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Numerical Analysis

Transparent boundary conditions for a class of boundary value problems in some ramified domains with a fractal boundary ☆

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Abstract

We consider some boundary value problems in self-similar ramified domains, with Laplace and Helmholtz equations. We discuss transparent boundary conditions. These conditions permit computing the restriction of the solutions to domains obtained by stopping the geometric construction after a finite number of steps. ***To cite this article: Y. Achdou et al., C. R. Acad. Sci. Paris, Ser. I 342 (2006).***

Résumé

Conditions aux limites transparentes pour des problèmes aux limites dans des domaines ramifiés à frontière fractale. On considère une classe de problèmes aux limites dans des domaines autosimilaires ramifiés, avec des équations de Laplace ou d'Helmholtz. On s'intéresse à l'obtention de conditions aux limites transparentes, permettant le calcul de la solution dans un domaine obtenu en arrêtant la construction après un nombre fini d'étapes. ***Pour citer cet article : Y. Achdou et al., C. R. Acad. Sci. Paris, Ser. I 342 (2006).***

Version française abrégée

Dans cette Note, on considère une classe de problèmes aux limites avec les équations de Laplace ou de Helmholtz dans un domaine auto-similaire ramifié de $\mathbb{R}^2$. Cette étude entre dans le cadre d'un projet sur la diffusion des aérosols médicaux dans les poumons, voir [3]. Le but de cette note est de donner un cadre fonctionnel rigoureux et surtout de montrer qu'on peut calculer la restriction des solutions aux domaines obtenus en arrêtant la construction géométrique après un nombre fini d'étapes. Pour cela, on doit utiliser des *conditions aux limites transparentes* mettant en jeu des opérateurs non locaux du type Dirichlet–Neumann.

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Le domaine est construit à partir d'un motif de base Y^0 et de deux transformations affines F_1 et F_2 donnés par (1). Pour $n \geqslant 1$, soit $\mathcal{A}_n$ l'ensemble des 2^n applications de $\{1, \ldots, n\}$ dans $\{1, 2\}$. Pour $\sigma \in \mathcal{A}_n$, on définit l'application affine $\mathcal{M}_\sigma(F_1, F_2)$ par (2). Le domaine Ω^0 est construit dans (3) en assemblant les domaines Y^0 et $\mathcal{M}_\sigma(F_1, F_2)(Y^0)$, $\sigma \in \mathcal{A}_n, n \geqslant 1$, voir Fig. 1. Sa frontière est décrite par (4). On appelle Y^N le domaine obtenu en arrêtant la construction de Ω^0 à la $N+1$-ème étape, voir (5), et $\Omega^\sigma = \mathcal{M}_\sigma(F_1, F_2)(\Omega^0)$.

On introduit l'espace de Sobolev $H^1(\Omega^0)$ des fonctions de carré sommable dans Ω^0 dont les dérivées partielles sont de carré sommable. On montre l'inégalité de Poincaré (6), et la compacité de l'injection de $H^1(\Omega^0)$ dans $L^2(\Omega^0)$. Pour $u \in H^{1/2}(\Gamma^0)$, on cherche d'abord $\mathcal{H}(u)$, solution du problème de Poisson (7), avec une condition de Neumann homogène généralisée sur Γ^∞. La forme variationelle (8) du problème est bien posée. L'autosimilarité implique l'estimation (9), qui dit que la contribution de $\Omega^0 \setminus Y^{p-1}$ à l'énergie de $\mathcal{H}(u)$ décroît exponentiellement avec p quand $p \to \infty$. La Proposition 3.4 dit que $\mathcal{H}(u)|_{Y^{n-1}}$ peut être calculé en résolvant successivement $1 + \cdots + 2^{n-1}$ problèmes aux limites dans Y^0 avec les conditions aux limites non locales (13) sur $F_1(\Gamma^0)$ et $F_2(\Gamma^0)$, appelées *conditions aux limites transparentes*, et mettant en jeu l'opérateur de Dirichet–Neumann T défini par (10). De plus, on montre que T est l'unique point fixe d'une application $\mathbb{M}$ définie par (14), et que T peut être approché par des itérations de point fixe de $\mathbb{M}$, avec l'estimation d'erreur (15). On aboutit donc à un programme complet pour calculer $\mathcal{H}(u)|_{Y^{n-1}}$.

