A metric-based adaptation for hybrid RANS/LES flow calculations

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Abstract

Ce document présente une approche d'adaptation de maillage pour les calculs utilisant des modeles de turbulence hybrid RANS/LES. On priviliégie les applications au calcul d'écoulements quasi-stationnaires et quasi-périodiques.

Keywords: Compressible flow, Hyperbolic, Euler flow, Finite volume, Error estimation, Mesh adaptation.

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Contents

1 Introduction

Large Eddy Simulation is a numerical tool for predicting turbulent flows. Unlike a statistical Navier-Stokes model which tends to discard all fluctuations into a statistical average, in many case by damping theses fluctuations. LES can be interpreted as damping only a part of unsteady turbulent structures, typically structures with a scale smaller than a prescribed filter size. The smallest structures being the most difficult to solve, LES consumes much less computational effort than a Direct Numerical Simulation which computes all turbulence structures. The idea of LES is to consider the Kolmogorov energy cascade and try to exclude from the computation the smallest scales of smallest energy by :
(i)- defining the neglected scales as smaller than a filter width Δ_f and adding a model of the action of neglected scales on the non-neglected ones. This define a continuous model parameterized by the filter width Δ_f,
(ii)- using, in order to approximate the continuous model built in (i), a mesh-based approximation with local mesh size Δ_g.

While, by construction, Δ_f should be larger than Δ_g, in order to approximate accurately the non-neglected scales, the research of the lowest computational cost motivates the practitioner to set $\Delta_f = \Delta_g$, with the consequence that the smallest unfiltered scales are the smallest scales computed on the grid and are then very poorly approximated, whatever be the accuracy of the numerical scheme.

When using a second-order accurate approximation, an important disadvantage comes from the fact that many LES models of Smagorinsky type are similar to second-order accurate truncation terms, in such a way that approximation errors are of same order as the filter model. According to an analysis of Ghosal [8] and to the outputs of many numerical computations, see e.g. [11], using a second-order accurate approximation may result in errors larger than the effect of LES modelling. I remains that second-order accurate approximations are much used and very useful for computinf LES flows in engineering. A good practise for increasing the confidence in second-order accurate LES computations is to compare (a) the LES-based computations with (b) their no-model counterpart in order two, see e.g. [12].

Let assume that an approximation of nominal order α [1] is used. An im-

[1] By nominal we mean the usual order of convergence which can be observed when no singularity occurs, typically second-order convergence with second-order codes and extremely fine meshes.

portant issue is the fact that the convergence at nominal order, is subject to the condition of using a sufficiently refined mesh: the mesh should be in any point sufficiently fine for capturing the smallest local detail of the flow computed, in order to start second-order or higher order convergence.
- Already in steady CFD, the convergence at nominal order is difficult to attain. A very efficient tool for this purpose is the convergent mesh adaptation double loop as described in [1, 6]. The inner loop is an anisotropic metric-based fixed-point *adaptation* working with a fixed number of unknowns. The outer loop is an anisotropic metric-based *enrichment* increasing progressively the total number of unknowns and controlling the actual convergence to the continuous solution. Thanks to this double loop, steady second-order RANS calculations are reaching a higher level of accuracy and fiability.
- As concerns unsteady RANS, mesh convergence with a double mesh adaptive loop is more difficult to apply, but effective in many cases. See for examples [3], [16], [15].
- At the contrary, with LES, the scenario consisting of a brute-force mesh convergence with LES by increasing simply the number of nodes generally may not succeed for the following reason. The filter term can be considered as a second order error. However refining diminishes the SGS term and introduces the arising of smaller and smaller new unstable scales in the solution which therefore cannot be accurately approximated until the process simply solves the corresponding DNS flow.

Therefore, in contrast to laminar and RANS modeling, mesh adaptation for LES and hybrid models cannot have as goal the faster/fastest convergence to a continuous field. The designing of a mesh adaptation criterion for LES is an important and difficult issue, addressed by a large quantity of works, among which we have selected the following typical ones.

In [4], The approach is a numerical one, related to truncature. The error estimator identifies the regions lacking in accuracy, improving their resolution by either decreasing the size of the element or increasing the polynomial degree which approximates locally the solution. A smoothness indicator guides the hp-decision, leading to p-enrichment for smooth regions and h-refinement for non-smooth regions.

