



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 may be exposed to intense X-rays in outer space, leading to severe damage. The reinforcement of these objects to reduce the damage caused by X-ray irradiation is a significant concern. The blow-off impulse (BOI) is a crucial physical quantity for investigating material damage induced by X-ray irradiation. However, the accurate calculation of BOI is challenging, particularly for large deformations of materials with complex configurations. In this study, we develop a novel two-dimensional particle-in-cell code, *Xablation2D*, to calculate BOIs under far-field X-ray irradiation. This significantly reduces the dependence of the numerical simulation on the grid shape. The reliability of this code is verified by simulation results from open-source codes, and the calculated BOIs are consistent with the experimental and analytical results.

Keywords X-ray irradiation · Energy deposition · Blow-off impulse · Particle in cells

1 Introduction

High-energy-density X-ray irradiation induced by nuclear explosions in outer space can damage spacecraft and missiles [1–3]. If the X-ray source is located in the far field, the surface material of these objects may undergo sublimation. The vaporized material rapidly expands outward, causing a

blow-off impulse (BOI). The BOI loads the remaining solid material, generating a compressive stress wave that propagates inward, which is called vapor recoil loading. However, the pressure disturbance caused by nonuniform deposition energy as thermal stress loading generates a thermal shock wave characterized by compression at the front and tension at the rear [4]. These stress waves form one thermal shock wave that induce mechanical damage to material structures, and permanently disable space objects. Reinforcing space objects to reduce the damage caused by X-ray irradiation is a valuable issue that has been extensively investigated.

The BOI, as a measurable physical quantity, plays a crucial role in investigating material damage induced by X-ray irradiation [5–8]. The pulse duration of X-rays induced by a nuclear explosion and the time required for phase transition in the material are both $\mathcal{O}(0.1 \mu\text{s})$, which is significantly shorter than the time required for the dynamic response and stress wave propagation within the material. It is reasonable to decouple the energy deposition process from the entire X-ray irradiation process. In early research, several physical analytical models were proposed to calculate the BOI under the assumption of instantaneous deposition energy [9, 10], including the Whitener, BBAY, and the modified BBAY (MBBAY) models. These models have analytical formulas for BOI

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and have been extensively utilized in subsequent simulation and experimental studies [9, 11–14]. The predictive capabilities of these models are satisfactory for calculating the BOI for one-dimensional or simple configuration materials; however, their accuracy falls short when applied to materials with complex configurations and non-instantaneous deposition energy. Another approach for calculating the BOI is to combine the energy deposition process with the generation and propagation of stress waves and simulate the entire X-ray irradiation. With the rapid development of computational fluid dynamics, a series of codes, referred to this approach, have been developed to calculate the BOI for multidimensional materials, such as *PUFF-TFT* [15], *CTH* [16], *LS-DYNA* [17], *ABAQUS* [18], *RAMA* [19–21], and *TSHOCK3D* [22]. These codes employ either the finite difference or finite element method and incorporate Eulerian or Lagrangian descriptions for numerical simulation, which enables the calculation of the temporal evolution of the BOI and results in significant enhancements in computational accuracy. Nevertheless, there are certain disadvantages associated with these codes; that is, the Eulerian description has difficulty tracking fluid interfaces, whereas the Lagrangian description is prone to mesh distortion when encountering large material deformations. In addition to the mesh method mentioned above, another simulation tool is the Monte Carlo method [23, 24]. However, this method relies on statistics, has low efficiency, and requires significant computational resources.

Particle in cell (PIC) is a particle mesh method that is developed by F.H. Harlow et al. for the first time when studying gas dynamics problems at the Los Alamos National Laboratory in the USA [25, 26]. It is then widely generalized to computational plasma physics [27]. Harlow's PIC method discretizes the fluid into free-moving pseudo-particles in a spatial grid and combines Lagrangian and Eulerian descriptions, which has the advantage of simulating large deformation problems in materials with complex configurations. To the best of our knowledge, no reports have been published on a PIC code for BOI calculations. In this study, we develop a novel two-dimensional PIC code called *Xablation2D*. This code can be used to calculate the BOI produced by X-ray-irradiated materials.

The remainder of this paper is organized as follows. In Sect. 2, we discuss the theoretical basis and essential modeling techniques, including the fluid PIC scheme and the three main modules of the code. In Sect. 3, we describe the implementation of algorithm in detail, including the initialization, discretization, and parallelization. Section 4 is dedicated to presenting the reliability of the code, including the simulation of energy deposition, shear flow, and Kelvin-Helmholtz instability. Furthermore, a series of material simulations involving

X-ray irradiation are conducted to verify the simulation capabilities of the *Xablation2D* code for BOI. Finally, we present our conclusions in the final section.

2 Theoretical basis and modeling for simulation

2.1 Fluid PIC scheme

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

$$\frac{\partial \mathbf{q}}{\partial t} + \hat{\mathbf{A}}\mathbf{q} = 0, \quad (1)$$

where $\mathbf{q}(\mathbf{r}, t)$ is an arbitrary hydrodynamic quantity and $\hat{\mathbf{A}}$ is an abstract operator. According to the rule of operator decomposition, the solution of equation (1) at time step Δt is reduced to a sequential solution of the two auxiliary problems [28]

$$\begin{cases} \frac{\partial \tilde{\mathbf{q}}(\mathbf{r}, t)}{\partial t} + \hat{\mathbf{E}}\tilde{\mathbf{q}}(\mathbf{r}, t) = 0, \\ \frac{\partial \mathbf{q}(\mathbf{r}, t)}{\partial t} + \hat{\mathbf{L}}\mathbf{q}(\mathbf{r}, t) = 0, \end{cases} \quad (2)$$

where $\hat{\mathbf{A}} = \hat{\mathbf{E}} + \hat{\mathbf{L}}$. The first equation in Eq. 2 corresponds to the “Euler step” and the second one corresponds to “Lagrange step” in the Harlow's splitting scheme, respectively. In the “Euler step,” the operator $\hat{\mathbf{E}}$ does not incorporate the spatial divergence operator with respect to hydrodynamic quantity. Thus, 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 can be obtained on the grids by summing the pseudo-particles. The “Lagrange step” can be seen as a computational procedure for modeling particle migration, which compensates for the transport effect that is neglected in the “Euler step.”

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

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot (\mathbf{q}\mathbf{U}) = 0, \quad (3)$$

where $\mathbf{U}$ is the flow velocity, and $\mathbf{q} = (\rho, \rho\mathbf{U}, pe)$ represent the mass, momentum and internal energy density, respectively. Equation 3 is in the form of the conservation equation, the solution of which can be written as a summation of pseudo-particles.

$$\mathbf{q}(\mathbf{r}, t) = \sum_{j=1}^N \mathbf{Q}_j R(\mathbf{r}, \mathbf{r}_j(t)). \quad (4)$$

The total number of pseudo-particles is denoted by N , and $\mathbf{Q}_j$ represents the hydrodynamic quantities carried by the j th pseudo-particle. The value of $\mathbf{Q}_j$ remains constant in one “Lagrange step.” The kernel function of the pseudo-particle denoted as $R(\mathbf{r}, \mathbf{r}_j(t))$, depends on the current space coordinate $\mathbf{r}$ and the radius vector $\mathbf{r}_j$ of the j th pseudo-particle center. This kernel function satisfies certain universal properties of typical

$$\begin{cases} R(\mathbf{r}_1, \mathbf{r}_2) = R(\mathbf{r}_2, \mathbf{r}_1) \geq 0, \\ \frac{\partial R}{\partial \mathbf{r}_1} = -\frac{\partial R}{\partial \mathbf{r}_2}, \\ \int_{\Omega} d\mathbf{r}_1 R(\mathbf{r}_1, \mathbf{r}_2) = 1, \end{cases} \quad (5)$$

where Ω denotes the full space. Given the aforementioned characteristics and any smooth finite function, the representation $\mathbf{q}(\mathbf{r}, t)$ in Eq. 4 simplifies Eq. 3 to satisfy the equations of motion for pseudo-particles,

$$\frac{d\mathbf{r}_j}{dt} = \mathbf{U}(\mathbf{r}_j(t)), \quad j = 1, 2, \dots, N. \quad (6)$$

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

2.2 Energy deposition

The energy deposition module is responsible for estimating the energy transfer between the X-rays and matter. At a microscopic level, X-rays primarily interact with matter through electrons. Initially, the energy of the photons is transferred directly to the electrons, which then interact with the atoms in the matter, resulting in energy deposition. The photoelectric effect is dominant in the low-energy region. As the photon energy increases, Compton scattering contributes to the energy deposition [29]. In far-field X-ray irradiation, the degree of ionization of the material is so low that the effects of the plasma can be disregarded. The energy flux for parallel X-rays incident on the target material can be estimated by considering the distance x traveled in the direction of incidence

$$\Phi(x) = \Phi_0 \frac{\int_0^\infty f(\lambda, T) \exp[-\mu(\lambda)\rho x] d\lambda}{\int_0^\infty f(\lambda, T) d\lambda}, \quad (7)$$

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

$$\Phi(x) = \Phi_0 \sum_j w_j \exp[-\mu(\lambda_j)\rho x], \quad (8)$$

where the subscript j is the discretized energy group index and w_j represents the proportion of the incident energy flux of monochromatic light with a specific wavelength λ_j . The quantity e_R represents the amount of photon energy deposited due to the interaction between X-rays and matter per unit mass and per unit time within the region $x \sim x + \Delta x$

$$e_R = \frac{\Phi(x) - \Phi(x + \Delta x)}{\rho \Delta x \tau}, \quad (9)$$

where τ denotes a time increment. It is postulated in the subsequent discussion that all the deposited energy is converted into internal energy.

