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MULTISCALE MATHEMATICAL AND PHYSICAL MODEL FOR THE STUDY OF NUCLEATION PROCESSES IN METEOROLOGY

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ABSTRACT. The development of numerical models for meteorological analysis is often based on nonlinear equations systems describing complex fluids, having more components and for which generalized Navier-Stokes equations are used. In several real cases it is necessary to use numerical calculation approaches in which the equations are discretized. The aim of this contribution is working out results regarding the optimization of the performance of a mathematical-physical model, formulated for meteorology forecasts in limited and high resolution area, and obtained by interdisciplinary studies. In particular, in order to test the validity of the presented model, different microphysical parameterizations have been analyzed, every one taking into account different hydrometeor nucleation processes.

1. Introduction

Dynamic meteorology represents the study of the physical laws that govern the behavior of the atmosphere. These laws can be expressed by means of a system of differential equations, whose resolution allows to provide a description of the future state of the atmosphere starting from a present state. However, the problem is not easy to solve, both from a mathematical and a physical point of view. The number and quality of information on the initial values of the investigated physical fields, the adequacy of the approximations introduced in the equations in order to obtain a mathematically solvable system, and the efficiency of the numerical integration algorithm of the system thus obtained, are parameters fundamental for the reliability of a numerical meteorological forecast. The references for the Numerical Weather Prediction (NWP) are made up of Global Models (GM) and Limited Area Models (LAM). Global Models are used to simulate the evolution of the dynamic state of the atmosphere of the entire planet on a spatial grid with a horizontal pitch of tens of kilometres. The initialization data of the Global Models are provided by the observing synoptic terrestrial stations (about 15000) to which the approximately 3300 boe are added and by the data coming from satellite analyzes, radio soundings. The Limited Area Models, also called "mesoscale" models, allow to enrich the information on a large scale with those provided on mesoscale by a higher resolution forecast (Orlanski 1975;

Wallace and Hobbs 1977; Pielke 2002). The original purpose of the limited area modelling consists in a more accurate description of the phenomena of scale than that provided by the Global Models. In recent years, the further development of LAM, associated with a greater description of physical processes, the introduction of schemes that allow to explicitly deal with microphysics, as well as the implementation of non-hydrostatic schemes, has made it possible to widen the field of applicability of these models.

2. The WRF model

The limited area model Weather Research Forecast (WRF) (Skamarock 2008) is a numerical prediction system realized in collaboration between the National Center for Atmospheric Research (NCAR), the National Center for Environmental Prediction (NCEP) and the Earth System Research Laboratory (ESRL) of the National Oceanic and Atmospheric Administration (NOAA). The WRF has both scientific purposes (for example for the numerical simulation of atmospheric dynamics), and for more operative purposes, such as the operative numerical prediction. The structure of the model is a central core, called the WRF Software Framework (WSF), constituted of different assimilation and parameterization schemes of the physical variables. The pre and post processing modules are connected to it. The phase of pre-processing (WPS) includes three calculation routines, Geogrid, Ungrib and Metgrid that in sequence are responsible for processing the data that feeds the model. In particular, Geogrid creates static data that includes geographic data and land use data, Ungrib assimilates the meteorological data in GRIB format collected by the global calculation centers, and finally Metgrid interpolates the horizontal meteorological data, scaling them on the domain originally defined. The data thus pre-processed, are passed to other calculation routines, and specifically to the WRF-REAL software that vertically interpolates the data in the spatial coordinates of the model. The final phase of the process is the production of output data originated from the software WRF and the subsequent graphic production (post-processing). Two different "core" govern the dynamics of the WRF model: Advanced Research WRF (ARW), calculation code developed by NCAR, able to simulate different types of meteorological events with different spatial resolutions, and Non-hydrostatic Mesoscale Model (NMM), developed by NCEP, able to operate in both hydrostatic and non-hydrostatic modes. The ARW "core" is generally dedicated to research applications and requires more computing resources, while the latter has finality operative.