The physical approach is discuted in [5]: Arguments based on the ratio of subgrid to viscous dissipation or viscosity are meaningful only in the buffer layer of wall-bounded turbulence since LES should be ap- plicable to free shear flows at any Reynolds number. Measuring the sufficiency of a grid in LES by the ratio of modeled to resolved (or total) turbulence kinetic energy has been found to correlate poorly to the known behavior of length scales in wall-bounded flows. Methods that approximate a local turbulent spec- trum have some basis for isotropic flows, but fail for more relevant cases.

The most well-grounded approach to date is that by Toosi and Larsson [17] which can be viewed as an estimate of the LES modeling residual, i.e., the source term in an error transport equation. In Toosi and Larsson proposition, a process analog to the dynamic Germano calculus identifies the coarsest resolution for which the LES solution is sufficiently accurate and exhibits minimal sensitivity to the resolution.

In [13] the approach relies on a Discontinuous Galerkin hifg-order approximation. The ideal DG-LES solution is defined as the result of the application of two successive filter- ing operations. A first convolution filter is applied to the DNS data which filters out frequencies beyond the LES grid cut-off. Next, a L 2 -projection of this filtered field is performed on the hp-discretization space (referred to in the following as DG-projection). +VMS.DG-VMS. Pas vraiment adaptatif.

In [7], a field-inversion machine-learning (FIML) framework is introduced. It only requires unsteady primal solutions. Two error estimates are compared in this work, (E1) Time-averaged unsteady residual weighted by a time-averaged adjoint, (E2) an Augmented-system residual weighted by the augmented-system adjoint

The work in [10] compares three indicators. The first indicator is based on the unsteady residual. The second indicator is based on a local smoothness indicator. The third indicator is based on an estimate for small scale turbulent kinetic energy. Comparisons with DNS tend to show that the first indicator is the best.

Similarly, in [9] several indicators are studied

. The classic residual based error indicator and the newly introduced heuristic indicator perform best. If an indicator is based on the eddy viscosity v 1 , we assume that both error types the discretisation and the modeling error are tracked. In this sense we define TJmax := TJmax (l!t). For comparison only the presumably weak performing indicator T/max (u), which measures the maximum value of the veloci- ties, is introduced as well. Wall jet.

In contrast to the above approaches, our approach starts from the successful adaptation of steady RANS flows. In order to extend it to LES/hybrid, we try to combine (a) an adaptation of mesh to the flow in a similar manner to (RANS or non-turbulent) steady flow with (b) a special adaptation for turbulence. Focusing on hybrid modeling, we could hope (1) a rather good quasi-convergent capturing in RANS regions, to be combined with (2) a suffficiently predictive resolution in LES region. The balance between both criteria is a central question which we shall discuss.

In this work, we focus on flows which are of a somewhat intermediate difficulty. These turbulent flows are assumed to be quasi-periodic with a rather well identified Strouhal number, and possibly quasi-steady in a large part of the computational domain. For an thin airfoil at small angle of attack for example, RANS calculation will produce a steady flow. VLES calculations with medium meshes will produce a flow which is mainly steady, but which presents an unsteady region with vortices. Our standpoint is to try to derive a sufficiently efficient adapted mesh for this flow.

2 Recall: mesh adaptation double loop for transient flows

2.1 Riemannian metric

The Riemannian metric $(\mathcal{M}(\mathbf{x}))_{\mathbf{x}\in\Omega}$ is a symmetric positive matrix 3×3 field on computational domain Ω yielding a local description of any "unit mesh" following the mesh sizes specified by $\mathcal{M}$:

$$\mathcal{M}: \ \mathbf{x}\in\Omega \mapsto \mathcal{M}(\mathbf{x}) \ = \ \mathcal{R}(\mathbf{x})\,\Lambda(\mathbf{x})\,{}^t\mathcal{R}(\mathbf{x}), \tag{1}$$

where diagonal matrix $\Lambda(\mathbf{x})$ is

$$\begin{bmatrix} \lambda_1(\mathbf{x}) & & \\ & \lambda_2(\mathbf{x}) & \\ & & \lambda_3(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} h_1^{-2}(\mathbf{x}) & & \\ & h_2^{-2}(\mathbf{x}) & \\ & & h_3^{-2}(\mathbf{x}) \end{bmatrix}. \tag{2}$$

