Two-dimensional Particle-in-Cell modeling of blow-off impulse by X-ray irradiation

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Abstract

Space objects, such as spacecraft or missiles, might be exposed to intense X-rays in outer space, leading to severe damage. How to reinforce these objects to reduce damage from X-ray irradiation is a significant concern. Blow-off impulse (BOI) is a crucial physical quantity for investigating the material damage induced by X-ray irradiation. However, the accurate calculation of the BOI is a challenge, particularly for the large deformation of materials with complex configurations. In this paper, we develop a novel two-dimensional Particle-in-Cell (PIC) code, Xablation2D, to calculate the BOIs under far-field X-ray irradiation. This significantly reduces the dependence on grid shape for numerical simulation. The reliability of this code is verified by the simulation results from the open-source codes, and the calculated BOIs are consistent with experimental and analytical results.

Full Text

Preamble

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Space objects such as spacecraft or missiles may be exposed to intense X-rays in outer space, leading to severe damage. How to reinforce these objects to reduce damage from X-ray irradiation represents a significant concern. Blow-off impulse (BOI) is a crucial physical quantity for investigating material damage induced by X-ray irradiation. However, accurate calculation of BOI presents a challenge, particularly for materials undergoing large deformation with complex configurations. In this paper, we develop a novel two-dimensional Particle-in-Cell (PIC) code, Xablation2D, to calculate BOIs under far-field X-ray irradiation. This approach significantly reduces the dependence on grid shape for numerical simulation. The reliability of this code is verified through comparison with simulation results from open-source codes, and the calculated BOIs show consistency with experimental and analytical results.

Keywords: X-ray irradiation, Energy deposition, Blow-off impulse, Particle-in-Cell

INTRODUCTION

High energy-density X-ray irradiation induced by nuclear explosions in outer space can damage spacecraft or missiles [**?**, **?**, **?**]. When the X-ray source is located in the far field, surface materials of these objects may undergo sublimation. The vaporized material rapidly expands outward, causing a blow-off impulse (BOI) that loads onto the remaining solid material and generates a compressive stress wave propagating inward—a phenomenon called vapor recoil loading. Meanwhile, pressure disturbances caused by non-uniform energy deposition as thermal stress loading generate a thermal shock wave characterized by compression at the front and tension at the rear [**?**]. These stress waves form a thermal shock that induces mechanical damage to material structures and can permanently disable space objects. Reinforcing space objects to reduce damage from X-ray irradiation represents a valuable issue that has been investigated extensively.

The BOI, as a measurable physical quantity, plays a crucial role in investigating material damage induced by X-ray irradiation [**?**, **?**, **?**, **?**]. Since the pulse duration of X-rays from a nuclear explosion and the time for phase transition in the material are both O(0.1 μs)—significantly shorter than the time required for dynamic response and stress wave propagation within the material—it is reasonable to decouple the energy deposition process from the overall X-ray irradiation problem. Early research proposed several physical analytical models to calculate BOI under the assumption of instantaneous energy deposition [**?**, **?**], including the Whitener model, the BBAY model, and the modified BBAY (MBBAY) model. These models provide analytical formulas for BOI and have been extensively utilized in subsequent simulation and experimental works [**?**, **?**, **?**, **?**, **?**]. Their predictive capabilities prove satisfactory for one-dimensional or simple configuration materials, but accuracy falls short when applied to complex configurations and non-instantaneous energy deposition.

An alternative approach combines the energy deposition process with stress wave generation and propagation to simulate the complete X-ray irradiation event. With rapid developments in computational fluid dynamics, a series of codes employing this approach have been developed for multi-dimensional materials, including PUFF-TFT [**?**], CTH [**?**], LS-DYNA [**?**], ABAQUS [**?**], RAMA [**?**, **?**, **?**], TSHOCK3D [**?**], and others. These codes use either finite difference or finite element methods and incorporate Eulerian or Lagrangian descriptions for numerical simulation, enabling calculation of the temporal evolution of BOI and yielding significant enhancements in computational accuracy. Nevertheless, certain disadvantages exist: the Eulerian description struggles to track fluid interfaces, while the Lagrangian description suffers from mesh distortion when encountering large material deformations. Beyond mesh-based methods, the Monte Carlo method [**?**, **?**] serves as another simulation tool, though it relies on statistics, exhibits low efficiency, and requires substantial computational resources.

Particle-in-Cell (PIC) is a particle-mesh method first developed by F. H. Harlow' s team at Los Alamos National Laboratory for studying gas dynamics problems [**?**, **?**] and later widely generalized to computational plasma physics [**?**]. Harlow' s PIC method discretizes fluid into free-moving pseudo-particles within a spatial grid, combining Lagrangian and Eulerian descriptions, which offers advantages for simulating large deformation problems in materials with complex configurations. To our knowledge, no PIC code has been reported for BOI calculation. In this paper, we develop a novel two-dimensional PIC code, Xablation2D, capable of calculating the BOI produced by X-ray irradiation of materials.

The paper is organized as follows. Section II discusses the theoretical basis and essential modeling techniques, including the fluid PIC scheme and the three main modules of the code. Section III describes the algorithm implementation in detail, including initialization, discretization, and parallelization. Section IV presents the code' s reliability through simulations of energy deposition, shear flow, and Kelvin-Helmholtz instability. Furthermore, a series of material simulations involving X-ray irradiation are conducted to verify Xablation2D' s capabilities for BOI calculation. Finally, conclusions are presented in the last section.

