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Adaptive time-stepping algorithms for molecular beam epitaxy: Based on energy or roughness

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ABSTRACT

Due to the small parameter, high order derivatives and nonlinear term, it takes a long time to reach the steady state in the simulation of the molecular beam epitaxy (MBE) model. In this work, based on the numerical scheme in Qiao et al. (2011) and the good properties it holds, we introduce two types of adaptive time-stepping methods, in which the physical quantities like energy or roughness are involved to produce time steps. Similarly to the spatial adaptive method, we take equidistribution of the physical quantities in time direction to control the simulation error. The numerical experiment shows that the computational time is significantly saved by these methods.

1. Introduction

The dynamic of molecular beam epitaxy (MBE) growth has been widely concerned recently. In this work, we consider the continuum model for the evolution of MBE growth. The governing partial differential equation is:

$$\begin{cases} \frac{\partial \phi}{\partial t} = -\varepsilon \Delta^2 \phi - \nabla \cdot [(1 - |\nabla \phi|^2)\nabla \phi] & \text{in } \Omega \times (0, T), \\ \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}) & \text{in } \Omega, \end{cases} \tag{1.1}$$

where $\Omega := [0, L]^2$. ϕ is a periodic height function and ϵ is a constant. The equation of MBE is the gradient flow associated with the following energy functional

$$E(\phi) = \int_\Omega \left(\frac{1}{4}(1 - |\nabla \phi|^2)^2 + \frac{\epsilon^2}{2} |\Delta \phi|^2 \right) d\mathbf{x}, \tag{1.2}$$

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where the nonlinear second-order term models the Ehrlich–Schwoebel effect, which leads to a preference of the structures with slope $|\nabla\phi| = 1$, and the fourth-order term represents the surface diffusion effect.

There have been extensive works for the MBE model. On the finite difference method, approaches based on convex splitting can be found in [1,2], where the unconditional energy stability is given. In [3,4] some implicit–explicit methods are introduced to deal with the problem. On the finite element method, [5] introduces a mixed finite element method combining the Crank–Nicolson (CN) scheme, and gets optimal order in space and time. [6] applies Local discontinuous Galerkin method to the problem. [7] proposes a scalar auxiliary variable (SAV) for gradient flows. For more details, please see [8].

How to reduce the computational time in simulating the long term behavior is also widely considered. In [3], an adaptive time-stepping technique is developed based on the energy derivative in time and was also used in [9] for the Cahn–Hilliard problem. In [4], based on the stabilization method there, the large time step is allowed in computation. [10] proposes the spectral deferred correction methods, and [11] applies this method to the phase field problems. In this work, we mainly focus on finding some new adaptive time-stepping methods to shorten the simulation time. Based on the second order CN scheme, we first propose an *adaptive time-stepping method: based on the energy* (**ATSBE**) similar to that in [12]. Then we also propose a new type of *adaptive time-stepping method: based on the roughness* (**ATSBR**). With the help of the two methods, we propose the adaptive time-stepping algorithm for the MBE problem and use the numerical example to illustrate the algorithm.

2. Difference scheme and some properties

In this section, we briefly introduce some properties of the equation and also the difference scheme for the completeness of the paper because the focus of the paper is on the time step variance. You can find more details in [3].

Define $\|\cdot\|$ as the standard L^2 norm in Ω, and $\|\cdot\|_{L^p}$ as the L^p norm. First, we list some known results for the continuum MBE model about the mass conservation, energy decay and stability.

Lemma 2.1 (*Mass Conservation*)**.** *The solution ϕ of MBE problem (1.1) is of mass conservation:*

$$\frac{d}{dt}\int_{\Omega}\phi(\mathbf{x},t)d\mathbf{x} = 0. \tag{2.1}$$

Proof. Integral the first equation of (1.1) with respect to spatial variables, and apply the period boundary condition and Gauss–Green Formula. We prove the result. □

