OPERATOR-SPLITTING METHODS RESPECTING EIGENVALUE PROBLEMS FOR CONVECTION-DIFFUSION AND WAVE EQUATIONS.

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Abstract.

We discuss iterative operator-splitting methods for convection-diffusion and wave equations motivated from the eigenvalue problem to decide the splitting process. The operator-splitting methods are well-know to solve such complicated multi-dimensional and multi-physical problems. Often the problem, how to decouple the underlying operators, is not understood well enough. We propose a method based on computing the eigenvalues for the simpler problem to decide the splitting operators and the time steps. We present the analysis and the numerical results.

Keywords: partial differential equations, operator-splitting methods, iterative methods, consistency analysis.

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1. Introduction. We are mitigated by simulating a three-dimensional wave equation for an anisotropic material with stress-free boundary conditions. The applications are suited in the earthquake simulation that is fundamental to seismic model problems, see [1], [3], and [10]. In this paper we discuss the efficiency of a higher-order time-discretization method that is based on an iterative operator-splitting method. The main contributions are the scale decoupling based on the eigenvalue problem. We propose an algorithm to compute such pre-eigenvalues for the scale separations. To apply the scale separations we have to discuss a Runge-Kutta method as a higher-order time-discretization to approximate the coarser scales into the finer scales. The efficiency of different time scales due to each operator allows improved simulation times. We verify our numerical methods with computational results based on our software tool OPERA - SPLITT. We present 2D wave equations with different higher-order splitting ideas. Finally we discuss the next works.

The paper is organized as follows. A mathematical model based on the wave equations is introduced in Section 2. The discretization methods are explained in Section 3. The decomposition method as an iterative operator-splitting method is presented in Section 4. In Section 5, the error estimates are discussed. The decoupling method based on the eigenvalue problems is discussed in Section 6. We introduce the numerical results in Section 7. Finally we discuss our future works in the area of splitting and decomposition methods.

2. Mathematical model. The motivation to our model problem comes from the earthquake simulations done with an elastic wave propagation. We concentrate on the simpler wave equations, which represent the propagation of linear waves. Due to this motivation we analyze the following model problem:

$$\partial_{tt}c(t) = D_1(c, x, y, t)\partial_{xx}c(x, y, t) + D_2(c, x, y, t)\partial_{yy}c(x, y, t), \text{ in } \Omega \times (0, T), \quad (2.1)$$

 $c(x, y, 0) = c_0(x, y), c'(x, y, 0) = c_1(x, y), \text{ on } \Omega,$ (2.2)

$$c(x, y, t) = c_2(x, y, t), \text{ on } \partial\Omega \times (0, T),$$

$$(2.3)$$

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where the initial functions $c_0(x, y)$ and $c_1(x, y)$ and the Dirichlet boundary condition $c_2(x, y, t)$ are given. We deal with nonlinear diffusion operators D_1 and D_2 with sufficient smoothness.

The simulation of such models is studied in [2], [3]. We propose the decomposition with respect to its spatial directions to obtain efficient methods, which take into account the different time scales of the operators. In such a case the discretization methods might be adapted to the decomposition methods. Our contributions can be found in the following sections.

3. Discretization methods for the wave equation. For the time- and spacediscretization we first underly finite difference schemes for the discretization.

For a classical wave equation we treat the well-known discretization in time and space.

Based on this discretization, the time is discretized as:

$$U_{tt,i} = \frac{U_i^{n+1} - 2U_i^n + U_i^{n-1}}{\Delta t^2},$$
(3.1)

$$U(0) = u_0, U_t(0) = u_1, (3.2)$$

where *i* is the space point x_i and $\Delta t = t^{n+1} - t^n$ is the time step.

The space is discretized as:

$$U_{xx,n} = \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{\Lambda r^2},$$
(3.3)

$$U(0) = u_0, U_t(0) = u_1, (3.4)$$

where n is the time point t_n and $\Delta x = x_{i+1} - x_i$ is the grid width.

The underlying equation,

$$u_{tt} = D_1 u_{xx} + D_2 u_{yy} \text{ in } \Omega, \qquad (3.5)$$

$$u(x, y, 0) = u_0(x, y), u_t(x, y, 0) = u_1(x, y),$$
(3.6)

$$u(x, y, t) = u_2 \text{ on } \partial\Omega, \tag{3.7}$$

is discretized with the unconditional stable implicit η -method, see [4].