3. The prognostic equations of the model

Limited area models are mostly non-hydrostatic. Under these conditions the vertical equation does not follow the hydrostatic approximation:

$$dp = -p\rho dz \tag{1}$$

Therefore the vertical speed turns out to be an unknown factor of the system. To overcome this problem it is possible to use the terrain-following coordinates η as a vertical coordinate (Laprise 1991):

$$\eta = \frac{p_h - p_{ht}}{\mu} \tag{2}$$

where:

- $\mu = p_{hs} - p_{ht}$ it is directly associated with the mass of the air column per surface unit;
- p_h it is the hydrostatic component of pressure
- p_{ht} it is the pressure at the upper (fictitious) edge of the atmosphere;
- p_{hs} it is the pressure at the surface.

The WRF model integrates differential equations to the nonlinear partial derivatives defined as follows (Ooyama 1990). Introducing the appropriate flux form variables:

$$V = \mu v = (U, V, W) \quad ; \quad v = (u, v, w) \quad ; \quad \Omega = \mu \dot{\eta} \quad ; \quad \Theta = v\theta \tag{3}$$

where:

- $v = (u, v, w)$ it is the covariant velocities in the two horizontal and vertical directions, respectively;
- $\omega = \dot{\eta}$ is the contra variant vertical velocity;
- θ it is the potential temperature, that is the temperature of an air particle that is adiabatically brought to the altitude of 1000 hPa.

and considering the following variables:

- $\phi = gz$ is the geo-potential, that is the work necessary to overcome the force of gravity and move upwards, at a given height, a unitary mass of air;
- $\alpha = \frac{1}{\rho}$ is the inverse of the density;
- $p = p_0(R_d\theta/p_0\alpha)^\gamma$ is the equation of state with R_d constant of the dry air gases, $\gamma = \frac{c_p}{c_V} = 1,4$ and p_0 the pressure reference, typically 10^5 Pa;
- $\partial_n\phi = -\alpha\mu$ is the diagnostic relationship for density;

it is possible to derive the differential equations to the partial, non-linear, fundamental derivatives of the model:

$$\partial_t U + (\nabla \cdot Vu) - \partial_x(p\phi_\eta) + \partial_\eta(p\phi_x) = F_U \tag{4}$$

$$\partial_t V + (\nabla \cdot Vv) - \partial_y(p\phi_\eta) + \partial_\eta(p\phi_y) = F_V \tag{5}$$

$$\partial_t W + (\nabla \cdot Vw) - g(\partial_\eta p - \mu) = F_W \tag{6}$$

$$\partial_t \Theta + (\nabla \cdot V\theta) = F_\Theta \tag{7}$$

$$\partial_t \mu + (\nabla \cdot V) = 0 \tag{8}$$

$$\partial_t \phi + \mu^{-1}[(V \cdot \nabla\phi) - gW] = 0 \tag{9}$$

where F_U, F_V, F_W, F_Θ represent forcing terms arising from model physics, turbulent mixing, spherical projections, and the earth's rotation.

The Eqs.(4)-(9) have been calculated not taking into account a fundamental parameter from the meteorological point of view, the moisture. In fact it is responsible for the most important effects on atmospheric dynamics to which the release of latent heat is associated. Furthermore, water vapor and clouds play a fundamental role in the reflection, absorption and emission of both solar and terrestrial radiation. Therefore, it is necessary to reformulate the previous equations taking into account the effect of moisture, but keeping the prognostic variables and the vertical coordinate coupled with the mass of dry air.

The appropriate flux form variables considering the terms of dry air (subscript d) can be written as follows:

$$V = \mu_d v \quad ; \quad \Omega = \mu_d \dot{\eta} \quad ; \quad \Theta = \mu_d \theta \quad ; \quad \eta = \frac{p_{dh} - p_{dht}}{\mu_d} \quad ; \quad \mu_d = p_{dhs} - p_{dht} \tag{10}$$

Adding an additional conservation equation to include water mixing ratios in all of its phases:

$$\partial_t Q_m + (\nabla \cdot V q_m) = F_{Qm} \tag{11}$$

where:

$$Q_m = \mu_d q_m \tag{12}$$

and

$$q_m = q_v, q_c, q_i, q_r, q_s \tag{13}$$

are the mixing ratio of water vapor (q_v), liquid water of the cloud (q_c), ice (q_i) and of all the hydrometeors that the model considers.

