RePLaT–Chaos-edu

Illustration of the chaotic behavior of atmospheric pollutant spreading

Theoretical background and user guide

Tímea Haszpra

Department of Theoretical Physics, Eötvös Loránd University
MTA–ELTE Theoretical Physics Research Group

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Content

1. Introduction

The main aim of RePLaT-Chaos-edu is to make the simulation of global-scale atmospheric spreading of pollutant clouds and the studying of the so-called chaotic features of the advection easy. The pollutant clouds consist of aerosol particles or gas particles. The software is a simpler version of the previously developed RePLaT (Real Particle Lagrangian Trajectory) model [1, 2]. RePLaT-Chaos-edu determines the motion of the particles by taking into account the advection by the wind components in the horizontal direction and and its vertical motion is, in addition, influenced by its terminal velocity due the gravity.[1].

In three-dimensional flows, as it is the case in the atmosphere, the advection of pollutants is chaotic. The advection dynamics of pollutants shows typical characteristics of the chaos, such as sensitivity to the initial conditions (the trajectories of initially nearby particles diverge within short time), irregular motion, and complex but regular (fractal) structures. It can be easily observed in the RePLaT-Chaos-edu simulations that pollutant clouds do not disperse in the atmosphere like dye blobs on clothes, rather an initially compact pollutant cloud becomes soon strongly stretched, its length grows rapidly, while becoming filamentary, tortuous and folded. The software can also calculate two quantities which describe the chaoticity of the advection. The stretching rate characterizes the rate of the exponential stretching of pollutant clouds, while the life time quantifies the deposition rate of particles falling out from the atmosphere to the surface [3].

2. User guide

2.1. Short description

RePLaT-Chaos-edu simulates the atmospheric spreading of pollutant clouds in time interval 04.14.2010 00 UTC–04.30.2010 12 UTC and with different simulation setups given by the user. Pollutant clouds consist of individual particles the number of which is determined by the user. For the spreading calculations meteorological files containing the appropriate meteorological data overlapping the defined time interval are required. The initial position, size and other properties of the pollutant cloud (and its particles) can be given in the user interface. RePLaT-Chaos-edu determines the new position of each particle of the pollutant cloud in each time step based on the meteorological data and writes the particle data to file in every 6 hours. Furthermore, it computes the length of the pollutant cloud and the ratio of the particles not deposited from the atmosphere. These data are needed for the calculation of two quantities describing the chaoticity of the spreading: one of them is the stretching rate characterizing the stretching rate of the length of the pollutant clouds and the other one is the life time quanitifying the rapidity of the particle deposition. RePLaT-Chaos-edu provides an opportunity to determine the above-mentioned two chaotic measures.

2.2. Launch RePLaT-Chaos-edu

Depending on the operation system the software can be downloaded and installed in different ways described in detail on the webpage http://hatimi.web.elte.hu/RePLaT/index.html.

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[1] Neglecting the impact of other processes (e.g., turbulent diffusivity and the scavenging of particles by precipitation).

On the **welcome** page and on the **Additional eruptions** page animations of the spreading of particles from different, hypothetical volcano eruptions can be seen. One may design his/her own pollutant spreading simulations on the **Design eruption** or on the **Measure chaos** pages by clicking the **Start** button. A brief explanation about the calculated chaos quantities with colored illustrations can be found on the **Chaos quantities** page. On the **Interesting** page one can find the main conclusions and lessons about the phenomena demonstrated by the software.