2.3 Equation of state

X-ray irradiation induces significant changes in the state of matter, including phase transitions, thermal expansion, and shock compression, which results in a wide range of material parameters. Consequently, it is necessary to employ distinct equations of state to characterize the expansion and compression regions of a material. For the thermal expansion region, the PUFF EOS [15] is adopted.

$$p = \rho \left[\gamma - 1 + (\Gamma_0 - \gamma + 1) \sqrt{\frac{\rho}{\rho_0}} \right] \left[e - e_s \left\{ 1 - \exp \left[\frac{N\rho_0}{\rho} \left(1 - \frac{\rho_0}{\rho} \right) \right] \right\} \right], \quad \rho < \rho_0, \quad (10)$$

where ρ_0 and ρ are the initial density and current mass densities, respectively, p is the material pressure, Γ_0 is the Güneisen 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 a solid material with postshock velocity u and another Hugoniot parameter λ . The relation is

$$D = C_0 + \lambda u. \quad (11)$$

For the compression zone, the Güneisen EOS on the Hugoniot line is used, which is expressed as [30]

$$p = p_H(v) + \rho_0 \Gamma_0 (e - e_H), \quad \rho \geq \rho_0, \quad (12)$$

where $p_H(v)$ and e_H are

$$p_H(v) = \frac{\rho_0 C_0^2 (1 - v/v_0)}{[1 - \lambda(1 - v/v_0)^2]} \quad (13)$$

and

$$e_H = \frac{1}{2} p_H(v_0 - v), \quad (14)$$

respectively, representing the postshock pressure and specific internal energy when the preshock is stationary; $v = 1/\rho$ is the specific volume, and v_0 is the initial specific volume.

In addition to the analytic expression of the EOS, an open-source code, *FEOS*, provides the EOS for a wide range of temperatures and densities in tabular form [31]. The *FEOS*, based on the quotidian equation of state (QEOS) model [32], calculates the material-specific Helmholtz free energy $F(\rho, T)$ directly, which is widely used in computational fluid dynamics codes.

2.4 Ideal hydrodynamics

In the hydrodynamic module, the effects of thermal radiation and heat conduction can be ignored. The far-field X-ray flux with respect to these issues is $\mathcal{O}(100 \text{ J/cm}^2)$. In this case, the material temperature is $\mathcal{O}(1 \text{ eV})$ and the corresponding radiation pressure is only $\mathcal{O}(1 \text{ Pa})$, which is far lower than the material pressure. The velocity of the thermal shock wave in solid materials is approximately $\mathcal{O}(1 \text{ km/s})$, which is much faster than the heat conduction; therefore, these effects can be ignored. Furthermore, our code aims to calculate the blow-off impulse occurring in the thermal expansion-vaporized region. This region is characterized by a significantly lower material stress than the material pressure; thus, we can also ignore the stress for the impulse calculation in the following.

The 2D governing equations for ideal hydrodynamics are as follows:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u_x) + \frac{\partial}{\partial y}(\rho u_y) = 0, \\ \frac{\partial}{\partial t}(\rho u_x) + \frac{\partial}{\partial x}(\rho u_x^2) + \frac{\partial}{\partial y}(\rho u_x u_y) = -\frac{\partial p}{\partial x}, \\ \frac{\partial}{\partial t}(\rho u_y) + \frac{\partial}{\partial y}(\rho u_y^2) + \frac{\partial}{\partial x}(\rho u_x u_y) = -\frac{\partial p}{\partial y}, \\ \frac{\partial w}{\partial t} + \frac{\partial}{\partial x}(w u_x) + \frac{\partial}{\partial y}(w u_y) = e_R, \end{cases} \quad (15)$$

where ρ is the mass density, $\mathbf{u} = (u_x, u_y)$ is the fluid velocity, p is the pressure, e is the specific internal energy,

$w = \rho(e + \mathbf{u}^2/2)$ is the total energy, and e_R is the energy deposited by X-ray irradiation per unit mass per unit time. According to Harlow's splitting scheme, the 2D governing equations can be divided into the following distinct groups:

$$\begin{cases} \frac{\partial \rho_1}{\partial t} = 0, \\ \frac{\partial}{\partial t}(\rho_1 u_{x,1}) = -\frac{\partial p}{\partial x}, \\ \frac{\partial}{\partial t}(\rho_1 u_{y,1}) = -\frac{\partial p}{\partial y}, \\ \frac{\partial w}{\partial t} = -\frac{\partial}{\partial x}(p u_{x,1}) - \frac{\partial}{\partial y}(p u_{y,1}) + e_R, \end{cases} \quad (16)$$

and

$$\begin{cases} \frac{\partial \rho_2}{\partial t} + \frac{\partial}{\partial x}(\rho_2 u_{x,2}) + \frac{\partial}{\partial y}(\rho_2 u_{y,2}) = 0, \\ \frac{\partial}{\partial t}(\rho_2 u_{x,2}) + \frac{\partial}{\partial x}(\rho_2 u_{x,2}^2) + \frac{\partial}{\partial y}(\rho_2 u_{x,2} u_{y,2}) = 0, \\ \frac{\partial}{\partial t}(\rho_2 u_{y,2}) + \frac{\partial}{\partial x}(\rho_2 u_{x,2} u_{y,2}) + \frac{\partial}{\partial y}(\rho_2 u_{y,2}^2) = 0, \\ \frac{\partial w_2}{\partial t} + \frac{\partial}{\partial x}(u_{x,2} w_2) + \frac{\partial}{\partial y}(u_{y,2} w_2) = 0, \end{cases} \quad (17)$$

where subscripts 1 and 2 denote "Euler step" and "Lagrange step", respectively.

2.5 Blow-off impulse calculation

When X-rays irradiate the surface of a material, the material undergoes sublimation, forming an evaporation layer. The vaporized material is violently ejected outward into the surroundings, generating a blow-off impulse. According to the impulse theorem, the specific impulse in a given direction is equal to the momentum change

$$I = \int_{P_0}^P dP = P - P_0 = m(u - u_0), \quad (18)$$

where P , u , P_0 and u_0 represent the final momentum, final flow velocity, initial momentum, and initial flow velocity, respectively, in a certain direction, and m is the material mass. Typically, the initial velocity of the vaporized material is zero, that is $u_0 = 0$. For the numerical calculations, Eq. 18 can be written in summation form [33]

$$I = \sum_{u_j < 0, e_j > e_s} m_j |u_j|, \quad (19)$$

where m_j and u_j are the material mass and velocity in the j th grid, respectively, and BOI is the sum of the momentum in all grids in which the vaporized material ejects outward. However, BOI can also be computed using the definition:

$$I = \int_{t_0}^t p_g dt, \quad (20)$$

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

$$I = \sum_n p_g \Delta t. \quad (21)$$

where n represents the n th vaporized grid.

3 Algorithm implementation

According to the theoretical framework outlined in Sect. 2, we develop a two-dimensional code named *Xablation2D* to calculate the blow-off impulse of a material under far-field X-ray radiation. This section provides a detailed description of the algorithm implemented in *Xablation2D*. In the following discussion, we omit subscript 1, 2 that distinguishes “Euler step” and “Lagrange step,” for convenience.

3.1 Initialization

We discretize the simulation domain into rectangular grids in Cartesian coordinates. The physical quantities of the fluid, except for the mass density, are initialized by manually assigning them to grid points. The mass density is initialized by summing the weights of the pseudo-particles, as follows:

$$\begin{aligned} \rho_{ij} &= \rho_{ij} + \rho_p \cdot \omega_{ij}, \\ \rho_{i+1,j} &= \rho_{i+1,j} + \rho_p \cdot \omega_{i,j}, \\ \rho_{i,j+1} &= \rho_{i,j+1} + \rho_p \cdot \omega_{i,j}, \\ \rho_{i+1,j+1} &= \rho_{i+1,j+1} + \rho_p \cdot \omega_{i,j}, \end{aligned} \quad (22)$$

where ρ_{ij} denotes the mass density of the grid, ρ_p denotes the mass density of the pseudo-particle, and ω_{ij} denotes the weight factor. Notably, in our code, the value of ρ_p remains constant throughout the simulation. The area-weighting method illustrated in Fig. 1 is employed to distribute the mass density in the 2D simulation, and weight factors are expressed as

$$\begin{aligned} \omega_{ij} &= \frac{A_1}{A_1 + A_2 + A_3 + A_4}, \\ \omega_{i+1,j} &= \frac{A_2}{A_1 + A_2 + A_3 + A_4}, \\ \omega_{i,j+1} &= \frac{A_3}{A_1 + A_2 + A_3 + A_4}, \\ \omega_{i+1,j+1} &= \frac{A_4}{A_1 + A_2 + A_3 + A_4}, \end{aligned} \quad (23)$$

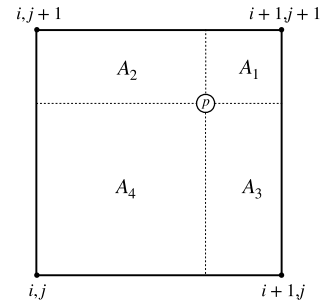


Fig. 1 Area-weighting method for the pseudo-particle in 2D simulation. The circle p represents the pseudo-particle center, and the black dot (i, j) is the grid point

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

3.2 Euler step

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

$$e_{R,ij}^n = \frac{\Phi_{i-1,j-1}^n - \Phi_{ij}^n}{\rho_{ij}^n h_1 \tau}, \quad (24)$$

and

$$\begin{cases} p_{ij}^n = p_{H,ij}^n + \Gamma_0 \rho_0 \left[e_{ij}^n - \frac{1}{2} p_{H,ij}^n (v_0 - v_{ij}^n) \right], & \rho_{ij} \geq \rho_0, \\ p_{ij}^n = \rho_{ij}^n \times \left[\gamma - 1 (\Gamma_0 - \gamma + 1) \sqrt{\frac{\rho_{ij}^n}{\rho_0}} \right] e_{A,ij}^n, & \rho_{ij} < \rho_0, \end{cases} \quad (25)$$

where $p_{H,ij}^n$ and $e_{A,ij}^n$ are:

$$p_{H,ij}^n = \frac{\rho_0 C_0^2 (1 - v_{ij}^n / v_0)}{[1 - \lambda (1 - v_{ij}^n / v_0)^2]}, \quad (26)$$

and

$$e_{A,ij}^n = e_{ij}^n - e_s \left\{ 1 - \exp \left[\frac{N \rho_0}{\rho_{ij}^n} \left(1 - \frac{\rho_0}{\rho_{ij}^n} \right) \right] \right\}, \quad (27)$$

respectively. Subsequently, the hydrodynamic equations (Eq. 16) in the “Euler step” can be discretized as

$$\begin{cases} u_{x,i,j}^{n+1} = u_{x,i,j}^n - \frac{\tau}{h_1 \rho_{i,j}^n} (p_{i+1/2,j}^n - p_{i-1/2,j}^n), \\ u_{y,i,j}^{n+1} = u_{y,i,j}^n - \frac{\tau}{h_2 \rho_{i,j}^n} (p_{i,j+1/2}^n - p_{i,j-1/2,j}^n), \\ e_{i,j}^{n+1} = e_{i,j}^n - \frac{\tau p_{i,j}^n}{\rho_{i,j}^n} \left(\frac{u_{x,i+1/2,j}^n - u_{x,i-1/2,j}^n}{h_1} \right. \\ \left. + \frac{u_{y,i,j+1/2}^n - u_{y,i,j-1/2}^n}{h_2} \right) + e_{R,i,j}^n, \end{cases} \quad (28)$$

