Hydrodynamic simulation of laser-induced shock waves using the Turbulence Problem Solver software package

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Abstract. The problem of irradiation of a semi-infinite bulk metal target by a single laser pulse, being important for many laser technology applications, is considered. The model for simulating the propagation and attenuation of shock waves, occurring when metals are irradiated with single laser pulse, is presented. The paper describes the computational algorithm based on the model and features of its implementation in C++ in a software package Turbulence Problem Solver (TPS) for modeling a wide class of problems described by hyperbolic equations. The problem is modeled using different approaches and the results are compared. The object-oriented polymorphic architecture of the software complex accelerates and facilitates the process of model development and calibration, allowing for flexible configuration and combination of elements of numerical models: Riemann solvers, various types of and reconstructions, and equations of state of matter.

1. Introduction

Figure 1. Samples of ASTM A262 stainless steel before and after various types of impact hardening.
The picture is taken from the review [1].
Laser technologies have been developing very intensively in recent decades. This growth is accompanied by an increase in the number of their application areas, and the number of application areas is also growing. For example, laser ablation to liquid (LAL) [2] is used to form nanoparticles in the form of a colloidal solution, formed by nanoparticles of irradiated metal with the liquid. Another example is laser shock wave peening of metals (LSP) [1]. As a result of peening, anti-corrosion properties, wear resistance and fatigue resistance of metal parts are improved. The lifespan of the parts due to this treatment may increase 2–5 times. Figure 1 shows photos of surfaces and sections of steel samples before and after LSP. The treated samples show significantly fewer surface irregularities, cavities, and microcracks.

The main driver of these and many other laser technology applications is laser-induced shock waves. The considered problem of irradiation of a volume target is particularly important for the problems of laser shock hardening, since in fact LSP occurs as a result of residual deformations after the past shock wave. The study of the laws of propagation and attenuation of laser-induced shock waves will allow more accurately identifying the criteria and restrictions on the initial conditions under which LSP occurs.

Due to the growth rate of the nanosecond and femtosecond laser industry, the demand for accurate mathematical models of the processes occurring during the irradiation of substances with laser pulses is also increasing. The paper describes a physical and mathematical model created for numerical simulation of metal irradiation mainly by short and ultrashort laser pulses.

2. Problem statement and scheme

Thick aluminum target is irradiated with a single laser pulse of nano- (1 ns = 10⁻⁹ s) or femtosecond (1 fs = 10⁻¹⁵ s) duration. The laser beam is directed along the normal line to the target surface, and falls from top to bottom. On top, the target is adjacent to a layer of rarefied medium-air or vacuum. Both environments are initially at rest, \( u_{Al} = u_{vac} = 0 \), \( v_{Al} = v_{vac} = 0 \).

![Figure 2. Scheme of irradiation of a volume target by a single ultrashort laser pulse.](image-url)
The laser beam falls along the normal to the target surface, and the origin is at the intersection of the beam symmetry axis with the target surface. The x-axis is directed along the surface, and the y-axis is directed along the beam incidence.
The metal target has dimensions $2L_x \times L_y$, where $L_x = 1280 \text{ nm}$, $L_y = 800 \text{ nm}$. and the vacuum region has dimensions $2L_x \times L_{\text{vac}}$, where $L_{\text{vac}} = 200 \text{ nm}$. The point of coordinates origin is selected at the intersection of the laser launch axis and the target surface. The problem has a symmetry with respect to the axis of the laser beam, so in the calculations we will consider only the right half of the target. Thus, the entire simulation box is a rectangle $[0, 1280 \text{ nm}] \times [-800 \text{ nm}, 200 \text{ nm}]$ being the right half of the area in Fig. 1. In terms of time, the calculation is carried out from 0 to 115 ps, which roughly corresponds to the time of the passage of the shock wave front to the rear boundary of the target.

The two-temperature effects [3] accompanying the first few picoseconds (ps, $1 \text{ ps} = 10^{-12} \text{s}$) are quite well studied, and there is no need to model them here. So, assumingly, only a rectangular area in the center of the target with dimensions $2L_T \times L_R$, where $L_T = 800 \text{ nm}$, $L_R = 200 \text{ nm}$, is heated at the initial time. The heating area is indicated in Fig. 2 with orange color. The density of aluminum in the entire target is $\rho_{\text{Al}} = 2413 \text{ kg/m}^3$, and the pressure in the heating zone is $p_{\text{heat}} = 35.6 \text{ GPa}$, $1 \text{ GPa} = 10^9 \text{ Pa}$.

