# PyBox: a Python tool for simulating the kinematics of Pyroclastic density currents with the box-model approach Reference and User's Guide 

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This report describes the physical principles, numerical method and implementation into a Python code of an integral (box) model to simulate the kinematics of pyroclastic density currents (PDCs) and the PDC invasion maps over a rugged topography.

The kinematic model analyzed here is based on the box model formulation described in many previous papers (Huppert and Simpson, 1980; Dade and Huppert, 1995a; Bonnecaze et al., 1995; Hallworth et al., 1998; Esposti Ongaro et al., 2016). It describes the propagation of a turbulent particle-laden gravity current, generated by the sudden release of a homogeneous fluid with suspended particles into a still atmosphere. Inertial effects are assumed to have a leading role with respect to viscous forces and particleparticle interactions. Particle sedimentation, which modifies the current inertia during propagation, is also taken into account.

The procedure to incorporate the effects of the topography on the PDC box model is based on the energy conoid approach proposed by Neri et al. (2015); Bevilacqua (2016); Bevilacqua et al. (2017).

In Section 1, we first briefly recall the main characteristics of PDCs, from a physical and geological point of view basing upon Roche et al. (2013); Dufek et al. (2015).

In Section 2, we derive the differential equations of the box model, for channelized (Cartesian) and axisymmetric geometries and for particle-laden gravity currents. The model is based on some simplifying assumptions, already discussed in previous works Bevilacqua (2016); Esposti Ongaro et al. (2016); Bevilacqua et al. (2017).

Section 3 deals with PDCs hazard assessment in active volcanic regions. In particular, the distribution of areas exposed to PDCs invasion is discussed and is the focus of the following subsections 4.5-4.6.

Finally, a new Python-3.x implementation of the box model is described and attached to these notes. Section 4 contains some discussion on the implementation of the pybox.py code.

## 1 Phenomenological aspects of PDCs

PDCs are horizontal, gravity-driven currents composed of a hot mixture of volcanic gas and solid particles, generated by explosive volcanic phenomena. They are typically generated by the gravitational collapse of lava domes or explosive eruption columns. PDCs display a coexistence of different flow regimes, ranging from a basal, dense pyroclastic flow (originating by the progressive sedimentation of granular particles) to an upper, dilute, turbulent pyroclastic surge (Roche et al., 2013; Esposti Ongaro et al., 2016).

The following Figure 1 schematically represents the above concepts.


Figure 1: Examples and schematic representations of PDCs different generation mechanisms: lava dome collapse ( $a, b$ ) and volcanic plume collapse ( $c, d$ ). Basal dense granular avalanche and upper pyroclastic surge are labeled $F$ and $S$, respectively (from Roche et al. (2013)).

The transition between the two regions with aforementioned regimes can be rough or progressive and can occur at different heights. Naturally, the concentrated flow at the current base is strongly influenced by topography (since it is commonly up to a few tens of meters thick), whereas the upper ash-laden cloud is not. Pyroclastic density currents can travel over distances up to tens of kilometres, at speed of up to $\sim 200 \mathrm{~m} \cdot \mathrm{~s}^{-1}$ (Roche et al., 2013). However, dense pyroclastic flows can have relatively low speeds of $\sim 5-20 \mathrm{~m} \cdot \mathrm{~s}^{-1}$, as discussed in Roche et al. (2016).

### 1.1 Density currents and PDC regimes

Gravity currents originate whenever a density difference between two fluids results in one laterally flowing into the other one. For PDCs, such a density difference arises
from the presence of suspended particles and hot gas in the flow, due to the turbulence generated by the flow. PDCs contain pyroclasts (deriving from magma fragmentation), whose size varies from the order of microns (ashes) to the order of centimeters (lapilli), up to meters (blocks).

Typically, density currents dynamics can be described in three distinct phases (Huppert and Simpson, 1980; Roche et al., 2013):

- the slumping phase, in which the gas-particle mixture collapses, intruding into the ambient fluid: herein, the flow dynamics is controlled by the release conditions and geometry;
- the inertial phase, during which the flow motion is governed by the balance of inertia and buoyancy forces;
- the stopping phase, wherein the buoyancy force of the intruding fluid is balanced by viscous forces and this balance leads to the stop of the current.

The box model presented in this report is suited for the simulation of the intertial phase of a particle-laden gravity current. In our model, based on numerical experiments by Esposti Ongaro et al. (2016) we assume that the basal flow has not a controlling role in the current kinematics.