On suit le même programme pour l'équation de Helmholtz (17). On peut introduire les conditions aux limites transparentes (20) permettant de calculer la restriction de la solution à Y^0 (ou Y^n), voir Proposition 4.2. On utilise de manière cruciale l'autosimilarité géométrique pour calculer les opérateurs de Dirichlet–Neumann. La construction, qui peut être utilisée pour des simulations numériques (voir [2]), n'est pas aussi simple que pour l'équation de Laplace, car l'équation de Helmholtz n'est pas invariante par changement d'échelle : les effets diffusifs deviennent de plus en plus importants dans les petites structures du domaine ramifié, et l'onde est amortie exponentiellement. C'est précisément ce qui rend possible l'approximation des opérateurs de Dirichlet–Neumann par une formule de récurrence. La méthode est esquissée dans la fin de la note (voir [1] pour l'algorithme complet, ainsi que pour une estimation d'erreur). Le programme proposé a été appliqué numériquement avec succès, voir [2]. Les preuves des résultats annoncés dans cette Note sont contenues dans [1].

1. Introduction

In this Note, we deal with a class of boundary value problems in a ramified self-similar domain of $\mathbb{R}^2$ with a fractal boundary. This work was motivated by a challenging project aiming at simulating the diffusion of medical sprays in the lungs, (see [3]). Here, the geometry of the problems (two dimensions only) and the underlying physical phenomena are much simpler. The first goal is to study a class of boundary value problems with Laplace or Helmholtz equations. The second goal is to propose a method for computing the solutions in subdomains obtained by stopping the fractal's construction after a finite number of steps. This is important, because, in numerical simulations, it is not possible to represent the whole domain, for this would require infinite memory and computing time. The abovementioned method involves new boundary value problems with nonlocal boundary conditions, see (13) and (20) below. These will be called *transparent boundary conditions*, because they permit computing the solutions in subdomains without error. Transparent boundary conditions were originally proposed for linear partial differential equations in unbounded domains, see e.g. [5]. In the present context, the nonlocal operators involved in the transparent conditions can be computed, more precisely approximated up to an arbitrary accuracy, by taking advantage of the self-similarity in the geometry, see Theorem 3.5 below and [1] for Helmholtz equation.

The method developed here is reminiscent of some of the techniques involved in the theoretical analysis of ramified fractals (see [10,9]). For PDEs in domains with fractal boundaries, see [8,6]. The content of this note can be generalized to other geometries (for example, the Koch flake), and equations (for example, $\mathrm{div}(\kappa \nabla \mathrm{u}) = 0$, where κ is a suitable constant tensor). The results below are proved in [1] and the discrete counterparts of the methods have been successfully implemented in [2].

2. The geometry

Let Y^0 and F_i, $i = 1, 2$, be respectively the T-shaped subset of $\mathbb{R}^2$ and the affine maps defined by:

$$Y^0 = \mathrm{Interior}\big(\big([-1,1] \times [0,2]\big) \cup \big([-2,2] \times [2,3]\big)\big), \qquad F_i(x) = \left((-1)^i \frac{3}{2} + \frac{x_1}{2}, 3 + \frac{x_2}{2}\right), \quad i = 1, 2. \tag{1}$$

