The worm lattice Boltzmann method: the case of diffusive-ballistic phonon transport

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Abstract

The lattice Boltzmann method (LBM) is a numerical approach for tackling problems described by a Boltzmann type equation, where time, space and velocities are discretized. The method is widely used in fluid dynamics, radiation transfer, neutron transport, and more recently for studying diffusive-ballistic heat transport [1, 2, 3, 4]. The main disadvantage of the method is the ray effect problem, caused by the finite set of propagation directions used to discretize the angular space. A higher number of propagation directions would potentially solve the problem, but at the expense of increasing the computational cost of the scheme. Here, we propose the worm-lattice Boltzmann method (worm-LBM), which allows to implement multiple (as much as necessary) propagation directions, by alternating the directions given by the standard next neighbor schemes in time. The method is demonstrated for a 2D square scheme of the type D2Q$[M \times 8]$ ($M > 1$), and can be straight for-

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ward generalized for the 3D case. Moreover, to overcome the inherent problem of non-isotropic speed of propagation in square schemes, we introduce a time adaptive scheme to impose a circular propagation. The method, indeed, allows any angular distribution for the propagation velocities. The new worm-LBM is introduced in the framework of phonon transport, and its suitability for addressing both the diffusive and ballistic regimes is demonstrated. More generally, we show that it does not suffer from the long-standing problems of direct discretization methods namely, numerical smearing, angular false scattering, and ray effect. The worm-LBM, thus, has the potential to be at the forefront of the methods for addressing transport studies.

**Keywords:** Phonon transport, Boltzmann transport equation, lattice Boltzmann method

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**Highlights**

- Multiple directions in a D2Q[\(M \times 8\)] LBM scheme (\(M > 1\)) for the Boltzmann transport equation.
- Time adaptive scheme allows isotropic and arbitrary angular dependent velocity in the LBM.
- Low cost per propagation direction, as for the conventional D2Q8-LBM scheme.

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**1. Introduction**

In the quest to develop smaller devices with improved performance, the problem of thermal management has become increasingly crucial. Computer simulations, addressing the underlying physics of thermal transport in materials, are indeed a priceless tool for designing thermal management strategies in nanodevices [5, 6, 7, 8, 9].

At length scales comparable to the mean free path of the thermal energy carriers, or at time scales shorter than their relaxation times, the diffusive picture of heat transport is replaced by the so-called ballistic transport [10, 11]. In this regime, as long as the particle nature of the heat carriers prevails, the Boltzmann transport equation (BTE) must be used.
The different regimes for thermal transport can be classified by using the Knudsen number

\[ K_n = \frac{\Lambda}{l}, \]  

where \( l \) is the characteristic length of the system, and \( \Lambda \) is the mean free path (MFP) of the carriers. The diffusive transport regime is characterized by \( K_n \ll 1 \), while the ballistic regime by \( K_n \gg 1 \). Those cases in which the MFP is of the same order of magnitude as \( l \) are in the quasi-ballistic regime, and feature Knudsen numbers in the range between \( 0.1 \leq K_n \leq 10 \).

The BTE can be used to describe both the continuum (diffusive) and sub-continuum (ballistic) regime, but it is computationally demanding as it involves seven independent variables accounting for space, time and velocity. Monte Carlo (MC) methods have been used traditionally to tackle the high dimensionality issue of the Boltzmann transport equations. However, they are less effective for thermal transport studies, where in most of the cases one deals with problems close to equilibrium. In this case, MC methods spent too much time sampling the equilibrium distribution. This issue was overcome with the energy-based variance-reduced Monte Carlo formulation [12]. This method is highly efficient, if a linearization of the BTE is justified, and if the superposition principle can be used to propagate the particles independently of each other through the system. Conversely, for a temperature dependent scattering and strong thermal gradients, a direct discretization of the BTE is desirable. Among the discretization based methods to tackle this problem, the discrete ordinates method (DOM), and the finite volume method (FVM) are widely implemented [13, 14, 15, 16, 8]. The accuracy of these methods, however, is limited by three types of numerical errors triggered by the spatial and angular discretization, namely: ray effect, numerical smearing, and angular false scattering [17, 13]. An alternative and rather inexpensive discretization method, that overcomes the latter two problems, is the so called Lattice Boltzmann Method (LBM) [13].