## 2 The box model

The model consists of a set of ordinary differential equations, that provide the time evolution of the PDC front velocity, $u(t)$, together with the current height $h(t)$ and the solid particle volume fraction ${ }^{1} \epsilon_{i}(t), i=1, \ldots, N, N$ being the number of particle classes considered.
We assume the classical dam break configuration, in which a column of fluid instantaneously collapses and propagates, under gravity, in a surrounding atmosphere with uniform density $\rho_{\text {atm }}$. Several examples are available in literature and significant cases are provided by various Computational Fluid Dynamics toolboxes (e.g., Breaking of a dam, in CFD Direct OpenFOAM v6 User Guide (2018), available at https://cfd.direct/ openfoam/user-guide/v6-damBreak/.) Other authors (Bonnecaze et al., 1995; Dade and Huppert, 1995b, 1996) have considered gravity currents produced by the constantflux release of dense suspension from a plane source. Extension of the model presented here to such a configuration is straightforward and will be implemented in the next version of the model.

PDCs are driven by their density excess with respect to the surrounding air: the density of the current $\rho_{\mathrm{c}}$ is defined as the sum of the density of an interstitial gas, $\rho_{\mathrm{g}}$,

[^0]and the bulk densities of the pyroclasts carried by the flow, i.e.,
\[

$$
\begin{equation*}
\rho_{c}=\left(1-\epsilon_{\mathrm{tot}}\right) \rho_{\mathrm{g}}+\sum_{i=1}^{N} \epsilon_{i} \rho_{i}^{s}, \quad \epsilon_{\mathrm{tot}}=\sum_{i=1}^{N} \epsilon_{i} \tag{1}
\end{equation*}
$$

\]

where $\rho_{i}^{s}, i=1, \ldots, N$, is the density of the $i$-th particle class. We assume $\rho_{\mathrm{c}}>\rho_{\text {atm }}$ and $\rho_{\mathrm{atm}}>\rho_{\mathrm{g}}$, since at PDCs temperatures (typically $300-700^{\circ} \mathrm{C}$ ) the density of the interstitial gas is lower than the atmospheric one (Dufek et al., 2015).
A proper way to express the density contrast between the current and the ambient fluid is given by the reduced gravity

$$
g^{\prime} \stackrel{\text { def }}{=} \frac{\rho_{\mathrm{c}}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}} g
$$

that can be rewritten as

$$
\begin{equation*}
g^{\prime}=\frac{\left(1-\sum_{i=1}^{N} \epsilon_{i}\right) \rho_{\mathrm{g}}+\sum_{i=1}^{N} \epsilon_{i} \rho_{i}^{s}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}} g=\frac{\rho_{\mathrm{g}}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}} g+\sum_{i=1}^{N} \epsilon_{i} \frac{\rho_{i}^{s}-\rho_{\mathrm{g}}}{\rho_{\mathrm{atm}}} g . \tag{2}
\end{equation*}
$$

That said, we make some additional simplifying hypotheses.
First of all, we assume that the mixture flow regime is incompressible and inviscid. The hypothesis of inviscid fluid is reasonable since we assume that the dynamics of the current is dominated by the balance between inertial and buoyancy forces, as previously stated: this allow us to neglect viscosity. Note that the assumption of incompressibility implies that the current volume $V(t)$ remains constant, i.e., $V(t)=V_{0}$ (see Figure 2). Neglecting compressibility effects is acceptable because velocity is much lower than the speed of sound (Esposti Ongaro et al., 2016).
Moreover, we assume that, within the current, the vertical mixing, due to turbulence, produces a vertically uniform distribution of particles. The particles are assumed to sediment out of the current at a rate proportional to their (constant) terminal (or settling) velocity $w_{i}^{s}, i=1, \ldots, N$. Once deposited, they cannot be re-entrained by the flow. Finally, surface effects of the ambient fluid are neglected.

Under these hypotheses, the box model for particle-laden gravity currents states that the velocity of the current front is related to the average depth of the current by the von Kármán equation for density currents (Benjamin, 1968; Huppert and Simpson, 1980; Dade and Huppert, 1995a; Bonnecaze et al., 1995; Hallworth et al., 1998; Bevilacqua, 2016)

$$
\begin{equation*}
u=\operatorname{Fr} \sqrt{g^{\prime} h} \tag{3}
\end{equation*}
$$

where Fr is the Froude number, a dimensionless number expressing the ratio between inertial and buoyancy forces.