II. THEORETICAL BASIS AND MODELING FOR SIMULATION

A. Fluid PIC scheme

We use Harlow' s splitting PIC scheme to solve the hydrodynamic equations. Without loss of generality, the equations can be written in abstract operator form as

$$\frac{\partial q}{\partial t} + \hat{A}q = 0,$$

where $q(r,t)$ is an arbitrary hydrodynamic quantity and $\hat{A}$ is an abstract operator. According to the rule of operator decomposition, the solution of equation (1) at time step Δt reduces to the sequential solution of two auxiliary problems:

$$\frac{\partial \tilde{q}(r,t)}{\partial t} + \hat{E}\tilde{q}(r,t) = 0,$$

$$\frac{\partial q(r,t)}{\partial t} + \hat{L}q(r,t) = 0,$$

where $\hat{A} = \hat{E} + \hat{L}$. The two equations in Eq. (2) correspond to the "Euler step" and "Lagrange step" in Harlow' s scheme, respectively. In the "Euler step," the operator $\hat{E}$ does not incorporate the spatial divergence operator, so the equation is easily solved on a fixed spatial grid. In the "Lagrange step," pseudo-particles are introduced to carry mass density, momentum density, and specific internal energy density. In one time step, as pseudo-particles move to new positions, new hydrodynamic quantities are obtained on grids by summing pseudo-particles. The "Lagrange step" can be seen as a computational procedure for modeling particle migration, which compensates for the transport effect neglected in the "Euler step."

Without loss of generality, the second equation in Eq. (2) can be written as

$$\frac{\partial q}{\partial t} + \nabla \cdot (qU) = 0,$$

where U is the flow velocity and $q = (\rho, \rho U, \rho e)$ represents the mass density, momentum density, and internal energy density, respectively. Equation (3) takes the form of a conservation equation, whose solution can be written as a summation of pseudo-particles:

$$q(r,t) = \sum_{j=1}^{N} Q_j R(r, r_j(t)).$$

The total number of pseudo-particles is denoted as N, and Q_j represents the hydrodynamic quantities carried by the j-th pseudo-particle. The value of Q_j remains constant during one "Lagrange step." The kernel function of the pseudo-particle, denoted as $R(r, r_j(t))$, depends on the current space coordinate r and the radius-vector r_j of the j-th pseudo-particle center. This kernel function satisfies certain universal properties:

$$\begin{cases} R(r_1, r_2) = R(r_2, r_1) \geq 0, \\ \int_\Omega dr_1 R(r_1, r_2) = 1, \end{cases}$$

where Ω denotes the full space. With these characteristics and any smooth finite function, the representation $q(r,t)$ in Eq. (4) enables the simplification of Eq. (3) to fulfill the equations of motion for pseudo-particles:

$$\frac{dr_j(t)}{dt} = U(r_j(t)), \quad j = 1, 2, \ldots, N.$$

Our code comprises three primary modules: an energy deposition module, an equation of state (EOS) module, and an ideal hydrodynamics module, complemented by a post-processing script for blow-off impulse calculation to constitute the complete Xablation2D code.

B. Energy deposition

The energy deposition module estimates energy transfer between X-rays and matter. At the microscopic level, X-rays primarily interact with matter through electrons. Initially, photon energy transfers directly to electrons, which then interact with atoms in the material, resulting in energy deposition. The photoelectric effect dominates in the low-energy region, while Compton scattering contributes as photon energy increases [**?**]. For far-field X-ray irradiation, the degree of material ionization is so low that plasma effects can be disregarded.

The energy flux for parallel X-rays incident on target material can be estimated by considering the distance x traveled in the incident direction:

$$\Phi(x) = \Phi_0 \frac{\int_0^\infty f(\lambda, T) \exp[-\mu(\lambda)\rho x] d\lambda}{\int_0^\infty f(\lambda, T) d\lambda},$$

where Φ_0 and $\Phi(x)$ are the energy flux at the initial position and at position x, respectively; $f(\lambda, T)$ is the X-ray energy spectrum, which depends on photon wavelength λ and radiation temperature T; ρ is the mass density; and $\mu(\lambda)$ is the mass absorption coefficient associated with photon wavelength. The energy spectrum $f(\lambda, T)$ approximates a black-body spectrum for X-rays produced by nuclear explosions. In numerical simulation, it is necessary to truncate and discretize the energy spectrum. Hence, the expression for energy flux in computation can be written as:

$$\Phi(x) = \Phi_0 \sum_j w_j \exp[-\mu(\lambda_j)\rho x],$$

where subscript j is the discretized energy group index and w_j represents the proportion of incident energy flux for monochromatic light with specific wavelength λ_j.

The quantity e_R signifies the amount of photon energy deposited through X-ray-matter interaction, per unit mass and per unit time, within the region $x \sim x + \Delta x$:

$$e_R = \frac{\Phi(x) - \Phi(x + \Delta x)}{\rho \Delta x \tau},$$

where τ is the time increment. It is postulated that the entirety of this deposited energy converts into internal energy in subsequent discussion.