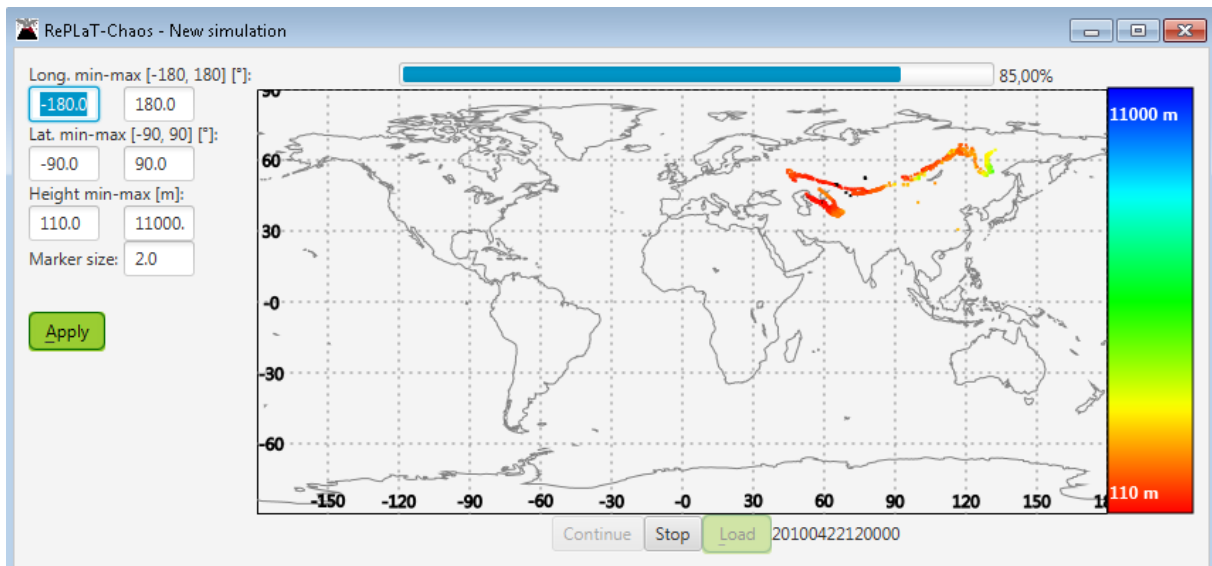## 2.3. Setting the display properties of the simulation

Figure 1: Tracking the calculation of the simulation with displaying the particle positions.

