bar{q} \) appearing in eqs. (1.10) to (1.14), which is characterized by the following relations:

\[
\begin{align*}
q_A \neq 0 & \quad \text{only if } \frac{\partial \bar{u}^2}{\partial a} \neq 0, \\
q_B \neq 0 & \quad \text{only if } \frac{\partial \bar{u}^2}{\partial b} \neq 0.
\end{align*}
\]  

(1.15)

Such a definition of \( \bar{q} \) is necessary for assuring the continuity of the velocity component parallel to a shock front (only the normal component should be affected by the artificial viscosity). In general, \( q_A \) and \( q_B \) may be specified as functions of the respective velocity gradients. Schulz used the product of the first and second derivatives of the velocity components for defining \( q_A \) and \( q_B \). Such an approximation seemed tedious and rather approximate at the boundaries of the region occupied by the fluid owing to the difficulties associated with the discretization of second derivatives in generalized coordinates at a fluid-vacuum interface. Hence only combinations of the first derivatives were used for defining \( \bar{q} \) in the present computations. The resulting numerical system functioned well also with rather large cell deformations.

Note that equations (1.10) and (1.13) differ from the respective equations of Schulz. Splitting the artificial viscosity into individual constituents, i.e. the arbitrary replacement of a scalar quantity by a tensor one has the undesired effect that eq. (1.13) is no longer invariant with respect to Galilean transformation, i.e. it is no longer an exact analogue of eq. (1.3). For preserving the invariance of the energy equation with respect to Galilean transformation Schulz changed simultaneously the structure of eqs. (1.10) and (1.13) in a rather arbitrary manner, but still conserving the total energy per unit mass, i.e. leaving eq. (1.14) unchanged. Following
Schulz, eqs. (1.10) and (1.13) should be written in the following form:

\[
\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{m} \left( \mathbf{a} \frac{\partial \mathbf{u}}{\partial \mathbf{a}} - \mathbf{a} \frac{\partial \mathbf{u}}{\partial \mathbf{b}} \right) - \frac{1}{m} \left[ \frac{\partial}{\partial \mathbf{a}} \left( \mathbf{q}_A \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{b}} \right) - \frac{\partial}{\partial \mathbf{b}} \left( \mathbf{q}_B \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{a}} \right) \right], \tag{1.16}
\]

\[
\frac{\partial \mathbf{q}}{\partial t} = -\nabla \cdot \mathbf{q} - \mathbf{q} \frac{\partial \mathbf{V}}{\partial t} - \frac{1}{m} \left( \mathbf{q}_A \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{a}} - \mathbf{q}_B \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{b}} \right). \tag{1.17}
\]

In this representation, the invariance of the energy equation is assured.

For the sake of clarity, computations were performed following both approaches, i.e. by means of eqs. (1.10) to (1.13) as well as by eqs. (1.16) to (1.17). The results were found to be qualitatively about the same in both cases (the shape of the expanding gas cloud, the form of the crater developing in the ice layer, etc.), but the quantitative difference between the local gas parameter values amounted to 25% to 30% in some cases. Since, as shall be seen, the application of eqs. (1.10) and (1.13) yielded results that are in good agreement with theoretical predictions, it has been decided to use these equations irrespective of their Galilean transformation properties.

In the computations described here 100% laser energy damping was assumed to take place at a particular gas density value, i.e. in the last mass-cell whose density is just below a given threshold value (following the direction of propagation of the laser light). In most of the calculations this threshold value was defined in terms of the electron density at which the laser beam frequency is equal to the electron plasma frequency, i.e. \( \omega_{\text{e}} = \omega_{\text{p}} = (m_e c^2 / e) \nu \). In a fully ionized deuterium plasma, the electron density may then be replaced by the respective gas density, i.e. \( m_e = \zeta / M_0 \). In the case of deuterium gas, \( \rho_{\text{lat}} / \rho_o \approx 1 / 50 \), where \( \rho_o \) denotes
deuterium ice density \( \varrho_0 \approx 0.196 \text{ gr/cm}^3 \), measured value [15]). Such an approach made it rather simple to discretize the term \( \nabla \cdot \varphi^2 \) appearing in the energy equation.

