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DISCONTINUOUS DATA ASSIMILATION

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Data Assimilation is important in meteorology, oceanography and climatology because it is a way to improve the models with newly measured data, statically or dynamically. The problem is well known in control and system theory and a large number of methods applied to environmental sciences are issued from Kalman filters, optimal control etc. In this paper, we give a short review of data assimilation by least squares and optimal control and then concentrate on the problem of finding a discontinuity known to be present in the data but of unknown position in space, such as a meteorological front. As standard control theory assumes differentiability, there are new mathematical difficulties here: if gradient methods are to be used computationally, one needs to establish that derivatives exists in the sense of L^1 instead of L^2. We show on simple examples the difficulties and give some numerical solutions for some flows with shocks.

Key Words: Inverse Problems; Data Assimilation; Meteorology; Optimal Control; Discontinuities

1 Introduction

For obvious reasons, it is of prime importance to improve the numerical models for meteorology, oceanography and climatology. The fundamental equations of fluids are known and need no improvements. The numerical mesh for their discretisation are usually not adequate for lack of computing resource and turbulence modelling must be done. However even if the mesh could resolve all the scales in these flows, there would still be a problem of stability: however accurate the initial state, errors grow to an unacceptable level after some time. The numerical models need to be reinitialized or adjusted with new observations, a process which is called data assimilation.

For example, denote by Ω the domain occupied by the fluid (air or water), by $W(x,t)$ the vector field of the dynamic flow variables (density ρ flux velocities ρu temperature θ or pressure p, and possibly humidity, salinity) and let the set of equations for the fluid be the Euler equations

$$\partial_t W + \nabla . F(W) = 0 \text{ for all } x \text{ in } \Omega, \text{ all } t \text{ in } (0,T) \quad ...(1)$$

with initial and boundary conditions

$$\text{for all } x \text{ in } \Omega : W(x,0) = V(x). \text{ on the boundary } \Gamma = \partial\Omega : (AW).\ n = \upsilon \quad ...(2)$$

where the outer normal to Γ is denoted by n. The matrix field $A(x, t)$ selects components of $W(x, t)$ which have to be given to ensure uniqueness.

Assume now that we have a new set of data BW_d where $B(x,t)$ is a matrix field which selects the components of $W(x,t)$ which are measured at time t and point x (B would contain Dirac masses if W is measured at isolated points). Then one would like to reset V and/or v so as to fit the new data. One way to do this is to solve

$$\min_{V,\upsilon} J_o(V,\upsilon) = \int_{\Omega\times(0,T)} \left| B(W-W_d) \right|^2 \text{ subject to eq. (1)} \quad ...(3)$$

Since this is a least square procedure, Sasaki[1] proposed to adapt the norm to the probability measure of the state and observation variable because, after all, data assimilation is necessary because of random error on data. The so-called *4D-Var* method (cf refs. [2-4], proposes to replace J_0 by

$$J_1(V,\upsilon) = \int_{\Omega\times(0,T)} ((W-W_d)^T B^T \mathbf{R} B(W-W_d) + (W-W_1)^T S(W-W_1)) \quad ...(4)$$

where **R** is the covariance probability matrix on the measurements and **S** is a covariance matrix on the predictive error to realize W_1.

2 Data Assimilation

There are important programmes to acquire oceanic data by satellite (TOPEX/POSEIDON, ENVISAT in France) and the problem is to input this constant stream of new data into the numerical models for meteorology, oceanography and climatology[5]. This has brought forth the necessity of a data assimilation programme, the

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Global Ocean Data Assimilation Experiment (GODAE); the French contribution to GODAE is called MERCATOR and the coupling module is called PALM, a collaboration between the research centre CERFACS in Toulouse, France, and the French meteorology agency. Various numerical methods have been tested and the 4D-Var is currently in use. Following the ref. [6], we proceed to present some of the methods available.