Depending on whether the user has chosen this option or not, during the simulation calculation the current position of the particles of the pollutant cloud is displayed colored according to the vertical coordinate of the particles on a map or only a progressbar is visible to show the percentage of the progress of the calculation and the corresponding date and time. The user can stop and continue the calculation by clicking the **Stop** or **Continue** buttons, respectively. The longitudinal and latitudinal boundaries of the map, the vertical boundaries of the coloring and the marker size of the particles can be changed on the left side (formats: real numbers in the given intervals). The settings are applied by clicking the **Apply** button. If there is a wrong or empty textfield, the problem is indicated by an alert window and the wrong fields are marked by red.
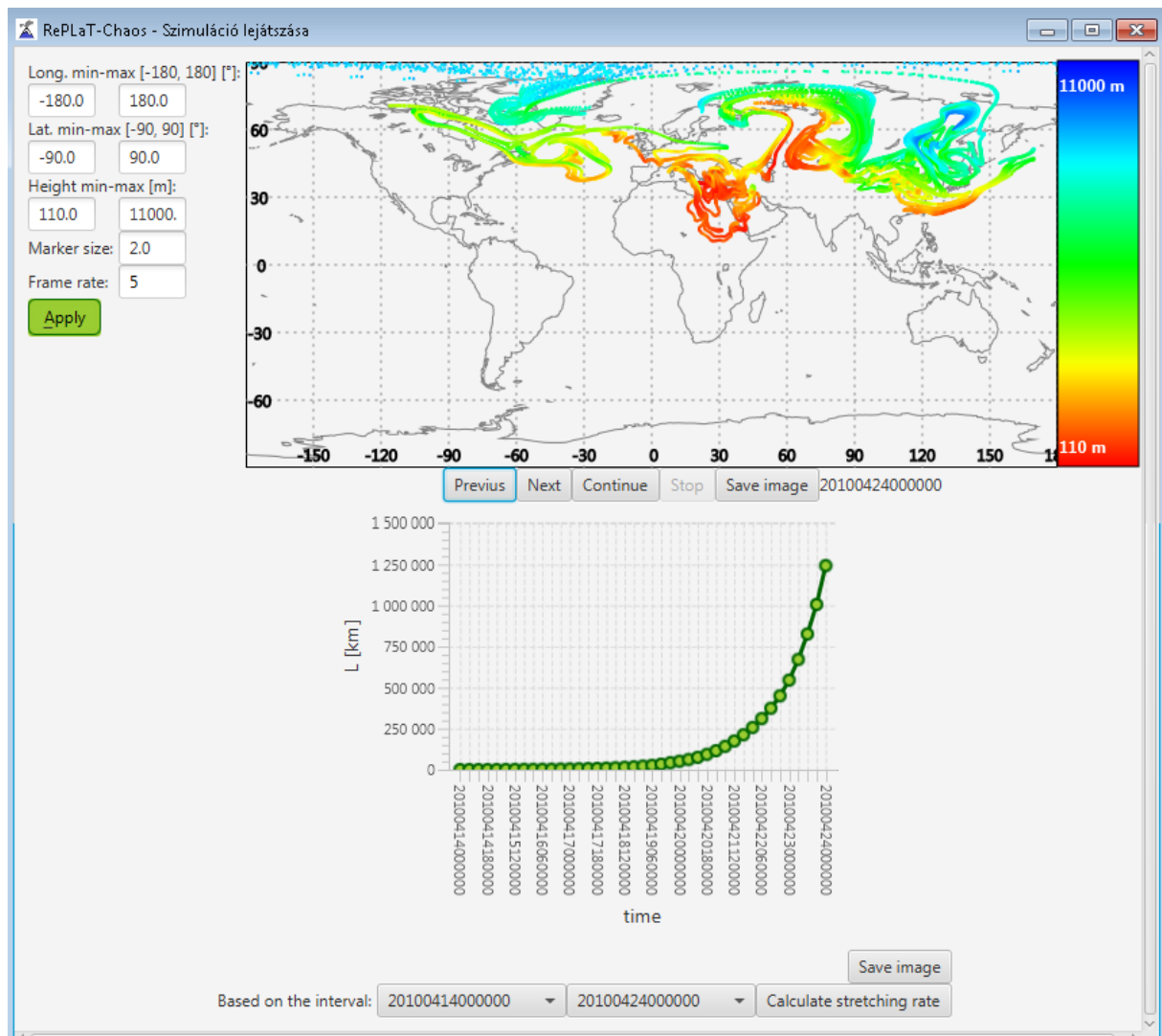
2.4. Replaying a simulation

Figure 2. Displaying saved simulation and the time dependence of the lengh of the pollutant cloud.

After the end of the simulation calculation, the simulation is loaded and its replay starts. Depending on the page (**Design eruption**, **Measure chaos**: **Volcanic gas** / **Volcanic ash**) where the user started the simulation the time dependence of the natural logarithm of the length of the pollutant cloud / the time dependence of the natural logarithm of the ratio of the non-escaped particles is also appear on the panel (Figure 2, Figure 3). By default, the forward loop of the spreading of pollutant cloud is displayed according to the given **Frame rate**. The user can stop and continue the replay by clicking the **Stop** and **Continue** buttons, respectively, and can move the replay one by one frame forward/backward by clicking the **Previous**/**Next** buttons. The instantenous position of the pollutant cloud can be saved by clicking the **Save image** button. The properties of the display can be changed similarly as described in section 2.3 by clicking the **Apply** button. Beyond those options the speed of the animation (**Frame rate**) can be modified, too.

If the user loaded length data / data for the ratio of the non-escaped particles from file, she/he can select a start and end date and time from the two lists in the bottom of the panel.