For the scale-dependent cases we propose explicit Runge-Kutta methods for the coarser scales to approximate the intermediate values.

The second-order differential equation is transformed into a system of first-order derivatives:

$$u_1' = u_2 , u_1(x_0) = c_0, (3.8)$$

$$u_2' = (A+B)u_1, u_2(x_0) = c_1.$$
(3.9)

The explicit Runge-Kutta method is given as

or with the 3/8-rule as 4th-order RK method:

4. Iterative operator-splitting methods for wave equations. In the following we present the iterative operator-splitting method as an extension of the traditional splitting method for wave equations.

We deal with the second-order Cauchy problem, derived from applying a semidiscretization in space with our finite difference methods. We concentrate on the abstract equation

$$\frac{d^2 c(t)}{dt^2} = (A+B) \ c(t), \text{ for } t \in [0,T],$$
(4.1)

where the initial conditions are $c_0 = c(0)$ and $c_1 = \frac{dc}{dt}(0)$. The operators A, B are a matrices given with rank(A) = rank(B) = m, and we assume them to be bounded operators.

The idea is to repeat the splitting steps with the improved computed solutions. At least we have to solve a fixed-point iteration and we obtain higher-order results. The iterative splitting method is given as

$$\frac{d^{2}c_{i}(t)}{dt^{2}} = Ac_{i}(t) + Bc_{i-1}(t) + f(t), \quad t \in [t^{n}, t^{n+1}],$$
with $c_{i}(t^{n}) = c_{\rm sp}^{n}, \quad \frac{dc_{i}(t^{n})}{dt} = \frac{dc_{\rm sp}^{n}}{dt},$

$$\frac{d^{2}c_{i+1}(t)}{dt^{2}} = Ac_{i}(t) + Bc_{i+1}(t) + f(t), \quad t \in [t^{n}, t^{n+1}],$$
with $c_{i+1}(t^{n}) = c_{\rm sp}^{n}, \quad \frac{dc_{i+1}(t^{n})}{dt} = \frac{dc_{\rm sp}^{n}}{dt},$
(4.2)

for $i = 1, 3, 5, \ldots, 2m + 1$, where $c_0(t), \frac{dc_0(t)}{dt}$ are fixed functions for each iteration. (Here, as before, $c_{\rm sp}^n, \frac{dc_{\rm sp}^n}{dt}$ denote known split approximations at the time level $t = t^n$.) The time step is given as $\tau = t^{n+1} - t^n$. The split approximation at the time level $t = t^{n+1}$ is $c_{\rm sp}^{n+1} = c_{2m+2}(t^{n+1})$. For the discrete version of the iterative operator-splitting method, we apply the

second-order discretization of the time derivations and obtain:

$$c_{i} - 2c(t^{n}) + c(t^{n-1}) = \tau_{n}^{2}A(\eta c_{i} + (1 - 2\eta)c(t^{n}) + \eta c(t^{n-1}))$$

$$+ \tau_{n}^{2}B(\eta c_{i-1} + (1 - 2\eta)c(t^{n}) + \eta c(t^{n-1}))$$

$$+ \tau_{n}^{2}(\eta f(t^{n+1}) + (1 - 2\eta)f(t^{n}) + \eta f(t^{n-1})),$$

$$c_{i+1} - 2c(t^{n}) + c(t^{n-1}) = \tau_{n}^{2}A(\eta c_{i} + (1 - 2\eta)c(t^{n}) + \eta c(t^{n-1}))$$

$$+ \tau_{n}^{2}B(\eta c_{i+1} + (1 - 2\eta)c(t^{n}) + \eta c(t^{n-1}))$$

$$+ \tau_{n}^{2}(\eta f(t^{n+1}) + (1 - 2\eta)f(t^{n}) + \eta f(t^{n-1})),$$

$$(4.4)$$

where we iterate for i = 1, 3, 5, ... and the starting solutions $c_0(t), \frac{dc_0(t)}{dt}$ are any fixed functions for each iteration, for example $c_0(t) = \frac{dc_0(t)}{dt} = 0$. The result is given as

 $c(t^{n+1})$ with the initial conditions $c(t^n) = c_{sp}^n$ and $\frac{dc(t^n)}{dt} = \frac{dc_{sp}^n}{dt}$, and $\eta \in [0, 0.5]$, using the fully coupled method for $\eta = 0$ or the decoupled method for $0 < \eta \le 0.5$, which is a mixing of explicit and implicit Euler methods.