Finally, it is possible to rewrite the modified fundamental equations of model, taking into account the moisture, as follows:

$$\partial_t U + (\nabla \cdot V u) + \mu_d \alpha \partial_x p + (\alpha/\alpha_d) \partial_\eta p \partial_x \phi) = F_U \tag{14}$$

$$\partial_t V + (\nabla \cdot V v) + \mu_d \alpha \partial_y p + (\alpha/\alpha_d) \partial_\eta p \partial_y \phi) = F_V \tag{15}$$

$$\partial_t W + (\nabla \cdot V w) - g[(\alpha/\alpha_d) \partial_\eta p - \mu_d] = F_W \tag{16}$$

$$\partial_t \Theta + (\nabla \cdot V \theta) = F_\Theta \tag{17}$$

$$\partial_t \mu_d + (\nabla \cdot V) = 0 \tag{18}$$

$$\partial_t \phi + \mu_d^{-1} [(V \cdot \nabla \phi) - gW] = 0 \tag{19}$$

$$\partial_t Q_m + (\nabla \cdot V q_m) = F_{Qm} \tag{20}$$

where:

- $\alpha_d = \frac{1}{\rho_d}$ is the inverse of the density of dry air;
- α is the inverse of density, and takes into account the mixing ratios of the various entities present in the volume of air considered.

Analytically we have that:

$$\alpha = \alpha_d (1 + q_v + q_c + q_i + q_r + q_s + \ldots) \tag{21}$$

being:

- $\partial_\eta \phi = -\alpha_d \mu_d$ the diagnostic relationship for density;

- $p = p_0(R_d\theta_m)/(p_0\alpha_d)^\gamma$ the diagnostic equation for total pressure (vapor plus dry air).

In (20), which represents the diagnostic equation for total pressure (vapor plus dry air), the potential temperature θ_m is given by:

$$\theta_m = \theta[1+(R_v/R_d)q_v] \quad \approx \quad \theta(1+1.61q_v) \tag{22}$$

Such systems of non-linear equations to partial derivatives can not be solved analytically. The solution is obtained by numerical calculation methods in which the equations are discretized and resolved on a grid.

There are numerous numerical techniques but most LAM models use finite difference schemes. This technique approximates the spatial and time derivatives by means of a series development of Taylor appropriately truncated, in which the increments are represented by the spatial and time grid pitch.

4. Model physical parametrization

The presence of sources and wells energy associated with flows heat, water vapor and momentum, near the Earth's surface, in the Planetary Boundary Layer (PBL), and finally in the free atmosphere above PBL, are physical aspects that must be considered and schematized in the structure of a numerical model for meteorological simulation (Skamarock 2008).

Furthermore, radiative effects and water phase changes must be schematized. Many of these physical processes occur on scales smaller than that defined by the spatial grid (subgrid scale processes). It is therefore necessary to treat them with a different methodology from that of explicit simulation, which goes by the name of "parametrization".

The terms to be parametrized appear in the prognostic equations either as terms of source or well, or as terms with unresolved scale, or as terms of correlation between sub-grid variables. This is a direct consequence of the non-linearity of the equations integrated by the model. In order for the equation system to be "closed" in the unknowns it is necessary that the terms of sub-grid correlation are expressed as a function of the unknowns themselves.

A schematics of such a parametrization is depicted in Figure 1.

5. Microphysics

When a portion of moist air reaches the condensation level, the formation of the liquid phase takes place through an intermediate passage, called nucleation (Fletcher 1962; Lin *et al.* 1983; Walko *et al.* 1995; Ryan 1996; Hong *et al.* 2004; Morison and Pinto 2005; Hong and Lim 2006; Hong *et al.* 2008; Morrison and Thompson 2009; Lim and Hong 2010). Nucleation can be homogeneous or heterogeneous.

In the first case (often negligible) there is the formation of droplets without the intervention of external elements. In the second case there is the intervention of an external element (atmospheric aerosol) that acts as an aggregator.

Consider the case in which a sufficient quantity of water is deposited around a wettable aerosol, so as to form a film that envelopes it. From that point on, the aerosol is approximated to a drop of water. When the drop reaches the size of a few microns then come into play a series of processes that influence the subsequent evolution of these droplets.