By clicking the **Calculate stretching rate** / **Calculate life time** button an exponential function is fitted to the graph between the given time instants using the least squares approach and its slope (i.e. the topological entropy (Figure 2)) / (-1)×slope (i.e., the escape rate (Figure 3) is also presented. The graphs can be saved by clicking the **Save image** button.
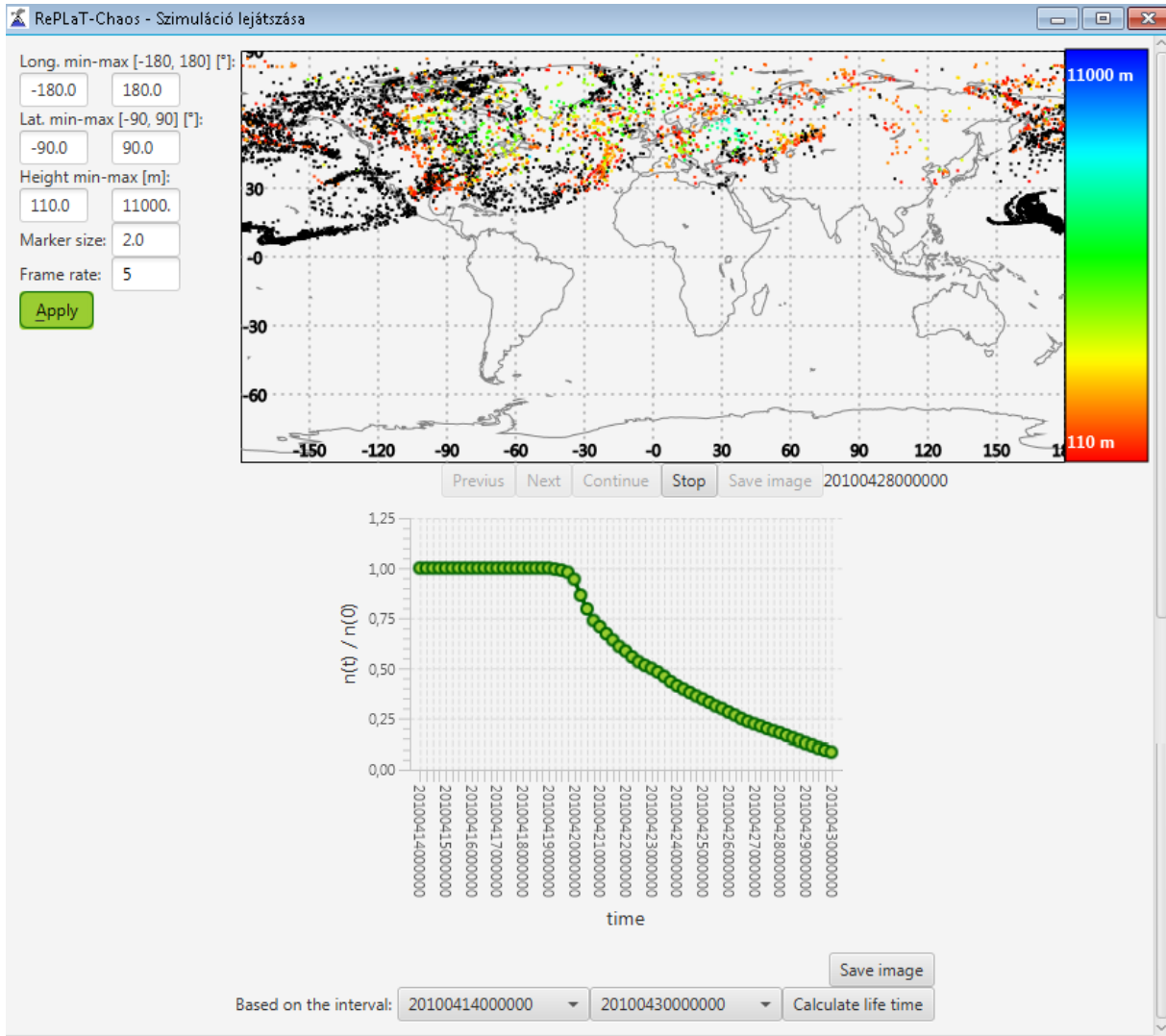

Figure 3. Displaying saved simulation and the time dependence of the ratio of non-escaped particles.