The stop criteria is given as

 $|c_{\tilde{i}+2} - c_{\tilde{i}}| \le \epsilon,$

where $\tilde{i} \in 1, 3, 5, \ldots \epsilon \in \mathbb{R}^+$.

Therefore the solution is given as $c(t^{n+1}) = c_{\tilde{i}+2}$.

The consistency result is given in the following Theorem 4.1.

THEOREM 4.1. Let $A, B \in \mathcal{L}(\mathcal{X})$ be given linear bounded operators. Then the abstract Cauchy problem (4.1) has a unique solution and the iterative splitting method (4.2)–(4.2) with i = 1, 3, ..., 2m + 1 is consistent with the order of the consistency $\mathcal{O}(\tau_n^{2m})$.

The error estimate is given as:

$$||e_i|| = K||B||\tau_n||e_{i-1}|| + \mathcal{O}(\tau_n^2),$$
(4.6)

where $e_i = \max\{|e_{1,i}|, |e_{i,2}|\}.$

Proof. The proof is outlined in [9]. \Box

In the next section we discuss the strategies to compute the efficient starting vector.

5. Error estimates. For the error estimates we derive the *a priori* and *a posteriori error* estimates with respect to the iterative solutions.

The a priori error estimate is given as:

THEOREM 5.1. Let $A, B \in \mathcal{L}(\mathcal{X})$ be given linear bounded operators. Then the abstract Cauchy problem (4.1) has a unique solution and the iterative splitting method (4.2)–(4.2) with i = 1, 3, ..., 2m + 1 is consistent with the order of the consistency $\mathcal{O}(\tau_n^{2m})$.

The error estimate is given as:

$$\|u_i(t^{n+1}) - u_{i-1}(t^{n+1})\| = \frac{1}{i!}\tau^i \lambda^i_{A+B,1} u(t^n),$$
(5.1)

where $i = 1, 3, \ldots, 2m + 1$.

Proof. By starting with $u_0(t^{n+1}) = 0$ as initialization of our iterative method we can derive the iterative solutions as

$$u_i(t^{n+1}) = \left(\sum_{j=0}^i \frac{1}{j!} \tau^j (A+B)^j\right) u(t^n),$$
(5.2)

where i = 1, 3, ..., 2m + 1 and $u(t^n)$ is the solution at t^n . The time step is given as τ , see also [5].

Therefore we can calculate the error estimate as

$$u_{i}(t^{n+1}) - u_{i-1}(t^{n+1}) = \left(\sum_{j=0}^{i} \frac{1}{j!} \tau^{j} (A+B)^{j}\right) u(t^{n}) - \left(\sum_{j=0}^{i-1} \frac{1}{j!} \tau^{j} (A+B)^{j}\right) u(t^{n}),$$

$$= \frac{1}{i!} \tau^{i} (A+B)^{i} u(t^{n}),$$
(5.3)

where we assume an equidistant time step τ and the exact initial condition $u(t^n)$.

If we assume the diagonalization of the operators to the eigenvalues λ_A and λ_B , the error estimate is given as

$$\|u_i(t^{n+1}) - u_{i-1}(t^{n+1})\| = \frac{1}{i!}\tau^i \lambda^i_{A+B,1} u(t^n),$$
(5.4)

where $\lambda_{A+B,1}$ is the maximal eigenvalue for the operator A+B.

REMARK 5.1. The a priori error estimate is dominated by the maximal eigenvalues of A and B. With more iterations we can take control of the eigenvalues, because we can decrease the error. So the balance between the time step, which is given as τ , and the number of iterations i is important to control the error of the underlying methods.

The a posteriori error estimate is discussed in the following theorem.

