LAGRANGIAN TRANSPORT MODELING

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ABSTRACT

Numerical simulations of Lagrangian tracer dynamics in ocean or atmosphere need a particular care, and some important issues must be considered. First, the finite resolution of general circulation models imposes severe limitations on the reconstruction of the velocity fields below certain scales of motion. Second, the unresolved small-scale components should be somehow replaced by suitable sub-grid parameterizations. Non linear multi-scale flows may generate chaotic, turbulent-like, Lagrangian trajectories, even at low Reynolds numbers. We exploit this property to build up deterministic kinematic models of sub-grid turbulent diffusion. We present applications for tracer transport in the Mediterranean Sea and for marine aerosol deposition over Salento peninsula.

Key words: Lagrangian chaos, turbulence, ocean modeling, tracer transport .

1. INTRODUCTION

Transport phenomena in fluids like the ocean or the atmosphere play a relevant role in applicative issues like diffusion and mixing of bio-chemical reactive species, pollutant dispersion, search and rescue (SAR) operations, etc, as well as in studies addressing questions connected to the theory of turbulence. To model and measure Lagrangian dispersion properties we exploit established mathematical tools, developed and refined in the framework of the dynamical system theory. On one hand, relative dispersion, i.e. the rate of separation between two fluid particles, since it is inherently a scale-dependent process, is characterized by computing the Finite-Scale Lyapunov Exponent (FSLE), i.e. the generalization of the maximum Lyapunov exponent to finite-size perturbation. On the other hand, turbulent trajectories, i.e. fluid particles that statistically fulfill the properties of turbulent dynamics, are simulated by means of deterministic, non linear kinematic fields, containing a series of independent spatial modes. The kind of kinematic models we have developed are not affected by "sweeping effects", thanks to the use of a quasi-Lagrangian reference frame, and allow one to explain the turbulent properties of the trajectories in more physical terms with respect to other methods. In numerical simulations, large-scale dynamics is reconstructed, with good accuracy, by general circulation models. Sub-grid motions, instead, must be necessarily parameterized and we adopt, for this task, our kinematic models calibrated on observative data. This modeling apparatus forms a Lagrangian Tracking System which can be employed in several contexts. The FSLE technique not only allows one to measure the scale-dependent dispersion rates, but also provides an instrument to check and validate model current fields from a Lagrangian point of view. We present applications in oceanography and atmospheric dynamics. As regards to the marine environment, we addressed the problem of characterizing the effects of the Lagrangian transport, in the Sicily Channel, on the dispersal of Anchovy larvae from a spawning area to a recruitment area. In particular, the interannual fluctuations of the transport efficiency have been characterized by means of a Lagrangian Transport Index (LTI). Another study concerns the localization of the release point of a set of tracers in the Mediterranean sea, with the backward trajectory simulation technique. Reverse drifter motion is used as paradigm for source localization problem. The first-kind FSLE, or FSLE-I, is commonly used to measure relative dispersion rates of model or experimental trajectories. The second-kind FSLE, or FSLE-II, instead, is specifically defined to measure the scale-dependent error between model and observation. At this regard, we have tested the Mediterranean Forecasting System (MFS) model against actual drifter motion, and have implemented a 2D parameterization of mesoscale dynamics which restores the effects of poorly resolved velocity modes on the tracer dispersion in the sea upper layer. As far as the atmosphere is concerned, we show the results of a preliminary Lagrangian simulation where marine aerosol particles, released along the coastlines of Salento peninsula, are advected in a double-breeze regime simulated by the WRF model [1]. Planetary Boundary Layer (PBL) turbulence is modeled by means of a 3D kinematic multi-scale convective model which avoids unrealistic particle clustering due to the lack of small-scale mixing of the WRF model.

