THE IMPACT OF CLIMATE CHANGE ON ATMOSPHERIC DISPERSION PROCESSES – A DYNAMICAL SYSTEMS APPROACH

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Final report

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(i) In the first part of the research, the question of how a changing climate influences the spreading of atmospheric pollutant clouds on continental and global scale was investigated by the Real Particle Lagrangian Trajectory (RePLaT) dispersion model, developed earlier by Tímea Haszpra (Haszpra and Tél, Nonlin. Proc. Geophys. 20(5), 867–881, 2013). In these simulations pollutant clouds consist of a large number of ideal tracers, corresponding to inert gases. For such particles, the velocity of a particle coincides with the velocity of the air at the location of the particle at any time instant. Due to the chaotic nature of advection, pollutant clouds spread in a filamentary, fractal structure, and the length of these filaments grows in an exponential manner in time. Thus, the intensity of large-scale spreading can be quantified by a measure of chaotic systems, by the so-called topological entropy (also called stretching rate in the atmospheric context), which describes the rate of the exponential increase. The larger the stretching rate, the faster the length of the pollutant cloud grows, and the more complicated and tortuous the shape of the filament is. As a measure of folding, it is also closely related to the predictability of the spreading of pollutant clouds.

We investigated the changes in the stretching rate utilizing the reanalysis fields of the ERA-Interim database for 1979–2015 (Haszpra, 2017). In order to study the geographical dependence of the stretching rate, 1-D pollutant clouds (line segments) were initialized uniformly distributed over the globe. The zonal-seasonal mean stretching rate displays a typical zonal distribution in each year with smaller values in the tropics and larger values in the extratropics. We showed that the largest stretching rates appear in the respective winter season of the hemispheres due to the more enhanced cyclonic activity. A slight increase of 3-10% in the values of the mean stretching rates from 1979 to 2015 is found. Larger stretching rate values indicate more intense spreading, more foldings and larger geographical areas reached by the pollutants. The increased mean stretching rate of the analyzed decades, therefore, implies the risk of larger polluted regions from particular pollution events.

Finding a relationship between the stretching rate and some meteorological variable could help estimate the changes of large-scale transport properties of the atmosphere in different climate projections without the necessity to carry out computationally costly extra spreading simulations. The largest correlation for the stretching rate (0.6-0.9) was found with the area-mean of the absolute value of the relative vorticity. Changes in the spreading intensity were also investigated using an ensemble of climate realizations produced by the intermediate-complexity climate model Planet Simulator (PlaSim, Fraedrich et al., Meteorol. Zeitschrift 14, 299–304, 2005) (Haszpra and Herein, 2019; Tél et al., 2020) to separate the effect of climate change and the fluctuations due to the internal variability of climate. By utilizing single ensemble members there are regions where the existence of a trend cannot be identified for the time interval of a surface temperature increase of 6 °C over 100 years, however, the ensemble mean of the stretching rate shows a clear decrease of 5-10%. The typical decrease of -0.05 day^{-1} implies that in year 100 the length of 10-day-old filaments is 61% of the length of the filaments initialized at the beginning of the temperature increase, thus, the length changes considerably.

Since PlaSim is sometimes criticized for being only an intermediate-complexity climate model, beyond the plans described in the research proposal, simulations were carried out using the 35-member ensemble of the state-of-the-art Community Earth System Model – Large Ensemble Project (CESM-LE, Kay et al., Bull. Am. Meteorol. Soc. 96, 1333–1349, 2015) (Haszpra and Herein, 2019; Tél et al., 2020). The zonal distribution of the stretching rate, the magnitude and decreasing nature of the trends are in harmony with the results obtained using the PlaSim meteorological data. Why this conclusion is different from that obtained from reanalysis data shall be studied in future work. The numerical results confirm the earlier conclusion that the changes in the intensity of spreading in arbitrary climate simulations can be estimated utilizing meteorological variables (i.e. relative vorticity or velocity data) operationally computed and stored by the climate models, without carrying out numerous computationally demanding dispersion simulations.