2.1 Kalman Filter

The most natural method is to use the Kalman filter[7]. It applies to any time dependent model predicting a state x_i at time t_i and solution of a (possibly non-linear) discrete or continuous state equation with random errors η_i. To correct these errors we have observations y_i up to errors ε_i. So the system is

$$x_{i+1} = A_i(x_i) + \eta_i \qquad y_i + H(x_i) + \varepsilon_i.$$

Then, based on statistical informations on η and ε, it is possible to correct the model so as to improve the mean response and replace x_i by x_i^c given by

$$x_{i+1}^c = x_{i+1} + K_{i+1}\left(y_{i+1} - H_{i+1}(x_{i+1})\right)$$

where the gain matrix K_{i+1} is given by a recurrence equation involving the covariance matrix of the modelling error Q_i and the covariance of the data measurement error R_i:

$$K_i = P_i H_i^T (H_i P_i H_i^T + R_i)^{-1} P_{i+1} = A_i^T (P_i - K_i H_i P_i) A_i + Q_i$$

Application to meteorology can be found in Budgell[8], Blanchet[9] and Evensen[10].

2.2 Nudging

Nudging is an intuitive technique which consist in a fixed point like correction of the state by the prediction error:

$$x_i^c = x_i + K(y_i - H_i(x_i)) \qquad \text{...(5)}$$

where K is a correction matrix. In ref. [11] some indications are given to choose the matrix K. There is a priori no theoretical justification for such methods, however "feedback control", combined with variational methods, somehow justifies equations like (5), as shown in ref. [12].

2.3 Variational Methods

Data assimilation by variational methods and least squares has been recognized to be among the best methods. Earlier studies include Talagrand[13] Moore[14] and Zou *et al.*[15] and the bibliography therein. It assumes that there are some control parameters v_i to adjust the model by

$$\min_{\upsilon}\left\{E(y_i - H_i))^2 : x_{i+1} = A_i(x_i, \upsilon_i) + \eta_i\right\}$$

It is a stochastic discrete optimal control problem and the best solution method is Bellman's dynamic programming. A simplified version can be obtained by ignoring the random errors. Then it is a standard discrete control problem which can be solved by differentiable optimization and for which there is a huge literature.

2.4 Automatic Differentiation

Gradient and conjugate gradient methods (see Polak[16] for instance) like other differentiable optimization methods require the computation of derivatives with respect to the control parameters v. This can be difficult and tedious for meteorology or oceanography, for which most models use finite difference schemes. Automatic differentiation of computer program is a very powerful idea to handle this difficulty. Popularised by Andreas Griewank[17], it is based on the observation that any computer programme is exactly differentiable because each line is a differentiable function. Therefore a function represented by its computer programme is differentiable except perhaps at some discrete points such as those where a branching statements occur; its derivative is represented by the computer programme in which each line is differentiated and written above the original line. For example x^n, represented by the C++ function

```
float npower(float x)
{float y=1; for(int i=0; i<n; i++) y=y*x; return y;}
```

has its x-derivative generated by

```
class dfloat {float val,dx;};

dfloat dx_npower(float x)
{dfloat y; y.val=1; y.dx = 0;
for(int i=0; i<n; i++)
{y.dx = y.dx * x + y.val; y.val=y.val*x;}
return y;}
```

A few tools are available for this type of automatic differentiation: Adolc[17], Adifor[18], Odyssee[19], or even home made libraries[20] based on operator overloading in C++. The availability of such tools for meteorology and oceanography for data assimilation is not to be underestimated[2].

2.5 Gradient Methods

Problem given by eqs.(1)-(4) is of the type

$$\min_{\upsilon\in V} J(w,\upsilon): A\omega = f(\upsilon). \quad ...(6)$$

where J is a real valued function, A a linear operator from the state spaceW into its dual W'. It is a special type of optimization problem in infinite dimensional space. In Polak[16], for example, a comprehensive reference on optimization techniques can be found. In Lions[21] the mathematical framework necessary to study problems like in eq. (6) is presented, together with the computation of derivatives and optimality conditions (calculus of variations). In this short review we can present only the guidelines of such analysis.