$\mathcal{R}(\mathbf{x})$ is an orthonormal matrix providing the local orientation of mesh stretching through the eigenvectors $(\mathbf{v}_i(\mathbf{x}))_{i=1,3}$, $(\lambda_i(\mathbf{x}))_{i=1,3}$ are the local eigenvalues. $(h_i(\mathbf{x}))_{i=1,3} = (\lambda_i(\mathbf{x})^{-\frac{1}{2}})_{i=1,3}$ are the local mesh sizes along the principal directions of $\mathbf{M}$. The density d of $\mathcal{M}$ is defined from its eigenvalues as

$$d(\mathbf{x}) = det\big(\mathcal{M}(\mathbf{x})\big)^{\frac{1}{2}} = (\lambda_1(\mathbf{x})\,\lambda_2(\mathbf{x})\,\lambda_3(\mathbf{x}))^{\frac{1}{2}} = (h_1(\mathbf{x})\,h_2(\mathbf{x})\,h_3(\mathbf{x}))^{-1}.$$

We decompose $\mathcal{M}$ as follows:

$$\mathcal{M}(\mathbf{x}) = d^{\frac{2}{3}}(\mathbf{x})\,\mathcal{R}(\mathbf{x}) \begin{bmatrix} r_1^{-\frac{2}{3}}(\mathbf{x}) & & \\ & r_2^{-\frac{2}{3}}(\mathbf{x}) & \\ & & r_3^{-\frac{2}{3}}(\mathbf{x}) \end{bmatrix} {}^t\mathcal{R}(\mathbf{x})$$

where the r_i's define the stretching strength and where the density d controls the local level of accuracy of $\mathcal{M}$. The *complexity* $\mathcal{C}$ of $\mathcal{M}$ is defined by:

$$\mathcal{C}(\mathcal{M}) = \int_\Omega d(\mathbf{x})\,d\mathbf{x} = \int_\Omega \sqrt{\det(\mathcal{M}(\mathbf{x}))}\,d\mathbf{x}.$$

This real-value parameter quantifies the global level of accuracy of $(\mathcal{M}(\mathbf{x}))_{\mathbf{x}\in\boldsymbol{\Omega}}$.

A discrete mesh $\mathcal{H}$ is *unit* for the metric $\mathcal{M}$ if any of its edges $\mathbf{ab}$ has a length in the metric sufficiently close to unity :

$$\frac{1}{\sqrt{2}} \leq \int_0^1 \sqrt{{}^t\mathbf{ab}\ \mathcal{M}(\mathbf{a} + t\,\mathbf{ab})\ \mathbf{ab}}\,\mathrm{d}t \leq \sqrt{2}$$

Then the complexity can also be interpreted as the continuous counterpart of the *number of vertices of a discrete unit mesh* while d can be interpreted as the continuous counterpart of the *number of vertices per volume unit of a discrete unit mesh*.

We call *refinement* the process which replaces a unit mesh of a given metric $\mathcal{M}$ with local mesh size $(h_1(\mathbf{x})\, h_2(\mathbf{x})\, h_3(\mathbf{x}))$ by a unit mesh of $\mathcal{M}/\beta^2$ with local mesh size $(\beta h_1(\mathbf{x})\, \beta h_2(\mathbf{x})\, \beta h_3(\mathbf{x}))$ and complexity $\mathcal{C}(\mathcal{M}/\beta^2) = \beta^3 \mathcal{C}(\mathcal{M})$ where refinement factor β is smaller than one [2] .

2.2 Metric-based mesh adaptation of an unsteady flow

The flows under study are unsteady. In order to apply mesh adaptation, we shall use a version of the Transient Fixed Point introduced in [2]. A sketch of this algorithm is given by Algorithm 1.