Lemma 2.2 (*Energy Identities [13]*)**.** *For the solution ϕ of MBE problem (1.1), the following energy identities hold:*

$$\frac{d}{dt}\|\phi\|^2 + 4E(\phi) + \|\nabla\phi\|_{L^4}^4 = |\Omega|, \tag{2.2}$$

$$\frac{d}{dt}E(\phi) + \|\phi_t\|^2 = 0. \tag{2.3}$$

Lemma 2.3 (L^2 *Stability [3]*)**.** *The solution $\phi(\mathbf{x},t)$ is L^2 stable under the sense that*

$$\|\phi(\cdot,t)\|^2 \le e^{t/2\epsilon}\|\phi(\cdot,0)\|^2. \tag{2.4}$$

Then, we use the CN scheme proposed in [3] to discretize the continuum MBE model. The CN scheme enjoys properties including energy decay, unconditional stability and second order accuracy in both time and space dimension.

Suppose a square domain Ω is divided uniformly with size $\Delta x = L/N_x$ and $\Delta y = L/N_y$, where L is side length of the square and N_x, N_y are the integers used to divide the sides. The set of the grid

points is $\Omega_h = \{(x_i, y_j), x_i = i\Delta x, y_j = j\Delta y\}$. In time direction, Δt is used to denote the time steps. The discrete difference operator is defined for any function f as $\nabla_h f_{i+\frac{1}{2},j+\frac{1}{2}} = (\frac{f_{i+1,j}-f_{i,j}}{\Delta x}, \frac{f_{i,j+1}-f_{i,j}}{\Delta y})^T$, $\Delta_h f_{i,j} = \frac{f_{i+1,j}+f_{i-1,j}-2f_{i,j}}{(\Delta x)^2} + \frac{f_{i,j+1}+f_{i,j-1}-2f_{i,j}}{(\Delta y)^2}$, where $f_{i,j} = f(x_i, y_j)$. The second order CN scheme for MBE model (1.1) is

$$\frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = -\mu_{i,j}^{n+\frac{1}{2}}, \tag{2.5}$$

where

$$\mu_{i,j}^{n+\frac{1}{2}} = (\epsilon\Delta_h^2 + \Delta_h)\frac{\phi_{i,j}^{n+1} + \phi_{i,j}^{n}}{2} - \nabla_h \cdot \left(\frac{|\nabla_h \phi_{i,j}^{n+1}|^2 + |\nabla_h \phi_{i,j}^{n}|}{2} \frac{\nabla_h(\phi_{i,j}^{n+1} + \phi_{i,j}^{n})}{2} \right). \tag{2.6}$$

The discrete L^2 inner product and L^2 norm for the grid function f, g are defined as $(f, g)_h = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} f_{i,j}g_{i,j}\Delta x\Delta y$, $\|f\|_h^2 = (f, f)_h$, and the discrete H^1 norm is $\|f\|_{H^1,h} = \big[\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}(|f_{i,j}|^2 + |\nabla_h f_{i-\frac{1}{2},j-\frac{1}{2}}|^2)\Delta x\Delta y\big]$.

The CN scheme preserves a discrete version of the properties held by the continuum model. These properties are important ingredients for the adaptive time-stepping algorithms.

Lemma 2.4 (*Mass Conservation*). *For any solution of (2.5), the discrete form of mass conservation holds*

$$\sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \phi_{i,j}^{s}\Delta x\Delta y = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \phi_{i,j}^{t}\Delta x\Delta y, \qquad \forall s, t. \tag{2.7}$$

Proof. Multiply $\Delta x\Delta y\Delta t$ on both sides of (2.5), and sum on all of the spatial grid, we have the left hand side

$$\sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \Delta x\Delta y\Delta t\frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \phi_{i,j}^{n+1}\Delta x\Delta y - \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \phi_{i,j}^{n}\Delta x\Delta y.$$

By the definition of the discrete operator ∇_h and Δ_h and the periodic boundary condition, the right-hand side equals zero. So the conclusion holds for two consecutive steps and thus for any two solutions. □