C. Equation of state

X-ray irradiation induces significant changes in material state, including phase transitions, thermal expansion, and shock compression, rendering a large range of material parameters. Consequently, distinct equations of state are required to characterize the expansion and compression regions of the material. For the thermal expansion region, the PUFF EOS [**?**] is adopted:

$$p = \rho \left[(\gamma - 1) + (\Gamma_0 - \gamma + 1) \frac{\rho_0}{\rho} \right] \left[e - e_s \exp\left(-\frac{N \rho_0}{\rho} \right) \right], \quad \rho < \rho_0,$$

where ρ_0 and ρ are the initial and current densities, respectively; p is material pressure; Γ_0 is the Grüneisen coefficient; γ is the specific heat ratio of vaporized gas; e_s is the sublimation energy; and $N = C_0^2 / \Gamma_0 e_s$. C_0 is a Hugoniot parameter that determines the shock wave velocity D in solid material with post-shock velocity u and another Hugoniot parameter λ by $D = C_0 + \lambda u$.

For the compression zone, the Grüneisen EOS on the Hugoniot line is used, expressed as [**?**]:

$$p = p_H(v) + \rho_0 \Gamma_0 (e - e_H), \quad \rho \geq \rho_0,$$

where $p_H(v)$ and e_H represent the post-shock pressure and specific internal energy when the pre-shock is stationary, respectively; $v = 1/\rho$ is the specific volume; and v_0 is the initial specific volume. These are given by:

$$p_H(v) = \frac{\rho_0 C_0^2 (1 - v/v_0)}{[1 - \lambda(1 - v/v_0)]^2},$$

$$e_H = \frac{1}{2} p_H (v_0 - v).$$

In addition to analytic EOS expressions, the open-source code FEOS provides tabular EOS data across wide temperature and density ranges [**?**]. FEOS, based on the QEOS (quotidian equation of state) model [**?**], calculates the material-specific Helmholtz free energy $F(\rho, T)$ directly and is widely used in computational fluid dynamics codes.

D. Ideal hydrodynamics

In the hydrodynamics module, we ignore thermal radiation and heat conduction effects. The far-field X-ray flux of concern in these issues is O(100 J/cm^2). In this case, material temperature is O(1 eV), and the corresponding radiation pressure is only O(1 Pa), which is far lower than material pressure. The velocity of thermal shock waves in solid materials is about O(1 km/s), much faster than heat conduction. Therefore, ignoring these effects is reasonable. Additionally, our code aims to calculate the blow-off impulse occurring in the thermal expansion vaporized region. This region is characterized by significantly lower material stress compared to material pressure, allowing us to also ignore stress for impulse calculation.

The 2D governing equations of ideal hydrodynamics are written as:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} = 0, \\ \frac{\partial(\rho u_x)}{\partial t} + \frac{\partial(\rho u_x^2)}{\partial x} + \frac{\partial(\rho u_x u_y)}{\partial y} = -\frac{\partial p}{\partial x}, \\ \frac{\partial(\rho u_y)}{\partial t} + \frac{\partial(\rho u_x u_y)}{\partial x} + \frac{\partial(\rho u_y^2)}{\partial y} = -\frac{\partial p}{\partial y}, \\ \frac{\partial(\rho e)}{\partial t} + \frac{\partial(u_x w)}{\partial x} + \frac{\partial(u_y w)}{\partial y} = e_R, \end{cases}$$

where ρ is mass density, $u = (u_x, u_y)$ is fluid velocity, p is pressure, e is specific internal energy, $w = \rho(e + u^2/2)$ is total energy, and e_R is the deposited energy from X-ray irradiation per unit mass per unit time. According to Harlow' s splitting scheme, the 2D governing equations can be divided into distinct groups for the Euler and Lagrange steps, respectively.

E. Blow-off impulse calculation

When X-rays irradiate a material surface, the material undergoes sublimation, forming an evaporation layer. The vaporized material violently ejects outward and generates a blow-off impulse. According to the impulse theorem, the specific impulse in a given direction equals the change in momentum:

$$P - P_0 = m(u - u_0),$$

where P, u, P_0, and u_0 represent final momentum, final flow velocity, initial momentum, and initial flow velocity in a certain direction, respectively, and m is material mass. Typically, the initial velocity of vaporized material is zero ($u_0 = 0$). For numerical calculations, Eq. (18) can be written in summation form [**?**]:

$$I = \sum_j m_j |u_j|, \quad u_j < 0, e_j > e_s,$$

where m_j and u_j are material mass and velocity in the j-th grid, respectively, accounting for the sum of momentum in all grids where vaporized material ejects outward. Alternatively, BOI can be computed by its definition:

$$I = \int_{t_0}^{t} p_g dt,$$

where p_g represents the pressure exerted by ejected gas on the surface of the solid material at rest, and t and t_0 are the final and initial times, respectively. For numerical calculations, the discrete form of Eq. (20) is:

$$I = \sum_{n} p_g \Delta t,$$

where n represents the n-th vaporized grid.

III. ALGORITHM IMPLEMENTATION

Based on the theoretical framework outlined in Section II, we develop a two-dimensional code named Xablation2D to calculate the blow-off impulse of materials under far-field X-ray radiation. This section provides a detailed description of the algorithm implementation. For convenience, we omit the subscripts 1 and 2 that distinguish "Euler step" and "Lagrange step" in the following discussion.