The rest of the heating zone is occupied by cold metal. The target is homogeneous, and its density in the cold zone is also $\rho_{\text{Al}} = 2413 \text{ kg/m}^3$. Pressure in the cold zone is $p_{\text{cold}} = 0$. Since we use uniform simulation scheme through all the area physically occupied by two media (metal and vacuum), we will take a metal rarefied to a density of $\rho_{\text{Al}} = 200 \text{ kg/m}^3$ as a vacuum. Such a difference in densities is sufficient to correctly describe the decay of the initial heating region and the further propagation of the shock wave. We do not need an exact description of the laser plume and the accompanying effects at the metal-vacuum interface. Pressure in the vacuum area is also $p_{\text{vac}} = p_{\text{cold}} = 0$.

On the left boundary, being the axis of symmetry of the problem, symmetric boundary conditions are set. Transmissive boundary condition is set on the upper, right, and lower boundaries.

### 3. Model and computational methods

The Euler equations, which express the laws of conservation of mass, momentum, and energy of matter, in planar two-dimensional geometry have the form:

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} + \frac{\partial \vec{G}}{\partial y} = 0, \quad (1)$$

$$\vec{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho \nu \\ \rho E \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ u(p + \rho E) \end{pmatrix}, \quad \vec{G} = \begin{pmatrix} \rho \nu \\ \rho uv \\ p + \rho \nu^2 \\ v(p + \rho E) \end{pmatrix}, \quad (2)$$

where $\vec{U}$ is the vector of conservative variables, $\vec{F}, \vec{G}$ are the fluxes, $\rho$ is the density, $u, \nu$ are the velocity vector components, $p$ is the pressure, $E = e + \frac{1}{2}(u^2 + \nu^2)$ is the specific full energy of the substance, and $e$ is the specific inner energy of the substance.

The system is closed by the Mi-Gruneisen equation of state for aluminum [4], which is uniform in the entire computational domain. The vacuum region is replaced in our case by a highly rarefied metal. It has the form:
\[ p(\rho, e) = p_c(\rho) + Gp(e - e_c). \]  

(3)

where \( \rho \) is the density, \( p_c, e_c \) are the pressure and energy depending on density at a temperature close to absolute zero (cold curves), and \( G=2 \) is the dimensionless Gruneisen parameter. Expressions for cold energy and pressure are as follows:

\[ p_c(\rho) = \frac{B}{\gamma} \left( \frac{\rho}{\rho_0} \right)^\gamma - 1, \]  

(4)

\[ e_c(\rho) = \frac{B}{\gamma(\gamma - 1)} \left( \frac{\rho}{\rho_0} \right)^\gamma - \frac{B}{\gamma - 1} \frac{\rho}{\rho_0} + \frac{B}{\gamma}, \]  

(5)

where \( B=76 \text{ GPa} \) is the aluminum bulk modulus, \( \rho_0 = 2750 \text{ kg/m}^3 \) is the constant denoting undisturbed density of the metal, and \( \gamma = 3.9 \) is the additional approximation parameter.

The speed of sound for this equation is calculated by the formula:

\[ c^2(p, \rho) = \rho \left( B \left( \frac{\rho}{\rho_0} \right)^\gamma \left[ p - \frac{B}{\gamma} \left( \frac{\rho}{\rho_0} \right)^\gamma \right] + (G + 1) \right). \]  

(6)

The parameters of the equation are selected and adjusted on the basis of one-step approximation of the metal cold curve and shockwave experiments. Note that, unlike tabular semi-empirical dependences, it can be explicitly resolved with respect to energy. It can also be explicitly differentiated, which allows obtaining a simple analytical expression for the speed of sound.

For the numerical solution of the model equations in the computational domain, an explicit and conservative unsplit 2D Godunov-type scheme is used [5]:

\[ \frac{\bar{U}_{i+1,j}^{n+1} - \bar{U}_{i,j}^{n}}{\tau} + \frac{\bar{F}_{i+1/2,j}^{n+1} - \bar{F}_{i-1/2,j}^{n}}{h_x} + \frac{\bar{G}^{n+1}_{i,j+1/2} - \bar{G}^{n}_{i,j-1/2}}{h_y} = 0, \]  

(7)

where \( \tau \) is the time step, and \( h_x, h_y \) are the grid cell \( x \)- and \( y \)- sizes.