THEOREM 5.2. Let $A, B \in \mathcal{L}(\mathcal{X})$ be given linear bounded operators. Then the abstract Cauchy problem (4.1) has a unique solution and the iterative splitting method (4.2)–(4.2) with i = 1, 3, ..., 2m + 1 is consistent with the order of the consistency $\mathcal{O}(\tau_n^{2m})$.

The error estimate is given as:

$$\|u_i(t^{n+1}) - u_{i-1}(t^{n+1})\| \le \|u_{i-1}(t^{n+1}) - u_{i-2}(t^{n+1})\|, \frac{1}{i}\tau\lambda_{A+B,1}\epsilon_i \le \epsilon_{i-1}, \quad (5.5)$$

where $i = 1, 3, \ldots, 2m + 1$.

Proof. We also start with $u_0(t^{n+1}) = 0$ as initialization of our iterative method and obtain the iterative solution as

$$u_i(t^{n+1}) = \left(\sum_{j=0}^i \frac{1}{j!} \tau^j (A+B)^j\right) u(t^n),$$
(5.6)

where i = 1, 3, ..., 2m + 1 and $u(t^n)$ is the solution at t^n . The time step is given as τ , see also [5].

We assume the diagonalization of the operators to the eigenvalues λ_A and λ_B . So we can derive the error estimate as

$$u_i(t^{n+1}) - u_{i-1}(t^{n+1})| \le |u_{i-1}(t^{n+1}) - u_{i-2}(t^{n+1})|, \tag{5.7}$$

$$\left|\frac{1}{i!}\tau^{i}\lambda_{A+B,1}^{i}u(t^{n})\right| \leq \left|\frac{1}{(i-1)!}\tau^{i-1}\lambda_{A+B,1}^{i-1}u(t^{n})\right|,\tag{5.8}$$

$$\frac{1}{i}\tau\lambda_{A+B,1} \le 1,\tag{5.9}$$

where we assume an equidistant time step τ and the exact initial condition $u(t^n)$. $\lambda_{A+B,1}$ is the maximal eigenvalue for the operator A+B.

Therefore the error reduction between two iterations is given as

$$\frac{1}{i}\tau\lambda_{A+B,1}\epsilon_i \le \epsilon_{i-1},\tag{5.10}$$

where $\epsilon_i = u_i(t^{n+1}) - u_{i-1}(t^{n+1})$ and $\epsilon_{i-1} = u_{i-1}(t^{n+1}) - u_{i-2}(t^{n+1})$.

6. DECOUPLING IDEAS BASED ON EIGENVALUE PROBLEMS

REMARK 5.2. The a posteriori error estimate is given by the maximal eigenvalues of A and B and also by the underlying iterations and time steps. The stability condition is given with $\frac{1}{i}\tau\lambda_{A+B,1} \leq 1$. Thus more iterations stabilize the scheme. A balancing between time steps and iterations can be done to optimize the computational time.

6. Decoupling ideas based on eigenvalue problems. To detect the operators in the differential equation as stiff or non-stiff operators, we can apply the eigenvalues of each operator and use them as reciprocal time scales.

The operator equations are analyzed with the eigenvalue problem:

$$\partial_{tt}c(t) = (A+B)c(t) = (\lambda_A + \lambda_B)c(t), \ t \in (t^n, t^{n+1}), \qquad (6.1)$$
$$c(t^n) = g(t), \ c'(t^n) = f(t),$$

where the operators A and B result form the spatial discretization.

The eigenvalues are detected in the decoupled equations:

$$\partial_{tt}c(t) = Ac(t) = \lambda_A c(t), \ t \in (t^n, t^{n+1}), \ c(t^n) = g(t), \ c'(t^n) = f(t),$$
(6.2)

$$\partial_{tt}c(t) = Bc(t) = \lambda_B c(t), \ t \in (t^n, t^{n+1}), \ c(t^n) = g(t), \ c'(t^n) = f(t).$$
(6.3)

Based on the eigenvalues λ_A , λ_B we can propose the time steps $\Delta t_A \approx 1/\lambda_A$ and $\Delta t_B \approx 1/\lambda_B$.

