Electron beam absorption algorithms for electron beam melting processes simulated by a three–dimensional thermal free surface lattice Boltzmann method in a distributed and parallel environment

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Abstract

This paper introduces two electron beam absorption algorithms for a three–dimensional thermal free surface lattice Boltzmann method simulating electron beam melting processes. The algorithms use a state-of-the-art volume of fluid free surface method of the lattice Boltzmann multi–distribution approach to handle the interaction between the electron beam and the material. Modeling the electron beam gun properties, such as absorption and energy dissipation, is explained in detail. Special emphasis is given to an implementation in a distributed and parallel environment due to the high computational costs of three–dimensional simulations. Finally, a thorough validation for the beam absorption behavior against the analytical solution is proceeded and a concluding example in a powder bed shows the capability of the approach to simulate and support understanding the electron beam melting process.

Keywords: Electron beam melting; Electron beam absorption; Thermal lattice Boltzmann method; Free surface

1. Introduction

Electron beam melting (EBM) is an additive manufacturing method used to produce metallic structures layer by layer from metal powder. A schematic of an EBM system and the process is shown in Fig. 1. Before the process starts a three–dimensional CAD model is sliced into certain thin layers. These slices determine where the electron beam melts the powder. During the EBM process the current layer of metal powder is preheated and afterwards the electron beam melts the powder according to the layer data. Once the layer is melted the build platform is lowered by one layer thickness and the rake distributes a new powder layer.

There are numerous products generated by EBM: medical implants like hip joints or artificial spinal discs [2], [3] or components for aerospace or automotive industry. Advantages of the EBM manufacturing are the possibilities to construct very complex structures which are strong and flexible.

The objective is to accelerate the build process and the production accuracy. Therefore, a better understanding of the beam–powder interaction is necessary, which is gained by three–dimensional simulations of the process. Based on a two–dimensional model [4] we developed a thermal three–dimensional free surface lattice Boltzmann method...
model (LBM) where powder particles are taken into account. The model includes hydrodynamic physical effects, like the flow of the melt pool, capillarity and wetting, as well as thermal effects, like heat conduction and transport, electron beam absorption and solid–liquid phase transitions.

In this paper we describe in detail the derivation of absorption algorithms basing on electron beam properties. Two acceleration voltages are considered and the resulting penetration behavior leads to the corresponding absorption algorithms. Both are derived suitable for parallel computation and validated by analytical solutions and numerical examples. Our results show the high potential of the LB approach in combination with the electron beam integration to understand and develop complex processes like EBM depending on thermodynamic as well as on fluid dynamic considerations.

The remainder of the paper is organized as follows. Section 2 describes the numerical method of a thermal LBM used for discretization and its parallel implementation. Section 3, the main part of this paper, amplifies the aspects belonging to the modeling of the EBM process, i.e. definition of the electron beam and different absorption types. Section 4 provides information about the implementation and validates the derived absorption algorithms. Finally, the numerical results of the absorption in a powder bed are shown and aspects and targets of future work are described.

2. Numerical Methods

The single phase-continuum conservation equations to simulate incompressible thermodynamic fluid transport including melting and solidification are given by:

\[ \nabla \cdot \mathbf{u} = 0, \]

\[ \frac{\partial (\mathbf{u})}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{F}, \]

\[ \frac{\partial (E)}{\partial t} + \nabla \cdot (\mathbf{u} E) = \nabla \cdot (k \nabla E) + \Phi, \]

where \( t \) is the time and \( \mathbf{u} \) the macroscopic velocity. Further hydrodynamic quantities are the density \( \rho \), pressure \( p \), body forces \( \mathbf{F} \) like the gravity and kinematic viscosity \( \nu \). The thermal energy density \( E \) depends on the fluid temperature, specific heat capacity and also latent heat for the phase transition and is related to the thermal diffusivity \( k(E) \). Energy sources, like the electron beam, are summarized in \( \Phi \). Fluid compression and viscous heat dissipation are neglected by this model.
The electron beam absorption marks the starting point for the simulation of the EBM process. The absorbed energy introduced as a volumetric energy source in $\Phi$ heats the material and finally leads to a phase transition from solid to liquid. Mainly the surface tension is the reason behind the melt pool flow which affects heat conduction and further electron beam absorption.