Let q be a Lagrange multiplier associated to $Aw = f(\upsilon)$. By duality theory one may solve

$$\min_{\upsilon\in V} \max_{q} L(w,q,\upsilon) = J(w,\upsilon) + < q, A\omega = f(\upsilon) >. \quad ...(7)$$

where <, > denotes the duality product in W. When the hypotheses for the min-max theorem are met, a solution of eq. (7) will be found by solving the *optimality conditions*

$$\partial_w L(w,q,\upsilon) = 0,\ \partial_q L(w,q,\upsilon) = 0,\ \partial_\upsilon L(w,q,\upsilon) = 0. \quad ...(8)$$

When A is invertible, more information can be extracted from eq. (8) because one can look at eq. (6) as a minimisation of $\upsilon \to J(w(\upsilon),\upsilon)$ without constraint and apply calculus of variations:

$$\delta J: J(w(\upsilon+\delta\upsilon),\upsilon+\delta\upsilon) - J(w(\upsilon),\upsilon):$$
$$= \partial_\omega J(w,\upsilon)\delta w + \partial_\upsilon J(w,\upsilon)\delta\upsilon + o\,(|\delta\iota \quad ...(9)$$

where $\delta w := w(\upsilon+\delta\upsilon) - w(\upsilon)$ satisfies the linearized state equation

$$A\delta w = \partial_\upsilon f(\upsilon)\delta\upsilon + o\,(|\delta\upsilon|) \quad ...(10)$$

Then, using the adjoint trick[21]

$$< q, \partial_\upsilon f(\upsilon)\delta\upsilon > = < q, A\delta w > = < A^* q, \delta w >$$
$$= \partial_w J(w,\upsilon)\delta w + o(|\delta\upsilon|) \quad ...(11)$$

provided q is the solution of the adjoint equation

$$A^* q = \partial_w J(w,\upsilon). \quad ...(12)$$

So finally

$$\delta J = < q, \partial_\upsilon f(\upsilon)\delta\upsilon > + o\,(|\delta\upsilon|) \quad ...(13)$$

This calculus is helpful to set up a gradient method to solve the problem numerically because an iterative scheme of the type (where w^m means $w(v^m)$)

$\upsilon^{m+1} = \upsilon^m - \mu q^m \partial_\upsilon f(\upsilon^m)$ with $\mu > 0$ a small step size parameter ...(14)

generates a decreasing sequence of cost function values $\{J(w^m, \upsilon^m)\}$, independently of the initial guess v^0.

3 Discontinuous Data Assimilation

Gradient methods applied to the Euler system of equations can be difficult for several reasons:

1. The solution W can be discontinuous (shocks).
2. The system is controllable but not the linearized one

Controllability is necessary because one is precisely looking for an initial state V which drives the system to a desired state W_I. This problem has been studied by Coron *et al.*[22]. However in the *4D-Var* approach[6] strictly speaking, exact controllability is not necessary since we search for a minimum of J_I, but there may be stability problems without it.

Shocks is a more serious difficulty as we shall show on the following example.

3.1 An Example with a Shock

Consider the shock tube problem with a constant state on each side of the shock denoted by W^+ on the right and W^- on the left of the shock. The Euler equations for a perfect gas are given by eq. (1) with, in dimension d,

$$W = (\rho, \rho u, \rho(\tfrac{|u|^2}{2} + \tfrac{\gamma}{\gamma-1}\tfrac{p}{\rho}))$$

$$F_i(w) = (\rho u_i, \rho u_1 u_i + \delta_{1i} p, \ldots, \rho u_3 u_i$$
$$+\delta_{di} p, u_i(\tfrac{|u|^2}{2} + \tfrac{\gamma}{\gamma-1}\tfrac{p}{\rho}))^T \quad ...(15)$$

Assume that W^- is given and equal to (A,B,C), that the geometry is a tube of length L, and that the Rankine-Hugoniot conditions are satisfied, so that the flow is at rest and

$$A = \rho^- u^- = \rho^+ u^+$$
$$B = \rho^- u^{-2} + p^- = \rho^+ u^{+2} + p^+$$
$$C = \rho^- u^- (\tfrac{|u^-|^2}{2} + \tfrac{g}{g-1}\tfrac{p^-}{r^-}) = \rho^+ u^+ (\tfrac{|u+|^2}{2} + \tfrac{g}{g-1}\tfrac{p+}{r^-}) \quad ...(16)$$

An equation for $\rho^\pm$ can be obtained:

$$2C(\gamma-1)\rho^\pm - 2\gamma AB + A^3(\gamma+1)\tfrac{1}{\rho\pm} = 0 \quad ...(17)$$

With appropriate choice of A,B,C there are two admissible solutions (the entropy inequality needs to be satisfied also), one corresponding to ρ^s and the other to ρ^+. The position of the discontinuity is not fixed; this is because we are looking at the stationary problem.