In the next part of the research the algorithmic precision of the RePLaT dispersion model has been improved (Haszpra, 2019). Another version of the improved RePLaT model was also created, called RePLaT-Chaos, applicable to educational purposes mainly for university students (http://theorphys.elte.hu/fiztan/volcano/index.html) (Haszpra, 2018a; Haszpra, 2020). Its main aim is an easy demonstration of the chaotic behavior of atmospheric pollutant spreading. The user-friendly graphical user interface helps the user carry out spreading simulations with several different parameters. In the spreading simulations, one can observe the typical characteristics of chaos, such as sensitivity to initial conditions, irregular motion, and complicated but well-organized (fractal) structures. It can be easily observed in the RePLaT-Chaos simulations that an initially compact pollutant cloud soon becomes strongly stretched; its length grows rapidly, while it becomes filamentary, tortuous and folded. RePLaT-Chaos can also compute two quantities that describe the chaoticity of the advection and the investigations of which are the main topics of this project. One of them is the stretching rate, and the other is the escape rate which quantifies the deposition rate of particles falling out from the atmosphere to the surface.

The RePLaT-Chaos-edu application (http://theorphys.elte.hu/fiztan/volcano/index.html#edu) is a version of RePLaT-Chaos with simplified user interface designed especially for secondary school education (Haszpra, 2018b; Haszpra et al., 2019). By means of RePLaT-Chaos-edu they can design their own "volcano eruptions". Here only those parameters can be set which students are familiar with, and the application includes eye-catching animations, more explanation and description for the observable phenomena. The RePLaT-Chaos-edu application was successfully used by students to become acquainted with the main features of the chaotic behavior and of the large-scale spreading of atmospheric pollutants during Physics classes at the Berzsenyi Dániel Grammar School and during two project weeks on chaotic phenomena at the Szent István Grammar School.

Beyond stretching, chaotic features in the lifetime distribution and deposition of atmospheric aerosol particles of realistic density (2000 kg/m^3) and radius (1–10 μm) were also investigated (Haszpra, 2019). Such particles emanate, e.g., from volcano eruptions, and, unlike for inert gases, a settling velocity is added to the background velocity field in their equation of motion. Due to this new term which represents gravity, the particles move downwards on average and remain in the atmosphere for a finite time. The number of particles not yet deposited from the atmosphere decays exponentially after a while, which is characteristic to transient chaos. The exponent is called escape rate. It describes the rapidity of the decrease, and its reciprocal can be used to estimate the average lifetime of the particles. We demonstrated that the geographical distribution of the individual lifetimes shows a filamentary, fractal distribution, typical for chaos: the lifetime of particles may be quite different at very close geographic locations (e.g., a few days vs. 150 days within 10 km for particles of radius of 5 μm). These maps can serve as atlases for the potential fate of volcanic ash clouds or of particles distributed for geoengineering purposes. We showed that the trajectories of nearby particles with similar lifetimes remain close to each other for a long time and they deposit at nearby locations. Thus, the boundaries between these types of coherent particle groups can be considered to form repelling Lagrangian coherent structures. The escape rate is associated with the exponential decrease in the number of long-living particles only. It was found to show a quadratic dependence on the particle size, but to be independent of initial altitude. The latter finding indicates the existence of a single global value of the escape rate and thus that of a unique chaotic saddle in the atmosphere. We reconstructed this saddle and its stable and unstable manifolds, and followed their time dependence. For a local finite-time characterization of chaotic escape, see research area (ii).

Our results also reveal that changing climate does not involve considerable changes in the escape rate and average lifetime, as opposed to the stretching. However, the average lifetime has a clear annual cycle with a larger maximum in July and a smaller one in January. This cycle proved to be related to the displacements of the Intertropical Convergence Zone.

The study of the escape rate and lifetime (Haszpra, 2019) was chosen to be promoted as an "Editor's Pick/Featured" article, and one of its figures was selected to be the cover image for the July 2019 issue of Chaos. An interview about the research was also published on the web page of the American Institute of Physics Publishing. Besides the topic of the research it mentions the RePLaT-Chaos computer "game" as well. Parts of the interview were published in other international media as well.