Lemma 2.5 (*Equality Between Two Steps [3]*). *Let ϕ^n and ϕ^{n+1} be two consecutive numerical solutions of (2.5) and define $\phi^{n+\frac{1}{2}} := \frac{\phi^n+\phi^{n+1}}{2}$, then we have*

$$\frac{\|\phi^{n+1}\|_h^2 - \|\phi^{n}\|_h^2}{\Delta t} = - \left(2\epsilon\|\Delta_h\phi^{n+\frac{1}{2}}\|_h^2 + \Big(\frac{|\nabla_h\phi^n|^2 + |\nabla_h\phi^{n+1}|^2}{2}, |\nabla_h\phi^{n+\frac{1}{2}}|^2\Big) - 2\|\nabla_h\phi^{n+\frac{1}{2}}\|_h^2 \right). \tag{2.8}$$

Moreover, we have $\|\phi^n\|_h^2 \le C_1\|\phi^0\|_h^2$, with condition $\Delta t \le 4\epsilon$, where C_1 is independent of h and Δt, but depends on $1/\epsilon$.

Define the discrete energy functional of (1.2) as

$$E_h(\cdot) = \frac{1}{4}\|1 - |\nabla_h \cdot|^2\|_h^2 + \frac{\epsilon^2}{2}\|\Delta_h \cdot\|_h^2. \tag{2.9}$$

Lemma 2.6 (*Energy Stability [3]*). *The scheme (2.5) is unconditionally energy stable, which means for any time step Δt, it holds $E_h(\phi^{n+1}) \le E_h(\phi^n)$. More precisely, a similar energy identity as (2.3) holds*

$$\frac{E_h(\phi^{n+1}) - E_h(\phi^n)}{\Delta t} = -\|\mu^{n+\frac{1}{2}}\|_h^2, \tag{2.10}$$

where $\mu^{n+\frac{1}{2}}$ is defined in (2.6).

3. Adaptive time-stepping algorithms

We introduce two types of adaptive time-stepping methods in this section. First, there are two ways to build the adaptive time step. Then with some uniform notation, we proposed the adaptive time-stepping algorithms.

(a) An adaptive time step: based on energy (ATSBE)

We follow the method in [12] for the Cahn–Hilliard equation to use the energy decay to control the variance of the time steps. A transform of discrete energy identity (2.10) is $\Delta t = -\frac{E_h(\phi^{n+1})-E_h(\phi^n)}{\|\mu^{n+\frac{1}{2}}\|_h^2}$. As we aim at equidistribution of the energy decrease, let the numerator $|E_h(\phi_h^{n+1}) - E_h(\phi_h^n)|$ be a constant δE. Then it turns to $\Delta t = \frac{\delta E}{\|\mu^{n+\frac{1}{2}}\|_h^2}$. There is still an unknown term ϕ_h^{n+1} in the denominator. We replace ϕ_h^{n+1} by ϕ_h^n in (2.6) to denote μ^n and get a computable adaptive time step δt

$$\delta t = \frac{\delta E}{\|\mu^n\|_h^2}. \tag{3.1}$$

(b) An adaptive time step: based on roughness (ATSBR)

The roughness changes according to the phase changes, and it is bounded by initial data. Thus, it is reasonable to consider using it to produce time steps.

The roughness, noted as $M(t)$, for the height function at t is defined as

$$M(t) = \sqrt{\frac{1}{|\Omega|}\int_\Omega (\phi(\mathbf{x},t) - \bar{\phi}(t))^2 d\mathbf{x}}, \text{ where } \bar{\phi}(t) = \frac{1}{|\Omega|}\int_\Omega \phi(\mathbf{x},t) d\mathbf{x}.$$

Since we have conservation law in both continuous form (2.1) and discrete form (2.7), and when the initial value is chosen to satisfy the $\bar{\phi}(t) = 0$, we have $|\Omega|M(t)^2 = \|\phi\|^2$ and the identity (2.8) can be viewed as the relationship between roughness and time steps.