The LBM, in spite of its advantages, suffers from the ray effect problem intrinsic of any direct discretization method, which results in an inadequate description of the ballistic regime [18]. To overcome this problem, it is necessary to resolve more directions over which the heat carriers can travel on the grid.

In the framework of LBM, the 2D grid with the highest number of propagation directions (six directions) with isotropic velocity is the hexagonal D2Q6, which is insufficient to tackle ray effect and ballistic transport [18]. A
square D2Q8 scheme would allow to resolve more directions (eight in total),
but it suffers of non-isotropic speed of propagation [18]. Here we propose
the time adaptive scheme lattice Boltzmann method (TAS-LBM) to remedy
this problem. The TAS-LBM allows to describe an isotropic speed of prop-
agation within a square scheme, and can be easily extended to account for
a high number of propagation directions. It can also be extended beyond
the isotropic speed of propagation to describe any angle dependent velocity.
Finally, and most importantly, we extend the TAS-LBM to the worm lat-
tice Boltzmann method (worm-LBM). A simple and powerful approach to
reduce the computational cost and complexity that results from increasing
the number of propagation directions [19, 20]. In the following, the proposed
methods will be explained in detail, tested and compared to the standard
LBM and DOM.

The paper is organized as follows: In Sec. 2 the Boltzmann transport
equation and the LBM are briefly described. In Sec. 3 the TAS-LBM ap-
proach is introduced, and in Sec. 4 is generalized for an arbitrary number of
propagation directions. In Sec. 5 the worm-LBM is introduced and tested.
In the last section of the paper, Sec. 6 the new worm-LBM is compared to
the DOM. Finally we summarize and conclude our work.

2. Numerical methods

2.1. Boltzmann transport equation

In semiconductors and dielectric materials the phonon contribution to the
thermal transport dominates, the electron contribution is negligible, and the
heat transport problem reduces to solving the phonon BTE:

$$\frac{\partial f}{\partial t} + \vec{v}_g \cdot \nabla f + \vec{F} \cdot \nabla f = \left( \frac{\partial f}{\partial t} \right)_{\text{collision}}, \quad (2)$$

where $f = f(\vec{r}, t)$ is the phonon distribution function of a phonon state $(\vec{k}, p)$
at position $\vec{r}$ and time $t$, being $\vec{k}$ the wave-vector and $p$ the polarization. $\vec{v}_g$
is the group velocity, related to the phonon frequency $\omega_{k,p}$ through the dis-
persion relation $\vec{v}_g = \nabla_{\vec{k}} \omega$. The second term on the left side describes the
advection of phonons, and the third term their change of momentum due to
an external force $\vec{F}$. The term on the right side describes the phonon scat-
tering (phonon-phonon, phonon-electron, phonon-defect). In the absence of
external forces acting on the phonons, and using the relaxation time approx-
imation (RTA), the BTE can be written as:

$$\frac{\partial f}{\partial t} + \vec{v}_g \cdot \nabla f = \frac{f_{eq} - f}{\tau},$$

where $\tau$ is the phonon relaxation time, and

$$f_{eq} = \frac{1}{\exp(h\omega_{k,p}/k_BT) - 1}$$

is the equilibrium phonon distribution function defined by the Bose-Einstein
statistics, and the phonon band structure given by $\omega_{k,p}$. Here $h$ is the Planck
constant divided by $2\pi$, and $k_B$ is the Boltzmann constant. The BTE in
the gray approximation, which makes use of the Debye model and considers
a single phonon propagation speed, can be expressed in terms of a single
phonon energy density,

$$e(T) = \sum_p \int f \hbar \omega_p D_p(\omega) d\omega,$$

where the sum runs over the polarization, $p$, of the phonons, and $D_p(\omega)$ is
the phonon density of states per unit volume. Accordingly, the BTE can be
written as:

$$\frac{\partial e}{\partial t} + \vec{v}_g \cdot \nabla e = \frac{e_{eq} - e}{\tau}.$$  

This equation represents an infinite set of coupled differential equations. Note
that the advection term allows for an arbitrary number of propagation di-
rections. Therefore, aside of time and space, angular discretization has to be
included.