Nevertheless, since (3) is a single equation relating the unknown variables $u(t)$ and $h(t)$, we have to specify other equations to completely determine the current kinematics. So, we assume that particles can settle to the ground and this process changes the solid


Figure 2: Evolution of channelized currents through a series of equal-area rectangles, according to the model (hence the name "box model").
particle fractions $\epsilon_{i}(t), i=1, \ldots, N$. In particular, the rate of the $i$-th particulate class volume loss is due to sedimentation over the current base surface $B$, i.e.,

$$
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\epsilon_{i} V_{0}\right)=-w_{i}^{s} \epsilon_{i} B, \quad i=1, \ldots, N
$$

which reduces to

$$
\frac{\mathrm{d} \epsilon_{i}}{\mathrm{~d} t}=-w_{i}^{s} \epsilon_{i} \frac{B}{V_{0}}=-\frac{w_{i}^{s} \epsilon_{i}}{h}, \quad i=1, \ldots, N
$$

Cartesian currents. Hence, the box model for channelized particle-laden gravity currents can be written as:

$$
\begin{align*}
& \frac{\mathrm{d} l}{\mathrm{~d} t}=\operatorname{Fr} \sqrt{g^{\prime} h}  \tag{4}\\
& l h=l_{0} h_{0}=V_{0}  \tag{5}\\
& \frac{\mathrm{~d} \epsilon_{i}}{\mathrm{~d} t}=-\frac{w_{i}^{s} \epsilon_{i}}{h}, \quad i=1, \ldots N \tag{6}
\end{align*}
$$

where $l_{0}$ and $h_{0}$ are, respectively, the length and the height of the current before being released.

Axisymmetric currents. When considering radially spreading currents, Eqns. (4) and (6) are unaltered (Huppert and Simpson, 1980) whereas the constant-volume condition is expressed by

$$
\xi \pi l^{2} h=\xi \pi l_{0}^{2} h_{0}=V_{0}
$$

where $\xi$ is a spreading factor, $\xi=\frac{\theta}{2 \pi}$, which allow us to consider currents spreading within a circular sector of central angle $\theta$, measured in radians (for isotropic currents,
$\xi=1)$. In such a way, we can describe the propagation of PDCs originating from the gravitational collapse of a portion of the eruption column (hence an asymmetric collapse). The box model for axisymmetric currents thus reads:

$$
\begin{align*}
\frac{\mathrm{d} l}{\mathrm{~d} t} & =\operatorname{Fr} \sqrt{g^{\prime} h}  \tag{7}\\
l^{2} h & =l_{0}^{2} h_{0}=\frac{V_{0}}{\xi \pi}  \tag{8}\\
\frac{\mathrm{~d} \epsilon_{i}}{\mathrm{~d} t} & =-\frac{w_{i}^{s} \epsilon_{i}}{h}, \quad i=1, \ldots N . \tag{9}
\end{align*}
$$

### 2.1 Analytical expression for the maximum current runout

In the case of monodisperse systems, we can determine analytical solutions for both cartesian and radially spreading currents, assuming the presence of either a buoyant interstitial gas or the neutrally buoyant interstitial ambient fluid (Neri et al., 2015; Bevilacqua, 2016).

In particular, an explicit expression for the maximum flow runout $l_{\infty}$, i.e., the distance at which $\rho_{\mathrm{c}}=\rho_{\mathrm{atm}}$, is available in the above mentioned cases (Bonnecaze et al., 1995; Esposti Ongaro et al., 2016; Bevilacqua, 2019). Note that, when considering monodisperse systems, from (1) we have that

$$
\frac{\rho_{\mathrm{c}}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}}=\frac{\epsilon \rho^{s}+(1-\epsilon) \rho_{\mathrm{g}}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}}=\epsilon \frac{\rho^{s}-\rho_{\mathrm{g}}}{\rho_{\mathrm{atm}}}+\frac{\rho_{\mathrm{g}}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}}=\left(\epsilon-\epsilon_{\mathrm{cr})} \frac{\rho^{s}-\rho_{\mathrm{g}}}{\rho_{\mathrm{atm}}},\right.
$$

where $\epsilon_{\mathrm{cr}} \stackrel{\text { def }}{=} \frac{\rho_{\mathrm{atm}}-\rho_{\mathrm{g}}}{\rho^{s}-\rho_{\mathrm{g}}}$. Note that, when the interstitial fluid is the ambient air, $\epsilon_{\mathrm{cr}}=0$. Hence, the current flow stops when $\epsilon=\epsilon_{\text {cr }}$.
The analytical expressions for the maximum runout are summarized below. We use the notation

$$
g_{p}^{\prime} \stackrel{\text { def }}{=} \frac{\rho^{s}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}} g \quad \text { and } \quad g_{p}^{\prime \prime} \stackrel{\text { def }}{=} \frac{\rho^{s}-\rho_{\mathrm{g}}}{\rho_{\mathrm{atm}}} g .
$$