From the discrete identity (2.8), with a slight transformation, it turns to

$$\Delta t = -\frac{\|\phi^{n+1}\|_h^2 - \|\phi^n\|_h^2}{\nu^{n+\frac{1}{2}}}, \tag{3.2}$$

where

$$\nu^{n+\frac{1}{2}} = \left(2\epsilon\|\Delta_h\phi^{n+\frac{1}{2}}\|_h^2 + \left(|\nabla_h\phi^n|^2 + |\nabla_h\phi^{n+1}|^2, |\nabla_h\phi^{n+\frac{1}{2}}|^2\right) - 2\|\nabla_h\phi^{n+\frac{1}{2}}\|_h^2\right). \tag{3.3}$$

Since the roughness is concerned here, we set a constant change constraint on $\|\phi\|_h^2$ by $\delta M = |\|\phi^{n+1}\|_h^2 - \|\phi^n\|_h^2|$, and replace the unknown term ϕ_h^{n+1} in (3.3) with ϕ_h^n to denote ν^n and form a second computable adaptive time step

$$\delta t = \frac{\delta M}{|\nu^n|} \tag{3.4}$$

where the absolute value is taken since the time step should be positive.

Based on the discussion, an adaptive time stepping algorithm on equidistribution of the energy decay or the roughness change is proposed as below. For the convenience, we use a triple $(W, \delta W, \gamma)$ in the algorithm

defined as $(W, \delta W, \gamma) := (E, \delta E, \mu)$ or $(M, \delta M, \nu)$.

Algorithm 3.1. (adaptive time-stepping algorithm)
1. Set Δt_{min} and Δt_{max}, compute the problem (2.5) with the minimal time step Δt_{min} for some step. Set δW as the average of the energy decay or the roughness change, and set $m, n = 1$.
2. At the time t_n, compute the time step with formula $\delta t = \frac{\delta W}{|\gamma^n|}$, and compute the problem (2.5) with time step $\Delta t = \min(\Delta t_{max}, \max(\delta t, \Delta t_{min}))$.
3. Check if energy decay or the roughness change between two step $\leq \delta W$ and $\Delta t = t_{min}$. If neither, return to 2 with time step $\Delta t = \min(t_{max}, \max(\frac{\Delta t}{2}, \Delta t_{min}))$.
4. If $\Delta t = \Delta t_{min}$, adjust δM with an arithmetic average

$$\delta W = \frac{m \times \delta W + \text{energy decay or the roughness change}}{m+1} \tag{3.5}$$

and set $m := m + 1$.
5. Set $t_{n+1} = t_n + \Delta t$, set $n := n + 1$ and go to 2.

Remark 3.1. The time step in **ATSBE** or **ATSBR** could have a similarly accurate mechanism to adjust result δt. When the phase changes fast which means the energy or the roughness changes fast, the methods can produce small time steps. When the phase change slows down, time steps turn to bigger.

Remark 3.2. It is noted that in roughness based adaptive method (3.4), only the first and second order derivatives are involved, compared to the higher order derivatives in the energy based one (3.1).

Remark 3.3. In the adaptive time-stepping strategy Algorithm 3.1, we *get rid of the artificial choice of the parameters*, except the $\Delta t_{\min}, \Delta t_{\max}$.

4. Numerical experiments

In this section, we implement two adaptive time-stepping methods for the MBE problem. The constant time steps are used to compute a comparable solution. The Newton iteration method is used to solve the nonlinear discrete system, and multigrid solver is used to solve the linear system that arises at each Newton iterative step. The tolerances for the Newton iteration method and for the multigrid method are set to be 10^{-9}.

Example. Consider the two-dimensional isotropic symmetry current model,

$$\begin{cases} \frac{\partial \phi}{\partial t} &= -\varepsilon \Delta^2 \phi - \nabla \cdot [(1 - |\nabla \phi|^2) \nabla \phi] \quad \text{in } [0, 2\pi]^2 \times (0, T), \\ \phi(\mathbf{x}, 0) &= \phi_0(\mathbf{x}) \qquad\qquad\qquad\qquad\quad \text{in } [0, 2\pi]^2, \end{cases} \tag{4.1}$$

with periodic boundary condition and parameter $\epsilon = 0.1$. The initial condition is $\phi_0(x) = 0.1(\sin 3x \sin 2y + \sin 5x \sin 5y)$ and $T = 30$.