A. Initialization

We discretize the simulation domain into rectangular grids on Cartesian coordinates. Fluid physical quantities, except mass density, are initialized by manual assignment to grid points. Mass density is initialized by summing the weight of pseudo-particles as follows:

$$\begin{cases} \rho_{i,j} = \rho_{i,j} + \rho_p \cdot \omega_{i,j}, \\ \rho_{i+1,j} = \rho_{i+1,j} + \rho_p \cdot \omega_{i,j}, \\ \rho_{i,j+1} = \rho_{i,j+1} + \rho_p \cdot \omega_{i,j}, \\ \rho_{i+1,j+1} = \rho_{i+1,j+1} + \rho_p \cdot \omega_{i,j}, \end{cases}$$

where $\rho_{i,j}$ is mass density on the grid, ρ_p denotes mass density carried by the pseudo-particle, and $\omega_{i,j}$ is the weight factor. Notably, in our code, ρ_p remains constant throughout the entire simulation. The area-weighting method shown in Fig. 1 [Figure 1: see original paper] is employed for mass density distribution in 2D simulation, with weight factors expressed as:

$$\omega_{i,j} = \frac{A_1}{A_1 + A_2 + A_3 + A_4}, \quad \omega_{i+1,j} = \frac{A_2}{A_1 + A_2 + A_3 + A_4},$$

$$\omega_{i,j+1} = \frac{A_3}{A_1 + A_2 + A_3 + A_4}, \quad \omega_{i+1,j+1} = \frac{A_4}{A_1 + A_2 + A_3 + A_4},$$

where A_i $(i = 1, 2, 3, 4)$ represents the area of overlap between the pseudo-particle and the grid.

B. Euler step

The radiative deposition energy and equation of state are discretized on the grid as follows:

$$e_{R,i,j} = \frac{\Phi_{i-1,j-1} - \Phi_{i,j}}{h_1 \tau},$$

where the energy flux $\Phi_{i,j}$ is given by:

$$\Phi_{i,j} = \Phi_0 \sum_j w_j \exp[-\mu(\lambda_j)\rho_{i,j}x].$$

The pressure $p_{i,j}$ is determined by:

$$p_{i,j} = \begin{cases} p_{A,i,j}, & \rho_{i,j} < \rho_0, \\ p_{H,i,j}, & \rho_{i,j} \geq \rho_0, \end{cases}$$

with the PUFF EOS for the expansion region:

$$p_{A,i,j} = \rho_{i,j} \left[(\gamma - 1) + (\Gamma_0 - \gamma + 1) \frac{\rho_0}{\rho_{i,j}} \right] \left[e_{i,j} - e_s \exp\left(-\frac{N\rho_0}{\rho_{i,j}} \right) \right],$$

and the Grüneisen EOS for the compression zone:

$$p_{H,i,j} = p_{H,i,j} + \Gamma_0 \rho_0 \left[e_{i,j} - e_{H,i,j}(v_0 - v_{i,j}) \right],$$

where:

$$p_{H,i,j} = \rho_0 C_0^2 \frac{(1 - v_{i,j}/v_0)}{[1 - \lambda(1 - v_{i,j}/v_0)]^2},$$

$$e_{H,i,j} = \frac{1}{2} p_{H,i,j}(v_0 - v_{i,j}).$$

The hydrodynamic equations (Eq. 16) in the "Euler step"can then be discretized as:

$$\begin{cases} u_{x,i,j}^{n+1} = u_{x,i,j}^{n} - \frac{\tau}{\rho_{i,j}} \frac{p_{i+1/2,j} - p_{i-1/2,j}}{h_1}, \\ u_{y,i,j}^{n+1} = u_{y,i,j}^{n} - \frac{\tau}{\rho_{i,j}} \frac{p_{i,j+1/2} - p_{i,j-1/2}}{h_2}, \\ e_{i,j}^{n+1} = e_{i,j}^{n} - \frac{\tau}{\rho_{i,j}} \left[\frac{(u_x w)_{i+1/2,j} - (u_x w)_{i-1/2,j}}{h_1} + \frac{(u_y w)_{i,j+1/2} - (u_y w)_{i,j-1/2}}{h_2} \right] + e_{R,i,j}, \end{cases}$$

where subscript (i, j) denotes the grid index in the spatial coordinate system, superscript n represents the n-th time step, τ is the time increment, and h_1 and h_2 are grid sizes in the x and y directions, respectively. Note that mass density remains constant as shown in Eq. (16), meaning $\rho_{i,j}^{n+1} = \rho_{i,j}^{n}$.

C. Lagrange step

In the "Lagrange step,"the fluid is divided into many pseudo-particles with finite sizes. We assume an internal distribution function of fluid quantities within a pseudo-particle:

$$q(\xi, \eta) = \{(q_{i+1,j+1} - q_{i+1,j})(2\eta - \delta\eta) + q_{i+1,j}\}(2\xi - \delta\xi) - \{(q_{i,j+1} - q_{i,j})(2\eta - \delta\eta) + q_{i,j}\}(2\xi - \delta\xi - 1),$$

where the pseudo-particle size is normalized, $q(\xi, \eta)$ represents physical quantities carried by pseudo-particles, coordinates (ξ, η) denote internal position within the pseudo-particle with the origin at the bottom left-hand corner, and $(\delta\xi, \delta\eta)$ are intervals from the origin of the internal coordinate system to grid boundaries in the x and y directions, respectively. These are illustrated in Fig. 2 [Figure 2: see original paper], where red lines represent grids, the red dot represents the pseudo-particle center, and the blue square represents pseudo-particle size. The physical quantity q_p carried by the pseudo-particle at the internal coordinate center can be obtained by integrating $q(\xi, \eta)$ from 0 to 1:

$$q_p = \int_0^1 \int_0^1 q(\xi, \eta) d\xi d\eta = q_{i+1,j+1}(1 - \delta\xi)(1 - \delta\eta) + q_{i+1,j}(1 - \delta\xi)\delta\eta + q_{i,j+1}\delta\xi(1 - \delta\eta) + q_{i,j}\delta\xi\delta\eta.$$