If this stationary state is a limit of a transient state then, invariants such as $I=\int_0^L \rho$, being independent of time, are fixed by the initial conditions. Therefore it is I which fixes the position $x = a$ of the shock:

$$I=\int_0^L \rho=\rho^- a+\rho^+(L-a) \qquad ...(18)$$

An analysis of the transient case in dimension one, done in the pioneering work of Godlewski *et al.*[23], confirms the role of eq. (18) to fix the shock.

3.2 Analysis

From eq. (16) it is clear that knowing ρ^-, u^-, p^+, I, for instance, is enough to determine a, the number of equations being equal to the number of unknowns (but of course there may not be any physical solution). However any iterative algorithm will change a as well, so the solution $\rho^\pm$, $u^\pm$, $p^\pm$, a will be found as the limit of $\{\rho^{\pm m}, u^{\pm m}, p^{\pm m}, a^m\}$. One then expects for instance $\rho^{m+1}-\rho^m \to 0$, but this cannot be true pointwise (but true in $L^1(0, L)$ only) because ρ^{m+1} and ρ^m are both discontinuous but not at the same point.

The same difficulty is found when Calculus of Variation is applied to eqs. (1)-(4); the meaning of the little o function in eqs.(9) and (11) is subtle and it is very easy to make a mistake.

3.3 The Stationary Case

Going back to eqs. (1)-(4) but in the stationary case, assume that we wish to solve

$$min_\upsilon \{J(\upsilon)=\int_\Omega |B(w-w_d)|^2$$

$$\text{subject to } \nabla.F(W)=0,\ n^T AW=\upsilon, \int_\Omega w_1\} \qquad ...(19)$$

by a gradient method. At some stage the derivative of J with respect to a parameter s of υ will be needed and it will require to differentiate the stationary Euler equation with respect to s.

3.4 Derivatives for Euler's Equations

All primes denoting derivatives with respect to s, the equation of conservation of mass could be differentiated by the chain rule

$$\nabla.(\rho u)=0 \Rightarrow \nabla.(\rho' u+\rho u')=0 \qquad ...(20)$$

However this makes no sense! This is because the position of the shock Σ varies with s too and so a discontinuous function like ρ is the sum of a smooth part $\bar{\rho}$ and a jump $[\rho]$:

$$\rho(x)=\bar{\rho}(x)+[\rho]I_{\Sigma-} \qquad ...(21)$$

where $I_{\Sigma-}$ is the indicator function of the domain before the shock (this representation is not unique). So when eq. (21) is differentiated with respect to s, the derivative of an indicator function being a Dirac function, we obtain:

$$\rho'(x)=\bar{\rho}'(x)-[\rho]x'_\Sigma.n_\Sigma\delta_\Sigma(x) \qquad ...(22)$$

where $x = x_\Sigma$ is the equation of $\Sigma (x'_\Sigma := dx_\Sigma / ds)$ and n_Σ outward normal. Plugging eq. (22) in eq. (20) gives terms like $u[\rho]\delta_\Sigma$ which make no sense because u is also discontinuous at Σ (no hint to choose between $[\rho]u^-$ and $[\rho]u^+$ when they appear in an integral).

When understood in the sense of distribution theory, eq. (20) contains two informations: the pointwise divergence of ρu is zero almost everywhere, and $\rho u.\ n$ is continuous on any curve/surface of normal n if ρ or u or both are discontinuous. In eq. (22) the first information is kept correctly but the second information is lost. The only way to differentiate eq. (20) correctly is to introduce the conservative variable $v = \rho u$ and write (assuming v is continuous across Σ, not just $v.\ n_\Sigma$, i.e. that the shock is normal to the flow)

$$\nabla.v=0 \Rightarrow \nabla.v'=0. \qquad ...(23)$$

Similarly, the momentum equation,

$$\nabla.(\rho u \otimes u)+\nabla p=0. \qquad ...(24)$$

ought to be rewritten in terms of products of variables where only one of them jumps (and preferably with the augmented pressure $q := p + \rho u^2$ which is continuous across the shock):

$$\nabla.(\tfrac{1}{\rho}(v\otimes v-v^2))+\nabla q=0 \qquad ...(25)$$

In this form it is correct to write

$$\nabla.(\tfrac{1}{\rho}(v'\otimes v+v\otimes v'-2vv'))$$

$$+\nabla.((\frac{1}{\rho})'(v\otimes v-v^2))+\nabla q'=0 \qquad ...(26)$$

One must be careful not to expand $(\rho^{-1})'$ because the result would be illicit in the distribution sense.