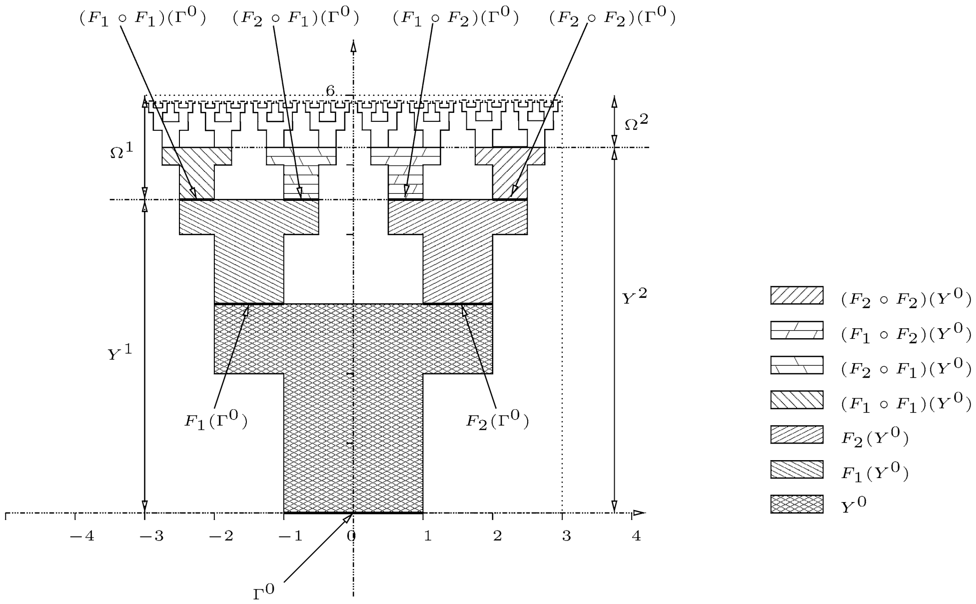

Fig. 1. The ramified domain Ω^0 (only a few generations are displayed).

Fig. 1. Le domaine Ω^0.

For $n \geqslant 1$, we call $\mathcal{A}_n$ the set containing all the 2^n mappings from $\{1, \dots, n\}$ to $\{1, 2\}$. We define

$$\mathcal{M}_\sigma(F_1, F_2) = F_{\sigma(1)} \circ \cdots \circ F_{\sigma(n)} \quad \text{for } \sigma \in \mathcal{A}_n, \tag{2}$$

and the ramified open domain, see Fig. 1,

$$\Omega^0 = \text{Interior}\left(\overline{Y^0} \cup \left(\bigcup_{n=1}^{\infty} \bigcup_{\sigma \in \mathcal{A}_n} \mathcal{M}_\sigma(F_1, F_2)\big(\overline{Y^0}\big)\right)\right). \tag{3}$$

It is important to observe that Ω^0 is not an (ϵ, δ) domain, see e.g. [4,7]. Thus, some usual results on Sobolev spaces may not hold (see [1]).

We split the boundary of Ω^0 into

$$\Gamma^0 = [-1, 1] \times \{0\}, \quad \Gamma^\infty = [-3, 3] \times \{6\}, \quad \text{and} \quad \Sigma^0 = \partial\Omega^0 \setminus \big(\Gamma^0 \cup \Gamma^\infty\big). \tag{4}$$

For what follows, it is important to define the translated/dilated copies Ω^σ ($\sigma \in \mathcal{A}_n$, $n > 0$) of Ω^0 and the polygonal open domain Y^N obtained by stopping the above construction at step $N + 1$,

$$\Omega^\sigma = \mathcal{M}_\sigma(F_1, F_2)\big(\Omega^0\big), \quad \text{and} \quad Y^N = \text{Interior}\left(\overline{Y^0} \cup \left(\bigcup_{n=1}^{N} \bigcup_{\sigma \in \mathcal{A}_n} \mathcal{M}_\sigma(F_1 F_2)\big(\overline{Y^0}\big)\right)\right). \tag{5}$$

We have $Y^N = \Omega^0 \setminus (\bigcup_{\sigma \in \mathcal{A}_{N+1}} \overline{\Omega^\sigma})$. We also define the sets $\Gamma^\sigma = \mathcal{M}_\sigma(F_1, F_2)(\Gamma^0)$, and $\Gamma^N = \bigcup_{\sigma \in \mathcal{A}_N} \Gamma^\sigma$.

3. A class of Poisson problems and transparent boundary conditions

Let $H^1(\Omega^0)$ be the space of functions in $L^2(\Omega^0)$ with first order partial derivatives in $L^2(\Omega^0)$.

Theorem 3.1. *There exists a constant $C > 0$, such that*

$$\forall u \in H^1\big(\Omega^0\big), \quad \|u\|^2_{L^2(\Omega^0)} \leqslant C\big(\|\nabla u\|^2_{L^2(\Omega^0)} + \|u|_{\Gamma^0}\|^2_{L^2(\Gamma^0)}\big). \tag{6}$$

The imbedding of $H^1(\Omega^0)$ in $L^2(\Omega^0)$ is compact.