As an outlook for investigating climate ensembles we took part in a research in which teleconnections were investigated in the ensemble approach using large ensembles with different forcing scenarios (Bódai et al. 2020a; 2020b; Haszpra et al., 2020a; 2020b; 2020c; Tél et al., 2020; Topál et al., 2020). We argue that an appropriate description of teleconnections is provided by correlation coefficients between the index of the main oscillatory mode and the remotely connected quantity evaluated over the ensemble at any time instant. Similarly, if an ensemble is available, the pattern of the AO and ENSO, and their time dependence should be studied through a reconsidered empirical orthogonal function (EOF) analysis (snapshot EOF, SEOF analysis) carried out across the ensemble at any time instant. We have shown that the traditional method for computing the AO index, which uses a single climate realization, results in values that strongly depend on the choice of the reference period. Our results emphasize that both the AO and ENSO and the related surface temperature/precipitation patterns are non-stationary and their time evolution depends on the forcing. We have identified an essential contributor to September sea ice loss in the Arctic to be a regional barotropic atmospheric process over Greenland and the Arctic Ocean in summer, and it features either a year-to-year change or a low-frequency variability in geopotential height. We have found all the investigated models to exhibit limitations in replicating the correct magnitude of the observed local atmosphere–sea ice coupling and its sensitivity to remote tropical sea surface temperature variability.

As another utilization of the ensemble framework, the effect of solar constant scenarios, consisting of an abrupt decrease, a plateau and thereafter a rapid increase, on the climate was investigated in ensembles of climate simulations of PlaSim (Kaszás et al., 2019). In individual simulations, depending on the scenario parameters (the reduction rate of the solar constant, the length of the plateau), the system is either found to stay stuck in the so-called snowball state (Earth covered entirely by ice and snow) or to return to the current climate. However, using an ensemble, results show that within certain intervals of the parameters, at the end of the scenario both stable states permitted by the current value of the solar constant are present simultaneously with certain probabilities. In addition, a third, unstable state (referred to as the edge state) is also recovered in the simulations.

(ii) The second main aim of our research was to establish a relationship between local and global properties of chaotic dispersion phenomena in incompressible flows, with an emphasis on Earth's atmosphere.

Even in closed flows, local properties are governed by a chaotic saddle of fractal dimension D_0. If local chaos is concentrated to a small region of the phase space, global chaos emerges via subsequent passings of a trajectory through this region (Drótos et al., Phys. Rev. E 87, 063017, 2013). Each passing leads to the appearance of a new component of a global chaotic set. We have analytically shown, by analyzing the stable and the unstable manifolds of the local saddle, that each passing increases the dimension of the global chaotic set by D_0. This increase continues until a space-filling pattern is reached.

We were planning to investigate the relationship between local and global dispersion properties in our model flow of a point vortex pair on a rotating sphere (Drótos et al., Phys. Rev. E 87, 063017, 2013). We have carried out a thorough analysis, by which we have revealed that the few qualitatively different vortex trajectory shapes permitted in our setup can be described in terms of an effective potential, i.e., a potential function for the meridional motion defined through a constant of motion.

In particular, the independence of the equations of motion of the longitude λ gives rise to an (angular momentum-like) second constant of motion N beyond the kinetic energy and the distance of the two vortices, which are conserved for infinitely small and finite-size vortex pairs, respectively (Drótos and Tél, 2020). For the former, a second-order equation of motion can be expressed in terms of N for the latitude φ alone, from which the construction of an effective potential is straightforward for the meridional motion. The transition point between meandering and circle-shaped trajectories (travelling eastward and westward, respectively) can be analytically computed as the position of a pitch-fork bifurcation in this potential. A few novel trajectory shapes are also revealed in short parameter ranges after one of the trajectory's meridional extrema reaches either of the poles for decreasing N. The meridional motion of finite-size vortex pairs can also be described via a similar construction but only through numerical computation. Nevertheless, similar trajectory shapes are systematically found.