In a series of calculations performed, allowance was made for heat conduction, i.e. the term

\[
- \nabla \cdot \varphi \text{ cond} = \text{Cond} \cdot \text{div} (\varrho \text{ grad} e), \quad \varrho \alpha e^{5/2} \tag{1.18}
\]

has been introduced into the energy equation. Owing to the temperature-dependence of \( \varrho \), heat conduction was found to affect primarily the high-temperature expansion fan of the gas blob produced: at sufficiently high laser flux intensities the expansion fan became nearly isothermal. In the low-temperature shock-heated gas region ahead of the absorption zone the conduction effect was found to be negligible.

Note that in view of eqs. (1.5) and (1.6) the right-hand side of eq. (1.18) consists of eight second-order derivatives, four of them being of the mixed-type. The recurrence formula for the internal energy of a particular mass-cell contains terms with the internal energies of the eight adjacent cells. In view of the temperature-dependence of the thermal conductivity the finite difference version of this equation can only be solved by means of rather crude approximations. In the present calculations, an explicit time-splitting scheme was used and the temperature-dependence of \( \varrho \) was accounted for by an iterative procedure. Since the computer time required for such a solution was found to be rather long and the yield rather low (the distributions computed with and without thermal conduction showed no other difference than the one described above) it was decided to abandon thermal diffusion until a more effective way of computing it is found.
RESULTS

A deuterium ice layer of thickness $l_0/2$, density $\rho_0$, and temperature $T_0$ was heated by a cylindrical laser beam whose diameter was equal to the ice thickness: $D_0 = l_0/2$. The radial (lateral) dimension of the target-layer $R_0$ was chosen so as to assure complete burn-through before the bow shock reaches the lateral side of the ice layer. The ratio $R_0/l_0 = 2/1$ was found to be satisfactory in most of the computational cases considered. For simulating absorption at a certain "critical" density value, an expansion fan was attached to the side of the ice layer exposed to the laser beam. The thickness of this layer was $l_0/2$ as well. The density was assumed to vary cubically in the expansion fan from zero to $\rho_0$. The initial parameter values were selected to correspond to measured data: $\rho_0 = 0.196 \text{ gr/cm}^3$, and $c_s = 2 \times 10^5 \text{ cm/sec}$ (density and sonic velocity in deuterium ice [14]). Hence assuming a total ice thickness of $l_0 = 200 \mu$, the characteristic time associated with the propagation of sonic disturbance over $l_0$ is $t_s = 100 \text{ ns}$. The dimensionless times displayed in the plots that follows are given in fractions of this time (all computations were performed in dimensionless coordinates by means of reduced variables). The dimensionless quantity $Q^*$ appearing in the figures is related to the laser flux $\phi_0$ by means of the expression $Q^* = Y(1-\text{I})/(\phi_0/\phi_{\text{cr}}), (\rho_0/\rho_{\text{c}})l_0/c_0$, where $\phi_0 = \rho_0 c_0^3$ and $\Delta_0$ denotes the "absorption length". Note that different combinations of initial values may yield the same input parameter $Q^*$.

The plots shown in Fig. 1 correspond to $\phi_0 = 5 \times 10^{12} \text{ W/cm}^2$ and $t_{\text{pulse}} = 200 \text{ ps}$. The pictures in the left-side column show the cell deformation, i.e. the development of a shock wave in the undisturbed material, and the rapid expansion of the gas cloud on the vacuum-side of the surface irradiated. The plots in the right-side column are vector plots.
\[ \tau = 0.004 \quad Q = 4 \times 10^6 \quad \tau_{\text{pulse}} = 0.002 \]

\[ \tau = 0.022 \]

\[ \tau = 0.063 \]