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

3.3 Lagrange step

In the ‘‘Lagrange step’’, the fluid is divided into many pseudo-particles with finite sizes. We assume an internal distribution function of the fluid quantities within a pseudo-particle [34]

$$\begin{aligned} q(\xi, \eta) = & \{(q_{i+1,j+1} - q_{i+1,j})(2\eta - \delta\eta) + q_{i+1,j}\}(2\xi - \delta\xi) \\ & - \{(q_{i,j+1} - q_{i,j})(2\eta - \delta\eta) + q_{i,j}\}(2\xi - \delta\xi - 1), \end{aligned} \quad (29)$$

where the pseudo-particle size is normalized and $q(\xi, \eta)$ is the physical quantity carried by the pseudo-particles,¹ the coordinates (ξ, η) represent the internal position within the pseudo-particle with the origin located at the bottom-left corner and $(\delta\xi, \delta\eta)$ are intervals from the origin of the internal coordinate system to the boundaries of the grid in the x and y directions, respectively. The results are shown in Fig. 2, where the red lines represent the grids, the red dot represents the pseudo-particle center, and the blue square represents the pseudo-particle size.

q_p represents the physical quantity carried by the pseudo-particle located at the center of the internal coordinates, which can be obtained by integrating $q(\xi, \eta)$ from 0 to 1.

$$\begin{aligned} q_p &= \int_0^1 \int_0^1 q(\xi, \eta) d\xi d\eta \\ &= q_{i+1,j+1}(1 - \delta\xi)(1 - \delta\eta) \\ &\quad + q_{i+1,j}(1 - \delta\xi)\delta\eta + q_{i,j+1}\delta\xi(1 - \delta\eta) + q_{i,j}\delta\xi\delta\eta \\ &= q\left(\frac{1}{2}, \frac{1}{2}\right). \end{aligned} \quad (30)$$

¹ q only represents the velocity $\mathbf{u} = (u_x, u_y)$ and the specific internal energy e of the pseudo-particle, not the mass density ρ , which is set to constant ρ_p in the initialization.

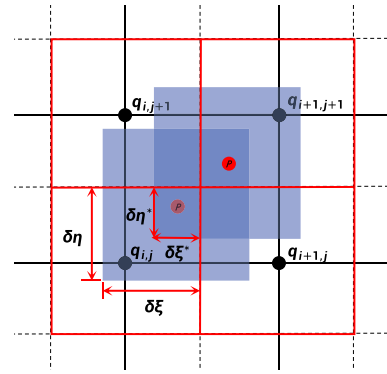


Fig. 2 Distribution of quantities within a pseudo-particle. The red dot p represents the pseudo-particle center, the blue square represents the pseudo-particle size, and the black dot is the grid point. The label $*$ represents the interval when the pseudo-particle reaches a new position

The equations for pseudo-particle motion are

$$\begin{cases} x_p^{n+1} = x_p^n + \tau u_{p,x}, \\ y_p^{n+1} = y_p^n + \tau u_{p,y}, \end{cases} \quad (31)$$

where (x_p, y_p) denotes the position of the pseudo-particle center and $(u_{p,x}, u_{p,y})$ represents the velocity of the pseudo-particle center, as determined by Eq. 30. When the pseudo-particle reaches a new position as shown in Fig. 2, we recompute the new intervals from the origin of the internal coordinate, denoted as $(\delta\xi^*, \delta\eta^*)$. By summing the pseudo-particles at new positions, new fluid quantities can be derived on the grid. In this study, we present three algorithms for the summation process: the area-weighting method (AWM), integration-weighting method (IWM), and interpolation-integration-weighting method (IIWM), each of which exhibits different types of numerical diffusion [34]. The details of summation algorithms are shown in Appendix A. The three algorithms have different numerical diffusions and noise and can be selected according to the requirements of the actual problems.

3.4 Parallelization

The message-passing interface (MPI) is employed in the construction of the parallelization [35]. Details of the parallel communication are provided in Appendix B.

4 Simulation results

4.1 Far-field X-ray energy deposition

The X-ray energy deposition module is crucial to the calculation accuracy of the blow-off impulse in the *Xablation2D*

Table 1 Discretized blackbody spectrum from wavelength $\lambda = 0.1 \text{ \AA}$ to $10 \text{ \AA}$ and corresponding mass absorption coefficient μ in the Al material [19]

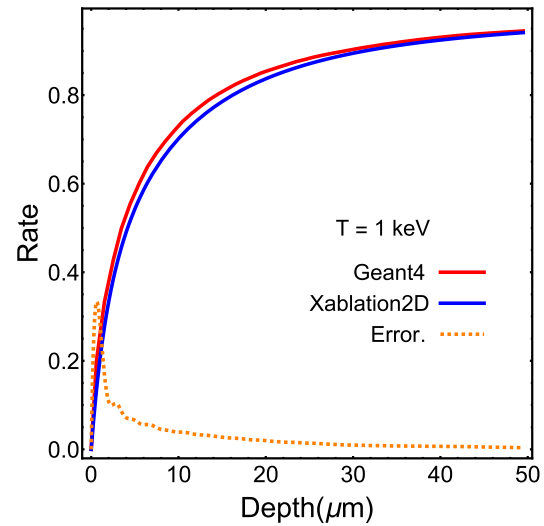
$\lambda \text{ (\AA)}$	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
$\mu \text{ (cm}^2\text{/g)}$	0.155	0.205	0.277	0.38	0.525	0.97	1.82	3.7	5.75	8.8	11.8	15.2
$\lambda \text{ (\AA)}$	1.5	2.0	2.5	3	4	5	6	7	8	9	10	
$\mu \text{ (cm}^2\text{/g)}$	41.5	87	235	360	780	1400	2250	3300	280	390	520	

code. To validate this module, we compare the energy deposition rate obtained from the *Xablation2D* code with that obtained from the Monte Carlo code *Geant4* [36–39]. In the *Xablation2D* simulation, parallel soft X-rays with an initial energy flux $\phi_0 = 418 \text{ J/cm}^2$ are incident perpendicularly on a 2D planar Al target with a density $\rho = 2.738 \text{ g/cm}^3$, and the pulse duration is 50 ns. The energy spectrum of the X-rays approximates a blackbody spectrum with a radiation temperature $T = 1 \text{ keV}$. The wavelength range of the energy spectrum is $\lambda = 0.1 \text{ \AA}$ to $10 \text{ \AA}$ discretized into 23 energy groups for the numerical simulation. The mass absorption coefficients μ in the Al material for the X-rays in each energy group are listed in Table 1.

In the *Geant4* code, a parallel blackbody spectrum photon beam with a radiation temperature of 1 keV is configured to simulate soft X-rays. The interaction between photons and materials is simulated using the Livermore low-energy electromagnetic physics model, which is effective within the energy range of photons from 250 eV to 1 GeV. By tracking the trajectory of photons within the Al target, it is possible to quantify the amount of the deposition energy in the material. The energy deposition rates calculated using the two codes are shown in Fig. 3, where the vertical axis corresponds to the energy deposition rate, which signifies the lost ratio of the incident energy flux after traversing corresponding distance in the material, and the horizontal axis represents the depth within the Al target, along with the direction of the incident X-rays. Figure 3 also shows the relative error of the two results by an orange dashed line. The largest deviation is observed near the material surface, which then rapidly decreased to $\mathcal{O}(5\%)$ along the incident depth. This is because the energy deposition rate is small at the material surface, where even a minor deviation in parameters such as the mass absorption coefficients in the database can result in a noticeable relative error. In addition, the depth required for 50% of the X-ray energy to be deposited in the material is $4.17 \text{ }\mu\text{m}$ for *Xablation2D* and $3.5 \text{ }\mu\text{m}$ for *Geant4*, which is consistent with $\mathcal{O}(5 \text{ }\mu\text{m})$ estimated in [19].

4.2 Shear flow simulation

We use plane shear flow simulations to verify the numerical diffusion from the algorithms of AWM, IWM, and IIWM.

**Fig. 3** (Color online) Energy deposition rate varying with the material depth along the X-rays incident direction

In the *Xablation2D* code, the size of the simulation domain is $L_x \times L_y = 0.4 \times 0.4 \text{ cm}^2$ and the domain is discretized into 400×400 grids. 10×10 pseudo-particles are allocated to each grid. The entire flow field is divided into two layers. The upper and lower fluids are denoted by *A* and *B*, respectively. The interface between the two fluids is located at $y = 0.2 \text{ cm}$. The mass density, velocity in the x direction, and velocity in the y direction of the upper fluid are $\rho_A = 2.738 \text{ g/cm}^3$, $u_{Ax} = 3 \times 10^5 \text{ cm/s}$ and $u_{Ay} = 0 \text{ cm/s}$, respectively. The lower fluid has the same mass density as the upper $\rho_B = \rho_A$, and the velocity is equal in magnitude but opposite in the x direction $u_{Bx} = -u_{Ax}$, and the same velocity in the y direction $u_{By} = u_{Ay}$. The simulation employs a periodic boundary condition in the x direction, and an open boundary condition in the y direction. In addition, the ideal gas EOS is adopted.

$$p = (\gamma - 1)\rho, \quad (32)$$

where $\gamma = 1.667$ is the ratio of the specific heat and the initial pressure p is set to 1 GPa. The fluid velocity distribution in the x direction (u_x) of shear flow is shown in Fig. 4.