3. Theoretical background

3.1. Calculation of particle trajectories

For small aerosol particles it can be shown that a particle is advected by the wind components in the horizontal direction and its vertical motion is influenced by its terminal velocity[2] and the vertical velocity component of air [2]. RePLaT-Chaos-edu utilizes meteorological data given on regular longitudinal–latitudinal grid in the horizontal direction and at different pressure levels in the vertical direction. Therefore, the equations of motion of the particles are written in spherical coordinates in the horizontal and in pressure coordinates in the vertical direction in agreement with the structure of the meteorological data:

$$\frac{d\lambda(t)}{dt} = u_{rad}(\lambda(t), \varphi(t), p(t), t) = \frac{u(\lambda(t), \varphi(t), p(t), t)}{R\cos(\varphi(t))},$$

$$\frac{d\varphi(t)}{dt} = v_{rad}(\lambda(t), \varphi(t), p(t), t) = \frac{v(\lambda(t), \varphi(t), p(t), t)}{R},$$

$$\frac{dp(t)}{dt} = \omega(\lambda(t), \varphi(t), p(t), t) + \omega_{term}(\lambda(t), \varphi(t), p(t), t),$$

where $\lambda(t)$, $\varphi(t)$, $p(t)$ denotes the longitude, latitude [rad] and pressure [Pa] coordinates of the particle at time instant t, u, v, ω are the zonal, meridional [m/s] and vertical [Pa/s] velocity components of air, u_{rad}, v_{rad} are the zonal and meridional wind components measures in [rad/s], $R = 6371$ km is the radius of the Earth, and ω_{term} is the terminal velocity of the particle. The terminal velocity is

$$\omega_{term} = \begin{cases} \dfrac{2}{9}\dfrac{\rho_p r^2 g^2}{\nu} & \text{if } \mathrm{Re} \ll 1, \\[2ex] \sqrt{\dfrac{8}{3}\dfrac{\rho_p \rho r}{C_D} g^3} & \text{if } \mathrm{Re} \gg 1, \end{cases}$$

where ρ_p is the density of the particle, ρ is the density of air, r is the radius of the particle, g is the gravitational acceleration, ν is kinamtic viscosity, C_D is the drag coefficient (for particles assumed to be spheres $C_D = 0.4$), $\mathrm{Re} = 2r\,V/\nu$ is the Reynolds number (where V denotes a the characteristic velocity about which it can be shown that converges to the terminal velocity). The limit of $r = 0$ μm can be considered as gas "particles", the terminal velocity of which is $\omega_{term} = 0$.

The required meteorological data for the above equations are the velocity components u, v, ω and the density ρ and kinematic viscosity ν of air. Since the latter two variables are not available in meteorological databases, we calculate them by means of temperature T. The density can be derived from the ideal gas law as follows:

$$\rho = \frac{p}{R_d T},$$

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[2] A particle falls through a motionless air with its terminal velocity if the sum of the drag force and the buoyancy is equal to the downward force of gravity.

where $R_d = 287$ J/kg/K is the specific gas constant of dry air. The kinematic viscosity can be expressed by means of the dynamic viscosity μ, where a μ depends again on the temperature T represented by Sutherland's law [4]:

$$\nu = \frac{\mu}{\rho}, \text{ where}$$

$$\mu = \beta \frac{T^{3/2}}{T + T_S}, \text{ that is}$$

$$\nu = \frac{\mu}{\rho} = \beta \frac{T^{5/2}}{T + T_S} \frac{R_d}{p},$$

where $\beta = 1.458 \times 10^{-6}$ kg m^{-1}s^{-1}K$^{-0.5}$ is Sutherland's constant and $T_S = 110.4$ K is a reference temperature.