Fig. 1  Crater formation in a deuterium ice layer.
\[ \phi_l = 5 \times 10^{12} \ \text{W/cm}^2, \ \tau_{\text{pulse}} = 200 \ \text{ns}. \]
\[ (Q, \hat{\xi} \ - \ \text{dimensionless quantities}, \ \hat{\xi}_o = 100 \ \text{ns}). \]
representing the momentary velocity distributions. Note that the first plot displayed corresponds to a time instant well after the pulse end. As can be seen, a shock wave propagates into the solid at an average velocity of approx. $5 \times 10^6$ cm/sec. As long as the shock wave remained quasi-steady the density increase across it (along the symmetry axis) was found to be identical with the classical value that could be predicted from the Rankine-Hugoniot relation. In about 5 ns the shock wave reaches the rear face of the ice layer and the gas starts to stream out on the back-side as well. Note the approximately linear dependence of the velocity on the radius (measured form the explosion center) in the asymptotic phase of the expansion. Such a dependence is characteristic of the asymptotic phase of spherical expansions, irrespective of the initial energy supply rates [16]. The absolute value decreases rapidly at any fixed radius as time goes on.

The pictures shown in Figs. 2a and 2b correspond to a laser flux intensity - pulse length combination of \( \Phi = 5 \times 10^{13} \, \text{W/cm}^2 \), \( t_{\text{pulse}} = 100 \, \text{ps} \). Since \( \Phi \) is now ten times larger than in the previous case, the initial phase of the expansion is characterized by considerably larger velocity values. The shock wave reached the back-face of the ice layer in about 2 ns in this case.

It is interesting to note that none of the sample calculations performed showed any mass-retardation at the symmetry axis as computed by Clarke [10] using the PIC method (the results are displayed also in [6]). It seems that this mass retardation in [10] was not caused by gas-dynamic effects.

The actual size of the gas cloud shortly before the moment of burn-through and shortly after it is shown for a representative case in Fig. 3. In this figure the fine structures of the respective craters are also given (the plot-scale has been changed). Note the good stability of the numerical system also at the relatively large cell deformations observed.
$Q^* = 4 \times 10^7$

$\tau_{\text{pulse}} = 0.001$

$\tau = 0.002$

$\tau = 0.004$

$\tau = 0.014$

**Fig. 2a** Crater formation in a deuterium ice layer.

$\phi_l = 5 \times 10^{13}$ W/cm$^2$, $t_{\text{pulse}} = 100$ ps.

($Q, \tau$ - dimensionless quantities, $\tau_0 = 100$ ns).
Fig. 2b  Burn-through of the deuterium ice layer shown in Fig. 2a.
Fig. 3. The size of the expanding gas cloud relative to the thickness of the deuterium ice layer. The fine structure of the developing crater is shown on the right side.
In a number of test runs, the effect of the assumed initial conditions (the form of the initial density distribution, the location of the critical density layer, etc.) on the dynamics of crater formation has been checked.

Figure 4 shows the effect of the location of the critical density layer: the three pictures on the left side correspond to a case where the critical density layer is located at about 4/10 of the total layer depth and the pictures on the right side correspond to an absorbing layer at 2/10 of the total depth. The second case is characterized by a smoother initial density profile (a nearly linear one) as compared with the first one. \( \Phi_0 = 5 \times 10^{13} \text{ W/cm}^2, t_{\text{pulse}} = 100 \text{ ps} \).

Absorption by a deeper-located critical density layer, i.e. energy deposition in the immediate vicinity of the high-density cold core, is characterized by a rounder crater geometry. Note the massive peripheral gas outflow appearing in the second case. The same effect can also be observed on the corresponding velocity vector diagrams shown in Fig. 5.

The effect of the energy deposition rate on the flow formation is shown in Fig. 6, where the time variations of the maximum temperature-pressure, and density in the crater are shown for two flux intensities associated with two different pulse durations. Note, however, that the total energy deposited (the product of \( Q^* \) and \( C_{\text{pulse}}^* \)) is the same in both cases.