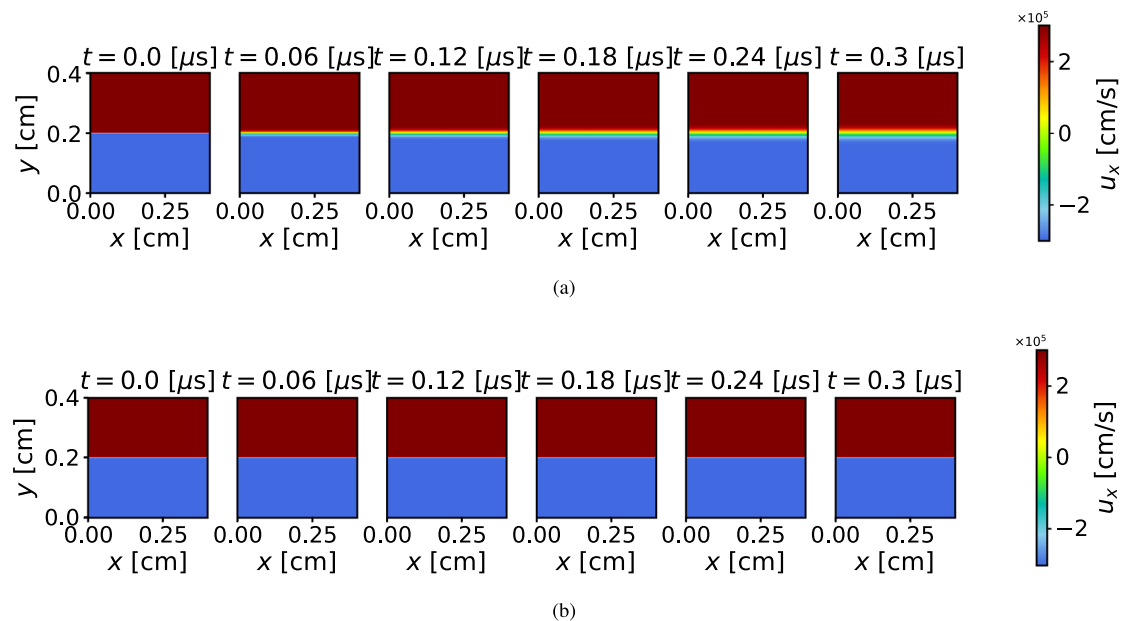


Fig. 4 (Color online) Fluid velocity distribution in the x direction in the simulation by two different algorithms at various time intervals. **a** AWM; **b** IIWM (or IWM)

In Fig. 4, it can be observed that the IIWM (or IWM) has a better suppression for numerical diffusion than that of the AWM. For the AWM in Fig. 4a, the jumped shear flow velocity becomes smooth, and this smoothness gradually saturates into the upper and lower layers owing to numerical diffusion, but for the IIWM (or IWM) in Fig. 4b, the jumped velocity can be maintained throughout the entire simulation time because of using the integration of the internal distribution function in the shear velocity direction.

4.3 Kelvin–Helmholtz instability simulation

When two contiguous fluids flow with shear velocities, instability can arise at the interface between the fluids if there is a small fluctuation. This phenomenon is known as the Kelvin–Helmholtz instability (KHI) [40, 41]. The KHI is widely observed in nature, including the turbulent mixing of fluids in jet streams, the formation of undulatus, and supernova explosions [42–44]. Here, we perform KHI simulations using the *Xablation2D* code and the open-radiation magnetohydrodynamic simulation code *FLASH4* [45], and compare the two simulation results. The initial parameters, including the size of the simulation domain, number of grids, and number of pseudo-particles for each grid, are the same as those in Sect. 4.2, except for the temperature. The initial material temperature is set as $T = 21.6$ eV, which corresponds to a specific internal energy $e = 1 \times 10^5$ J/g. The initial pressure determined by the EOS is 182.24 GPa. Initially, a velocity perturbation

in the y direction is introduced at the interface of the two fluids as a seed for the KHI in the following form [46]

$$u_y^1 = u_0 \sin\left(kx - \frac{\pi}{2}\right) e^{\left(k|y - \frac{L_y}{2}|\right)}, \quad (33)$$

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 the secondary unstable structures of KHI, it is necessary to reduce numerical diffusion; therefore, we adopt the IWM in the *Xablation2D* simulation. In the *FLASH4* simulation, we maintain consistency in the initialization parameters and perturbation but use adaptive mesh refinement (AMR).

Figure 5 illustrates the mass density of the evolution of the lower half fluid. The six subfigures in the first row are the results obtained from the *Xablation2D* code and those in the second row from the *FLASH4* code. Simulation results for the two codes are consistent. It can be observed that the disturbance at the fluid interface gradually increases, and eventually, the two fluids mix and show vortex structures. The IIWM is also employed to simulate the KHI process with the same parameters as in *Xablation2D*. The simulation results are consistent with those of *FLASH4*, except for some secondary structures, as shown in Fig. 6. This deviation can be attributed to the relatively higher numerical diffusion in the direction of convective velocity in the IIWM.

The mixing width η is defined as the difference between the maximum and initial positions of the lower half of the fluid as shown in Fig. 7a. The evolution of mixing width

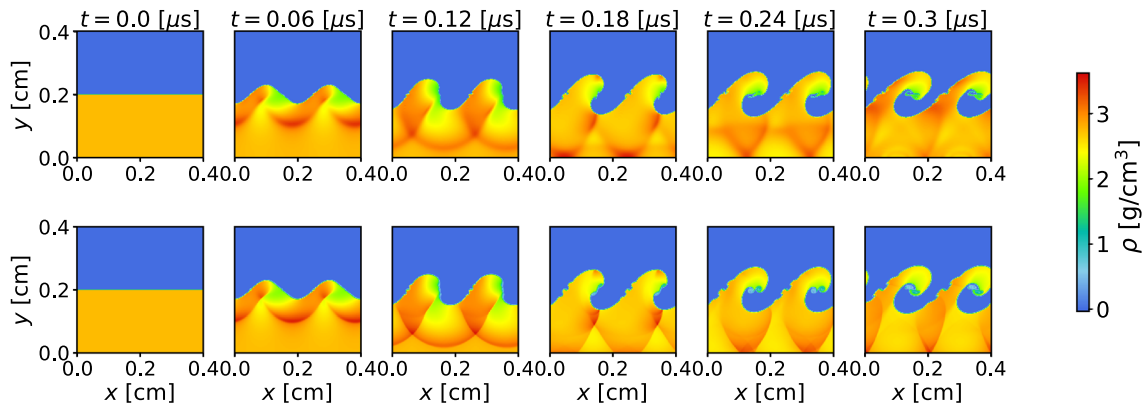


Fig. 5 (Color online) Mass density distribution of the lower half fluid at various time intervals in the *Xablation2D* and *FLASH4* simulations, respectively. The first row corresponds to the result from *Xablation2D*, and the second row corresponds to the result from *FLASH4*

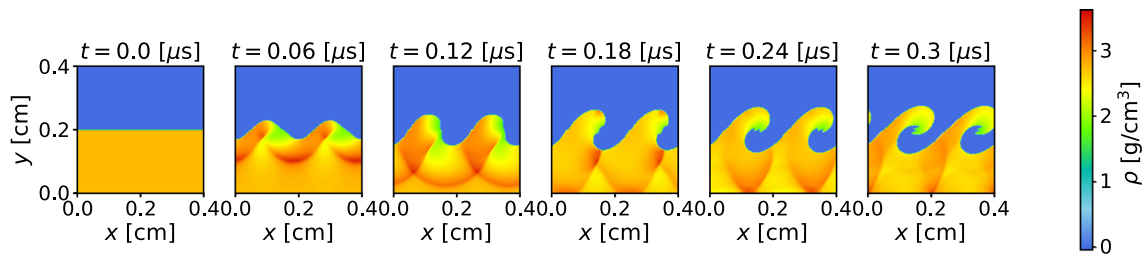


Fig. 6 (Color online) Mass density distribution of the lower half fluid at various time intervals in the *Xablation2D* simulation by IIWM

is shown in Fig. 7b, where the blue and cyan dashed lines correspond to the results obtained from the *Xablation2D*, and the magenta solid line corresponds to the *FLASH4*. The dotted lines indicate the relative errors between the two codes, which remain $\mathcal{O}(5\%)$, indicating a certain level of consistency between them. This minor deviation validates the reliability of the *Xablation2D* code. It is observed that the growth in the mixing width is significantly smaller than that predicted by the classical linear theory of the KHI. This is because the compressibility of the simulation and evolution of the fluid are nonlinear owing to the strong initial perturbation.

4.4 Vaporization blow-off impulse

When X-rays irradiate a solid material, a blow-off impulse load is applied to the material surface, as shown in Fig. 8. The energy of X-ray photons is primarily absorbed by the material through photoelectric effects and Compton scattering. The X-ray energy flux decreases exponentially as it penetrates the interior of the material from the surface. Consequently, the specific internal energy of the material at the surface increases rapidly, which leads to a phase transition and adiabatic expansion, and finally generates an ablation

layer. If the deposited energy exceeds the sublimation energy of the material, the solid material at the surface changes into a gas, forming a vaporization zone on the front. The vaporized material is violently sprayed into the vacuum to generate a recoil impulse loading on the remaining material, where the recoil impulse is known as the blow-off impulse (BOI).

In the BOI simulation case, the Al material is selected as the target material, and the IIWM algorithm is employed in the *Xablation2D* code. The expansion and compression of the material are described by the PUFF EOS (Eq. 10) and Güneisen EOS (Eq. 12) as discussed in Sect. 2.3, respectively. The physical properties of the Al used in the simulation are listed in Table 2. The size of the simulation domain is $L_x \times L_y = 0.8 \text{ cm} \times 0.8 \text{ cm}$, which is divided into 400×400 grids. We allocated 100×100 pseudo-particles to each grid near the surface of the target material and 5×5 pseudo-particles in other regions. Two geometric configurations of the target were simulated: a semi-infinite slab and a cylinder.