For discretization lattice Boltzmann models [5] using particle distribution functions (pdf) $f(x, v, t)$, describing the probability of finding a particle with velocity $v$ at position $x$ at time $t$, are used. The local values of density and momentum can be evaluated from known pdfs. The discretized pdf $f_i$ used by the lattice Boltzmann method is gained by dividing space into a regular lattice. Velocities are represented by a finite set of displacement vectors $e_i$ pointing to neighbor lattice sites. Resting particles are represented by a zero velocity vector.

There are mainly two approaches for solving the heat equation by LBM [6]. Thermal LBM using the multi-speed approach [7], [8], [9] can be seen as an extension of the isothermal LBM. Additional discrete velocities and momentum can be evaluated from known pdfs. The discretized pdf is obtained by dividing space into a regular lattice. Velocities are represented by a finite set of displacement vectors $e_i$ pointing to neighbor lattice sites. Resting particles are represented by a zero velocity vector.

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The basic idea for the derivation of the LBM [16], [17], [18] is to solve the linear transport equation for pdfs in the physical momentum space. Bhatagnar, Gross and Krook proposed an appropriate discretized approximation of the collision operator [19], which is used to retrieve the equations of motion:

$$f_i(x + e_i, t + \Delta t) = f_i(x, t) + \frac{\Delta t}{\tau_f} (f_{i\text{eq}}(x, t) - f_i(x, t)) + F_i(x, t),$$

$$h_i(x + e_i, t + \Delta t) = h_i(x, t) + \frac{\Delta t}{\tau_h} (h_{i\text{eq}}(x, t) - h_i(x, t)) + \Phi_i(x, t).$$

Body forces acting on the fluid are summarized in $F_i$, e.g. gravity [20], and energy sources, like the electron beam, are represented by $\Phi_i$. The polynomial equilibrium distribution functions, denoted by $f_{i\text{eq}}$ and $h_{i\text{eq}}$ are defined by:

$$f_{i\text{eq}}(x, t) = \omega_i \rho \left(1 + \frac{e_i \cdot u}{c_s^2} + \frac{(e_i \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2}\right).$$

$$h_{i\text{eq}}(x, t) = \omega_i E \left(1 + \frac{e_i \cdot u}{c_s^2}\right).$$

For the three-dimensional D3Q19 LBM the lattice weights $\omega_i$ and lattice displacement vectors $e_i$ are given by:

$$\omega_i = \begin{cases} \frac{1}{5} & i = 0 \\ \frac{1}{18} & i = 1, \ldots, 6 \\ \frac{1}{36} & i = 7, \ldots, 18 \end{cases}$$

$$e_i = \begin{cases} (0, 0, 0) & i = 0 \\ (\pm c, 0, 0), (0, \pm c, 0), (0, 0, \pm c) & i = 1, \ldots, 6 \\ (\pm c, \pm c, 0), (0, \pm c, \pm c), (\pm c, 0, \pm c) & i = 7, \ldots, 18 \end{cases}$$

The relaxation parameters $\tau_f$ and $\tau_h$, corresponding to the kinematic viscosity $\nu$ and the thermal diffusivity $k$ respectively, are defined by:

$$\nu = c_s^2 \Delta t (\tau_f - 0.5),$$

$$k = c_s^2 \Delta t (\tau_h - 0.5).$$

The lattice speed of sound $c_s^2$ is $c^2/3$ with cell length $c$ and $\Delta t$ is the time step. Under the incompressible flow limit, i.e. for small Mach numbers, the mass, momentum and energy conservation equations (1)-(3) can be derived through a Chapman–Enskog expansion [12], [21], [22]. The equations of motion (5) and (6) are solved in a two step approach. First the collision values on the right hand side are computed and then they are streamed to the neighbor cells.
2.1. Free Surface

The development of a free surface LBM is necessary for the simulation of moving interfaces between immiscible gas and liquid fluids. Therefore, each cell in the lattice has a cell type, e.g. wall, gas, liquid or liquid interface and solid or solid interface (Fig. 2). Furthermore it has to be guaranteed that the gas phase is separated by a closed interface layer from the fluid phase [23].