Finally, however, we did not utilize this velocity field. As discussed in topic (i), the dispersion of pollutants in Earth's atmosphere is most often a chaotic phenomenon with an escape (sedimentation) from the domain, i.e., an example of transient chaos itself. We have recognized that local properties of transient chaos are more naturally characterized, without rendering "local chaos" well defined via introducing artificial boundaries, by defining local quantifiers of transient chaos based on the escape from the global domain. Although coarse-graining must be involved in such a description, too, and a time span of interest must be defined, we avoid relying on the existence of a local chaotic set in this way, and identify local properties of the global chaotic set. We can thus explore differences within the global domain from the point of view of the most natural escape process: the escape process from the global domain itself, e.g., that from Earth's atmosphere.

We have defined coarse-grained local finite-time quantifiers of transient chaos (Lyapunov exponent Λ, escape rate κ and fractal dimensions D_k with k being any natural number) based on studies of elementary model problems (Drótos et al., 2020). In particular, we took the paradigmatic logistic map with leaks, and a leaked version of the double shear map. We have chosen the appropriate definitions by requiring the Kantz–Grassberger relation ($D_1 = 1 - \kappa/\Lambda$) between the three quantifiers to be fulfilled. We have concluded that the appropriate Lyapunov exponent is obtained as the box average of the well-known finite-time Lyapunov exponent. Surprisingly, the appropriate escape rate has been found to be the logarithm of the ratio of the number of trajectories not yet escaped within the given time span and their initial number, divided by the length of the given time span, as opposed to an instantaneous rate of escape. The fractal dimension has proven to be appropriately given simply by the fractal dimension obtained by increasingly fine sub-partitionings of the box in question. What is most interesting is that these quantifiers exhibit a considerable spread across the domain but satisfying the Kantz–Grassberger relation, which means that this spread describes true variations in the dynamical properties throughout the domain.

Maps of finite-time Lyapunov exponents in atmospheric dispersion problems are abundant in the literature. Maps of a local escape rate, however, had been impossible to plot in the absence of an appropriate definition. As a main result of our work, we provide here examples of such maps in Figure 1. A strength of such maps is that geographical regions where the influence of the chaotic saddle retains less or more of the released particles in the atmosphere are associated with some given time scale of interest. Geographical patterns also become clearer and better established than in an individual-trajectory-based representation: properties associated with individual trajectories are subject to an inherent uncertainty that originates from chaotic behavior, but aggregating such properties in some statistical quantifier of chaos (the local escape rate in our case) provides a robust representation. Figure 1 quantifies slow escape from the equatorial belt (identified by Haszpra, 2019) and further geographical details in this spirit. Furthermore, from comparing different time scales, one also learns how far the influence of escape dynamics associated with given geographical regions reaches, see, e.g., the increasing influence of the polar regions when comparing Figures 1a and 1b. Maps of this kind will most certainly be useful for a local dynamical characterization of atmospheric dispersion and for practical purposes in risk assessments of atmospheric pollutant dispersion and in designing geoengineering projects, cf. topic (i) in the present report with analogous and complementary results.

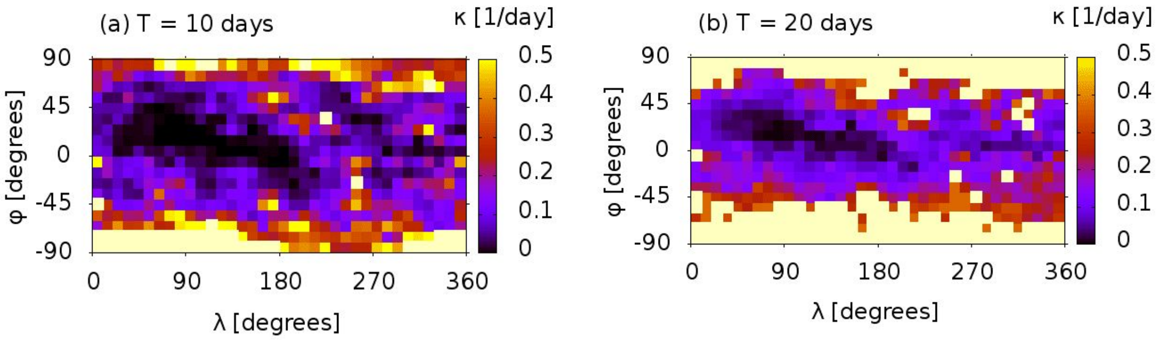

Figure 1: The local finite-time escape rate *κ* in different boxes of the globe for integration times *T* of (a) 10 and (b) 20 days. Pale yellow color corresponds to boxes from which all particles leave the domain during *T*. The 5-μm particles were initialized at 500 hPa on July 1, 2016 and were evolved by RePLaT in the ERA-Interim reanalysis field.