Now each quantity on the right-hand side of ordinary differential equation system describing the motion of the paricles is known. RePLaT-Chaos solves the differential equations by an explicit second-order Runge–Kutta method (applied often also in other dispersion models). Hence the position $\mathbf{r}(t + \Delta t) = [\lambda(t + \Delta t), \varphi(t + \Delta t), p(t + \Delta t)]$ of a particle at time instant $t + \Delta t$ using the velocity $\mathbf{v}(\mathbf{r}(t), t) = [u_{\mathrm{rad}}(\mathbf{r}(t), t), v_{\mathrm{rad}}(\mathbf{r}(t), t), \omega(\mathbf{r}(t), t) + \omega_{\mathrm{term}}(\mathbf{r}(t), t)]$ at time t can be written as:

$$\mathbf{r}_0 (t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(\mathbf{r}(t), t)\Delta t \qquad \text{and}$$

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \frac{1}{2}\Big[\mathbf{v}(\mathbf{r}(t), t) + \mathbf{v}(\mathbf{r}_0 (t + \Delta t), t + \Delta t)\Big]\Delta t.$$

The utlized meteorological data are available on a regular latitude–longitude grid on different pressure levels with a given (e.g., 3 or 6 hours) time resolution. Therefore, in order to solve the equations of motion of the particles and to calculate the particle trajectories, the quantites u, v, ω, T are interpolated to the location of the particles in each time step. RePLaT-Chaos-edu applies linear interpolation in each of the three directions and in time.

Each Δt time step for each particle is determined by the RePLaT-Chaos-edu model based on the grid size and the current atmospheric velocity components using the Courant–Friedrichs–Lewy condition:

$$\Delta t_{\mathrm{CFL}} = \mathrm{CFL} \cdot \min\left\{ \frac{\Delta \lambda_g}{\left|u_{\mathrm{rad}}(\mathbf{r}(t), t)\right|}; \frac{\Delta \varphi_g}{\left|v_{\mathrm{rad}}(\mathbf{r}(t), t)\right|}; \frac{\Delta p_g}{\left|\omega(\mathbf{r}(t), t) + \omega_{\mathrm{term}}(\mathbf{r}(t), t)\right|} \right\},$$

where $\Delta \lambda_g$, $\Delta \varphi_g$, Δp_g are the grid size in zonal, meridional [rad] and vertical [Pa] direction, CFL < 1 is the Courant number. The minimal time step $\Delta t_{\min}$ is 300 s. If the obtained Δt would be larger than the time interval $(t_{\mathrm{next}} - t)$ up to the next writing of particle data to file or up to the next reading of new meteorological fields then the time step is modified as:

$$\Delta t = \min\left\{t_{\mathrm{next}} - t; \max\left\{\Delta t_{\mathrm{CFL}}; \Delta t_{\min}\right\}\right\}.$$

3.2. Strecthing rate

The so-called stretching rate, which corresponds to a well-known quantity from dynamical systems theory, the topological entropy, quantifies the complexity, irregularity of the advection of pollutant clouds in the atmospheric context. According to a definition of

chaos, a system is chaotic if its topological entropy is positive [3]. It can be shown that an initially small pollutant cloud in the atmosphere becomes strongly stretched and folded; its length grows rapidly, while becoming filamentary and tortuous. The length L of the filament increases typically in an exponential manner in time t: $L(t) \sim \exp(h\,t)$ (Figure 4). The exponent h is called the stretching rate and it is the rate of the exponential increase of the filament length. The larger the stretching rate is, the faster the length grows and the more complex, tortuous shape the pollutant cloud forms [5]. Taking into account the potential highschool knowledge of students, here we do not call the stretching rate the exponent of $L(t) \sim e^{h\,t}$, rather than that of $L(t) \sim 10^{h\,t}$. The pollutant cloud stretches by a factor of 10 within the time of the reciproke of h.