The equations of pseudo-particle motion are:

$$\begin{cases} x_p^{n+1} = x_p^n + \tau u_{p,x}, \\ y_p^{n+1} = y_p^n + \tau u_{p,y}, \end{cases}$$

where (x_p, y_p) denote the position of the pseudo-particle center and $(u_{p,x}, u_{p,y})$ represent the velocity of the pseudo-particle center as determined by Eq. (30). When the pseudo-particle advances to a new position as shown in Fig. 2, we recompute new intervals from the origin of the internal coordinate, denoted as

$(\delta\xi^*, \delta\eta^*)$. By summing pseudo-particles at new positions, new fluid quantities on the grid can be derived.

In this paper, we present three algorithms—Area-weighting method (AWM), Integration-weighting method (IWM), and Interpolation-Integration-weighting method (IIWM)—for the summation process, each exhibiting different types of numerical diffusion [**?**]. The details of summation algorithms are shown in Appendix A. These three algorithms feature different numerical diffusion and noise characteristics and can be selected according to specific problem requirements.

D. Parallelization

The Message Passing Interface (MPI) is employed for parallelization [**?**]. Details of parallel communication are shown in Appendix B.

IV. SIMULATION RESULTS

A. Far-field X-ray energy deposition

The X-ray energy deposition module is crucial for calculation accuracy of the blow-off impulse in Xablation2D. To validate this module, we compared the energy deposition rate from Xablation2D with results obtained from the Monte Carlo code Geant4 [**?**, **?**, **?**, **?**]. In the Xablation2D simulation, parallel soft X-rays with initial energy flux $\phi_0 = 418$ J/cm^2 are incident perpendicularly into a 2D planar aluminum (Al) target with density $\rho = 2.738$ g/cm^3, and the pulse duration is 50 ns. The X-ray energy spectrum approximates a black-body spectrum with radiation temperature $T = 1$ keV. The wavelength range in the energy spectrum is $\lambda = 0.1$ Å to 10 Å, discretized into 23 energy groups for numerical simulation. The mass absorption coefficient μ for X-rays in each energy group in Al material is shown in Tab. 1 .

In the Geant4 code, a parallel black-body spectrum photon beam with radiation temperature 1 keV is configured to simulate soft X-rays. Photon-material interactions are simulated using the Livermore low-energy electromagnetic physics model, effective for photon energies from 250 eV to 1 GeV. By tracking photon trajectories within the Al target, the amount of deposited energy in the material can be quantified.

The energy deposition rates calculated by both codes are shown in Fig. 3 [Figure 3: see original paper], where the vertical axis corresponds to the energy deposition rate (signifying the lost ratio of incident energy flux after traversing corresponding distance in the material) and the horizontal axis represents depth within the aluminum target along the incident X-ray direction. Fig. 3 also shows the relative error between the two results as an orange dashed line. The largest deviation occurs near the material surface and rapidly decreases to O(5%) along the incident depth. This occurs because the energy deposition rate value is small at the material surface, where even minor deviations in parameters such as mass absorption coefficients can produce noticeable relative error.

Additionally, the depth required for 50% X-ray energy deposition is 4.17 µm for Xablation2D and 3.5 µm for Geant4, consistent with the O(5 µm) estimate in [?].

B. Shear flow simulation

We use plane shear flow simulations to verify numerical diffusion from the AWM, IWM, and IIWM algorithms. In Xablation2D, the simulation domain size is $L_x \times L_y = 0.4 \times 0.4$ cm^2, discretized into 400×400 grids with 10×10 pseudo-particles allocated per grid. The flow field is divided into two layers: upper fluid A and lower fluid B, with the interface located at $y = 0.2$ cm. The upper fluid has mass density $\rho_A = 2.738$ g/cm^3, x-direction velocity $u_{Ax} = 3 \times 10^5$ cm/s, and y-direction velocity $u_{Ay} = 0$ cm/s. The lower fluid has the same mass density $\rho_B = \rho_A$, x-direction velocity equal in magnitude but opposite in direction ($u_{Bx} = -u_{Ax}$), and the same y-direction velocity $u_{By} = u_{Ay}$. The simulation employs periodic boundary conditions in the x direction and open boundary conditions in the y direction. The ideal gas EOS $p = (\gamma - 1)\rho e$ is adopted with $\gamma = 1.667$, and initial pressure is set to 1 GPa.

The fluid velocity distribution in the x direction (u_x) of shear flow is shown in Fig. 4 [Figure 4: see original paper]. The IIWM (or IWM) exhibits better suppression of numerical diffusion than AWM. For AWM in Fig. 4(a), the discontinuous shear flow velocity becomes smoothed, and this smoothness gradually saturates into upper and lower layers due to numerical diffusion. In contrast, for IIWM (or IWM) in Fig. 4(b), the discontinuous velocity can be maintained throughout the entire simulation time due to using integration of the internal distribution function in the shear velocity direction.