We propose the vector iteration based on the Rayleigh quotient for the computation of the eigenvalues of the operators A and B:

$$Ac_{i+1,k} = c_{i+1,k+1}, (6.4)$$

$$Bc_{i+1,m} = c_{i+1,m+1}, (6.5)$$

where k, m = 0, 1, 2, ... and the eigenvalues are given as

$$\frac{c_{i+1,k+1}}{c_{i+1,k}} = |\lambda_{A,1}| + \mathcal{O}(p^k), \tag{6.6}$$

$$\frac{c_{i+1,m+1}}{c_{i+1,m}} = |\lambda_{B,1}| + \mathcal{O}(q^m), \tag{6.7}$$

where $\lambda_{A,1}$ and $\lambda_{B,1}$ are the maximal eigenvalues. The values are given as $p = \frac{\lambda_{A,2}}{\lambda_{A,1}}$ with $\lambda_{A,1} \ge \lambda_{A,2} \ldots \ge \lambda_{A,n}$, $q = \frac{\lambda_{B,2}}{\lambda_{B,1}}$ with $\lambda_{B,1} \ge \lambda_{B,2} \ldots \ge \lambda_{B,n}$. The following algorithm is used for separating the different scales of the operators

The following algorithm is used for separating the different scales of the operators A and B:

Algorithm 6.1.

- 1) We have the operators A, B.
- 2) We compute pre-eigenvalues with a given norm $|| \cdot ||$: ||Au||, ||Bu||,
- where u is a possible solution vector of the equations (4.4)-(4.5). 3) We compare the pre-eigenvalues:
- $||Au|| \le ||Bu||: A \text{ is stiff,}$ or $||Au|| \ge ||Bu||: B \text{ is stiff.}$
- 4) We initialize our splitting method.

REMARK 6.2. The efficiency of the method is given with the correct decomposition, which means the correct ordering of the underlying operators. With respect to the local error, the starting operator B in the first iterative equation dominates the error. Therefore the pre-processing to obtain the underlying eigenvalues is important and accelerates the solver process. Here we propose the vector iterations to compute the eigenvalues as a method that is embedded to our iterative splitting method. The declaration of the operators to be stiff or non-stiff results in the correct splitting operators.

In the next section we apply our theoretical results to a test example with respect to correct or incorrect decompositions.

7. Numerical examples of the splitting methods with respect to the eigenvalues of the operators. We discuss in the following the linear and nonlinear operator equations with respect to the approximation error and the computational benefits.

We deal with a two-dimensional example, where we can derive an analytical solution.

$$\partial_{tt}u = D_1^2 \partial_{xx}u + D_2^2 \partial_{yy}u, \tag{7.1}$$

$$c(x, y, 0) = c_0(x, y) = \sin(\frac{1}{D_1}\pi x)\sin(\frac{1}{D_2}\pi y), \ \partial_t c(x, y, 0) = c_1(x, y) = 0, \quad (7.2)$$

with
$$c(x, y, t) = 0$$
, $\operatorname{on}\partial\Omega \times (0, T)$, (7.3)

where $\Omega = [0, 1] \times [0, 1]$, $D_1 = 1$, $D_2 = 0.5$, and the initial conditions can be written as $c(x, y, t^n) = c_0(x, y)$ and $c(x, y, t^{n-1}) = c(x, y, t^{n+1}) = c(x, y, \Delta t)$.

The analytical solution is given as

$$u_{\text{analy}}(x, y, t) = \sin(\frac{1}{D_1}\pi x)\sin(\frac{1}{D_2}\pi y)\cos(\sqrt{2}\pi t).$$
(7.4)

The discretization is given with the implicit time-discretization and the finite difference method for the space-discretization.

Therefore have for the space-discretization:

$$Au(t) = D_1^2 \partial_{xx} u(t) \approx D_1^2 \, \frac{u(x + \Delta x, y, t) - 2u(x, y, t) + u(x - \Delta x, y, t)}{\Delta x^2}, \quad (7.5)$$

$$Bu(t) = D_2^2 \partial_{yy} u(t) \approx D_2^2 \, \frac{u(x, y + \Delta y, t) - 2u(x, y, t) + u(x, y - \Delta y, t)}{\Delta y^2}, \quad (7.6)$$

and the time-discretization is given as:

$$\partial_{tt}u \approx \frac{u(t+\Delta t) - 2u(t) + u(t-\Delta t)}{\Delta t^2}.$$
 (7.7)