Algorithm 1 Transient Fixed Point for URANS

Given a complexity $N_{prescribed}$, an initial metric, $\mathcal{M}_0$ of complexity c_0,
build a unit mesh $\mathcal{H}_0$ from $\mathcal{M}_0$
`For` $iadapt = 0, nadapt$

- Compute over $[0, T]$ the URANS flow W_{iadapt} from with mesh $\mathcal{H}_{iadapt}$
- Compute the k_{max} new metrics $\mathcal{M}^k_{iadapt+1}$ of complexity $N_{prescribed}$ each taking into account the flow over $[t_k, t_{k+1}]$.
- Compute the k_{max} new meshes $\mathcal{H}^k_{iadapt+1}$ from $\mathcal{M}^k_{iadapt+1}$
- $iadapt = iadapt + 1$

`End for` $iadapt$

[2] For $\beta = 2$ this refinement is equivalent to dividing mesh size by a factor 2 and multiplying the number of vertices in 3D by a factor 8.

Let us assume that Algorithm 1 iteratively converges (when *iadapt* increases to infinity) to a fixed point $(W_\infty, \mathcal{M}_\infty)$. Then this fixed point is a numerical flow computed on a succession of meshes $\mathcal{M}^k_\infty, k = 1, k_{max}$, each mesh $\mathcal{H}^k_\infty$ being adapted to the best approximation (in some sense) of the flow on time interval $[t_k, t_{k+1}]$. Further, the sum of the complexities of the different meshes for $k = 1, k_{max}$ is the global complexity $k_{max}N_{prescribed}$.
If we want to work with only one mesh for the whole time interval, we put:

$$k_{max} = 1 \ . \tag{3}$$

In next section, we work with a single mesh, $k_{max} = 1$, for identifying the best mesh (in some sense) for computing a quasi-steady quasi-periodic flow.

In the second study the problem of mesh convergence with $k_{max} = 1$ of a LES flow is considered.

3 Mesh-adapted LES for a quasi-periodic flow

The assumption is that the flow is essentially steady, with a rather small region of the computational domain in which we have a quasi periodic vortex shedding.

3.1 Grid filter and Riemannian metric

We restrict to a usual definition of the grid size:

$$\Delta_g = (\delta\xi\delta\eta\delta\zeta)^{\frac{1}{3}}.$$

It is expressed directly in terms of the local mesh size measured from the local mesh in three orthogonal directions. It can also be expressed locally in terms of the metric used for generating the mesh, cf. (2).

$$\Delta_{\mathcal{M}} = (h_1 h_2 h_3)^{\frac{1}{3}}.$$

We consider a LES formulation which replaces in the viscous term of Navier-Stokes the viscosity ν by the incremented viscosity $\nu + \nu_T$. We define ν_T according to the WALE model [14]:

$$\mu_{SGS} = \overline{\rho}(C_W\Delta)^2 \frac{\left(\tilde{S_{i,j}}^d \tilde{S_{i,j}}^d\right)^{3/2}}{\left(\tilde{S_{i,j}}\tilde{S_{i,j}}\right)^{5/2} + \left(\tilde{S_{i,j}}^d \tilde{S_{i,j}}^d\right)^{5/4}} \tag{4}$$

where $\tilde{S_{i,j}}^d$ is the symmetric part of tensor $g^2_{ij} = g_{ik}g_{kj}$, with $g_{ik} = \dfrac{\partial \tilde{v}_i}{\partial x_j}$:

$$\tilde{S_{i,j}}^d = \frac{1}{2}\left(g^2_{ij} + g^2_{ji}\right) - \frac{1}{3}\delta_{ij} g^2_{kk}. \tag{5}$$

In [14], the constant C_W is fixed to 0.5.

3.2 Adaptation sensor

In the case of a steady RANS calculation of a compressible flow, an efficient approach is to minimize the L^4 interpolation error on the Mach number. We follow the metric-based adaptation approach as in, e.g. [6]. The local interpolation error $e_{\mathcal{M}}$ (6) is evaluated in terms of the Hessian H_M of Mach number M and of the metric $\mathcal{M}$ used for generating the mesh:

$$e_{\mathcal{M}}(\mathbf{x}) = (M - \pi_{\mathcal{M}} M)(\mathbf{x}) \;=\; \frac{1}{10}\, trace\big(\mathcal{M}(\mathbf{x})^{-\frac{1}{2}}\, |H_M(\mathbf{x})|\, \mathcal{M}(\mathbf{x})^{-\frac{1}{2}}\big), \qquad (6)$$