C. Kelvin-Helmholtz instability simulation

When two contiguous fluids flow with shear velocities, instability can arise at the interface given small fluctuations. This phenomenon is known as Kelvin-Helmholtz instability (KHI) [?, ?]. KHI is widely observed in nature, including turbulent mixing in jet streams, formation of undulate clouds, and supernova explosions [?, ?, ?]. Here, we performed KHI simulations using both Xablation2D and the open radiation magnetohydrodynamics simulation code FLASH4 [?], comparing the results. Initial parameters including simulation domain size, number of grids, and pseudo-particles per grid are identical to Section IV B, except for temperature. The initial material temperature is $T = 21.6$ eV, corresponding to specific internal energy $e = 1 \times 10^5$ J/g. Initial pressure determined by EOS is 182.24 GPa. A velocity perturbation in the y direction is introduced at the fluid interface as a seed for KHI:

$$u_y = u_0 \sin(kx) \exp(k|y - L_y/2|),$$

where $u_0 = 1 \times 10^6$ cm/s is the initial amplitude and $k = 4\pi/L_x$ cm^{-1} is the

initial wave number [**?**]. To observe secondary unstable structures, numerical diffusion must be reduced, so we adopt IWM in Xablation2D. In FLASH4 simulation, we maintain consistent initialization parameters and perturbation but use adaptive mesh refinement (AMR).

Fig. 5 [Figure 5: see original paper] illustrates the mass density evolution of the lower half fluid. The six subfigures in the first row show Xablation2D results, and the second row shows FLASH4 results. The simulation results are consistent between codes. The disturbance at the fluid interface gradually increases, and eventually the two fluids mix and exhibit vortex structures. IIWM is also employed to simulate KHI with the same parameters in Xablation2D. The results are basically consistent with FLASH4, except for some secondary structures, as shown in Fig. 6 [Figure 6: see original paper]. This deviation is attributed to relatively higher numerical diffusion in the convective velocity direction in IIWM.

The mixing width η is defined as the difference between the maximum position and initial position of the lower half fluid, as shown in Fig. 7(a) [Figure 7: see original paper]. Fig. 7(b) shows mixing width evolution, where blue and cyan dashed lines correspond to Xablation2D results and the magenta solid line corresponds to FLASH4. Orange dotted lines indicate relative errors between the two codes, remaining O(5%), demonstrating consistency. This minor deviation validates Xablation2D' s reliability. The mixing width growth is significantly smaller than predicted by classical linear KHI theory because the simulation exhibits compressibility and nonlinear fluid evolution due to strong initial perturbation.

D. Vaporization blow-off impulse

When X-rays irradiate solid material, a blow-off impulse loads onto the material surface, as illustrated in Fig. 8 [Figure 8: see original paper]. Photon energy in X-rays is primarily absorbed through the photoelectric effect and Compton scattering. X-ray energy flux decreases exponentially as it penetrates from the surface into the material interior. Consequently, specific internal energy at the surface increases rapidly, leading to phase transition and adiabatic expansion that generates an ablation layer. If deposited energy exceeds material sublimation energy, surface solid material transforms into gas, forming a vaporization zone at the front. The vaporized material violently sprays into vacuum, generating a recoil impulse on remaining material known as the blow-off impulse (BOI).

In the BOI simulation case, aluminum (Al) is selected as the target material, and the IIWM algorithm is employed in Xablation2D. Material expansion and compression are described by PUFF EOS (Eq. 10) and Grüneisen EOS (Eq. 12) as discussed in Section II C. Physical property parameters of Al in the simulation are shown in Tab. 2 . The simulation domain has size $L_x \times L_y = 0.8 \times 0.8$ cm^2 divided into 400×400 grids. We allocate 100×100 pseudo-particles per grid

near the target material surface and 5×5 pseudo-particles in other regions. Two geometric configurations are simulated: a semi-infinite slab and a cylinder.

1. Semi-Infinite Slab The semi-infinite slab occupies the region where $x > 0.4$ cm, while the region where $x \leq 0.4$ cm is filled with low-density gas to maintain numerical stability. Periodic boundary conditions are applied in the y direction, and open boundary conditions in the x direction. Parallel X-rays have radiation temperature $T = 1$ keV and incident normally on the slab. The energy spectrum is discretized into 23 energy groups as in Tab. 1 , with initial fluxes $\Phi_0 = 209$ J/cm^2 and 418 J/cm^2. Fig. 9 [Figure 9: see original paper] illustrates mass density and pressure evolution. The material surface vaporizes under X-ray irradiation and expands outward, generating a blow-off impulse that drives a thermal shock wave propagating inward. Density accumulation in the left region results from the low-density gas initialization.