2. METHOD

2.1. Measuring Dispersion: FSLE

The Finite-Scale Lyapunov Exponent (FSLE) has become by now an established tool in Lagrangian studies. It is a non linear, scale-dependent indicator that accurately describes both the scaling properties and the physical parameters characterizing turbulent dispersion [4]. Historically, the FSLE was born as generalization of the maximum Lyapunov exponent to non infinitesimal perturbations. In a Lagrangian dynamics context, it becomes a natural measure of the dispersion rate at a given separation between particles. Given a series of n scales $\delta_1, \delta_2, ..., \delta_n$, such that $\delta_{m+1} = \rho\delta_m$ for $m = 1, 2, ..., n-1$, with $\rho > 1$, the FSLE $\lambda(\delta)$ is defined as:

$$\lambda(\delta) = \frac{\ln \rho}{\langle \tau(\delta) \rangle} \tag{1}$$

where $\tau(\delta)$ is the first exit time of the particle separation from the shell δ to the next-neighbour shell $\rho\delta$, and $\langle \cdot \rangle$ indicates the average over all the available phase space. We agree to distinguish between first-kind FSLE, or FSLE-I, and second-kind FSLE, or FSLE-II, depending on the nature of the "perturbation" δ: FSLE-I measures the separation rate of two homogeneous trajectories that belong to the same dynamical system; FSLE-II measures the separation rate of two heterogeneous trajectories that belong to different dynamical systems but sharing the same phase space. General scaling properties hold for both quantities. In a general scenario of 3D isotropic and homogeneous turbulence, in presence of direct energy cascade, the FSLE-I goes like:

$\lambda(\delta) \sim \lambda_L$=constant, for $\delta \to 0$, where λ_L is the Lagrangian maximum Lyapunov exponent;

$\lambda(\delta) \sim \epsilon^{1/3}\delta^{-2/3}$, inside the inertial range, where ϵ is the turbulent dissipation rate;

$\lambda(\delta) \sim K\delta^{-2}$, for $\delta \to \infty$, where K is the asymptotic eddy-diffusion coefficient.

Similar laws hold for 2D homogeneous and isotropic turbulence where energy is injected at a forcing scale δ_f:

$\lambda(\delta) \sim$constant, for $\delta < \delta_f$, in direct enstrophy cascade;

$\lambda(\delta) \sim \epsilon^{1/3}\delta^{-2/3}$, for $\delta > \delta_f$, in inverse energy cascade;

Again, standard diffusion $\lambda(\delta) \sim \delta^{-2}$ normally occurs for asymptotically large particle separations.

As regards to FSLE-II, it is assumed to diverge as δ^{-1} in the limit $\delta \to 0$, because of non zero model errors, while, on the other hand, it is expected to converge to the FSLE-I for sufficiently large δ, i.e. when the model error is "absorbed" by the instrinsic chaoticity of the system. Significant improvements of the model, e.g. change of resolution, refinement of parameterizations, etc, should imply a decreasing of the threshold scale at which FSLE-I and FSLE-II coincide, that is why this test can be used as a method to validate model fields against observations, at least from what concerns the Lagrangian transport properties.

2.2. Modelling Dispersion: KLM

When it comes to parameterize unresolved turbulent motions in large circulation models, one can adopt various techniques. One is based on stochastic diffusion models, in which particles velocity is driven by random noise in a suitable Langevin equation. Another one is based on deterministic, multiscale, nonlinear velocity fields, in which Lagrangian Chaos is the key mechanism that gives rise, ultimately, to turbulent-like trajectory evolution. This is the one we adopt in our applications, also defined as Kinematic Lagrangian Modelling, or KLM. For simplicity, we define a non divergent velocity field as the curl of a "potential vector function":