This example is used in [3,4,13] to study the stability, energy decay, roughness evolution and adaptive time stepping. Here we also do detailed research on this problem to show the usability of our algorithm. Since the true solution is unknown, a numerical result obtained on a 200×200 grid and with a uniform time step $\delta t = 0.0001$ is served as the "true solution". For two adaptive time stepping methods, we use the average energy decay in the time interval $[0.05, 0.1]$ as δM and set $\Delta t_{\min} = 0.0001$.

The comparison of the phase pictures.

Some phase pictures on special timelines are shown in Fig. 1. The upper three are with uniform step ($\Delta t = 0.0001$) , the middle three are with **ATSBE** and the lower three are with **ATSBR** (both adaptive

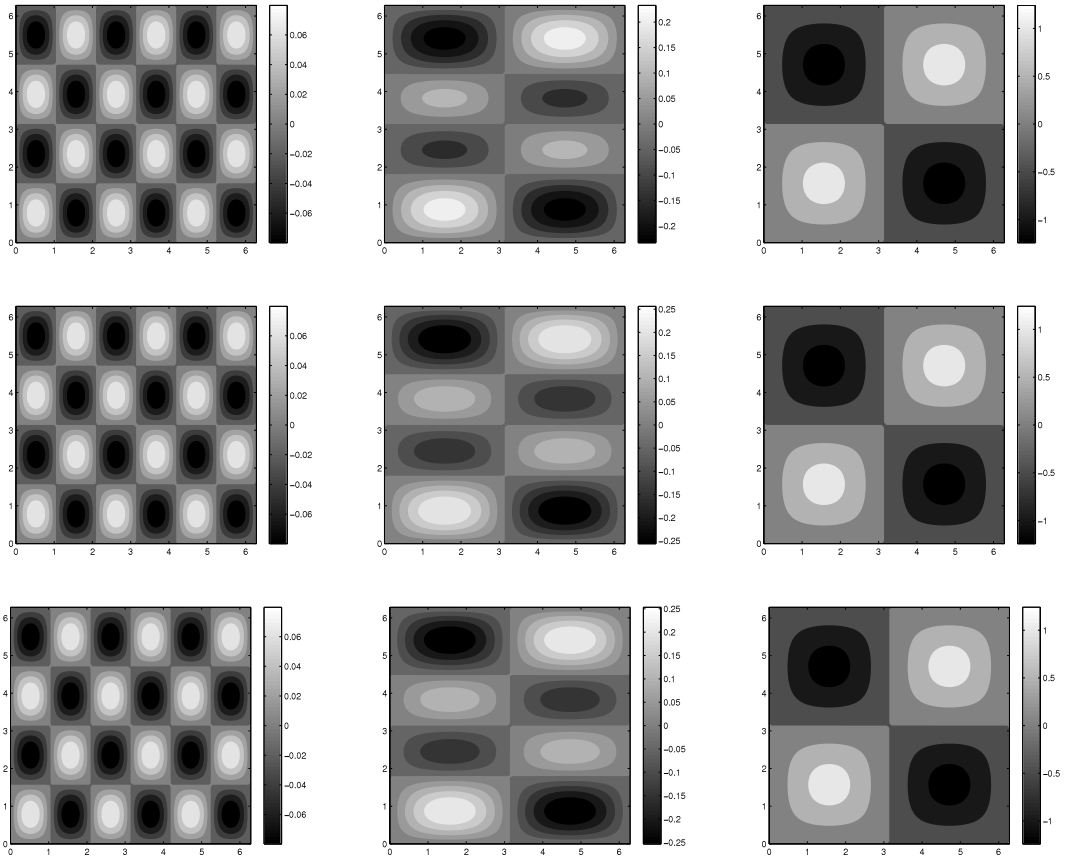

Fig. 1. Contour plots of height profiles: left to right, $t = 0.05s, t = 5.5s, t = 30s$; upper: with uniform Δt, middle: with **ATSBE**, bottom: with **ATSBR**.