Finally the energy equation is rewritten as

$$\nabla.(v(\tfrac{v^2}{\rho^2}-2\gamma\tfrac{q}{\rho}))=0 \qquad ...(27)$$

and its s-derivative is

$$\nabla.(v'(\tfrac{v^2}{\rho^2}-2\gamma\tfrac{q}{\rho})+v)2\tfrac{vv'}{\rho^2}+v^2(\tfrac{1}{\rho^2})'$$

$$-2\gamma\tfrac{q'}{\rho}-2\gamma q(\tfrac{1}{\rho})'))=0 \qquad ...(28)$$

4 Justification in a Simple Case

Consider the case of a potential flow

$$u = \nabla\phi, \nabla.(\rho\nabla\phi) = 0 in\Omega \ \frac{\partial\phi}{\partial n} = g \text{ on}\Gamma := \partial\Omega \quad ...(29)$$

Suppose that ρ is known to be piecewise constant equal to ρ^+ or ρ^- but the change from ρ^- to ρ^+ happens across Σ whose position is not known. We wish to identify Σ from the knowledge of $\nabla\phi$ in a subdomain D which does not intersect Σ. This will be done by solving

$$\min_{\Sigma} J(\rho) = \int_D |u_d - \nabla\phi|^2 \text{ subject to eq. (29)} \quad ...(30)$$

In order to update Σ so as to decrease J by a gradient method we need to compute the derivative of J with respect to parameters s defining Σ.

To do this we begin as usual:

$$J' = 2\int_D (\nabla\phi - u_d)\nabla\phi' \quad ...(31)$$

Then we write eq. (29) in mixed form with the conservation variable V= $\rho\nabla\phi$:

$$\nabla.V = 0, \frac{1}{\rho}V - \nabla\phi = 0. \quad ...(32)$$

and differentiate

$$\nabla.V' = 0, \ \frac{1}{\rho}V' - \nabla\phi' + \left[\tfrac{1}{\rho}\right]V_n \vec{n}_\Sigma x'_\Sigma . n_\Sigma \delta_\Sigma = 0. \quad ...(33)$$

where V_n means $V. n$. Therefore, setting the adjoint state to be solution of

$$-\nabla.(\rho\nabla q) = 2I_D(\nabla\phi - u_d)$$
$$\frac{\partial q}{\partial n}|\Gamma = 0, \ Q = \rho\nabla q \quad ...(34)$$

we obtain

$$J' = 2\int_D (\nabla\phi = u_d)\nabla\phi' = \int_\Omega \rho\nabla q \nabla\phi'$$
$$= \int_\Omega V'\nabla q + \int_\Sigma \left[\tfrac{1}{\rho}\right] V_n Q_n x'_\Sigma . n_\Sigma$$
$$= \int_\Sigma \left[\tfrac{1}{\rho}\right](\rho u_n)(\rho q_n) x'_\Sigma \cdot n_\Sigma \quad ...(35)$$

This calculus has been justified mathematically in ref. [24] for a similar problem on flow through porous media.

4.1 Numerical Simulation

The numerical implementation is done with freefem++[25]. To illustrate the theory we have solved the problem

$$-\nabla.(\rho\nabla\phi) = 0 \ in\Omega \quad \phi|\Gamma = xy \quad ...(36)$$

where Ω is the rectangle (-5,5)x (-2.5,2.5), ρ is 6 inside an ellipse in the middle of the rectangle and 1 outside.