$$\mathbf{u}(\mathbf{x}, t) = \nabla \times \psi(\mathbf{x}, t) \tag{2}$$

where $\psi = (\psi_1, \psi_2, \psi_3)$ is a sufficiently regular potential vector function, $\mathbf{x}$ is the position vector of a fluid particle and $\mathbf{u}$ its velocity in $\mathbf{x}$ at time t. The choice for the analytical expression of ψ, and therefore $\mathbf{u}$, is not unique. We define the kinematic velocity field as a series of N_m independent spatial modes, each one characterized by a regular pattern of convective cells of size l_n and turnover time t_n, for $n = 1, 2, ..., N_m$. Richardson law for particle dispersion, expected to hold in the $k^{-5/3}$ Kolmogorov spectral range, can be efficiently simulated by assigning the appropriate scaling rule to the mode velocity with the eddy size, i.e. $v_n \sim (\epsilon l_n)^{1/3}$, where ϵ is the turbulent dissipation rate. Lagrangian simulations of two particle dispersion must take into account the problem arising from the "sweeping effect", always present in models where the velocity field structures do not move from their initial positions, i.e. where the small-scale eddies do not follow the large-scale advection. This drawback can be overtaken if one adopts quasi-Lagrangian coordinates, i.e. computing the kinematic field in a reference frame anchored to the mass center of two moving particles. In the 2D approximation, the velocity field can be defined in a similar way, but in this case the Kolmogorov spectrum refers to the inverse mesoscale cascade regime. We will present and discuss applications of the kinematic modelling technique to problems related to the ocean upper layer and to the planetary boundary layer.

3. RESULTS: THE LTS

The full Lagrangian Tracking System, or LTS, consists in large-scale current fields given by some general cir-

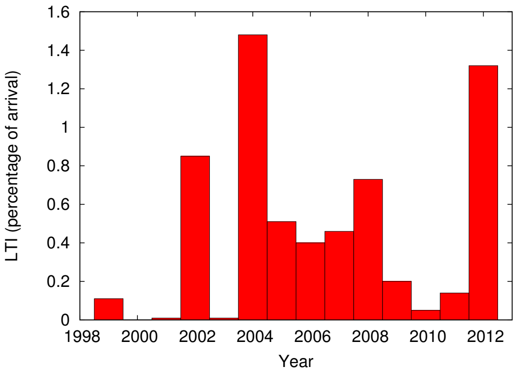

Figure 1. Lagrangian Transport Index year by year displaying high interannual variability.

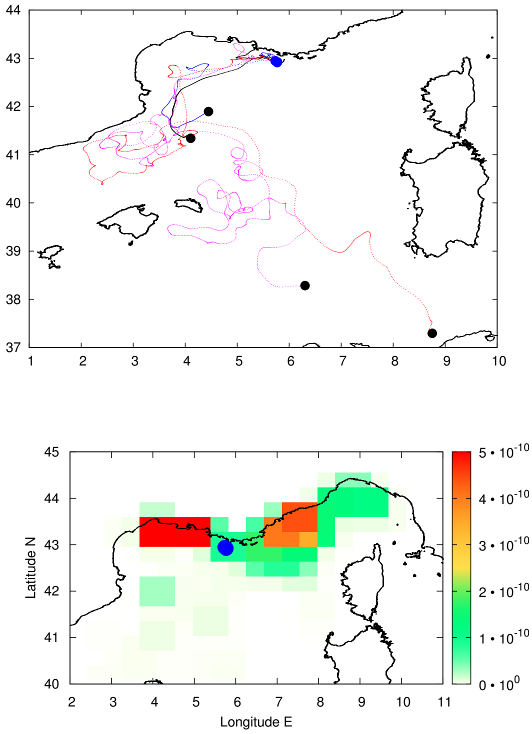

Figure 2. Top: four initially close drifters simulate tracer dispersion in various directions. Bottom: Intersection area of backward trajectory sets at the release date (MFS+KLM)

culation model; subgrid parameterization of unresolved, or poorly resolved motions; evolution equations for the Lagrangian trajectories associated to the considered flow. We present and discuss, briefly, some results related to applications in ocean and atmosphere.

3.1. Anchovy larva dispersal in the Sicily Channel

Using the Mediterranean Forecasting System current fields [2] and parameterizing the sub-grid scale dynamics in terms of kinematic fields we can define a Lagrangian Transport Index (LTI) which measures the Lagrangian Connectivity in the Sicily Channel, between an anchovy spawning area near Sciacca and a recruitment area near Cape Passero. Larvae are mixed by 3D and 2D turbulence and follow the Diel Vertical Motion (DVM) while large scale transport is mainly driven by meandering currents like the Atlantic ionian Stream (AIS). According to DVM, larvae go up near the surface during daytime while the sink to deeper water during night-time. The LTI is defined as the percentage of larvae arriving alive at the recruitment area. The average arrival time is estimated of the order of some days. We show the inter annual evolution of the LTI in Fig.1.