The implicit discretization is given as:

$$u(t^{n+1}) - 2u(t^n) + u(t^{n-1}) = \Delta t^2 (A + B)(\eta u(t^{n+1}) + (1 - 2\eta)u(t^n) + \eta u(t^{n-1})).$$

For the approximation error we choose the L_1 -norm. The L_1 -norm is given as

$$err_{L_1} := \sum_{i,j=1,\dots,m} V_{i,j} |u_{\text{num}}(x_i, y_j, t^n) - u_{\text{exact}}(x_i, y_j, t^n)|,$$
(7.9)

where $u(x_i, y_j, t^n)$ is the numerical and $u_{\text{analy}}(x_i, y_j, t^n)$ is the analytical solution, $V_{i,j} = \Delta x \Delta y.$

The model domain is given by an rectangle with $\Delta x = 1/16$ and $\Delta y = 1/32$. The time steps are given with $\Delta t = 1/16$, and we have $0 \le \eta \le 0.5$.

The eigenvalue problem is given as:

$$D_1^2 D_{xx} U = \Lambda_A U, \tag{7.10}$$

$$D_2^2 D_{yy} U = \Lambda_B U, \tag{7.11}$$

where $U = u_1, \ldots, u_n$, with *n* grid points, $D_{xx}U$ is the space-discretization of u_{xx} , $D_{yy}U$ is the space-discretization of u_{yy} , $\Lambda_A = diag(\lambda_{A_i})_{i=1,\ldots,n}$ contains the eigenvalues of the operator A and $\Lambda_B = diag(\lambda_{B_i})_{i=1,\ldots,n}$ contains the eigenvalues of the operator B.

We computed the underlying problem with the following values for the equation: $\Omega = [0,1] \times [0,1], D_1 = 1, D_2 = 0.5$, and the initial conditions $c(x, y, t^n) = c_0(x, y)$ and $c(x, y, t^{n-1}) = c(x, y, t^{n+1}) = c(x, y, \Delta t)$.

The computational results for the correct decomposition are given in Table 7.1.

D_1	D_2	$\operatorname{err} = u_{\operatorname{exact}} - u_{\operatorname{num}} $	$ \partial_{yy}u_{\mathrm{exact}} - \partial_{yy}u_{\mathrm{num}} $	
4.0	0.01	$1.878 \cdot 10^{-3}$	$1.8504 \cdot 10^{-4}$	
4.0	0.0001	$1.878 \cdot 10^{-3}$	$1.8502 \cdot 10^{-6}$	
TABLE 7.1				

Numerical results for the iterative splitting method with correct decomposition.

The computational results for the incorrect decomposition, while neglecting the eigenvalues of the operator, are given in Table 7.2.

D_1	D_2	$\operatorname{err} = u_{\operatorname{exact}} - u_{\operatorname{num}} $	$\left \partial_{yy}u_{\mathrm{exact}}-\partial_{yy}u_{\mathrm{num}}\right $	
0.01	1.0	$2.074 \cdot 10^{-1}$	$2.0433 \cdot 10^{0}$	
0.0001	1.0	$1.843 \cdot 10^{-1}$	$1.818 \cdot 10^{0}$	
TABLE 7.2				

Numerical results for the iterative splitting method with incorrect decomposition.

The visualization of the numerical results for the correct decomposition is shown in Figures 7.1 and 7.2.

8. Conclusions and discussions. We present an iterative operator-splitting method to solve partial differential equations with respect to their underlying time scales. The correct splitting into the underlying operators of the equations is important to reduce the splitting error and contribute an efficient method. Therefore we present an embedded eigenvalue solver. First numerical results can validate the correct splitting and the efficiency. In future it will be important to have efficient eigenvalue methods, which can be embedded into the splitting methods, to contribute the operator-splitting methods as efficient solver methods for large evolution equations.

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FIG. 7.1. Results for the iterative splitting method with RK method and parameters $D_1 = 4.0$, $D_2 = 0.01$.

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FIG. 7.2. Results for the iterative splitting method with RK method and parameters $D_1 = 4.0$, $D_2 = 0.0001$.

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