We are interested in the boundary value problem: for $u \in H^{1/2}(\Gamma^0)$, find $\mathcal{H}(u) \in H^1(\Omega^0)$ such that

$$\Delta \mathcal{H}(u) = 0 \quad \text{in } \Omega^0, \qquad \mathcal{H}(u)|_{\Gamma^0} = u, \qquad \frac{\partial \mathcal{H}(u)}{\partial n} = 0 \quad \text{on } \Sigma^0, \tag{7}$$

with an additional generalized homogeneous Neumann condition on Γ^∞, (see (8) below). Defining $\mathcal{V}(\Omega^0) = \{v \in H^1(\Omega^0);\ v|_{\Gamma^0} = 0\}$, the variational problem is to seek $\mathcal{H}(u) \in H^1(\Omega^0)$, s.t.:

$$\mathcal{H}(u)|_{\Gamma^0} = u, \quad \text{and} \quad \int_{\Omega^0} \nabla \mathcal{H}(u) \cdot \nabla v = 0, \quad \forall v \in \mathcal{V}(\Omega^0). \tag{8}$$

Proposition 3.2. *Problem* (8) *has a unique solution. The mapping $\mathcal{H}$ is bounded from $H^{1/2}(\Gamma^0)$ to $H^1(\Omega^0)$.*

The following result is the theoretical key to the method proposed below for approximating $\mathcal{H}(u)|_{Y^n}$:

Proposition 3.3. *There exists a constant $\rho < 1$ such that for any $u \in H^{1/2}(\Gamma^0)$, and for any $p > 0$,*

$$\sum_{\sigma \in \mathcal{A}_p} \int_{\Omega^\sigma} \left|\nabla \mathcal{H}(u)\right|^2 \leqslant \rho^p \int_{\Omega^0} \left|\nabla \mathcal{H}(u)\right|^2. \tag{9}$$

The Dirichlet–Neumann operator T:

$$Tu = -\frac{\partial \mathcal{H}(u)}{\partial x_2}\bigg|_{\Gamma^0}, \tag{10}$$

is characterized by $\langle Tu, v\rangle = \int_{\Omega^0} \nabla \mathcal{H}(u) \cdot \nabla \mathcal{H}(v)$, for any $v \in H^{1/2}(\Gamma^0)$, where $\langle , \rangle$ is the duality pairing between $(H^{1/2}(\Gamma^0))'$ and $H^{1/2}(\Gamma^0)$. We remark that $T \in \mathbb{O}$, the cone containing the self-adjoint, positive semi-definite, bounded linear operators from $H^{1/2}(\Gamma^0)$ to $(H^{1/2}(\Gamma^0))'$ which vanish on the constants.

If T is available, the self-similarity implies that $\mathcal{H}(u)|_{Y^0} = w$, where w is the weak solution of

$$\Delta w = 0 \quad \text{in } Y^0, \qquad \frac{\partial w}{\partial n}\bigg|_{\partial Y^0 \setminus (\Gamma^0 \cup \Gamma^1)} = 0, \tag{11}$$

$$w|_{\Gamma^0} = u, \tag{12}$$

$$\frac{\partial w}{\partial x_2}\bigg|_{F_i(\Gamma^0)} + 2\big(T(w|_{F_i(\Gamma^0)} \circ F_i)\big) \circ F_i^{-1} = 0, \quad i = 1, 2. \tag{13}$$

We call (13) a transparent boundary condition, because it permits the computation of $\mathcal{H}(u)|_{Y^0}$ without error. We stress the fact that (11)–(13) is well posed, from the observation on T above. The construction may be generalized to $\mathcal{H}(u)|_{Y^{n-1}}$, $n \geqslant 1$:

Proposition 3.4. *For $u \in H^{1/2}(\Gamma^0)$, $\mathcal{H}(u)|_{Y^{n-1}}$ can be computed by solving successively $1 + 2 + \cdots + 2^{n-1}$ boundary value problems in Y^0:*

- *Loop: for $p = 0$ to $n - 1$,*
  - *Loop: for $\sigma \in \mathcal{A}_p$, (at this point, if $p \geqslant 1$, $(\mathcal{H}(u))|_{\Gamma^\sigma}$ is known)*
    Find $w \in H^1(Y^0)$ satisfying the boundary value problem (11), (13), *and either* (12) *if $p = 0$, or $w|_{\Gamma^0} = \mathcal{H}(u)|_{\Gamma^\sigma} \circ \mathcal{M}_\sigma(F_1, F_2)$ if $p > 0$.*
    Set $\mathcal{H}(u)|_{Y^0} = w$ if $p = 0$. If $p > 0$, set $(\mathcal{H}(u))|_{\mathcal{M}_\sigma(F_1,F_2)(Y^0)} = w \circ (\mathcal{M}_\sigma(F_1, F_2))^{-1}$.