## Analytic expressions maximum flow runout

Cartesian current without interstitial buoyant gas
$l_{\infty}=\left(\frac{5 \operatorname{Fr}\left(\epsilon(0) g_{p}^{\prime} V_{0}^{3}\right)^{\frac{1}{2}}}{w^{s}}+l_{0}^{\frac{5}{2}}\right)^{\frac{2}{5}}$
Axisymmetric current without interstitial buoyant gas
$l_{\infty}=\left(8 \operatorname{Fr}\left(\epsilon(0) g_{p}^{\prime}\left(\frac{V_{0}}{\xi \pi}\right)^{3}\right)^{\frac{1}{2}} \frac{1}{w_{s}}+l_{0}^{4}\right)^{\frac{1}{4}}$
Cartesian current with interstitial buoyant gas
$l_{\infty}=\left(\frac{5 \operatorname{Fr}\left(\epsilon_{\mathrm{cr}} g_{p}^{\prime \prime} V_{0}^{3}\right)^{\frac{1}{2}}}{w^{s}}\left(\left(\frac{\epsilon(0)}{\epsilon_{\mathrm{cr}}}-1\right)^{\frac{1}{2}}-\arctan \left(\frac{\epsilon(0)}{\epsilon_{\mathrm{cr}}}-1\right)^{\frac{1}{2}}\right)+l_{0}^{\frac{5}{2}}\right)^{\frac{2}{5}}$

Axisymmetric current with interstitial buoyant gas

$$
l_{\infty}=\left(8 \operatorname{Fr}\left(\epsilon_{\mathrm{cr}} g_{p}^{\prime \prime}\left(\frac{V_{0}}{\xi \pi}\right)^{3}\right)^{\frac{1}{2}} \frac{1}{w^{s}}\left(\left(\frac{\epsilon(0)}{\epsilon_{\mathrm{cr}}}-1\right)^{\frac{1}{2}}-\arctan \left(\frac{\epsilon(0)}{\epsilon_{\mathrm{cr}}}-1\right)^{\frac{1}{2}}\right)+l_{0}^{4}\right)^{\frac{1}{4}}
$$

The box model has been intensively tested against laboratory experiments and multidimensional Eulerian multiphase flow models, able to describe the dynamics of stratified PDCs, providing fairly accurate results (Roche et al., 2013; Neri et al., 2015; Esposti Ongaro et al., 2016).

## 3 PDCs invasion maps

A potential use for the box model is represented by the definition of proper hazard maps, the hazard being the possibility of being reached by a PDC.
Set a vent location, we calculate the maximum flow runout over flat topographies, computed by the box model and then we assess the capability of topographic reliefs to block the current.

In particular, the invasion areas can be obtained by using the so-called energy-conoid model (Orsucci, 2014), based on the assumption of non-linear, monotonic decay of flow kinetic energy with distance (Bevilacqua, 2016).
In more detail, we determine the maximum height $h_{\max }$ of an obstacle the flow can overcome. Then we compare the kinetic energy of the current front and the potential energy associated to the obstacle top, i.e.,

$$
\frac{1}{2} \rho_{\mathrm{c}}\left(\frac{\mathrm{~d} l}{\mathrm{~d} t}\right)^{2}=\left(\rho_{\mathrm{c}}-\rho_{\mathrm{atm}}\right) g h_{\max } \Rightarrow h_{\max }=\frac{1}{2} \frac{\rho_{\mathrm{c}}}{\rho_{\mathrm{c}}-\rho_{\mathrm{atm}}} \frac{1}{g}\left(\frac{\mathrm{~d} l}{\mathrm{~d} t}\right)^{2}
$$

In the case of monodisperse mixtures without hot interstitial fluid, we can analytically solve the equation on the left, for both cartesian and cylindrical currents (Neri et al., 2015; Bevilacqua, 2016).
For simplicity, we are neglecting returning waves. Moreover, a sea surface, if present, is considered as a flat topography with no influence on a PDC traveling over (Bevilacqua et al., 2017).

## 4 Implementation of the PYroclastic BOX Model in the Python code pybox.py

The Python routine described in the sequel has been developed at Istituto Nazionale di Geofisica e Vulcanologia (INGV) - Sezione di Pisa. Its most important characteristics are summarized below.