Liquid cells (χ = 1)
Liquid Interface cells (χ ∈ [0; 1])
Solid cells (χ = 1)
Solid Interface cells (χ ∈ [0; 1])
Gas cells (χ = 0)
Wall cells
- Free Surface
- Solid–Liquid Phase Transition

Fig. 2. Example of a molten spot in compact material. Gas phase is separated from the fluid phase by an interface layer.

To ensure mass, momentum and energy conservation a volume of fluid approach is used, where a fill level χ ∈ [0; 1] is defined for each lattice cell.

We neglect the gas phase because of the high density difference to the fluid phase, i.e. there are no pdfs available in gas cells. Because of this fact missing pdfs after the streaming step in interface cells have to be reconstructed by the approach described in [24].

Because of the simulation of the EBM process, which includes phase transitions, each fluid lattice cell in the simulation domain is either liquid or solid [25], determined by the energy density E and a certain, material specific phase transition temperature.

Due to the high dynamics of the melt pool cell conversions between these states have to be done. All cells are able to change their state but a change from a gas to a liquid cell and vice versa are not allowed because of the free surface approach. Furthermore solid–liquid phase transitions [21] have to be considered.

3. Electron Beam Integration

In this part essential modeling aspects regarding the definition and behavior of the electron beam and its properties are described. The main focus is taken on two absorption algorithms for electron beams with different acceleration voltages. Both algorithms are derived from the physical absorption behavior and are reformulated to be executable in parallel.

3.1. Electron Beam Model

The electron beam energy $E_b$ on the surface area of one lattice cell is modeled by a two–dimensional Gaussian distribution

$$E_b(x) = \gamma \frac{UIC^2\Delta t}{2\pi\sigma^2} \exp \left( -\frac{1}{2\sigma^2} (x - x_b, x - x_b) \right), \quad (11)$$

where $x$ denotes the lattice cell center position in the x–y–plane, $x_b$ the current beam center position and $\sigma$ the standard deviation. The electron beam power is defined by the acceleration voltage $U$ and beam current $I$. Some electrons are lost due to reflection at the surface, so the remaining fraction of the electron beam energy penetrating the material is denoted by $\gamma \in [0; 1]$.

Regarding the EBM process it is necessary that the electron beam is mobile. Beam movements are defined by start, end and reference positions, start time and pulse duration. With these variables it is possible to describe stationary cases which are reached by equal positions, line, curve or circle melting by a suitable setup of the positions and multiplexing by defining a series of start positions with short pulse durations.
3.2. Electron Beam Absorption Model

The inclusion of beam energy has to be modeled by absorption, because absorption length of the electron beam is magnitudes higher than the thermal length [26]. The electron beam penetrates through the material nearly instantaneous. Therefore we model the energy source as a volumetric force of the first cells

\[ \Phi_i(x, t) = \omega_i \varphi(x, t) E_a(x, t), \]  

where \( x \) is the lattice cell center with the corresponding amount of absorbed energy \( E_a \) and \( \Phi_i \) the source term in equation (6).

Two different absorption approaches have to be compared and examined. The first is an exponential absorption type for an electron beam with an acceleration voltage of 60 kV and the second is a constant absorption type for a 120 kV electron beam. The lower voltage is typically used in EBM machines and the higher voltage is a current research topic.

In Fig. 3 the white marks show the absorption coefficient related to the penetration depth for both acceleration voltages [27] and the black marks visualize the approximated value functions. The 60 kV electron beam is approximated by a monotonically decreasing exponential function, meaning that most of the dissipated energy is consumed by the cells which are closer to the electron beam gun.