For one-dimensional pollutant clouds (line segments or filaments) the length of the pollutant cloud is calculated by the sum of the distances between its particles:

$$L(t) = \sum_{i=1}^{n-1} \left| \mathbf{r}_{i+1}(t) - \mathbf{r}_i(t) \right|,$$

where $\mathbf{r}_i(t)$ is the position of the ith particle. Since vertical stretching proved to be 10^{-2}–10^{-3} times smaller than the horizontal one [3], it can be neglected. Thus, the length of a filament is obtained from the horizontal distances between particle pairs, and the distance [km] is calculated along great circles by

$$\left| \mathbf{r}_{i+1}(t) - \mathbf{r}_i(t) \right|_{\mathrm{hor}} = \arccos\ \left[\sin\ \varphi_i \sin\ \varphi_{i+1} + \cos\ \varphi_i \cos\ \varphi_{i+1} \cos(\ \lambda_i - \lambda_{i+1}) \right] \times \frac{180}{\pi} \times 111\ .1\ ,$$

where λ_i and φ_i are the longitudinal and latitudinal coordinate of the ith particle, respectively, and $(180/\pi) \times 111.1$ converts the unit from radians to kilometers using the fact that the spherical distance of 1° along a great circle corresponds to a length of 111.1 km along the surface.
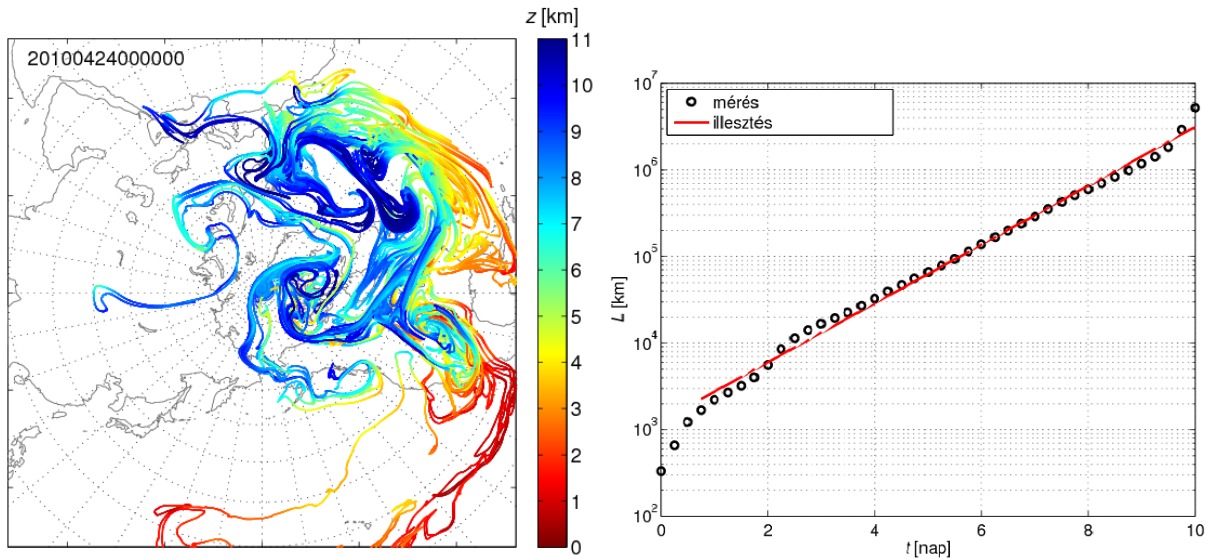

Figure 4. The length of pollutant clouds grows exponentially in the atmosphere. Left: A filament with an initial length of 300 km covers a large part of the Northern Hemisphere within 10 days. Right: The time-dependence of the length of the filament.