In order to compute T, we introduce the mapping $\mathbb{M} : \mathbb{O} \mapsto \mathbb{O}$: for any $Z \in \mathbb{O}$,

$$\forall u \in H^{1/2}(\Gamma^0), \quad \mathbb{M}(Z)u = -\frac{\partial w}{\partial x_2}\bigg|_{\Gamma^0}, \tag{14}$$

where $w \in H^1(Y^0)$ satisfies (11), (12) and $\frac{\partial w}{\partial x_2}|_{F_i(\Gamma^0)} + 2(Z(w|_{F_i(\Gamma^0)} \circ F_i)) \circ F_i^{-1} = 0$, $i = 1, 2$.

Theorem 3.5. *The operator T is the unique fixed point of $\mathbb{M}$. Moreover, if ρ, $0<\rho<1$, is the constant appearing in* (9)*, then, for all $Z\in\mathbb{O}$, there exists a positive constant C such that, for all $p\geqslant 0$,*

$$\left\|\mathbb{M}^p(Z)-T\right\|\leqslant C\rho^{p/4}. \tag{15}$$

The numerical computations in [2] show that ρ is very small, so the convergence of the fixed point method for computing T is extremely fast.

4. Helmholtz equation and transparent boundary conditions

For $k\in\mathbb{R}_+$, $u\in H^{1/2}(\Gamma^0)$, we look for $\mathcal{H}_k(u)\in H^1(\Omega^0)$ such that

$$\Delta\mathcal{H}_k(u)+k\mathcal{H}_k(u)=0\quad\text{in }\Omega^0,\qquad \mathcal{H}_k(u)|_{\Gamma^0}=u,\qquad \frac{\partial\mathcal{H}_k(u)}{\partial n}=0\quad\text{on }\Sigma^0, \tag{16}$$

with an additional generalized homogeneous Neumann condition on Γ^∞ as above. The weak form of this problem is written below, see (17).

Let us define the operator L_k and the closed subspace $(\ker(L_k))^\circ$ of $H^{1/2}(\Gamma^0)$:

$$L_k:\mathcal{V}(\Omega^0)\mapsto\left(\mathcal{V}(\Omega^0)\right)',\qquad \langle L_k(w),v\rangle=\int_{\Omega^0}\nabla w\cdot\nabla v-k\int_{\Omega^0}wv,$$

$$\left(\ker(L_k)\right)^\circ=\left\{u\in H^{1/2}(\Gamma^0)\text{ s.t. }\forall\tilde{u}\in H^1(\Omega^0)\text{ with }\tilde{u}|_{\Gamma^0}=u,\ \int_{\Omega^0}\nabla\tilde{u}\cdot\nabla v-k\tilde{u}v=0,\ \forall v\in\ker(L_k)\right\}.$$

Proposition 4.1. *There exists a countable subset of $\mathbb{R}_+$, $\mathrm{Sp}=\{\lambda_p,\ p\in\mathbb{N}\}$ with $0<\lambda_p\leqslant\lambda_{p+1}$ and $\lim_{p\to\infty}\lambda_p=+\infty$ such that* (a) *if $k\notin\mathrm{Sp}$, the operator L_k is one to one with a bounded inverse,* (b) *if $k\in\mathrm{Sp}$, $\ker(L_k)$ has a positive and finite dimension. One can obtain an Hilbertian basis of $\mathcal{V}(\Omega^0)$ by assembling bases of $\ker(L_k)$, $k\in\mathrm{Sp}$.*