The second absorption type for a 120 kV electron beam is approximated by a constant function. As a consequence of this, each cell in \( z \)-direction gets the same amount of energy until the complete energy is dissipated. The constant absorption type has a higher penetration depth.

The maximum penetration depth \( z_p \) is determined by minimizing the error of the approximated functions, which is used to derive the artificial absorption parameter \( \lambda \).

The approximations for a cell length of 1 \( \mu \text{m} \) in Fig. 3(a) are quite rough, but for a cell length of 5 \( \mu \text{m} \) in Fig. 3(b), which is the default case for our simulations, the approximations fit well. It is important to mention that they do not differ in the amount of energy which is absorbed, but rather in the depth. In both cases there is more energy deported into deeper cells.

Furthermore it has to be thought about the dependency of the absorption coefficient due to the fill level at the surface of the interface layer. Less filled cells should absorb less energy at the surface than completely filled cells.

Exponential Electron Beam Absorption. We approximate the absorption of \( E_b(x, y) \) for acceleration voltages at 60 kV by the exponential law. To apply the absorption on the lattice the spatial dimensions are discretized. For
the $x$–$y$–plane this is done in $E_b$ of equation (11) and the discretization of the $z$ direction leads to

$$E_a(x_i, y_j, z_k) = E_b(x_i, y_j) \cdot \left(1 - e^{-\lambda c}\right) \cdot e^{-\lambda z_k},$$

where $E_a$ denotes the beam energy absorbed in one lattice cell and $\lambda$ the material absorption parameter.

Here it is assumed that the electron beam energy is completely absorbed in a cell stack at $(x_i, y_j)$ and that this cell stack is filled with liquid cells. This assumption is not fulfilled for the EBM process, because powder layers with the material absorption parameter $\chi$ are used, which absorb the energy in a way that is not channelled. Therefore an equation within which the absorption is computable cell–by–cell without any of these global assumptions is needed.

The next step is to reformulate equation (13) in a recursive way. This is done by an auxiliary function $\psi(x_i, y_j, z_k)$ representing the exponential function:

$$E_a(x_i, y_j, z_k) = E_b(x_i, y_j) \cdot \psi(x_i, y_j, z_k),$$

$$\psi(x_i, y_j, z_k) = \left(1 - e^{-\lambda c}\right) \left(1 - \sum_{l=0}^{k-1} \psi(x_i, y_j, z_l)\right).$$

By induction equality of equation (13) and equations (14) and (15) is provable. The second step is to use the volume of fluid approach to determine the fraction of energy each cell can absorb. Therefore $\psi$ is replaced by

$$\chi(x_i, y_j, z_k) = \left(1 - e^{-\lambda c}\right) \left(1 - \sum_{l=0}^{k-1} \chi(x_i, y_j, z_l) \varphi(x_i, y_j, z_l)\right).$$

**Constant Electron Beam Absorption.** The electron beam energy absorption for acceleration voltages at 120 kV is approximated by a constant function, which is discretized spatially:

$$E_a(x_i, y_j, z_k) = \begin{cases} AE_b(x_i, y_j) \cdot c & k < n \\ AE_b(x_i, y_j) \cdot (z_p - z_k) & k = n \\ 0 & k > n \end{cases}, \quad \lambda = 1/z_p, \quad n = \lfloor z_p/c \rfloor,$$

with the material absorption parameter $\lambda$ and maximum penetration depth $z_p$.

For the same reason as for the exponential absorption a cell–by–cell computable equation without any global assumption is defined by the auxiliary function $\chi$, which uses the volume of fluid approach:

$$E_a(x_i, y_j, z_k) = E_b(x_i, y_j) \chi(x_i, y_j, z_k),$$

$$\chi(x_i, y_j, z_k) = \min\left\{\lambda c, 1 - \sum_{l=0}^{k-1} \chi(x_i, y_j, z_l) \varphi(x_i, y_j, z_l)\right\}.$$

**Fill Level Effects.** In Fig. 4 the absorption behavior for both algorithms for the first 12 lattice cells, each with a length of 5 $\mu$m, is shown. In both cases the graphs for a fill level of 1 equals the approximated graphs in Fig. 3.