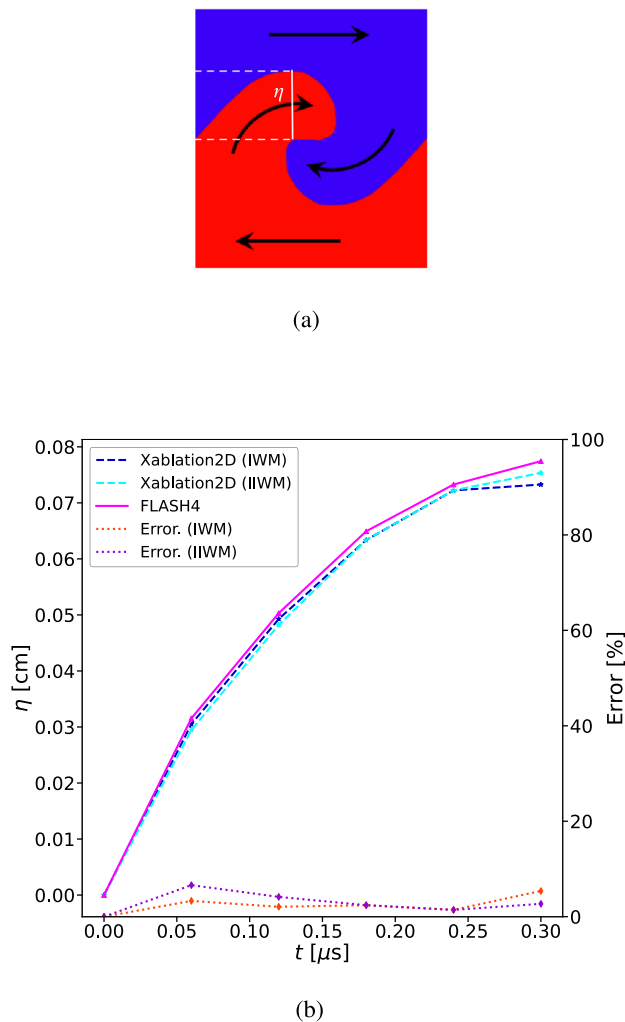


Fig. 7 (Color online) Evolution of the mixing width and relative error in the *Xablation2D* and *FLASH4* simulations, respectively. **a** The mixing width definition; **b** The mixing width at various time intervals

4.4.1 Semi-infinite slab

The semi-infinite slab is located in the region where $x > 0.4$ cm, whereas the region where $x \leq 0.4$ cm is filled with low-density gas to maintain the numerical stability of the code. A periodic boundary condition is applied in the y direction, and an open boundary condition is applied in the x direction. Parallel X-rays have a radiation temperature $T = 1$ keV and are incident on the slab in the normal direction. The energy spectrum is discretized into 23 energy groups, as shown in Table 1. The pulse duration and initial energy flux are 50 ns and 418 J/cm^2 , respectively. Figure 9 illustrates the evolution of the mass density and pressure. The

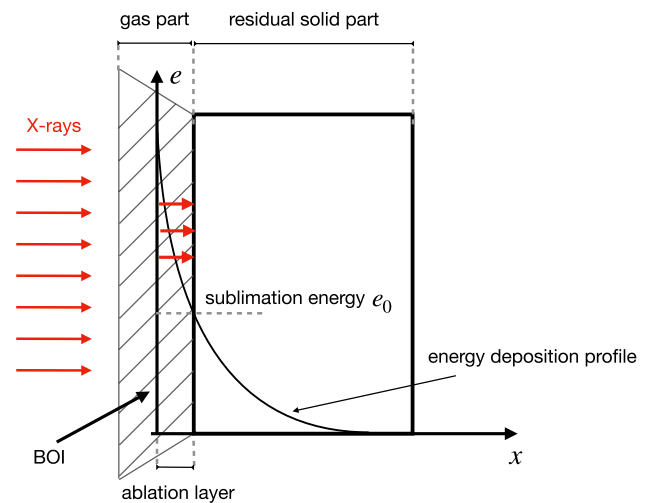


Fig. 8 Simple illustration of the far-field X-ray ablation. The shaded area represents the blow-off impulse, and the black solid curve is the energy deposition curve

Table 2 Physical property parameters of the Al material in the simulation

ρ_0 (g/cm ³)	2.738	Y_0 (GPa)	0.7	e_s (kJ/g)	10.89
C_0 (mm/μs)	5.328	G (GPa)	27	γ	1.667
λ	1.338	Γ_0	2.18	N	1.265

ρ_0 is the mass density at room temperature and atmospheric pressure, G is the shear modulus, Y_0 is the yield strength, e_s is the sublimation energy, γ is the specific heat ratio, Γ_0 is the Güneisen coefficient, λ , and C_0 are Hugoniot parameters, and $N = C_0^2/\Gamma_0 e_s$

material surface is vaporized by X-ray irradiation and then expands outward into the surroundings. Material expansion generates a blow-off impulse (BOI) and produces a thermal shock wave that propagates inward. The density accumulation in the left region is a consequence of the presence of low-density gas during initialization.

For the semi-infinite slab configuration, the impulse distribution is uniform in the y direction. It is possible to obtain the evolution of the one-dimensional average BOI by integrating it along the y direction and dividing it by the length L_y . This result is indicated by the dashed blue lines in Fig. 10. To verify its correctness, we use a one-dimensional Lagrangian code, referred to in Ref. [47] to calculate the BOI under the same parameters. The result is shown as a solid magenta line, which is consistent with the *Xablation2D* code. In addition, we compare the simulation results with the three BOI models, shown as dotted lines in Fig. 10. Their analytical formulas are as follows [9]:

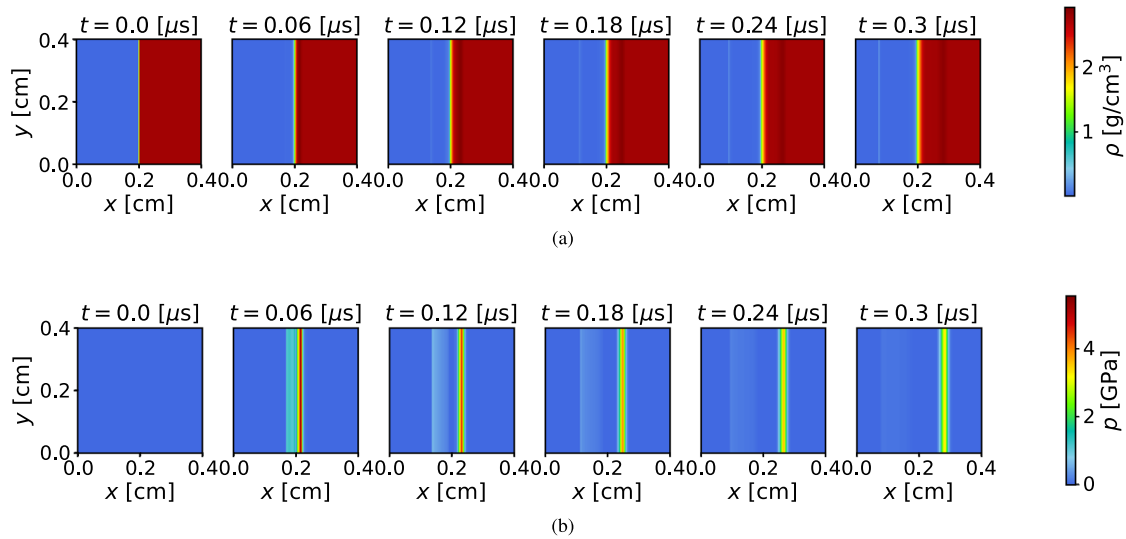


Fig. 9 (Color online) Mass density and pressure distribution in the semi-infinite slab at various time intervals. **a** Mass density varying with the simulation time; **b** Pressure varying with the simulation time

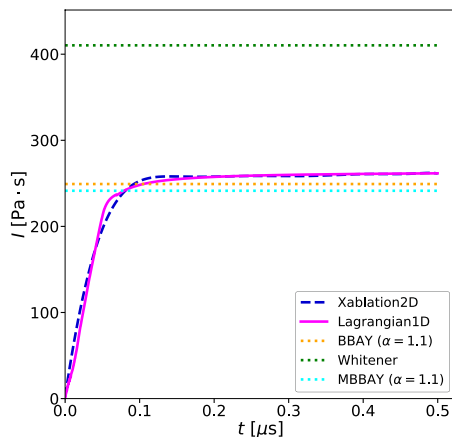


Fig. 10 (Color online) Blow-off impulse varying with the simulation time

$$\begin{aligned}
 \text{BBAY : } I &= \alpha \sqrt{2} \left\{ \int_0^{x_0} [e(x) - e_s] \rho_0 x \, dx \right\}^{1/2}, \\
 \text{Whitener : } I &= \sqrt{2} \int_0^{x_0} [e(x) - e_s]^{1/2} \rho_0 \, dx, \\
 \text{MBBAY : } I &= \alpha \sqrt{2} \left\{ \int_0^{x_0} e(x) - e_m \left[1 + \ln \frac{e(x)}{e_m} \right] \rho_0^2 x \, dx \right\}^{1/2},
 \end{aligned} \quad (34)$$

where $e(x)$ is the energy deposition profile, e_m is the melting energy, α is a correction parameter ranging from 1 to $\sqrt{2}$, and x_0 is the thickness of the sublimation layer determined by setting $e(x) = e_s$. In the simulation, we set $e_m = 3.975$ kJ/g and $\alpha = 1.1$, respectively. The BOI models estimated only the instantaneous deposition energy for irradiation, resulting

Table 3 X-ray parameters and measuring impulse in experiments

Number	01154	01170	01171
Radiation temperature T (keV)	0.21	0.227	0.211
Pulse duration τ_0 (ns)	53	36	44
Initial flux Φ_0 (J/cm ²)	163	181	192
Measuring impulse I (Pa · s)	99.1	118.5	162.2

in the horizontal dotted lines in Fig. 10. The BOIs calculated using the *Xablation2D* and 1D Lagrangian codes are shown as blue dashed and magenta solid lines in Fig. 10, having a growth time of $\mathcal{O}(0.1 \mu\text{s})$. It demonstrates a tendency to stabilize, which corresponds to the characteristic time in which the material completely sublimates at the surface. The results obtained from the BBAY model and MBBAY model align well with the stable values obtained from the numerical simulations.

Furthermore, we compare the simulation results of the *Xablation2D* code with the published experimental results to verify the reliability of the code. The Ref. [48] provides three measurements of the BOI produced by X-rays irradiating a flat Al material. The X-ray parameters and measured impulse values in experiments are presented in Table 3. We simulate these three experiments using *Xablation2D* with experimental parameters. The BOIs obtained in the simulations are shown in Fig. 11a. The stable values of these BOIs are 97.84, 121.82, and 125.36 Pa·s, respectively. Figure 11b shows the comparison between the simulation results and the measured BOIs in experiments. It can be observed that there are two consistent BOIs, and the relative errors between the simulation and experimental results are negligible for No.