Comparison with observative biological data supports the results obtained with the numerical simulations about the role of advection in modulating the abundance of juveniles in the selected area and, also, helps explain their origin [3].

3.2. Reverse drifter motion in Mediterranean Sea

The Mediterranean Forecasting System (MFS) ocean model is used, in this case, to test a technique based on reverse trajectory motion aimed at identifying the common source of various tracers observed in different places at different times. In this application, we restrict the study to 2D motion on the ocean surface layer. Large scale velocity fields are provided by MFS while mesoscale turbulent motions are parameterized by our kinematic Lagrangian model (KLM). The uncertainty in the trajectory position generally grows both forward and backward in time, and the correct growth rate of the error at small scales is granted by the presence of the KLM parameterization. Assigning a probability distribution function to each observed tracer at a given time, of initial size suitably determined, we can simulate backward motion up to the date of the release and look for the intersection of all the pdf's. If the method works, the release area is contained in the intersection area. For our test we consider four ocean drifters simultaneously released in the Mediterranean Sea at close distance from each other, order $\sim O(1)$ km. We take their final positions at different times from the release date (of the order of some months), we define an initial error distribution of size $\sim O(10)$ km and then integrate each numerical trajectory set with the MFS+KLM system back to the release date. We find that the release area is contained in the pdf intersection, with a localization uncertainty of order $\sim O(50)$ km, as shown in Fig. 2. This result is promising as regards to further applications in Search and Rescue (SAR) problems like, e.g., pollutant emissions, oil spill, wreckage recovery, etc.

3.3. Lagrangian predictability analysis of first and second kind

The Mediterranean Forecasting System (MFS) Ocean Model [2] , has been chosen as case study to analyze Lagrangian trajectory predictability by means of a dynamical systems approach. To this regard, numerical trajectories are tested against a large amount of Mediterranean drifter data, used as sample of the actual tracer dynamics across the sea. The separation rate of a trajectory pair is measured by computing the Finite-Scale Lyapunov Exponent (FSLE), of first and second kind, depending if the two trajectories belong to the same dynamical system or to two different dynamical systems sharing the same phase space. Our kinematic Lagrangian model (KLM), suitably treated to avoid "sweeping"-related problems, has been nested into the MFS in order to recover, in a statistical sense, the velocity field contributions to pair particle dispersion, at mesoscale level, smoothed out by finite resolution effects. The main results emerging from this work are [5]:

a) drifter pair dispersion displays Richardson's turbulent diffusion inside the [10-100] km range, while numerical simulations of MFS alone (i.e. without subgrid model) indicate exponential separation;

b) adding the subgrid model, model pair dispersion gets very close to observed data, indicating that KLM is effective in filling the energy "mesoscale gap" present in MFS velocity fields;

c) there exists a threshold size beyond which pair dispersion becomes weakly sensitive to the difference between model and "real" dynamics;

d) the whole methodology here presented can be used to quantify model errors and validate numerical current fields, as far as forecasts of Lagrangian dispersion are concerned.

As far as Lagrangian predictability is concerned, we recall that the second-kind Finite-Scale Lyapunov Exponent, FSLE-II, measures the growth rate of the error between a "model" trajectory and a "true" trajectory, sharing the same phase space. The scale where FSLE-II rejoins FSLE-I (if any) is the threshold after which the model error is absorbed by the instrinsic error growth due to the nonlinearities present in the model equations, i.e. when the "true" trajectory becomes undistinguishable from the "model" trajectories, as far as the dispersion process is concerned.

We present here a case study on the Mediterranean Sea. First we perform a Lagrangian analysis of the model current fields. Then we add the sub-grid model (KLM) as a multi-scale, deterministic 2D mesoscale field nested into MFS large-scale field. The sub-grid model is calibrated on the of the inverse cascade parameters obtained by means of the FSLE technique on real drifters. Results are shown in Fig.3. For more details see [5].