We studied specific, regular or chaotic local dispersion phenomena of sinking particles in incompressible flows as well. The first particular question concerned how such particles are distributed after sedimentation if particle inertia is negligible but gravity is not. Examples are the mesoscale motion of volcanic aerosol particles in the atmosphere and that of biogenic particles in the ocean.

In such situations, the equation of motion of a particle is incompressible. This implies that the spatial distribution of the particles cannot develop inhomogeneities if they are not already introduced in the initial condition. However, if one considers the density accumulated on (hyper-) surfaces of a dimensionality smaller than the full dimensionality of the fluid flow (e.g., on the bottom of the domain), and the particles are initially distributed uniformly but over a finite support, inhomogeneities will emerge due to advection in the flow.

We analytically derived, in the framework of an initially homogeneous particle sheet, the relationship between the geometry of the flow and the emerging accumulated density (Drótos et al., 2019). We identified the two relevant mechanisms to be stretching within the sheet, and projection of the deformed sheet onto the target surface. We pointed out that even caustics can develop for sheets. We exemplified our geometrical results with simulations in a simple kinematic flow, studied the dependence on various parameters involved, and illustrated that the basic mechanisms work similarly if the initial (homogeneous) distribution has a finite support with full dimensionality.

We also demonstrated that the identified processes lead to inhomogeneities in a realistic simulation of an oceanic flow in the Benguela region, including caustics for sheets of particles (Monroy et al., 2019). We explained the results in view of the strong anisotropy of the oceanic velocity field, and showed that submesoscale perturbations of the flow introduce negligible alterations. Furthermore, we illustrated that projection (stretching) becomes dominant in determining the inhomogeneities for small (high) values of the particles' settling velocity. Inhomogeneity has been found to be stronger for smaller particles and also in areas with stronger turbulent activity.

We continued the research by turning to isotropic homogeneous turbulent flows, representing small-scale turbulence in the ocean (Sozza et al., 2020). We analyzed sedimented inhomogeneity as a function of the Reynolds number and the settling velocity. We have identified two regimes that arise during the early and well-mixed stages of advection. In the former regime, more inhomogeneity is introduced for decreasing settling velocity or increasing Reynolds number, while the tendencies are opposite in the latter regime. We have pointed out the presumable applicability of our results to any turbulent flow, and have classified our Benguela setup to belong to the early regime.

Finally, motivated by a problem of oceanic microplastic pollution with immediate practical relevance, we continued our research on sinking behaviour by concentrating on the water column and investigating the vertical dispersion and distribution of negatively buoyant rigid microplastic particles in a realistic simulation of the Meditarranean velocity field (de la Fuente et al., 2020). In the framework of an idealized equation of motion, we have calculated the amount and vertical distribution of microplastic particles along the water column of the open sea supposing a continuous release from the sea surface at rates compatible with observations in the Mediterranean. The vertical distribution has been found to be practically uniform along depth for the majority of the practically relevant parameter range. Transient distributions from flash releases have revealed a non-Gaussian character of the dispersion and various diffusion laws, both normal and anomalous. The origin of these behaviors has been explored in terms of horizontal and vertical flow organization.

Changes in the participants: For the last project year Dániel Topál joined the project to partially take over the tasks of Tímea Haszpra.

Publication activity: The results were published in 14 articles in peer-reviewed journals (IF = 47.004) and 2 software descriptions, and presented in 4 solicited talks, 10 talks and 9 posters at international conferences, and in 9 miscellaneous talks. Another 4 manuscripts are currently under review, and 1 is in preparation.

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