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Since subsequent particles may travel far away from each other in time, the length of a pollutant cloud that consists of finite number of particles may be underestimated compared to a pollutant cloud with same initial conditions that consists of infinite number of particles (i.e. the pollutant cloud is continuous). This implies that after certain time when there are several "cut-off" segments among the particles the computed length differs from an exponential function, its values are lower than the expected ones. Hence to reduce the underestimation of the length if the distance of two neighboring particles becomes larger than a critical distance (here: 100 km), a new particle is inserted between them until the number of particles the maximum particle number defined as 100 000.

3.3. Life time

The particles of the pollutant clouds carry out the chaotic motion for finite duration because, e.g., reaching the surface of the Earth they may deposit on the ground. This type of chaos is called transient chaos [3]. Nevertheless, there also exists a null measure set, the so-called chaotic saddle, initialized on which the particles would never leave it and carry out chaotic motion for an inifinite amount of time. Being a null measure set the probability for the particles to be initially located on the chaotic saddle is zero and the particles sooner or later leave (i.e. "escape") any arbitrary preselected regions of the saddle. The rapidity of this leaving is characterized by the life time. After a sufficiently long time t_0, the decay in the ratio $n(t)/n(0)$ of survivors in the regions (in atmospheric spreading simulations in the region defined by the meteorological data) is generally exponential (similar to the law of radioactive decay): $n(t)/n(0) \sim \exp(-t/T)$, for $t > t_0$ (Figure 5), where T is the mean life time of the particles. [1]. Similarly to the stretching rate, the software does not calculate the T in the exponent of e, rather than T in $n(t)/n(0) \sim 10^{-t/T}$. In the quickly decaying stage merely a tenth of the particles remain in the atmosphere after time T. The value of T is longer for light particles, but depends on the atmospheric conditions, too.
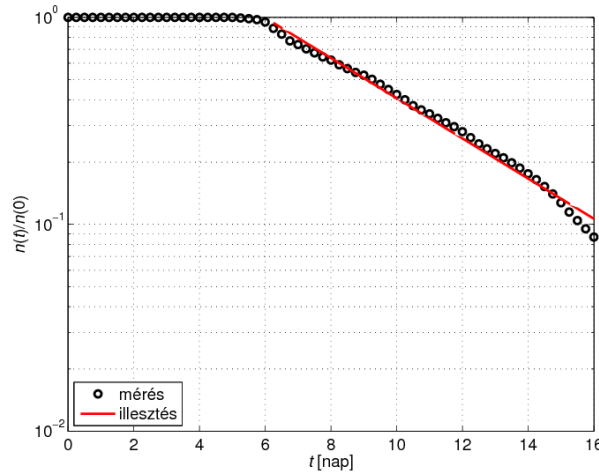

Figure 5. The ratio of non-deposited particles of the pollutant cloud decreases exponentially in time.

Acknowledgement

References

[1] Haszpra, T., Tél, T.: Escape rate: a Lagrangian measure of particle deposition from the atmosphere, Nonlin. Proc. Geophys. 20(5), 2013, 867–881.

[2] Haszpra, T., Horányi, A.: Some aspects of the impact of meteorological forecast uncertainties on environmental dispersion prediction. Időjárás, 118 (4), 2014, 335–347.

[3] Tél, T., Gruiz, M.: Chaotic dynamics: an introduction based on classical mechanics. Cambridge University Press, 2006, 415 p.

[4] Sutherland, W.: LII. The viscosity of gases and molecular force, Philosophical Magazine, Series 5, 36, 1893, 507–531.

[5] Haszpra, T., Tél, T.: Topological entropy: a Lagrangian measure of the state of the free atmosphere. Journal of the Atmospheric Sciences, 70(12), 2013, 4030–4040 (doi: 10.1175/JAS-D-13-069.1).

[6] http://www.oracle.com/technetwork/java/javase/downloads/jre8-downloads-2133155.html

[7] http://apps.ecmwf.int/datasets/

[8] http://nco.sourceforge.net