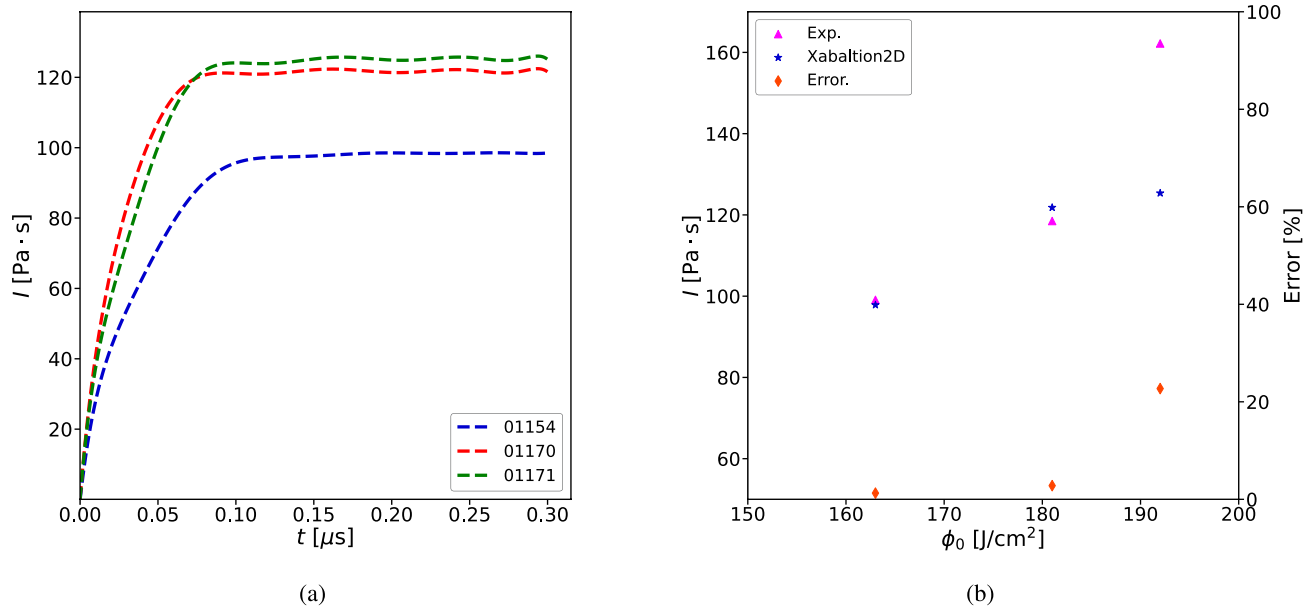


Fig. 11 (Color online) Comparison between the *Xablation2D* simulations and experiments. **a** Blow-off impulse varying with the simulation time; **b** Simulation results vs. the experiment results

01154 and No. 01170. Although the relative error in case No. 01171 is larger, it remains within $\mathcal{O}(20\%)$.

4.4.2 Cylinder

In the cylindrical configuration, the target is positioned at the center of the simulation domain. The central coordinates of the cylinder are $x = y = 0.4$ cm, and the radius of the target is 0.2 cm. The remaining areas of the simulation domain are filled with a low-density gas. The physical properties and X-ray parameters used in this configuration are identical to those employed in the semi-infinite slab configuration. The mass density and pressure distributions in the simulation are shown in Fig. 12. X-rays irradiate the left side of the cylinder. The vaporized material is produced on the left surface, ejected violently, and generates a BOI that drives a thermal shock wave moving toward the center of the cylinder.

When a parallel X-ray irradiates a curved surface, the density of the deposited energy on the material surface is nonuniform. The BOI is a function of the radial direction of the cylinder. Refs. [10, 11, 21, 49] propose that if the energy deposition density has a cosine profile on the cylinder surface, the variation of the BOI is proportional to the cosine of the polar angle

$$I = I_0 \cdot \cos \theta, \quad (35)$$

where θ denotes the polar angle defined in Fig. 13a, and I_0 represents the BOI at the $\theta = 0^\circ$.

Figure 13b–d shows the distribution of the BOI via the polar angle at different time intervals. The BOI profiles satisfy the cosine law; however, small deviations also exist. The main reason for this is that the thickness of the X-ray energy deposition layer cannot be completely ignored. The deviation between the BOI curve and the cosine function increases as the polar angle increases from 0° to 90° , particularly at $\theta = 90^\circ$, where the specific internal energy of the material is not zero because of the penetration of X-rays into the material; thus, the BOI is also not zero. The simulation results confirm this phenomenon.

5 Conclusion

We developed a novel parallel two-dimensional PIC code, *Xablation2D*, to calculate the BOI of far-field X-ray-irradiated materials. The code comprises three modules: an energy deposition module, an EOS module, and an ideal hydrodynamics module. In an ideal hydrodynamic model, the solution of hydrodynamic equations is divided into two steps: the “Euler step” and the “Lagrange step” according to Harlow’s splitting scheme. The introduced pseudo-particles compensate for the transport effect. We presented three new summation algorithms, AWM, IWM, and IIWM, to map the physical quantity carried by the pseudo-particles onto the grid. In contrast to conventional finite difference or finite element methods, the new PIC method significantly reduces the dependence on the grid shape and is well suited for the calculation of large deformation problems in materials with complex configurations. To

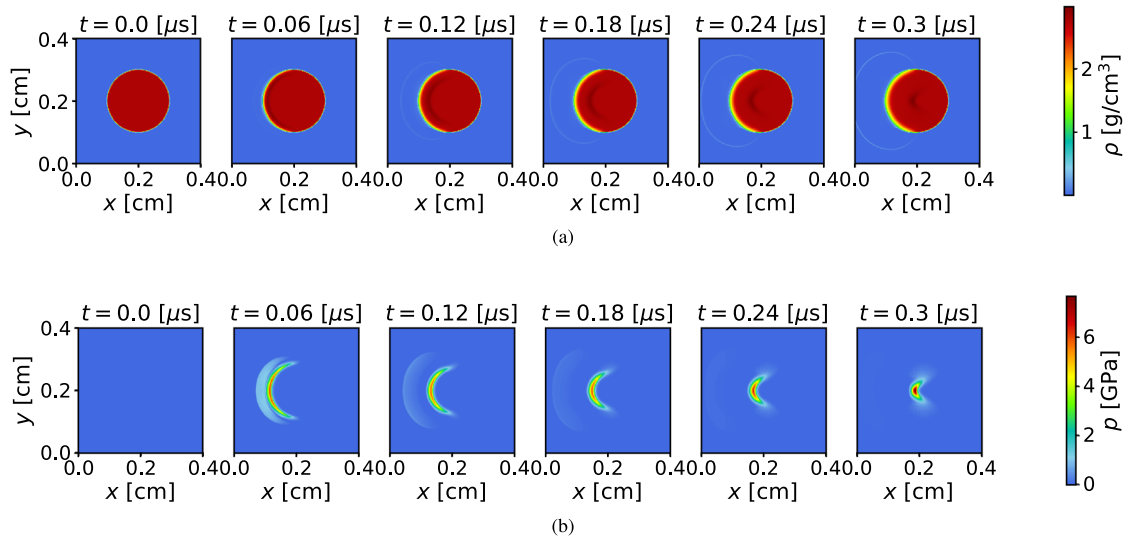


Fig. 12 (Color online) Mass density and pressure distribution in the cylinder at various time intervals. **a** Mass density varying with the simulation time; **b** Pressure varying with the simulation time

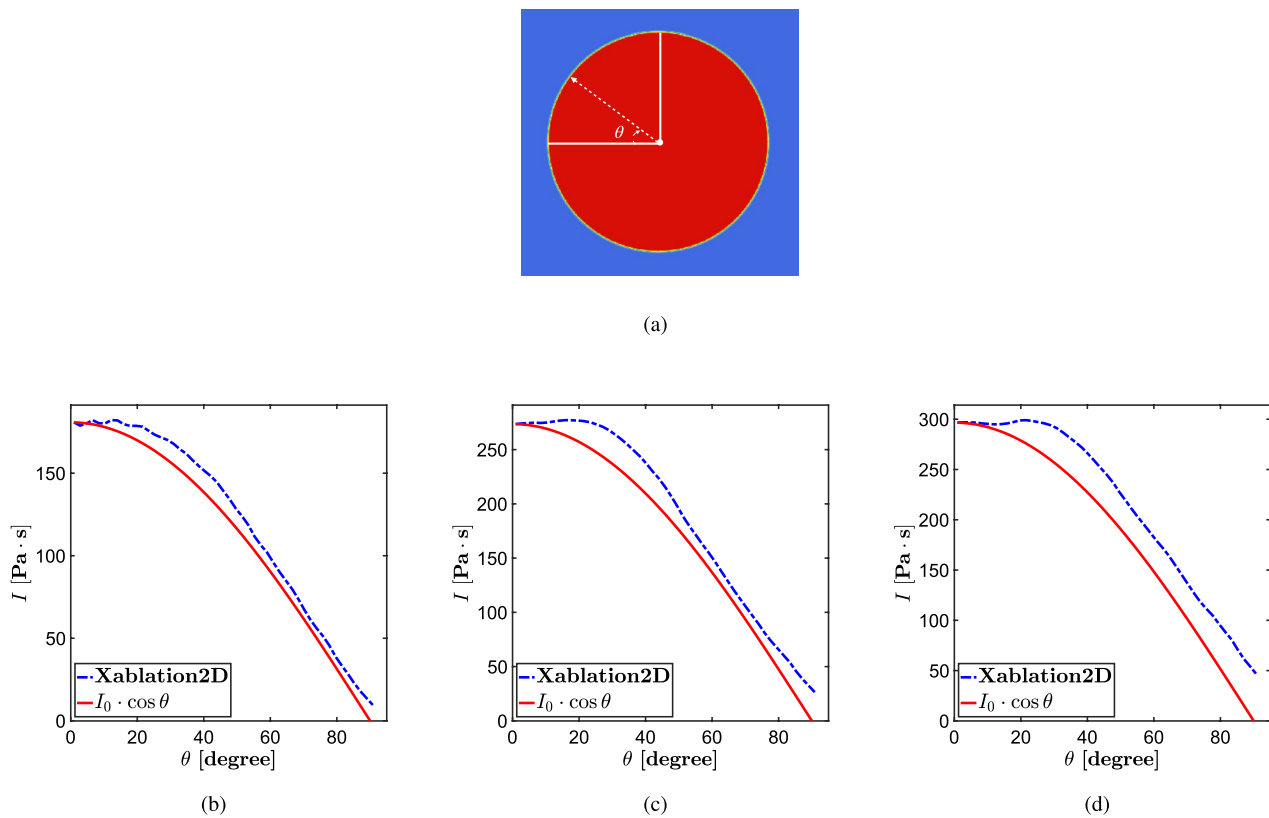


Fig. 13 Blow-off impulse varying with the polar angle at various time intervals. **a** Definition of the polar angle; **b** $t = 0.04 \mu\text{s}$; **c** $t = 0.10 \mu\text{s}$; **d** $t = 0.16 \mu\text{s}$

verify the reliability of *Xablation2D*, we used an open-source code for comparison. The soft X-ray energy deposition rate is

simulated using *Geant4*, and the shear flow and KHI problems are simulated using *FLASH4*. The simulation results exhibited

a minor discrepancy compared to our code. Finally, we calculated the BOI in two geometric configurations of Al materials under far-field X-ray irradiation. These results are consistent with the experimental, analytical, and other simulation results. It is also observed that a thermal shock wave propagates inside the material owing to X-ray irradiation.