2.2. Lattice Boltzmann method

Discretizing the first derivatives of the phonon energy density with respect
to time and space:

$$\frac{\partial e}{\partial t} = \frac{e(x, t + \Delta t) - e(x, t)}{\Delta t},$$

$$\frac{\partial e}{\partial x} = \frac{e(x + \Delta x, t + \Delta t) - e(x, t + \Delta t)}{\Delta x},$$

$$\frac{\partial e}{\partial t} = \frac{e(x, t + \Delta t) - e(x, t)}{\Delta t},$$

$$\frac{\partial e}{\partial x} = \frac{e(x + \Delta x, t + \Delta t) - e(x, t + \Delta t)}{\Delta x},$$

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$$\frac{\partial e}{\partial x} = \frac{e(x + \Delta x, t + \Delta t) - e(x, t + \Delta t)}{\Delta x},$$
and introducing an index $i$ to account for the phonon propagation in a discrete grid direction (see Fig. 1), Eq. (6) becomes:

$$
e_i(x,t + \Delta t) - e_i(x,t) + \Delta t \frac{\vec{v}_{g,i} e_i(x + \Delta x, t + \Delta t) - e_i(x, t + \Delta t)}{\Delta x} = \frac{e_{eq}^i(x,t) - e_i(x,t)}{\tau}.$$  

(7)

In the LBM approach the space domain is discretized by defining a grid of points separated by a distance $\Delta x_i$, along which the phonons propagate ballistically with a constant group velocity, resulting a set of BTE discretized equations:

$$e_i(x + \Delta x_i, t + \Delta t) = (1 - W_i) e_i(x,t) + W_i e_{eq}^i(x,t).$$  

(9)

Here $W = \Delta t/\tau$ is a weighting factor setting the contribution of ballistic (first term RHS) and diffusive transport (second term RHS). Bear in mind that $W$ can be expressed in terms of the Knudsen number. For the LBM on a regular grid, the distances $\Delta x_i$ depend on the lattice points separation:

$$\Delta x_i = \Delta t v_{g,i},$$  

(10)

thus, the weighting factors can be written as

$$W_i = \frac{\Delta t}{\tau} = \frac{\Delta x_i}{v_{g,i}} = \frac{1}{N_i K_{n,i}} \left( \frac{\Delta x_i = L_i}{N_i}, K_{n,i} = \Lambda L_i \right),$$  

(11)

where $L_i$ and $N_i$ are, respectively, the length of the domain size and the number of grid points in which the it is divided along the direction $i$.

The total phonon energy density at a grid site is then given by the sum of discrete energies calculated along each propagation direction:

$$e(x,t) = \sum_i e_i(x,t).$$  

(12)

Here, for simplicity, all the methods are introduced in the framework of the gray approximation. However, they can be straightforwardly extended to an arbitrary phonon band structure. This is known as the dispersion LBM \[21\] \[18\]. In this case, several phonon energy densities $e^j$, corresponding to linearly approximated intervals of the phonon dispersion, are simulated and coupled via the collision term of the BTE.
3. The adaptive time scheme lattice Boltzmann method

In the gray approximation, as well as in the isotropic dispersive regime (i.e. isotropic multi-mode), phonons travel with the same speed independent of the propagation direction. In the framework of the LBM, the two dimensional hexagonal scheme D2Q6 (Fig. 1) defines the grid with the highest number of propagation directions with isotropic speed (six directions). Although this grid is suitable to describe the diffusive regime [18], it poorly describes the ballistic one. An alternative would be to use the D2Q8 square grid which resolves two more propagation directions, but in this case the phonons would travel \(\sqrt{2}\) faster along the diagonal directions than along the axial ones, resulting in an unrealistic description of the problem [18]. For the diffusive regime this has been corrected by assigning different weights for the diagonals and axial directions [22]. However, in the gray approximation and isotropic dispersion LBM, the phonons travel at constant speed (i.e. with direction-independent velocity).