For $u\in(\ker(L_k))^\circ$, there exists a unique $\mathcal{H}_k(u)\in H^1(\Omega^0)/\ker(L_k)$ such that

$$\mathcal{H}_k(u)|_{\Gamma^0}=u\quad\text{and}\quad\forall v\in\mathcal{V}(\Omega^0),\quad\int_{\Omega^0}\nabla\mathcal{H}_k(u)\cdot\nabla v-k\int_{\Omega^0}\mathcal{H}_k(u)v=0. \tag{17}$$

In the most frequent case when $k\notin\mathrm{Sp}$, we define the Dirichlet–Neumann operator $T_k u=-\frac{\partial\mathcal{H}_k(u)}{\partial x_2}|_{\Gamma^0}$. In the general case, the mapping T_k from $(\ker(L_k))^\circ$ to the dual space $((\ker(L_k))^\circ)'$, is defined by:

$$\forall u,v\in\left(\ker(L_k)\right)^\circ,\quad\langle T_k u,v\rangle=\int_{\Omega^0}\nabla\mathcal{H}_k(u)\cdot\nabla\tilde{v}-k\int_{\Omega^0}\mathcal{H}_k(u)\tilde{v}, \tag{18}$$

for any $\tilde{v}\in H^1(\Omega^0)$ such that $\tilde{v}|_{\Gamma^0}=v$. If the operators $T_{4^{-p}k}$, $0\leqslant p\leqslant n$ are available, then $\mathcal{H}_k(u)|_{Y^{n-1}}$ can be found by solving successively $1+2+\cdots+2^{n-1}$ boundary value problems in Y^0 (which have solutions):

Proposition 4.2. *Assume for simplicity that $\forall p$, $0\leqslant p\leqslant n$, $4^{-p}k\notin\mathrm{Sp}$. For any $u\in H^{1/2}(\Gamma^0)$, the following algorithm produces $\mathcal{H}_k(u)|_{Y^{n-1}}$:*

- *Loop: for $p=0$ to $n-1$,*
  - *Loop: for $\sigma\in\mathcal{A}_p$, (at this point, if $p>0$, $(\mathcal{H}_k(u))|_{\Gamma^\sigma}$ is known)*
    Solve the boundary value problem in Y^0: find $w\in H^1(Y^0)$ such that

$$\Delta w+4^{-p}kw=0\quad\text{in }Y^0,\qquad \left.\frac{\partial w}{\partial n}\right|_{\partial Y^0\setminus(\Gamma^0\cup\Gamma^1)}=0, \tag{19}$$

$$\left.\frac{\partial w}{\partial x_2}\right|_{F_i(\Gamma^0)}+2\left(T_{4^{-p-1}k}\left(w|_{F_i(\Gamma^0)}\circ F_i\right)\right)\circ F_i^{-1}=0,\quad i=1,2. \tag{20}$$

$$\text{If }p=0,\quad w|_{\Gamma^0}=u,\quad\text{else}\quad w|_{\Gamma^0}=\mathcal{H}_k(u)|_{\Gamma^\sigma}\circ\mathcal{M}_\sigma(F_1,F_2). \tag{21}$$

Set $\mathcal{H}_k(u)|_{Y^0} = w$ *if* $p = 0$*, else set* $\mathcal{H}_k(u)|_{\mathcal{M}_\sigma(F_1,F_2)(Y^0)} = w \circ (\mathcal{M}_\sigma(F_1, F_2))^{-1}$.

The complete algorithm, omitted for brevity, involves additional finite dimensional systems if $4^{-p}k \in \mathrm{Sp}$, see [1]. There remains to compute the operators $T_{4^{-p}k}$, $p = 0, \ldots, n$. It is proved in [1] that

(i) $\lim_{p\to\infty} T_{4^{-p}k} = T$,
(ii) the operators $T_{4^{-p}k}$ satisfy a backward induction formula with respect to p, which has the following form in the simplest case when $4^{-p}k \notin \mathrm{Sp}$ and $4^{-p-1}k \notin \mathrm{Sp}$: for $u \in H^{1/2}(\Gamma^0)$, $T_{4^{-p}k}u = -\frac{\partial w}{\partial x_2}|_{\Gamma^0}$, where $w \in H^1(Y^0)$ is the weak solution of (19), (20) and $w|_{\Gamma^0} = u$.

These two observations yield an approximation method for the operators $T_{4^{-p}k}$, which is proposed in [1], along with error estimates.

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