in which $\mathbf{x} \in \Omega$, $(\mathbf{v}_i)_{i=1,3}$ are the local eigen-directions of $\mathcal{M}$, and $(h_i)_{i=1,3}$ are the local sizes of $\mathcal{M}$ along these directions. This local error [3] is a spatially second-order error. The metric based analysis would then use the following symmetric matrix:

$$H_1 = H_M \qquad (7)$$

In order to take into account boundary layers in good conditions, it has been observed (see e.g. [6]) that the error norm to be minimized is an L^4 norm. The mesh adaptation problem is then written:

$$\text{Find } \mathcal{M}_1 = \min_{\mathcal{M}} \int_{\Omega} \Big(trace\big(\mathcal{M}(\mathbf{x})^{-\frac{1}{2}}\, |H_M(\mathbf{x})|\, \mathcal{M}(\mathbf{x})^{-\frac{1}{2}}\big)\Big)^{\frac{1}{4}} \mathrm{d}\Omega \qquad (8)$$

under the constraint that the complexity, or integral of the metric density is equal to a specified number N:

$$\mathcal{C}(\mathcal{M}) = \int_{\Omega} d(\mathcal{M})\mathrm{d}\Omega = N.$$

Expressing via (6) the functional (8) in terms of H_M and assuming that this Hessian is sufficiently smooth, the solution of this constrained optimisation problem can be explicitly computed ([6]):

$$\mathcal{M}_1 = D_1 \ \det(|H_M|)^{\frac{-1}{11}}\, |H_M|, \ \text{with } D_1 = N^{\frac{2}{3}} \left(\int_{\Omega} \det(|H_M|)^{\frac{4}{11}} \mathrm{d}\Omega \right)^{-\frac{2}{3}}. \qquad (9)$$

Since the flow of interest is quasi steady in a large part of the computational domain, we keep this metric $\mathcal{M}_1$ as mean flow criterion of our novel method.

It remains to identify a good strategy for the quasi periodic unsteady region. Main structures are unsteady vortices. We do not want to follow these vortices with an unsteady mesh. Then we should try not to have strong

[3] $e_{\mathcal{M}}$ is an *a priori* error when we consider that M is the exact Mach number field. In practice, it will be an *a posteriori* error since $e_{\mathcal{M}}$ will be computed from a discrete solution through a recovery technique.

stretching, but, preferrably an isotropic mesh in this region. Then we have to build a second criterion for this region. At least two approaches can be applied:
(a)- physically based criterion, e.g. vorticity,
(b)- a criterion based on the LES mechanism.

Let us explain (b): LES can be considered as a cure to our unability to compute all the turbulent scales, at the price of a deviation with respect to the exact DNS flow. Then we can consider the filtering term in the Navier-Stokes equations

$$\nabla.\mathcal{T}_{SGS} = \nabla.\mu_{SGS} \left[(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}) - \frac{2}{3} \nabla.\, \mathbf{u}\, I \right] ,$$

as a local error to minimize.

According to the definition (4) of μ_{SGS}, an option is to consider this term as a spatially second-order error term. Taking the norm of $\nabla.\mathcal{T}_{SGS}$ in $\mathbb{R}^3$ we get a scalar number, allowing to build an *isotropic* second adaptation criterion

$$\bar{H}_2 = \frac{|\nabla.\mathcal{T}_{SGS}|}{\Delta x^2} \mathbf{Id}. \tag{10}$$

where $\mathbf{Id}$ is the identity 3×3 matrix. In general, $\bar{H}_2$ is a very irregular distribution and we shall work with a smoother representation of it:

$$H_2 = \mathcal{S}\Big(\frac{|\nabla.\mathcal{T}_{SGS}|}{\Delta x^2} \Big) \mathbf{Id}. \tag{11}$$

where $\mathcal{S}$ is a barycentering smoother. This allows to find a second "optimal" metric, computed, this time, by minimizing an L^2 norm of error:

$$\mathcal{M}_2 = D_2 \ \det(|H_2|)^{\frac{-1}{7}} \ |H_2|, \ \text{with} \ D_2 = N^{\frac{2}{3}} \left(\int_\Omega \det(|H_2|)^{\frac{2}{7}} \right)^{-\frac{2}{3}} . \tag{12}$$