Various calculation methods for this scheme differ in the ways of calculating intercell fluxes \( \bar{F}, \bar{G} \), i.e., they use different Riemann solvers. In this paper, HLL (Harten-Lax-van Leer) [6] and HLLC (HLL + contact) Riemann solvers are used. HLLC solver, developed by Toro and co-authors [7], is an improvement on the HLL solver. It is based on a more complex three-wave approximation, which provides additional resolution quality of shock waves and contact discontinuities comparable to the Roe solver [8]. An important feature of both of these Riemann solvers is the work with a general equation of state, provided that the correct estimates for the wave velocities are chosen. The implementation used in the TPS software package is based on Roe averaging.

Scheme (5) has the first-order temporal and spatial approximation. However, the order can be increased by using special techniques. In this paper, we use the MUSCL reconstruction and MUSCL-Hancock scheme [9] of the second-order temporal and spatial approximation with the minmod limiter, as well as the second-order spatial ENO [10] reconstruction.

Turbulence Problem Solver (TPS) software package [11] is written in C++ and has a polymorphic object-oriented architecture, which provides very simple and unified interface for problem setting. Volume target problem is represented in the package by HVVolumeTargetProblem class, which is inherited from the base general class of the HProblem problem. Abstract HRIemannSolver class is implemented to describe Riemann solvers. HLL and HLLC Riemann solvers are implemented using HHLLRiemannSolver and HHLLCRiemannSolver classes. Classes HGodunovTypeMethod for the
first-order Godunov-type approximation method and H2ndOrderMethod for the second-order reconstruction scheme are inherited from abstract HMethod class that defines the computational algorithm. Second-order reconstruction of MUSCL and ENO type are implemented by HMUSCL2Reconstruction and HENO2Reconstruction classes, inherited from HReconstruction base abstract class. Equation of state of aluminum is implemented by HEOSMieGruneisenAl class, inherited from base abstract HEOS class.

Thus, a method for solving a specific computational problem can be assembled in a software package, like a constructor, by varying the main components of the method, such as the Riemann solvers, the type and order of reconstructions, and equations of state.

4. Results
The simulations were carried out on a stationary rectangular homogeneous grid of 640x500 cells. The value of the CFL number in all calculations was taken to be 0.3.

Fig. 3 shows the results of two-dimensional modeling using the second-order MHM method with the Riemannian solver HLLC. In the process, we can distinguish the stages of plane propagation of the shock wave (a), the transition stage of spherization (b), and the hemispherical mode of propagation (c), accompanied by a faster attenuation. We can also notice that the shockwave front is followed by a rarefaction zone with strong negative pressure which denotes the corresponding stretching region in the metal.

Fig. 4. Comparison of various first- and second-order calculation methods by the example of a one-dimensional slice at time moment t=48 ps.
Fig. 4 shows one-dimensional pressure slices made on the y-axis (the symmetry axis of the target) obtained by calculations similar to the simulation in Figure 3. At time \( t=48 \) ps, the profiles obtained by modeling the problem using various first-and second-order approximation methods are shown. Among the first-order methods, there is a noticeable difference between the HLL and HLLC solvers, and the numerical dissipation of the first one is higher. But in terms of computational time, the HLL solver is approximately 20% faster.

For the second-order methods, the difference between Riemannian solvers becomes much less significant, giving way to the difference between the type of reconstruction. Thus, in terms of computational resources, it is probably not the most accurate, but the fastest and the most efficient method that is more advantageous for calculations with the second order of accuracy. Comparing the second-order reconstructions of ENO and MUSCL, we can note the greater dissipativity of the MUSCL approach, which makes it useful for modeling flows with strong shock waves. The ENO reconstruction is distinguished by a slightly clearer resolution of discontinuities, but it has stricter stability constraints and even at CFL=0.3 slightly oscillates in the right part of the profile.

For further development of the model, authors are planning to implement multiphase and multiphase liquid models in the TPS software package. They will allow for a more accurate resolution of the boundaries between substances and obtaining realistic descriptions of the processes occurring in the flare region, as well as phase transitions in the heating region and accompanying non-equilibrium phenomena, such as cavitation and breakaway. Adding elastic-plastic models to the code will provide a detailed description of the hardened areas of the metal, criteria and restrictions on the initial heating of the target, at which laser peening can occur.

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