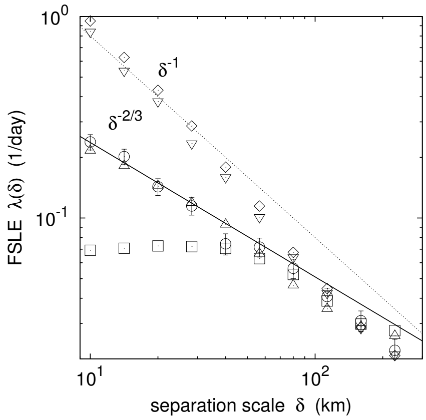

Figure 3. FSLE-I relative to: (◯) drifter data; (□) MFS data only; (△) MFS+KLM data. FSLE-II relative to: (▽) MFS vs drifters; (◇) MFS+KLM vs drifters. After [5]

3.4. Transport and deposition of marine aerosol over Salento

The mesoscale simulation is performed with the WRF model which solves the fully compressible, non hydrostatic Euler equations. The model uses the terrain-following, hydrostatic-pressure vertical coordinate with vertical grid stretching; the forty vertical levels used in the present study are more closely spaced in the boundary layer, with the first vertical level located below 100 m. The ECMWF analysis and forecasts (with resolution approximately equal to 0.351 in latitude/longitude) are used respectively as initial and 3-hourly boundary conditions; The period simulated with the WRF model lasts from 5 to 8 July 2005 and is characterized by a levelled pressure field and a weak synoptic forcing. The topography is nearly flat, and the region is influenced from spring to fall by complex breeze systems, caused by an intense diurnal heating cycle and modulated by the rough coastlines. The narrow extension of the region, combined with the presence of the sea along three of its sides, determines the convergence of two main breeze systems (a Ionian and an Adriatic SB) near the central axis of the peninsula in the central hours of the day in Summer.

Small-scale turbulence is parameterized by means of a 3D kinematic model simulating a direct cascade with dissipation rate of order 10^{-4} m^2 s^{-3}. In the Lagrangian simulation, aerosol production occurs at constant rate along the coastlines of Salento; the deposition velocity is set to 1 cm/s; the first hour after the emission is not taken into account for the statistics.

Since the grid mesh is irregular in the lon-lat domain, the Lagrangian simulation requires a non trivial interpolation procedure. We have adopted the Shepard's algorithm [6] restricted to the first next-neighbours points relative to the trajectory position. This allows to optimize the computational time taken by the numerical integration.

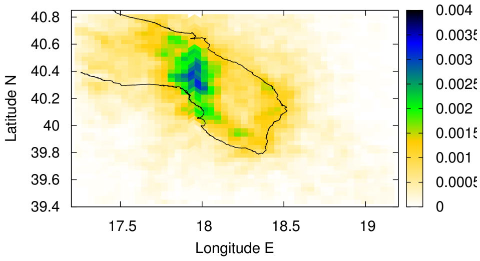

Figure 4. PDF of marine aerosol deposition after a 4-day simulation.

The case study we present concerns marine aerosol transport in a double-breeze regime. Aerosol particles are released at constant rate from the coastline of Salento peninsula and have a characteristic deposition velocity of 1 cm/s. The probability distribution function displays a preferential deposition over the hinterland of the peninsula, due to the convergence of the two sea breeze winds. Particle mixing at small scales is simulated by the action of the kinematic boundary layer turbulence.

4. CONCLUSIONS

Comparison with experimental data confirms that this kind of Lagrangian modelling is effective in simulating turbulent dispersion of tracers in ocean and atmosphere. The subgrid parameterization in terms of kinematic deterministic fields is effective in replacing, from a statistical point of view, the small-scale missing components in general circulation models, as far as Lagrangian motion is concerned. This kind of approach may have several applications also in biological connectivity, search and rescue issues and pollutant dispersion and source localization.

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