The discretisation is done with the finite element method on a mixed formulation of the problem by setting a system of equation for ϕ and Φ $\rho\Delta\phi$:

$$\int_\Omega \left(\tfrac{\Phi}{\rho} W + \phi\nabla.W\right) = 0 \quad \forall W \in W$$
$$\int_\Omega w\nabla.\Phi = 0 \quad \forall w \in L^2(\Omega) \quad ...(37)$$

where W is a subspace of the square integrable functions with square integrable divergence. These are approximated by piecewise linear discontinuous vector valued functions, continuous at the mid

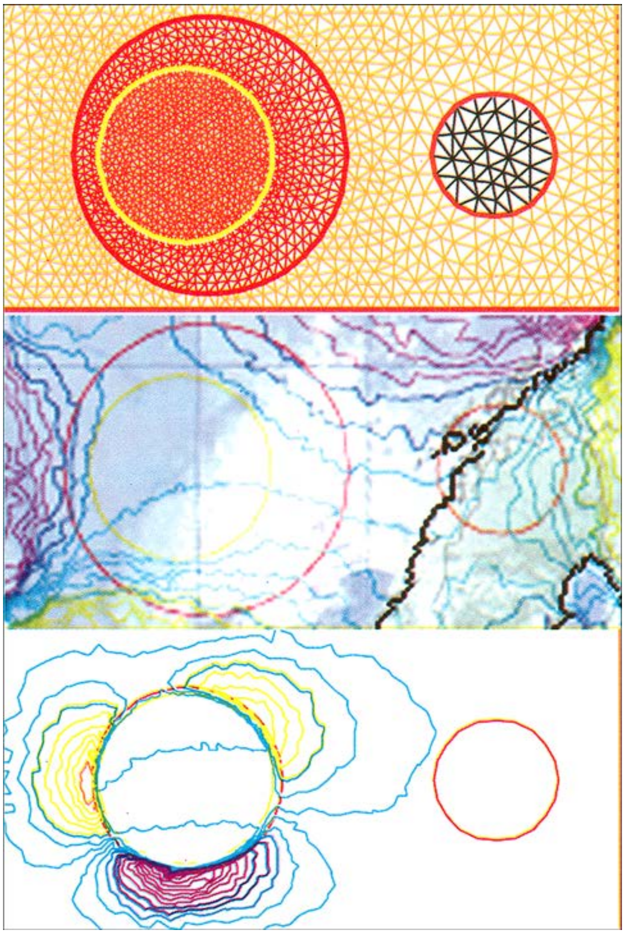

Fig. 1 ***Top***: The triangulation and the observation set (*disk on the right*), *the* initial guess (larger ellipse on the left) and the solution (smaller circle on the left). **Middle**: Illustration of a possible meteorology application in the north sea west of Scandinavia where the density of air is found above the sea from data in the observation set (right) above the land near the Spitzberg islands. The figure also shows the level lines of the calculated velocity potential ϕ. ***Bottom***: *After 10* iterations the discontinuity region has converged to a shape near to the analytical solution. The level line of the error are also shown (maximum error is about 10 *per cent.)*

side nodes and piecewise constant functions respectively. Convergence of the numerical method on problems such as eq. (34) is shown on the Table below. The numerical solution with a mesh size $h = c\varepsilon$ is compared with the ε-divided difference of two numerical solutions of eq. (32) on two geometries, the second one with Σ moved by

$$\left|x'_\Sigma . n_\Sigma\right| = \varepsilon$$

ε	0.1	0.05	0.025	0.0125
L^2-error	0.96	0.71	0.56	0.46

The data assimilation problem is eq. (30) where D is a disk on the right side of the domain and the discontinuity of ρ occurs on the left side of the domain in a domain which is to be found. Such situation could occur when measurements are available on land and lacking in the ocean, such as shown on Fig.1 with Scandinavia where a region of cold air in the ocean is to be identified.

The problem is simplified by taking only two parameters in the definition of the unknown shape:

$$x = -2+\left(\sqrt{2}+r+s\cos t\right)\cos t,$$

$$y = \left(\sqrt{2}+r+s\cos t)\sin t \; t\in(0,\ 2\pi\right).$$

The gradient method is applied to r and s starting from r=0.8 and s=0.4. After 10 iterations

$$r^{10} = 0.120625 \quad s^{10} = 0.01748$$

$$\frac{\partial J}{\partial r} = 0.00113 \quad \frac{\partial J}{\partial s} = 0.00079 \quad J = 0.0001516$$

while the exact solution is at r = s = 0.

Decreasing both ε and the mesh size gives convergence.

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