In case of a reduced fill level for all fluid cells, the absorption behavior changes. In the exponential case the first cells absorb less energy, but from the third cell on the remaining energy is high enough to eliminate the fill level effect and these cells absorb more energy than before. The absorption behavior for the constant case is similar. The first cells absorb the maximum amount of energy and the last cells the resulting energy. Here the maximum penetration depth is indirect proportional to the fill level.

### 3.3. Parallelization

To parallelize the numerical simulation the global domain is split in several blocks and those are distributed to different CPUs (Fig. 5). In a single streaming step of the LBM the pdfs to the direct neighbor cells have to be communicated (red). But for the absorption of the electron beam the iteration over the whole domain in $z$ direction in one time step is necessary. In general this is possible with equations (14), (16) and (18), (19), but then the computation of the absorption is completely sequential from top to bottom. This behavior will cause waiting times for other CPUs, so these equations are reformulated for parallel computation.
Fig. 4. Absorption behavior for different fill levels: in both figures the graph with a fill level of 1 equals the approximated graphs in Fig. 3(b); depending on the fill level lower energy is absorbed in the first cells and the electron beam penetrates deeper.

The main idea is to split the computation in a pre and post compute step which can be evaluated parallel on each block and a communication step between to exchange the necessary information. This communication (green) is a global top–to–bottom scheme, where each block sends its information to each lower block. With this technique each block can post compute the absorption coefficients.

This subsection concentrates on one special position $(x_i, y_j)$ and skip these parameters. Furthermore the indices of $z_k$ are extended to $z_{(k,m)}$ where $k$ denotes the index in the corresponding block $m$. The next step is to split up the auxiliary function $\chi$ into $\chi_{\text{pre}}$ and $\chi_{\text{post}}$ for the computation of the pre and the post absorption values, respectively.

For the exponential beam absorption these modifications lead to:

\begin{align}
E_a(z_{(k,m)}) &= E_b \chi_{\text{post}}(z_{(k,m)}) \\
\chi_{\text{post}}(z_{(k,m)}) &= \chi_{\text{pre}}(z_{(k,m)}) \prod_{n=0}^{m-1} \left(1 - \sum_{l} \chi_{\text{pre}}(z_{(l,n)}) \varphi(z_{(l,n)})\right) \\
\chi_{\text{pre}}(z_{(k,m)}) &= \left(1 - e^{-\lambda c}\right) \left(1 - \sum_{l=0}^{k-1} \chi_{\text{pre}}(z_{(l,m)}) \varphi(z_{(l,m)})\right)
\end{align}

Fig. 5. Communication schemes: local for pdf streaming (red); top–to–bottom for beam absorption (green)

The parallel computation starts from equation (22) which is computed on each block, then the second term of equation (21) is communicated and finally equations (21) and (20) can be evaluated in the post computation step.
A similar set of equations can be set up for the constant beam absorption:

\[
E_a(z_{k,m}) = E_b \chi_{\text{post}}(z_{k,m}) =\]

\[
\chi_{\text{post}}(z_{k,m}) = \min \left\{ \chi_{\text{pre}}(z_{k,m}), \max \left( 0, 1 - \sum_{n=0}^{m-1} \sum_{l=0}^{k-1} \chi_{\text{pre}}(z_{l,n}) \varphi(z_{l,n}) - \sum_{l=0}^{k-1} \chi_{\text{post}}(z_{l,m}) \varphi(z_{l,m}) \right) \right\} 
\]  (24)

\[
\chi_{\text{pre}}(z_{k,m}) = \min \left\{ \lambda_c, 1 - \sum_{l=0}^{k-1} \chi_{\text{pre}}(z_{l,m}) \varphi(z_{l,m}) \right\} 
\]  (25)

The parallel computation starts with the last equation (25) which is computed on each block, then the sum over the pre computation values of the maximum function of equation (24) is communicated and finally equations (24) and (23) are evaluated.