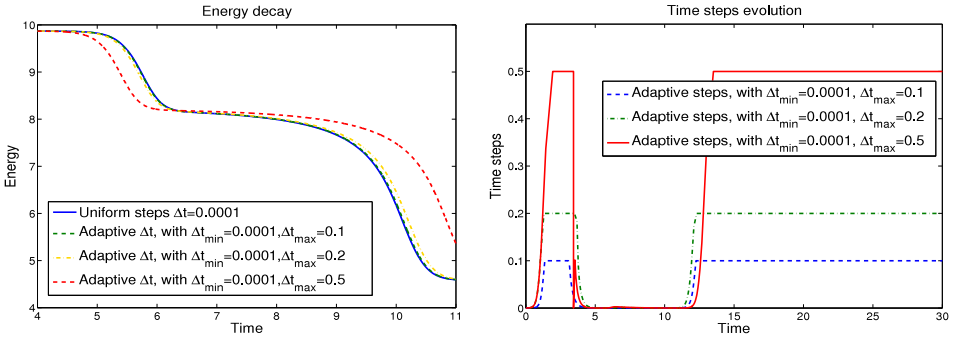

Fig. 2. ATSBE. Left: the energy evolution; Right: the Δt.

methods are with $\Delta t_{\min} = 0.0001, \Delta t_{\max} = 0.1$). From the pictures, we can see on every timeline the three look almost the same.

The evolution of M and the corresponding Δt. In order to show the sensitive of the adaptive method, we fix the $\Delta t_{\min} = 0.0001$, but use different $\Delta t_{\max} = 0.1, 0.2$ and 0.5. Fig. 2 shows the evolution of energy E, and the corresponding Δt of **ATSBE**, and Fig. 3 shows that of roughness M, and the corresponding Δt of **ATSBR**.

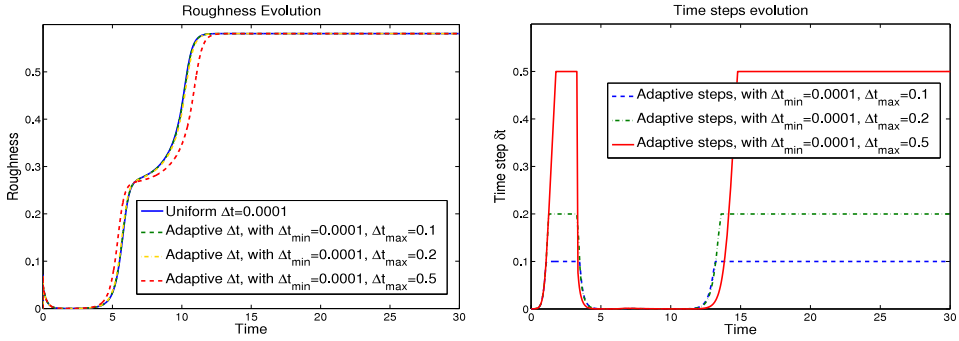

Fig. 3. ATSBR. Left: the roughness evolution; Right: the Δt.

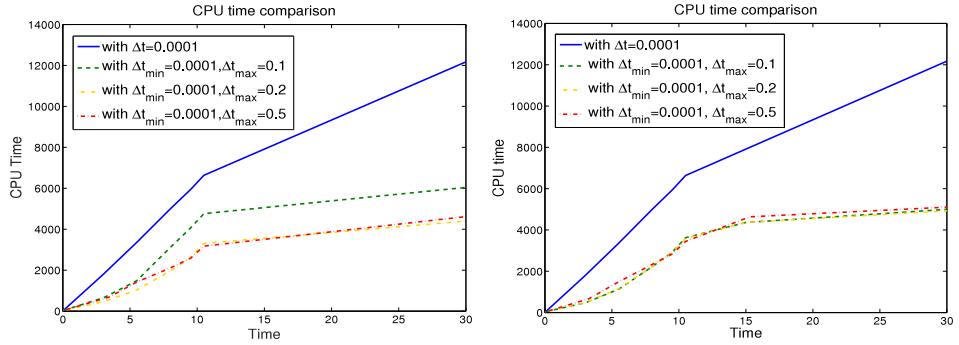

Fig. 4. The CPU time. Left: **ATSBE**; right: **ATSBR**.

The computational time. Finally, the CPU time is shown in Fig. 4, from which we can find both adaptive methods do actually save computational time and only take 1/3 to 1/2 of the time of the uniform method.

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