For the semi-infinite slab configuration, the impulse distribution is uniform in the y direction, allowing calculation of one-dimensional average BOI by integrating along y and dividing by length L_y. This result appears as the blue dashed line in Fig. 10 [Figure 10: see original paper]. To verify correctness, we developed a one-dimensional Lagrangian code based on Ref. [**?**] to calculate BOI under identical parameters. The result, shown as the magenta solid line, is consistent with Xablation2D. Additionally, we compare simulation results with three BOI models shown as dotted lines in Fig. 10. Their analytical formulas are [**?**]:

BBAY:

$$I = \alpha \left[\int_0^{x_0} [e(x) - e_s] \rho_0 x dx \right]^{1/2}$$

Whitener:

$$I = \int_0^{x_0} [e(x) - e_s]^{1/2} \rho_0 dx$$

MBBAY:

$$I = \alpha \left[\int_0^{x_0} \frac{e(x) - e_m}{1 + \ln\left(\frac{e(x)}{e_m}\right)} \rho_0 x dx \right]^{1/2}$$

where $e(x)$ is the energy deposition profile, e_m represents melting energy, α is a correction parameter ranging from 1 to 2, and x_0 is the sublimation layer thickness determined by $e(x) = e_s$.

In simulations, we set $e_m = 3.975$ kJ/g and $\alpha = 1.1$. The BOI models estimate only instantaneous deposition energy, resulting in horizontal dotted lines in Fig. 10. In contrast, BOIs calculated by Xablation2D and 1D Lagrangian codes (blue dashed and magenta solid lines) exhibit a growth time of O(0.1 μs) before stabilizing, corresponding to the characteristic time for complete surface

sublimation. Results from BBAY and MBBAY models align well with stable numerical simulation values.

Furthermore, we compared Xablation2D simulation results with published experimental data to verify code reliability. Ref. [**?**] provides three measurements of BOI produced by X-rays irradiating flat Al material. X-ray parameters and measured impulse values are presented in Tab. 3 . We simulated these three experiments using Xablation2D with experimental parameters. The BOIs from simulations are shown in Fig. 11(a) [Figure 11: see original paper], with stable values of 97.84, 121.82, and 125.36 Pa · s, respectively. Fig. 11(b) compares simulation results with measured BOIs. Two cases show consistent results with negligible relative error (cases No.01154 and No.01170). Although case No.01171 shows larger relative error, it remains within O(20%).

2. Cylinder In the cylinder configuration, the target is positioned at the simulation domain center with coordinates $x = y = 0.4$ cm and radius 0.2 cm. Remaining domain areas are filled with low-density gas. Physical property parameters and X-ray parameters are identical to those in the semi-infinite slab configuration. Mass density and pressure distributions are shown in Fig. 12 [Figure 12: see original paper]. X-rays irradiate the left side of the cylinder, producing vaporized material that ejects violently and generates BOI, which drives a thermal shock wave moving toward the cylinder center.

When parallel X-rays irradiate a curved surface, deposited energy density at the material surface is non-uniform, making BOI a function of the cylinder' s radial direction. Refs. [**?**, **?**, **?**, **?**] propose that if energy deposition density has a cosine profile on the cylinder surface, BOI variation is proportional to the cosine of the polar angle:

$$I = I_0 \cdot \cos\theta,$$

where θ is the polar angle defined in Fig. 13(a) [Figure 13: see original paper] and I_0 represents BOI at $\theta = 0^\circ$. Figs. 13(b), (c), and (d) show BOI distribution versus polar angle at different time intervals. The BOI profiles basically satisfy the cosine law, though small deviations exist. The primary reason is that X-ray energy deposition thickness cannot be completely ignored. Deviation between the BOI curve and cosine function increases as polar angle increases from 0° to 90°, especially at $\theta = 90^\circ$, where specific internal energy is non-zero due to X-ray penetration, resulting in non-zero BOI. Simulation results confirm this phenomenon.

V. CONCLUSION

We develop a novel parallel two-dimensional PIC code, Xablation2D, for calculating the BOI of far-field X-ray irradiating materials. The code comprises three primary modules: an energy deposition module, an EOS module, and an

ideal hydrodynamics module. In the ideal hydrodynamics module, the solution of hydrodynamic equations is divided into "Euler step" and "Lagrange step" according to Harlow' s splitting scheme. The introduced pseudo-particle compensates for transport effects. We present three new summation algorithms—AWM, IWM, and IIWM—to map physical quantities carried by pseudo-particles onto the grid.

In contrast to conventional finite difference or finite element methods, the new PIC method significantly reduces dependence on grid shape and is well-suited for calculating large deformation problems in materials with complex configurations. To verify Xablation2D' s reliability, we compare with open-source codes: Geant4 for soft X-ray energy deposition rate, and FLASH4 for shear flow and KHI problems. Simulation results exhibit minor discrepancies compared to our code. Finally, we calculate BOI in two geometric configurations of Al materials under far-field X-ray irradiation. Results show good consistency with experimental, analytical, and other simulation results. We also observe thermal shock wave propagation inside the material caused by X-ray irradiation.

For X-rays with increased energy flux, the overall process becomes more intricate. The material becomes highly ionized, and energy deposition involves interaction between the radiation field and plasma. In future work, we plan to develop a radiation transport module in Xablation2D for simulation of ultra-intense X-ray irradiating materials.

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Appendix A: Summation algorithms

(1) Area-weighting method (AWM): This approach assumes the distribution function of physical quantity $q(\xi, \eta)$ carried by the pseudo-particle collapses to the value at the internal coordinate center (q_p). New fluid physical quantities on the grid are obtained by simple summation of q_p multiplied by area:

$$\begin{cases} (\rho q)_{i,j} = \sum_{p\in(i,j)} \rho_p q_p \delta\xi^* \delta\eta^*, \\ (\rho q)_{i+1,j} = \sum_{p\in(i+1,j)} \rho_p q_p (1-\delta\xi^*) \delta\eta^*, \\ (\rho q)_{i,j+1} = \sum_{p\in(i,j+1)} \rho_p q_p \delta\xi^* (1-\delta\eta^*), \\ (\rho q)_{i+1,j+1} = \sum_{p\in(i+1,j+1)} \rho_p q_p (1-\delta\xi^*)(1-\delta\eta^*), \end{cases}$$

where $p \in (i, j)$ denotes pseudo-particles whose centers are located in the (i, j) grid. AWM is straightforward and computationally efficient but introduces zero-order numerical diffusion effects.