In order to deal with different propagation speeds (i.e. different lengths of propagation), in the proposed time adaptive scheme lattice Boltzmann method (TAS-LBM) a time condition for hopping along the diagonal sites is imposed: phonons are allowed to propagate along this direction only if they remain within a circle of radius \(x_{ax}\), which is set by the distance propagated along the axial direction (see Fig. 2). Otherwise, the propagation along the diagonal direction is paused until the condition is fulfilled.
Figure 2: TAS-LBM scheme: The non-isotropic propagation on a D2Q8 scheme is tackled by allowing hopping between lattice sites within a circle of radius $x_{\text{ax}}$, i.e. the distance propagated along the axial direction.

The upper panel of Fig. 3 shows the hopping evolution during the first five time steps along the D2Q8 grid. As it can be seen, diagonal hopping takes place just at time steps $n = 2, 3, 5$. As the simulation evolves in time, the propagation distance along the diagonal direction converges toward the distance travelled along the axial axis (lower panel Fig. 3), resulting over time in an isotropic speed of propagation.

Note that the diffusive part of the LBM is still executed for those phonons for which their ballistic propagation (along the diagonal) has been paused. Thus, the algorithm for the TAS-LBM along the diagonal directions can be written as:

$$e_i(x + \Delta x, t + \Delta t) = (1 - W) e_i(x, t) + We^{eq}_i(x, t) \quad \text{if} \quad x_{\text{diag}} \leq x_{\text{ax}}$$

$$e_i(x + \Delta x, t + \Delta t) = We^{eq}_i(x, t) \quad \text{if} \quad x_{\text{diag}} > x_{\text{ax}}$$

where $x_{\text{diag}}$ and $x_{\text{ax}}$ are, respectively, the cumulative distances propagated along the diagonal and axial directions at a time step $\Delta t$. For the axial directions, the first condition is always fulfilled. Note that $W$ does not depend here on the direction, as the gray approximation is used.

The performance of the LBM (D2Q8) and TAS-LBM (TAS-D2Q8) for the D2Q8 grid is compared in Fig. 4. The heat dissipation from a high temperature region into a cold infinite domain is shown. Five different Knudsen numbers encompassing regimes from the ballistic to the diffusive one are considered.
The differences between LBM and TAS-LBM are evident in the ballistic regime. Heat propagates faster along the diagonal directions within the D2Q8-LBM scheme, while it propagates isotropically within TAS-LBM. In the diffusive regime the non-isotropic speed of propagation effect is more subtle. It can be seen, however, that the different contours for the D2Q8-LBM case are more extended than those obtained with the TAS-LBM, as heat is propagated faster.

Thus, by the use of a simple time-scheme approach, the TAS-LBM allows to describe a circular propagation on a square grid, making the method particularly suitable for the gray approximation and for the isotropic dispersion case. The TAS-LBM, nonetheless, is not restricted to isotropic conditions, and can be used to impose any prescribed angle dependent velocity distribution.
Figure 4: Propagation of heat from a high temperature region into a cold infinite domain for five different Knudsen numbers, as obtained with the standard LBM (D2Q8) and the new TAS-LBM (TAS-D2Q8). The color map goes from maximum energy (red) to minimum energy (white). The simulations are performed for a square D2Q8 scheme. The initial temperature of the domain, except for a central region of radius 1/30 of the domain length, was set to 299.5 K. The central region was initialized at 300.5 K. In Eq. 11, the total number of grid points was \( N = 512 \), while the Knudsen number took values of \( \sim 1.40, 0.42, 0.14, 0.05 \) and 0.014.

4. Ray effect reduction: D2Q\([M \times 8]\)

In the previous section we have shown that the TAS-LBM can describe an isotropic speed of propagation along a D2Q8 grid. Nonetheless, as a consequence of the finite number of discrete propagation directions, the angular dependent heat flux profiles feature unrealistic bumps and oscillations as the Knudsen number increases (see heat profiles in Fig. 4). This problem is known as the ray effect, and is intrinsic of any direct discretization method [18].