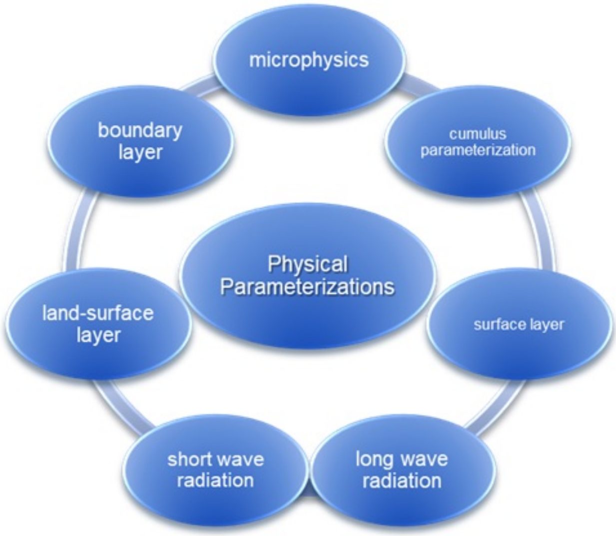

FIGURE 1. Scheme of the physical parametrization used in the limited area models.

These processes are:

- Coalescence: process of growth of the droplets by impact and by aggregation, strongly dependent on the diameter of the drops and their relative speed.
- Breakup: fractionation of the drops; experimentally the probability of breaking a drop is an exponential function of the ray of the drop itself.
- Evaporation: happens when some drops are transported on unsaturated areas; it is a function of air humidity, saturation humidity and the content of drops in the air.

This is generally valid for liquid drops. We now introduce the main processes that take place inside the clouds when it extends below 273 Kelvin (cold cloud). In case the temperature is below the freezing level, drops of liquid water can coexist with icy particles. This drop is in an unstable state but, in order to freeze it, similarly to the nucleation already seen, one must form within the drop an ice embryo large enough (with a radius greater than the critical ray) to grow. Because the number and size of these embryos grows as the temperature decreases, below a certain temperature, icing is a certain phenomenon. Also in this case, the heterogeneous nucleation is strongly advantageous compared to the homogeneous nucleation. The ice crystals formed, still too light to precipitate, can increase the size by diffusion or by aggregation. Based on the processes these particles undergo, various classes of solid hydrometeors are created. The residence time in the atmosphere of these liquid and solid particles is linked to the intensity of the ascension currents, to the state (solid / liquid), to the size of the particles, in turn related to the degree of over-saturation of the environment, as well as to the time of permanence in the atmosphere itself. It is also necessary keep in mind the heat fluxes coming from the outside of the cloud, both related to the state transitions that take place inside the cloud. It is therefore evident that it is not possible to accurately describe the various phenomena presented. For this purpose, in the numerical models of meteorological forecasting, the microphysical parametrization schemes were introduced, aimed at the representation of these processes. The goodness of the adopted scheme is connected to the model's ability to describe atmospheric water in its various states: there are usually six classes of hydrometeor, two liquids (liquid water in the cloud and rain) and four solids (ice crystals, snow, hail and graupel). The general approach in meteorological modelling is to define, for each hydrometeor class, m equations analogous to Eq.(11):

$$\partial_t Q_m + \partial_x (U q_m) + \partial_y (V q_m) = -\partial_\eta (\Omega_s q_m) + D_{q_m} + S_{q_m} \tag{23}$$

where the terms of sedimentation rate, Ω_s, and diffusion rate, D_{q_m}, are a function of the size of the particles and are calculated assuming a particular statistical distribution (generally gamma or exponential distribution) of the particle diameter. The source terms present in the Eq.(23), indicated collectively with S_{q_m}, describe each a particular microphysical process (nucleation, growth, fusion, etc ...) associated with the various classes of hydrometeors considered. Considering, for example, the diameters of a certain hydrometeora m distributed according to the exponential distribution function:

$$N_m(D) = N_{0m} e^{(-\lambda_m D_m)}, \tag{24}$$

in order to close Eq.(23), it is necessary to write the terms Ω_s, D_{q_m} and S_{q_m} as a function of the mixing ratio (prognostic variable of the equation). If N_{0m} in Eq.(24) is known, for example from experimental observations, integrating the distribution on all diameters, assuming the density ρ_m is known, it is possible to calculate the total mass M of each species in the volume considered, and therefore also the mixing ratio , as a function of λ_m:

$$M_m = \frac{\pi \rho_m}{6} \int_0^\infty D^3 N_m(D) dD = \frac{\pi \rho_m}{6} \int_0^\infty D^3 N_{0m} e^{(-\lambda_m D_m)} dD \tag{25}$$

Inverting the relation, λ_m can therefore be expressed as a function of the density (known quantity) and of the mixing ratio, and then obtain the distribution expressed in Eq.(24) as a function of the mixing ratio. The terms Ω_s, D_{q_m} and S_{q_m} can also be expressed as a function of Q_m. Similar considerations can be made in the presence of an additional prognostic equation for the concentration (double moment diagram) (Morison and Pinto 2005).