For X-rays with an increased energy flux, the overall process becomes more intricate. The material is highly ionized, and the energy deposition process involves an interaction between the radiation field and the plasma. In future work, we plan to develop a radiation transport module in the *Xablation2D* code for simulating ultraintense X-ray-irradiated materials.

Appendix: Summation algorithms

- (1) **Area-weighting method (AWM)**: This approach assumes that the distribution function of the physical quantity $q(\xi, \eta)$ carried by the pseudo-particle collapses into the value located at the internal coordinate center, that is, q_p . Therefore, the new fluid physical quantities on the grid can be simply obtained by a summation of the product of q_p and area as follows:

$$\begin{aligned}(\rho q)_{ij} &= \sum_{p \in (i,j)} \rho_p q_p \delta \xi^* \delta \eta^*, \\(\rho q)_{i+1,j} &= \sum_{p \in (i+1,j)} \rho_p q_p (1 - \delta \xi^*) \delta \eta^*, \\(\rho q)_{i,j+1} &= \sum_{p \in (i,j+1)} \rho_p q_p \delta \xi^* (1 - \delta \eta^*), \\(\rho q)_{i+1,j+1} &= \sum_{p \in (i+1,j+1)} \rho_p q_p (1 - \delta \xi^*) (1 - \delta \eta^*).\end{aligned}\quad (\text{A1})$$

where $p \in (i, j)$ denotes the pseudo-particle whose center is located in the (i, j) grid. The AWM is a straightforward approach and has high computational efficiency but introduces zero-order numerical diffusion effects.

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

$$\begin{aligned}(\rho q)_{ij} &= \sum_{p \in (i,j)} \rho_p \int_0^{\delta \xi^*} \int_0^{\delta \eta^*} q(\xi, \eta) d\xi d\eta, \\(\rho q)_{i+1,j} &= \sum_{p \in (i+1,j)} \rho_p \int_{\delta \xi^*}^1 \int_0^{\delta \eta^*} q(\xi, \eta) d\xi d\eta, \\(\rho q)_{i,j+1} &= \sum_{p \in (i,j+1)} \rho_p \int_0^{\delta \xi^*} \int_{\delta \eta^*}^1 q(\xi, \eta) d\xi d\eta, \\(\rho q)_{i+1,j+1} &= \sum_{p \in (i+1,j+1)} \rho_p \int_{\delta \xi^*}^1 \int_{\delta \eta^*}^1 q(\xi, \eta) d\xi d\eta.\end{aligned}\quad (\text{A2})$$

The IWM has second-order numerical diffusion, which is much better than that of the AWM. However, this approach would introduce some nonphysical numerical noise, causing the fluid motion to become somewhat unstable.

- (3) **Interpolation-Integration-weighting method (IIWM)**: The IIWM is a combination of the AWM (used in the convective velocity direction) and IWM (used in the shear velocity direction). For instance, if the $q(\xi, \eta)$ represents the fluid velocity in the x direction (u_x), then an inverse linear interpolation is employed to $q(\xi, \eta)$ in the x direction, and followed by the integration of $q(\xi, \eta)$ in the y direction. The specific procedures are as follows. Initially, we integrate the $q(\xi, \eta)$ over ξ from 0 to 1,

$$\begin{aligned}q(\eta) &= \int_0^1 q(\xi, \eta) d\xi \\&= \{[q_{i+1,j+1}(1 - \delta \xi) + q_{i,j+1}\delta \xi] \\&\quad - [q_{i+1,j}(1 - \delta \xi) + q_{i,j}\delta \xi]\}(2\eta - \delta \eta) \\&\quad + q_{i+1,j}(1 - \delta \xi) + q_{i,j}\delta \xi \\&= q\left(\frac{1}{2}, \eta\right).\end{aligned}\quad (\text{A3})$$

Then, we integrate $q(\eta)$ over the length of the pseudo-particle that overlaps the grid in the y direction, as shown in Fig. 2, to obtain two new intermediate physical quantities

$$q_1^* = \int_0^{\delta \eta^*} q(\eta) d\eta, \quad q_2^* = \int_{\delta \eta^*}^1 q(\eta) d\eta. \quad (\text{A4})$$

Finally, new physical quantities are determined by

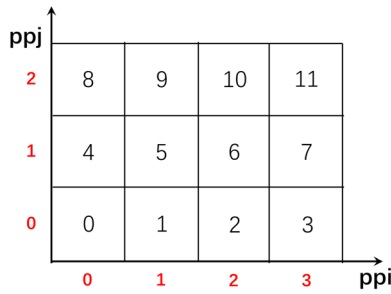


Fig. 14 Parallel division of the simulation region. A total of $N = 12$ processes, numbered from 0 to 11, are assigned to the simulation regions. The number of processes assigned to the grid along the x and y direction is 4 and 3, respectively

$$\begin{aligned}
 (\rho q)_{i,j} &= \sum_{p \in (i,j)} \rho_p q_1^* \delta \xi^*, \\
 (\rho q)_{i+1,j} &= \sum_{p \in (i+1,j)} \rho_p q_1^* (1 - \delta \xi^*), \\
 (\rho q)_{i,j+1} &= \sum_{p \in (i,j+1)} \rho_p q_2^* \delta \xi^*, \\
 (\rho q)_{i+1,j+1} &= \sum_{p \in (i+1,j+1)} \rho_p q_2^* (1 - \delta \xi^*).
 \end{aligned} \tag{A5}$$

Similarly, we can also implement this approach for the fluid velocity in the y direction (u_y).

Parallel communication

MPI adopts an explicit message-passing architecture, necessitating the explicit sending and receiving of messages to facilitate data exchange among processors, each of which has its own memory space. The processors access each other's memory space through explicit message passing. This design exhibited robust parallelism and is particularly suitable for the implementation of large-scale parallel algorithms.

In our code, the simulation region is divided into N parts based on the grid structure, and each part is assigned to an individual calculation process. The total number of processes $N = ppx \times ppy$, where ppx and ppy are the number of processes assigned to the grid along the x and y directions, respectively, as shown in Fig. 14. A grid layer called a guard grid or ghost grid is set up at the junction of adjacent parallel regions to store the physical quantities received from the adjacent processes. The exchange of physical quantities on the guard grids is achieved through two MPI communication subroutines, MPI_SEND and MPI_RECV, as illustrated in Fig. 15.

During initialization, all the pseudo-particles are placed within the parallel region and guard grids. When particles are pushed out of a parallel region, they are transferred to

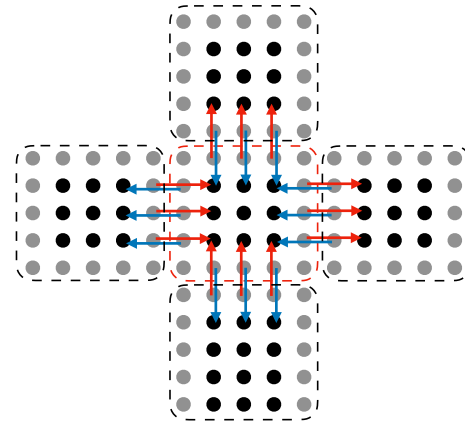


Fig. 15 MPI is utilized to update the guard grids. The dashed boxes represent parallel regions assigned to processors. The black and gray solid circles represent the grid points within the parallel region and guard points surrounding the parallel region, respectively. The red and blue arrow lines depict the communication that occurs between internal grid points and guard points across adjacent processors

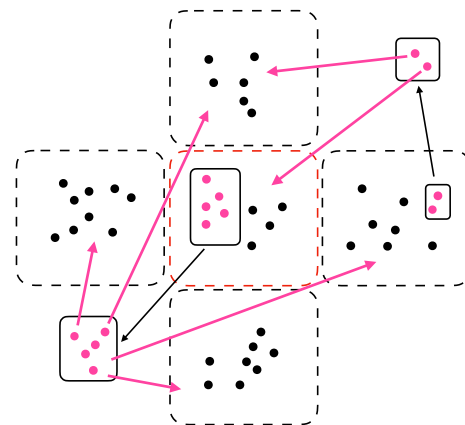


Fig. 16 MPI is utilized to facilitate the exchange of pseudo-particles. The magenta and black solid circles represent the pseudo-particles. The former indicates the pseudo-particles that require communication and the latter represents those that do not. The dashed boxes represent parallel regions. The black solid lines represent the link list containing all pseudo-particles to be communicated. The magenta and black arrow lines show the communication between different processors

another parallel region by MPI communication. Communication could be achieved between any two processors. First, all communicating pseudo-particles are gathered into a link list, then the processor grid in which each pseudo-particle falls 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