In order to make the TAS-LBM also accurate in the ballistic regime, it is then desirable to have more directions along which the phonons can travel on the grid. The number of directions on a square grid can be easily augmented by increasing the number of grid points used for hopping. For instance, by hopping to the next-next neighbour in the D2Q8 grid one can resolve eight additional propagation directions for the phonons [19] (D2Q16, Fig. 1). In total there are 16 directions that encompass three different hopping lengths, along the axial (1-4), diagonal (5-8) and intermediate (9-16) directions. In this case, the TAS-LBM will enable propagation along the diagonal and intermediate directions, as long as the propagated distance is
smaller than or equal to the distance traveled along the axial direction at a
given time step (i.e. the distance hopped along directions 1-4). Thus, the
TAS-LBM scheme can be easily generalized to enforce a circular propagation
for any D2Q[M × 8] grid, M being an integer. These grids would allow to
resolve M × 8 propagation directions, improving the ray effect problem and
providing a more accurate description of phonon transport in the ballistic
regime. It is important to remark again, that the method goes beyond the
isotropic condition, and can be used to describe any angular distribution of
velocities.

Note that for D2Q[M × 8] grids with M > 1, towards the diagonals the
angles between adjacent propagation directions get smaller. Thus, in the
vicinity of the diagonal directions the angular energy density gets higher the
more directions are added. An example of this artifact is provided for the
D2Q16 scheme (see upper panel Fig. 5). To compensate this effect one
can redistribute the energy among the different directions such that in the
directions closer to π/4 (i.e. the diagonal) there is less energy, depending on
how small is the angle in the adjacent direction \([19, 23]\) (e.g. lower panel
Fig. 5).

![Figure 5: Propagation of heat from a high temperature region into a cold infinite domain in a D2Q16 scheme, using the TAS-LBM approach with and without angular energy redistribution. The simulation conditions are the same as those used in Fig. 4.](image)

In practice, for a given scheme D2Q[M × 8], there will be a set of M × 8
angles,

\[ \theta_j = \tan^{-1}(j/M), \quad (j = 1, \ldots, M \times 8), \quad (13) \]
Figure 6: Example of weight distribution for the D2Q16 grid. Only the weights for the three first directions are listed, the remaining ones can be straightforward calculated by using Eq. 14. Note that, $\theta_1 = \theta_4 = \theta_5 = \theta_8 = \theta_9 = \theta_{12} = \theta_{13} = \theta_{16}$, and $\theta_2 = \theta_3 = \theta_6 = \theta_7 = \theta_{10} = \theta_{11} = \theta_{14} = \theta_{15}$.

that define $M \times 8$ weight factors:

$$W_j = \frac{\theta_{j-1} + \theta_j}{4\pi} \quad (1 < j < M \times 8),$$

(14)

where periodic boundary conditions are considered (i.e. $\theta_0 = \theta_{M \times 8}$). These weight factors are used for the initial and boundary conditions, and within the differential equation for the diffusive part. An example for D2Q16 grid is provided in Fig. 6.

Thus, accounting for the correct angular distribution of energy, the ray effect can be reduced by considering more propagation directions, improving the accuracy of the TAS-LBM in the ballistic regime.

5. Worm lattice Boltzmann method (worm-LBM): computational cost optimization

The TAS-LBM provides a reliable approach to correctly describe both the ballistic and the diffusive regimes of phonon transport. Nonetheless, the computational cost of the method scales quadratically with the size of the stencil in 2-D (cubic in 3-D), becoming expensive in the ballistic regime. An alternative to circumvent this problem is to encode the spatial propagation scheme on a square grid D2Q[M × 8] (with $M > 1$) into a time adaptive propagation on the D2Q8 scheme.
Figure 7: worm-LBM approach. Propagation on any grid $D2Q[M \times 8]$ is performed following the (a) propagation directions of the D2Q8 grid. Propagation directions in the (b) D2Q16 and (c) D2Q40 grids decomposed in hopping series along the axial and diagonal directions of the D2Q8 scheme. Note that the directions not shown are symmetrically equivalent to those depicted.

The D2Q8 scheme resolves eight propagation directions that allow phonon transport either along the axial (1-4 in Fig. 1) or along the diagonal directions (5-8, Fig. 1) of a square grid. It can be shown that any propagation direction in a D2Q[$M \times 8$] scheme can be achieved using the basic directions of D2Q8. Figure 7 shows an example of this approach for the case of the D2Q16 and D2Q40 grids. In the D2Q16 grid, the propagation along the directions 9-16 (Fig. 1) can be performed by combining one hopping along the axial direction plus one along the diagonal in a recurring way (Fig. 7b). The propagation, as in the TAS-LBM approach, is allowed if the hopping distance is within a radius defined by the hopped length along the axial direction of the grid space used (i.e. $M$ steps along the axial direction for the D2Q[$M \times 8$] grid). Conversely, scattering is allowed every time step at every lattice site. This method will be called in the following the worm-LBM. Note that the worm-LBM reduces to the TAS-LBM in the limit of the D2Q8 scheme.