4. Implementation and Simulation Results

In this section the implementation in the 	extsc{walberla} framework [28] is explained and the validation of the absorption algorithm is done with respect to the approximated solutions using a generated powder bed. Finally, the numerical results of these algorithms in a powder bed are shown.

4.1. Software frameworks

The implementation of the EBM process is done in the 	extsc{walberla} framework. It is a LBM based numerical fluid flow solver which can be used for the simulation of numerous physical applications, e.g. the simulation of blood flow in the human heart, the modeling of moving obstacles in a liquid or the simulation of bacteria in a fluid. Because of its modular architecture, the framework is well suited to be extended to simulate thermodynamic phenomena. The generation of powder particles are included into 	extsc{walberla} by coupling it with the PhysicsEngine 	extit{pe}, which enables massively parallel simulations of arbitrary shaped rigid bodies [29].

Both frameworks are coupled by the powder bed generation. First the free surface from the lattice cells of 	extsc{walberla} is approximated and transfered to 	extit{pe}, which then generates a new layer of powder particles consisting of different sized spheres. These particles are transfered back to the lattice cells, by changing the cell type and setting an appropriate fill level at the interface cells to approximate the body shape. After melting and solidification this process starts again for the next layer.

4.2. Absorption in powder bed

The previous section showed analytical results with a compact material, with artificially reduced fill levels. When the EBM process is simulated, the electron beam is absorbed in a powder bed, with completely and partly filled cells and empty gas cells.

Fig. 6 shows a slice through a generated powder bed, whereby the colors represent the absorption coefficient from a maximum value (red) to zero (blue) in fluid cells. Gas cells and the lattice grid are not shown. For this example we used the exponential algorithm with a maximum absorption coefficient of 0.38. The left subfigure represents the absorption coefficients in the pre computation step of a domain split into three blocks.
The right subfigure shows the absorption coefficients after the communication and post computation step. The values at the top of the lower blocks are correct and the values show a monotonous decrease from top to bottom.

In both figures it is obvious that the gas cells have no influence on the absorption behavior. Furthermore the absorption coefficients of interface cells are not affected by their fill levels, because $E_a$ is the absorbed energy per lattice cell volume. For the computation of the energy source term in equation (12) the fill level is taken into account.

4.3. Melting of a spot

The melting spot example shows the combination of the electron beam absorption with phase transitions and the LBM. In Fig. 7 are snapshots of melting a spot in a powder bed at different time steps shown.

![Snapshots of spot melting in a powder bed at different time steps](image)

The light gray cells are solid powder cells and the colored cells show the temperature gradient from the maximum temperature (red) to the phase transition temperature (blue). The simulation starts with a small melt pool (a), which grows (b) until time step 7500, when the beam pulse ends. Then the melt sink down in the powder bed while cooling and begin to solidify (c). This example shows a good agreement to experimental data and the potential to simulate the EBM process.

5. Conclusion

This paper describes a parallel, thermal free surface LBM which can be used for simulating the EBM process. The implementation is included in the waLBerla framework and uses the pe for the generation of powder particles. Particular importance was placed on the development of parallel absorption algorithms to take account of the high computational costs of three–dimensional simulations.

The model for the electron beam consists of a definition of the electron beam by the acceleration voltage and the current and enables us to define different movements of it. Two different absorption types, constant and exponential, are derived and their relation due to penetration depth and dissipated energy is explained. Both models are compared to the approximated solution and the implementation is also validated within a powder bed by numerical simulations.

Future research topics will be the validation of the melt pool behavior, i.e. the comparison of its lifespan and size with experimental data. First numerical simulations of melting spots and lines in powder beds will show the interaction of the electron beam with the powder particles and the energy absorption in the melt pool to calibrate the numerical model for a sufficient match with experiments. Then we will focus on the simulation of larger domain sizes and more powder layers to take into account the influence of the penetration depth due to the melt pool.

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