The schemes of parametrization of the microphysics of the clouds therefore play a key role in the refinement of forecast models.

6. Study Case: 6^{th} January 2017

A center of low pressure that, between the days of 5^{th} and 7^{th} January 2017, moved from the central south of the Italian peninsula to the coast of Greece, pushed cold air masses from Siberia causing the temperatures to collapse throughout Italy. The marked atmospheric instability and the strong icy winds coming from the northern quadrants, on 6^{th} January 2017, recorded heavy snowfalls throughout the Sicilian regional territory. Snowfalls at very low altitudes have also been recorded in the province of Messina. In particular, snowfalls were recorded on the Ionian coast of Messina.

In the present case study, the numerical simulations of the WRF limited area model are analyzed. The performances of the WRF model, appropriately optimized for Sicily (territory characterized by a complex orography) provide considerable support in various

FIGURE 2. Map of the spatial domain used by the WRF model. The domain is centered on Sicily. The model is configured with horizontal grid spacing of 5km and a time interval resolution of 1h.

multidisciplinary fields (Caccamo *et al.* 2017; Castorina *et al.* 2017; Colombo *et al.* 2017; Castorina *et al.* 2018).

The model is configured with horizontal grid spacing of 5km (see Figure 2) came out by a single-run. The model configuration uses 65 vertical levels with a maximum height of 50 hPa. The global model GFS at 0.25 degrees with a time interval resolution of 1h, processed for the 00Z run relative to the 24 November 2016 have generated the initial and boundary conditions. RTG sea surface temperature data with a resolution of 0.083 degrees were used. For long-wave and short-wave radiations the RRTMG scheme was used. In addition the above, were also used the schemes of Mellor-Yamada-Janjic for the boundary layer and Noah land surface model.

In the specific case, it is wanted to evaluate the performance of the model at the varies of a microphysicals parameterization. The parametric schemes for the ETA Ferrier microphysics (MP5), WSM6 (MP6) and Thompson (MP8) were examined. In both cases there are single moment schemes in which six classes of hydrometeors are considered. Specifically, the ETA Ferrier scheme considers the size of the hydrometeors as a function of temperature following Ryan's observations (Ryan 1996). Processes between one phase and another of water for temperatures above *243 K* are possible, while for lower temperatures only the solid phase is considered. The density of the various particles is considered a function of the growth processes to which the particles themselves are subjected. The WSM6 scheme pays particular attention to the concentration of ice crystals in relation to the temperature and to the total mass of ice present in the volume considered (Fletcher 1962). The distribution of the diameters is assumed exponentially and, during the precipitation of the particles, the melting / freezing processes are also calculated to increase the accuracy of the vertical profile relative to the release / absorption of heat (Hong *et al.* 2004).

Finally, in the Thompson scheme the snow size distribution is assumed to be a function both of the ice content of the volume considered, and of the temperature and is represented as a combination of the gamma and exponential distributions (Morrison and Thompson 2009), while for the distribution of the diameters of the other hydrometeors a generalized gamma distribution is used (Walko *et al.* 1995). The density of the snow is supposed to vary inversely proportional to the diameter, unlike what is assumed by many schemes, where it is considered constant.

Figure 3 shows the results of simulations in which only the microphysics parametrization scheme has been modified. To highlight the differences, the total rain recorded in the 24 hours and the Snow Water Equivalent (i.e. the international unit to measure the amount of snowpack expressed in kg/m^2) are shown.