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

References

1. M.H. Johnson, B.A. Lippmann, Electromagnetic signals from nuclear explosions in outer space. *Phys. Rev.* **119**, 827 (1960). <https://doi.org/10.1103/PhysRev.119.827>
2. W. Karzas, R. Latter, Electromagnetic radiation from a nuclear explosion in space. *Phys. Rev.* **126**, 1919 (1962). <https://doi.org/10.1103/PhysRev.126.1919>
3. M. S. Smith, R. T. Santoro, Initial effects of nuclear weapon x-radiation on the LAMPSHADE orbital debris satellite shield. Report, (Oak Ridge National Lab.(ORNL), Oak Ridge, TN (United States), 1989). <https://doi.org/10.2172/5549195>
4. K. Zhang, Constitutive relationship of anisotropic composites and its application in a FEM simulation of the dynamic response within the X-ray radiation in 3D condition. Dissertation, (Graduate School of National University of Defense Technology, 2018) (in Chinese)
5. S. Glasstone, P.J. Dolan, *The Effects of Nuclear Weapons* (US Department of Defense, Washington DC, 1977)
6. N.J. Rudie (ed.), *Principles and Techniques of Radiation Hardening* (Western Periodicals Company, North Hollywood, 1976)
7. Office of the Deputy Assistant Secretary of Defense for Nuclear Matters (ODASD(NM)), *Nuclear Matters Handbook*. (2020)
8. H. Wang, Y.-C. Lai, J.-J. Zhong et al., Correction of distorted X-ray absorption spectra collected with capillary sample cell. *Nucl. Sci. Tech.* **34**, 106 (2023). <https://doi.org/10.1007/s41365-023-01253-9>
9. R. W. Langley, Analytical relationships for estimating the effects of x-rays on materials. Report, (Huntington Beach, California: McDonnell Douglas Astronautics Company, 1974)
10. R.Q. Zhang, J.F. Tan, Blowoff impulse on the cylindrical shell caused by x-ray energy flux. *Acta Aerodynamica Sinica* **119**, 178 (1989). (in Chinese)
11. T. L. Cost, Dynamic Response of Missile Structures to Impulsive Loads Caused by Nuclear Effects Blowoff. Report, (Northport, AL, USA: Athena Engineering Company, 1976)
12. R. J. Lawrence, The equivalence of simple models for radiation-induced impulse. In *Shock Compression of Condensed Matter-1991*, (Elsevier, Amsterdam, 1992) pp. 785 – 788
13. J.L. Remo, M.D. Furnish, R.J. Lawrence, Plasma-driven Z-pinch X-ray loading and momentum coupling in meteorite and planetary materials. *J. Plasma Phys.* **97**, 121 (2013). <https://doi.org/10.1017/S0022377812000712>
14. J.L. Remo, R.J. Lawrence, S.B. Jacobsen et al., High energy density soft x-ray momentum coupling to comet analogs for neo mitigation. *Acta Astronaut.* **129**, 384 (2016). <https://doi.org/10.1016/j.actaastro.2016.09.02>
15. L. Seaman, D. R. Curran, Sri puff 8 computer program for one-dimensional stress wave propagation. SRI Report PYU-6802 (1978)
16. E. S. Hertel, R. L. Bell, M. G. Elrick, Cth: A software family for multi-dimensional shock physics analysis. In *Shock Waves@Marseille I*, (Springer, Berlin, Heidelberg, 1995) pp. 377 – 382. https://doi.org/10.1007/978-3-642-78829-1_61
17. Y. D. Murray et al., Users manual for ls-dyna concrete material model 159. Report, (United States: Federal Highway Administration, Office of Research, 2007)
18. Group Abaqus, Abaqus 6.11. Manual, (USA: Dassault Systemes Simulia Corporation, 2011)
19. N. Zhou, D. J. Qiao, *Materials dynamics under pulse beam radiation*. (National Defense Industry Press, Beijing, China, 2002) pp 13-21 (in Chinese)
20. D.J. Qiao, *Thermodynamic Effect and Reinforcing Technology under Pulse X-ray Radiation* (National Defense Industry Press, Beijing, China, 2012). (in Chinese)
21. D. Wang, Y. Gao, W. Chen et al., Equivalent analysis of thermodynamic blow-off impulse under x-ray irradiation. *Appl. Sci.* **11**, 8853 (2012). <https://doi.org/10.3390/app11198853>
22. D. Wang, K. Zhang, W.H. Tang, Numerical simulation of thermal shock waves induced by pulsed X-ray in C/PF materials. *J. Phys.: Conf. Ser.* **1865**, 022066 (2021). <https://doi.org/10.1088/1742-6596/1865/2/022066>
23. S.-C. Huang, H. Zhang, K. Bai et al., Monte Carlo study of the neutron ambient dose equivalent at the heavy ion medical machine in Wuwei. *Nucl. Sci. Tech.* **33**, 119 (2022). <https://doi.org/10.1007/s41365-022-01093-z>
24. D.-H. ShangGuan, W.-H. Yan, J.-X. Wei et al., Sample size adaptive strategy for time-dependent Monte Carlo particle transport simulation. *Nucl. Sci. Tech.* **34**, 58 (2023). <https://doi.org/10.1007/s41365-023-01202-6>
25. M.W. Evans, F.H. Harlow, E. Bromberg, *The particle-in-cell method for hydrodynamic calculations* (Report, Los Alamos Scientific Laboratory Los Alamos, 1957)
26. F. H. Harlow, The particle-in-cell method for numerical solution of problems in fluid dynamics. Report, (Los Alamos National Lab.(LANL), Los Alamos, NM (United States), 1962)
27. J.M. Dawson, Particle simulation of plasmas. *Rev. Mod. Phys.* **55**, 403 (1983). <https://doi.org/10.1103/RevModPhys.55.403>
28. Y.N. Grigoryev, V. Vshivkov, *Numerical “particle-in-cell” Methods: Theory and Applications* (Walter de Gruyter, Zeist, Netherlands, 2012)
29. N.A. Dyson, *X-rays in Atomic and Nuclear Physics* (Cambridge University Press, London, 1990)
30. E. Güneisen, Theorie des festen Zustandes einatomiger Elemente. *Ann. Phys.* **344**, 257 (1912). <https://doi.org/10.1002/andp.19123441202>. (in German)
31. S. Faik, A. Tauschwitz, I. Iosilevskiy, The equation of state package FEOS for high energy density matter. *Comput. Phys. Commun.* **227**, 117 (2018). <https://doi.org/10.1016/j.cpc.2018.01.008>
32. R. More, K. Warren, D. Young et al., A new quotidian equation of state (qeos) for hot dense matter. *Phys. Fluids* **31**, 3059 (1988). <https://doi.org/10.1063/1.866963>
33. G. Zhao, R.Q. Zhang, W.H. Tang, Blowoff impulse on material due to pulsed x-ray radiation. *Explos. Shock Waves* **16**, 260 (1996). (in Chinese)
34. A. Nishiguchi, T. Yabe, Second-order fluid particle scheme. *J. Comput. Phys.* **52**, 390 (1983). [https://doi.org/10.1016/0021-9991\(83\)90037-2](https://doi.org/10.1016/0021-9991(83)90037-2)
35. W. Gropp, E. Lusk, A. Skjellum, *Using MPI: Portable Parallel Programming with the Message-Passing Interface* (MIT press, United States, 1999)
36. S. Agostinelli, J. Allison, K.A. Amako et al., Geant4—a simulation toolkit. *Nucl. Instrum. Methods Phys. Res. Sect. A Acceler. Spectrom. Detect. Assoc. Equipm.* **506**, 250 (2003). [https://doi.org/10.1016/S0168-9002\(03\)01368-8](https://doi.org/10.1016/S0168-9002(03)01368-8)
37. J. Allison, K. Amako, J. Apostolakis et al., Geant4 developments and applications. *IEEE Trans. Nucl. Sci.* **53**, 270 (2006). <https://doi.org/10.1109/TNS.2006.869826>

38. J. Allison, K. Amako, J. Apostolakis et al., Recent developments in geant4. Nucl. Instrum. Methods Phys. Res., Sect. A **835**, 186 (2016). <https://doi.org/10.1016/j.nima.2016.06.125>
39. J.-L. Chen, S.-J. Yun, T.-K. Dong et al., Studies of the radiation environment on the Mars surface using the Geant4 toolkit. Nucl. Sci. Tech. **33**, 11 (2022). <https://doi.org/10.1007/s41365-022-00987-2>
40. W. Thomson, XLVI: hydrokinetic solutions and observations. Lond. Edinburgh Dublin Philos. Mag. J. Sci. **42**, 362 (1871). <https://doi.org/10.1080/14786447108640585>
41. Helmholtz, XLIII. On discontinuous movements of fluids. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science **36**, 337 (1868) (Published online 2009). <https://doi.org/10.1080/14786446808640073>
42. F.H. Ludlam, Characteristics of billow clouds and their relation to clear-air turbulence. Q. J. R. Meteorol. Soc. **93**, 419 (1967). <https://doi.org/10.1002/qj.497093398033>
43. G. Bodo, S. Massaglia, A. Ferrari et al., Kelvin-helmholtz instability of hydrodynamic supersonic jets. Astron. Astrophys. **283**, 655 (1994)
44. B.A. Remington, R.P. Drake, D.D. Ryutov, Experimental astrophysics with high power lasers and z pinches. Rev. Mod. Phys. **78**, 755 (2006). <https://doi.org/10.1103/RevModPhys.78.755>
45. K.B. Antypas, A.C. Calder, A. Dubey et al., *Parallel Computational Fluid Dynamics: Theory and Applications* (Elsevier, Oxford, 2006)
46. L.-F. Wang, W.-H. Ye, Z.-F. Fan et al., Kelvin-Helmholtz instability in compressible fluids. Acta Physica Sinica **59**, 6381 (2009). (in Chinese)
47. J. She, Research on the Thermal-dynamic Response of Multi-thin-layer Structure Materials Irradiated by X-ray. Dissertation, (Graduate School of National University of Defense Technology, 2009) (in Chinese)
48. C.-X. Peng, H.-M. Tan, P. Lin et al., Experimental studies of blowoff impulse in materials irradiated by pulsed soft X-ray. High Power Laser Particle Beams **15**, 89 (2003). (in Chinese)
49. G.M. Zhang, R.Q. Zhang, J.B. Chen, Two-dimensional dynamic calculation of X-ray thermal shock wave in cylindrical shell. J. Natl. Univ. Defense Technol. **17**, 105 (1995). (in Chinese)

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