In the first case (\( \Phi_0 \approx 10^{13} \text{ W/sec}, t_{\text{pulse}} = 1 \text{ ns} \)) the cell deformation is relatively small during the pulse time, and the temperature and pressure maxima coincide with the cutoff moment of the laser pulse. The compression lags considerably behind the pressure rise (density change is associated with cell deformation). The density build-up signalizes shock wave formation.
Q = 4 \times 10^7

\tau_{\text{pulse}} = 0.001

\tau = 0.0053

\tau = 0.0110

\tau = 0.0160

\tau = 0.0061

\tau = 0.0150

\tau = 0.0350

Fig. 4 Effect of the location of the absorbing layer on the form of the crater. Left: absorption at the surface of the dense core, right: absorption in a layer close to the vacuum surface.
Fig. 5  Effect of the location of the absorbing layer on the velocity vector distribution. Left: absorption at the surface of the dense core, right: absorption in a layer close to the vacuum surface.
In the second case ($\phi \approx 10^{12}$ W/sec, $t_{\text{pulse}} = 10$ ns) notable gasdynamic motion (i.e. cell deformation) sets on before the end of the laser pulse. The peak temperature and pressure values start to decrease before the laser pulse is cut-off. The temperature maximum reached is considerably lower than that in the previous case. There is no time delay between pressure change and density build-up.

In both cases, as soon as the shock wave formation has been completed, the density increase behind the flat part of the shock wave is in exact correspondence with the Rankine-Hugoniot value as long as the shock wave motion remains quasi-stationary. In this quasi-stationary phase, the pressure decays exponentially with time. The exponent characterizing the pressure decay is in good agreement with the analytical value given for spherical explosion waves ($\gamma = 1.2$).

The relation between the assumed laser flux intensity and the peak temperature value obtained in the crater is shown in Table 1 for two pulse durations $\tau = 1 \mu$s, $Q^* = 4 \times 10^5$ corresponds to $\phi = 5 \times 10^{11}$ W/cm$^2$). As can be seen, in the case of short pulses, where the effect of gasdynamic motion is negligible for the duration of the laser pulse, the temperature peak varies in almost direct proportion to the flux intensity.

In the case of longer pulses characterized by the onset of gasdynamic motion before the pulse end the exponent of the temperature variation reduces to about 0.67.

It can readily be shown (see, for example, the dimensional analysis performed by Bobin [17]) that the analytical value of the exponent relating the temperature to the laser flux intensity is 2/3 if only heat input and gasdynamic expansion are taken into account.
Fig. 6  Effect of pulse duration (by constant laser energy) on the build-up of shock waves and on the expansion dynamics ($\phi \cdot t_{\text{pulse}} = 10^4 \text{ J/cm}^2$ for both cases).
TABLE 1

TEMPERATURE PEAK OBSERVED IN THE CRATER AS A FUNCTION OF THE LASER FLUX INTENSITY FOR TWO DIFFERENT PULSE LENGTHS.

\[ \text{exp} = \frac{\ln(e_2^* / e_1^*)_{\text{peak}}}{\ln(Q^* / Q_1^*)} \]

<table>
<thead>
<tr>
<th>( \tau^* )</th>
<th>( Q^* )</th>
<th>( e^* )</th>
<th>( \text{exp} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^{-3} )</td>
<td>( 4 \times 10^5 )</td>
<td>( 2.10 \times 10^2 )</td>
<td>0.9829</td>
</tr>
<tr>
<td>( 8 \times 10^6 )</td>
<td>( 3.99 \times 10^3 )</td>
<td>0.9875</td>
<td></td>
</tr>
<tr>
<td>( 2 \times 10^7 )</td>
<td>( 9.86 \times 10^3 )</td>
<td>0.9023</td>
<td></td>
</tr>
<tr>
<td>( 4 \times 10^7 )</td>
<td>( 1.84 \times 10^4 )</td>
<td>0.9875</td>
<td></td>
</tr>
</tbody>
</table>

| \( 10^{-2} \) | \( 4 \times 10^5 \) | \( 1.16 \times 10^3 \) | 0.6633 |
| \( 8 \times 10^5 \) | \( 1.84 \times 10^3 \) | 0.6674 |
| \( 1 \times 10^6 \) | \( 2.13 \times 10^4 \) | 0.6665 |
| \( 4 \times 10^6 \) | \( 5.37 \times 10^4 \) | 0.6665 |

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