Each of metrics $\mathcal{M}_1$ and $\mathcal{M}_2$ has a complexity N. We can legitimately take the intersection of both (without scaling) for satisfying both criteria:

$$\overline{\mathcal{M}_{inter}} = \mathcal{M}_1 \cap \mathcal{M}_2.$$

The general operator for intersecting two metrics is defined in [6]. Its function is to provide the metric defining in any spatial direction the largest mesh size less than the two mesh sizes specified by the two metrics. But since $\mathcal{M}_2$ is isotropic, it specifies in each point $\mathbf{x}$ of the computational domain Ω a single mesh size $h_{\mathcal{M}_2}(\mathbf{x})$. Let us assume that at $\mathbf{x}$, the metric $\mathcal{M}_1$ specifies mesh sizes h_1, h_2, h_3 in its caracteristic directions $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$. Then the intersection is obtained in replacing

$$h_1, h_2, h_3$$

by

$$min(h_1, h_{\mathcal{M}_2}), min(h_2, h_{\mathcal{M}_2}), min(h_3, h_{\mathcal{M}_2}).$$

Note that the complexity $\int_\Omega det(\overline{\mathcal{M}_{inter}})^{\frac{1}{2}} d\Omega$ of this intersection is not anymore equal to N. Since applying our basic adaptation Algorithm 1 assumes that we maintain the complexity constant and equal to N, the final proposed metric is defined as:

$$\mathcal{M}_{inter} = \left(\frac{N}{\int_\Omega det(\overline{\mathcal{M}_{inter}})^{\frac{1}{2}} d\Omega} \right)^{\frac{2}{3}} \overline{\mathcal{M}_{inter}}. \quad (13)$$

3.3 Step 1: Fixed Point

In the usual LES strategy, a mesh is given, and a filter size derived from it at each local discretization node. In other words, giving the mesh is a mean for prescribing the local filter size.

In the proposed mesh adaptation method for LES, the user prescribes a global complexity, and the fixed point will iterate until an equilibrium is found between the adapted mesh, the related local filter, and the filtered RANS unsteady flow. This will be possible because we restrict the flows under consideration to quasi-periodic flows with a quasi-period T. Then the adaptation interval during which the mesh is frozen will be set to one periodicity interval $[0, T]$.

This gives Algorithm 2. We observe that when applied to a steady flow, Algorithm 2 will converge to an adapted solution of the flow, and convergence can be contained by increasing the complexity c_0. Similarly, when applied to an unsteady non turbulent flow, Algorithm 2 will converge to an adapted solution of the flow, and increasing both complexity c_0 and the number of time subintervals, convergence to the continuous flow will be obtained.$\square$

Let us consider the application to a turbulent flow. Let us assume that a fixed point of Algorithm 2 exists at least approximatively (two successive iterations produce very similar unsteady flows. Then we get a LES numerical

Algorithm 2 LES-Transient Fixed Point

`Given a complexity` $c_{prescribed}$, an initial metric $\mathcal{M}_0$ of complexity c_0

`Compute the local filter size` Δ_0 `from` $\mathcal{M}_0$

`Build a unit mesh` $\mathcal{H}_0$ `from` $\mathcal{M}_0$

`For` $iadapt = 0, nadapt$

- Compute over $[0, T]$ the LES flow from Δ_{iadapt} and $\mathcal{H}_{iadapt}$
- Compute a new metric $\mathcal{M}_{iadapt+1}$ of complexity c_0 taking into account the whole flow over $[0, T]$.
- Compute a new filter $\Delta_{iadapt+1}$ from $\mathcal{M}_{iadapt+1}$
- Compute a new mesh $\mathcal{H}_{iadapt+1}$ from $\mathcal{M}_{iadapt+1}$
- $iadapt = iadapt + 1$

`End for` $iadapt$

flow with a filter $\Delta_{nadapt+1}$ defined from to the mesh, the mesh being adapted to the best approximation (in some sense) of the flow.

4 What next?

We have described a new method permitting to get accuracy improvements by mesh adaptation for a class of LES calculations. This new method is being implemented in the mesh adaptative CFD platform Wolf (see[6]). Next step will produce numerical examples.

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