The visual analysis of the forecast maps shown in Figure 3 shows a substantial agreement in the total precipitation accumulated over the 24 hours. The MP6 microphysical scheme provided slightly higher pluviometric accumulations than the remaining schemes (MP5 and MP8). A substantial difference, however, is highlighted in the Snow Water Equivalent. The MP6 microphysical scheme, unlike the MP5 and MP8 schemes, was the only one to forecast, with 24 hours in advance, the snowfalls recorded on the Ionian coast of the province of Messina.

7. Conclusions

Systems of nonlinear equations, such as the generalized Navier-Stokes equations, and the parametrization of physical processes, form the basis of numerical models for meteorological analysis. The purpose of this contribution is to evaluate the performance of the meteorological model presented to the variation of the microphysical parameters, each of which takes into consideration different processes of nucleation of the hydrometeor. Specifically, a particular climatic event was considered as a case study. Between the days of 6 and 7 January 2017, frigid air masses from Siberia, caused a significant drop in temperatures throughout the Sicilian territory, making intense snowfalls recorded at very low altitudes.

The analysis of the forecast maps shows how the WSM6 microphysical scheme (MP6), unlike the ETA Ferrier microphysics (MP5), and Thompson (MP8), was the only one to forecast, with 24 hours in advance, the snowfalls recorded on the Ionian coast of the province of Messina.

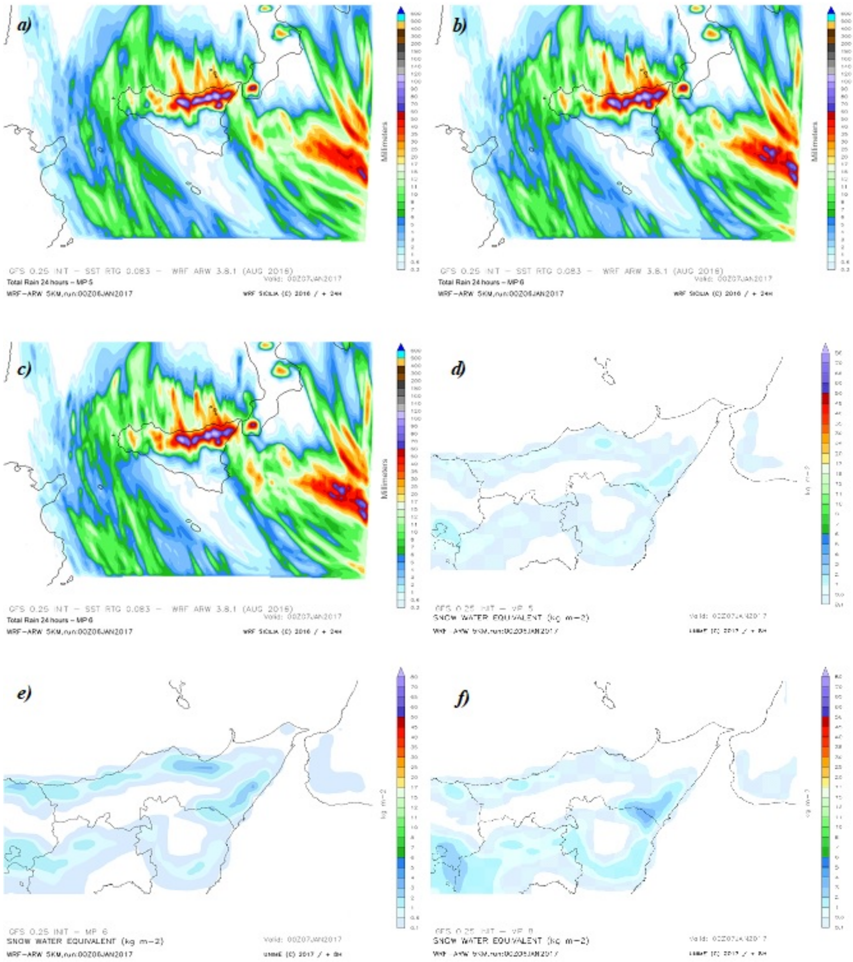

FIGURE 3. Simulations in which only the microphysics parametrization scheme has been modified. (a) Total rain recorded in the 24 hours through MP5, (b) Total rain recorded in the 24 hours through MP6, (c) Total rain recorded in the 24 hours through MP8, (d) Snow Water Equivalent through MP5, (e) Snow Water Equivalent through MP6, (f) Snow Water Equivalent through MP8.

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