Figure 8 shows the heat dissipation profile in a D2Q16 grid as obtained with the TAS-LBM and worm-LBM methods. As it can be seen both approaches provide the same solution for the heat distribution. However, the computational cost per direction of the worm-LBM has been reduced to that of a D2Q8 grid in the framework of the standard LBM.
Figure 8: Propagation of heat from a high temperature region into a cold infinite domain in a D2Q16 grid generated with the TAS-LBM and worm-LBM approaches. The simulation conditions are the same as those used in Fig. 6.

6. worm-LBM vs. DOM

Finally, we want to remark that the worm-LBM approach, as its LBM counterpart, does not suffer from the problems of numerical smearing and angular false scattering characteristic of other discretization methods as DOM. Figure 9 shows the time evolution of the temperature profiles in a D2Q8 scheme as calculated with the worm-LBM and DOM, and Figure 10 shows the corresponding heat profiles.

Although in the diffusive regime ($K_n = 0.014$) the difference between both methods is small, the DOM temperature profiles in the ballistic regime ($K_{inf}$) feature a progressive smoothing along the axial directions (numerical smearing), and tangential to the diagonals (angular false scattering). These effects are not observed in the temperature and heat profiles obtained with the worm-LBM.

The advantage of the LBM over DOM, is that it propagates the signal (heat) from one lattice site to another one, while DOM interpolates between grid points (since $\Delta x = v_g \Delta t$ cannot be fulfilled for all directions at the same time). The accuracy of DOM can be improved by increasing the spatial grid resolution and/or using higher order differencing schemes [24, 13], but at expenses of a more complex algorithm and a higher computational cost.
Figure 9: worm-LBM vs. DOM: Temperature profile at different time steps, along the diagonal and axial directions in a D2Q8 grid. Simulations were performed for $K_n = 0.014$ (difusive limit), and $K_n = \infty$ (ballistic limit). The profiles along the diagonal and axial directions in the case of the worm-LBM are the same. The simulation conditions are the same as those used in Fig. 4. The upwind scheme has been used for the spatial discretization in DOM.
7. Conclusions

In this work, the simple and powerful worm-LBM for solving Boltzmann-type transport equations is proposed. It is an improved lattice Boltzmann based method that does not suffer from the ray effect problem inherent of any direct discretization method (caused by a limited number of propagation directions), and is suitable for describing transport processes in the quasi-continuum regime. In practice, the method makes use of an adaptive time scheme that allows to implement isotropic as well as angular dependent propagation speeds within an square domain. Moreover, it provides a simple algorithm to implement multiple propagation directions within a square scheme of the type of D2Q$[M \times 8]$ ($M \geq 1$), at the same computational cost per direction as in a standard D2Q8 scheme.

The worm-LBM was introduced in the framework of thermal transport. Its suitability for describing both the ballistic and diffusive phonon transport was demonstrated. Moreover, it was shown that it does not suffer from the problems of numerical smearing and angular false scattering.

Overall, due to its efficiency, simplicity and advantages (i.e. reduced ray effect, no numerical smearing or angular false scattering), the worm-LBM has the potential of becoming the forefront methodology to tackle transport processes in a wide variety of fields.

\begin{table}
\begin{tabular}{|l|c|c|c|c|c|}
\hline
\textbf{SCHEME} & $K_n \approx 1.40$ & 0.42 & 0.14 & 0.05 & 0.014 \\
\hline
worm-LBM $D2Q8$ & & & & & \\
\hline
DOM Q8 & & & & & \\
\hline
\end{tabular}
\end{table}

Figure 10: Heat dissipation in a D2Q8 grid generated with the worm-LBM and DOM approaches. Note that the worm-LBM reduces to the TAS-LBM in the limit of the D2Q8 scheme. The simulation conditions are the same as those used in Fig. 4.
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