(2) Integration-weighting method (IWM): IWM maintains the internal distribution function $q(\xi,\eta)$ during pseudo-particle motion. New physical quantities on the grid are obtained by integrating $q(\xi,\eta)$ over each new area defined by overlap between pseudo-particle size and grid. For instance, the overlap area between pseudo-particle size and (i,j) grid is represented by $\delta\xi^*\times\delta\eta^*$ as shown in Fig. 2. The new fluid physical quantities on the grid are:

$$\begin{cases}(\rho q)_{i,j}=\sum_{p\in(i,j)}\int_0^{\delta\xi^*}\int_0^{\delta\eta^*}q(\xi,\eta)d\xi d\eta,\\(\rho q)_{i+1,j}=\sum_{p\in(i+1,j)}\int_{\delta\xi^*}^1\int_0^{\delta\eta^*}q(\xi,\eta)d\xi d\eta,\\(\rho q)_{i,j+1}=\sum_{p\in(i,j+1)}\int_0^{\delta\xi^*}\int_{\delta\eta^*}^1q(\xi,\eta)d\xi d\eta,\\(\rho q)_{i+1,j+1}=\sum_{p\in(i+1,j+1)}\int_{\delta\xi^*}^1\int_{\delta\eta^*}^1q(\xi,\eta)d\xi d\eta.\end{cases}$$

IWM has second-order numerical diffusion, much better than AWM, but introduces some non-physical numerical noise that can make fluid motion somewhat unstable.

(3) Interpolation-Integration-weighting method (IIWM): IIWM combines AWM (used in the convective velocity direction) and IWM (used in the shear velocity direction). For instance, if $q(\xi,\eta)$ represents fluid velocity in the x direction (u_x), inverse linear interpolation is applied to $q(\xi,\eta)$ in the x direction, followed by integration in the y direction. The specific procedure is as follows. First, integrate $q(\xi,\eta)$ over ξ from 0 to 1:

$$q(\eta)=\int_0^1 q(\xi,\eta)d\xi=\{[q_{i+1,j+1}(1-\delta\xi)+q_{i,j+1}\delta\xi]-[q_{i+1,j}(1-\delta\xi)+q_{i,j}\delta\xi]\}(2\eta-\delta\eta)+q_{i+1,j}(1-\delta\xi)+q_{i,j}\delta\xi.$$

Then integrate $q(\eta)$ over the length where pseudo-particle size and grid overlap in the y direction to obtain two new intermediate physical quantities:

$$\begin{cases}q_1=\int_0^{\delta\eta^*}q(\eta)d\eta,\\q_2=\int_{\delta\eta^*}^1q(\eta)d\eta.\end{cases}$$

Finally, new physical quantities are determined by:

$$\begin{cases}(\rho q)_{i,j}=\sum_{p\in(i,j)}\rho_p q_1(1-\delta\xi^*),\\(\rho q)_{i+1,j}=\sum_{p\in(i+1,j)}\rho_p q_1\delta\xi^*,\\(\rho q)_{i,j+1}=\sum_{p\in(i,j+1)}\rho_p q_2(1-\delta\xi^*),\\(\rho q)_{i+1,j+1}=\sum_{p\in(i+1,j+1)}\rho_p q_2\delta\xi^*.\end{cases}$$

This approach can similarly be implemented for fluid velocity in the y direction (u_y).

Appendix B: Parallel communication

MPI adopts an explicit message-passing architecture, necessitating explicit sending and receiving of messages to facilitate data exchange among processors. Each parallel process possesses its own memory space, and processors access each other' s memory through explicit message passing. This design exhibits robust parallelism and is particularly well-suited for implementing large-scale parallel algorithms.

In our code, the simulation region is divided into N parts based on a grid structure, with each part assigned to an individual process for calculation. The total number of processes $N = pp_x \times pp_y$, where pp_x and pp_y are the numbers of processes assigned to grids along the x and y directions, respectively, as shown in Fig. 14 [Figure 14: see original paper]. A layer of grid, called guard grid or ghost grid, is established at the junction of adjacent parallel regions to store physical quantities received from neighboring processes. Exchange of physical quantities on guard grids is achieved through two MPI communication subroutines: MPI_{SEND} and MPI_{RECV}, as illustrated in Fig. 15 [Figure 15: see original paper].

In initialization, all pseudo-particles are placed within parallel regions and guard grids. When pseudo-particles move out of a parallel region, they are transferred to another parallel region via MPI communication. This communication can occur between any two processors. First, all communicating pseudo-particles are gathered into a linked list, then the processor whose grid each pseudo-particle would fall into is determined, and finally the MPI communication subroutine is used to send the pseudo-particle to the corresponding processor. This procedure is illustrated in Fig. 16 [Figure 16: see original paper].

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Note: Figure translations are in progress. See original paper for figures.