### 4.1 Input parameters

The code requires the following parameters:

- 10 , h0 and theta0, i.e., the initial current front position, depth and temperature. Note that, if theta0 is equal to the ambient temperature of 300 K , the interstitial fluid density is assumed to be the ambient density, while values above it allow us to take into account the presence of a buoyant interstitial gas (see Section 2);
- eps0, rhos and ds, which are volume fraction, density and dimension for each grain size. Pyroclasts are assumed to be perfectly spherical, hence their representative size ds will be their diameter;
- Fr, g and rhoa, that are Froude number, gravitational acceleration value and air density (at standard conditions of pressure and temperature);
- alpha, the packing fraction, i.e., the volume fraction of solid particles in the deposit;
- flag_coords, by which we can select the geometry (channelized vs. axisymmetric currents): in particular, we can solve the box model equations in cartesian (Eqns. (4)-(6)) or cylindrical (Eqns. (7)-(9)) coordinates, simply by setting flag_coords to values greater or lower or equal than zero, respectively;
- flag_DEM, by which we can choose whether to read a Digital Elevation Model (DEM, see subsection 4.2) or not. Indeed, as previously said, it is possible to analyze the behaviour of PDCs both over flat topographies and over topographies with reliefs and obstacles. We allow either of these cases, depending on the value of flag_DEM: if flag_DEM is set to False, we consider the flow runout in absence of topographies, while, if flag_DEM is True, we account for the presence of a complex topography. In this last case, we have to set other parameters, that are:
- vertical_scale_factor, a scaling factor by which all the elevations registered in the DEM are multiplied. It must be consistent with the other data units;
- zone_number and zone_letter, that identify the UTM (Universal Transverse of Mercator) grid zone the volcanic area is in;
$-\mathrm{xv}, \mathrm{yv}$, the UTM coordinates of the volcanic vent location;
- rad_res, i.e., a resolution for the generation of a grid along each radial direction, centered on the vent;
- anglemin, anglemax, minimum and maximum angles defining a radial sector in which to study the collapse of an eruption column;
- differential_topography, that can be set to True or False, depending on whether we want to consider the current dynamics with respect to elevations above sea level or differential topographies, or not.
- a_tol, absolute tolerance for the control of the local error estimates when using Runge-Kutta 3(2) method to solve the differential problem (see subsection 4.3).


### 4.2 Operations on DEMs

## Reading a DEM

As already said, if flag_DEM is set to True, we are provided with a DEM (that is, a digital representation of the elevation of a given territory) of a volcanic area.
Before proceeding, we want to spend a few words about DEM files. In particular, we have a DEM in .asc format: it is a text file with the following entries in the header.

```
ncols 1900
nrows 1502
xllcorner 418015.70
yllcorner 4514318.30
cellsize 10.00
NODATA_value 0
```

Looking at the rest of the file, it as a matrix of "pixels" (below, also "cells"), each "pixel" recording an elevation value above sea level. The first two entries of the .asc file header represent the number of columns and rows of this matrix, whereas xllcorner and yllcorner indicate the UTM coordinates of the lowermost-leftmost point ${ }^{2}$ of the topographic domain. Besides, cellsize specifies the dimension (in meters) of each "pixel", while NODATA_value, in our case, establishes the elevation value for the cells at the sea level.

In the Python code, we define a subroutine read_dem for extracting information from a DEM in . asc format.
Then we define two vectors xdem and ydem, containing the coordinates of each "pixel" center, and a matrix zdem with cell elevations. Note that we read the elevation data from the upper-left component, so, since the UTM coordinates of each cell are based on the lower-left element ones, we need to flip the entries in each column in the up-down direction, with Python numpy command flipud.

## Writing a DEM

The subroutine write_dem allows us to a create a new file and write to it the above mentioned entries of a DEM in .asc format.

## Dividing a DEM into sectors

As we will explain later, ${ }^{3}$ hazard quantification can be improved by dividing the volcanic area, centered on the vent, in $N_{s}$ azimuthal sectors of central angle $\left(\frac{360}{N_{s}}\right)^{\circ}$.

In particular, we can divide each of these $N_{s}$ radial directions in a certain number of subintervals of fixed width $s_{r}$ (that is, the input parameter rad_res).

[^1]

Figure 3: Radial discretization of the space.

Assigned an angle $\vartheta$, starting from the vent, we construct two vectors, $\mathbf{x}_{r, \vartheta}$ and $\mathbf{y}_{r, \vartheta}$, the first elements being the vent coordinates and the other ones being given by

$$
\begin{aligned}
x_{r, \vartheta}^{(i)} & =x_{r, \vartheta}^{(0)}+i \cdot s_{r} \cos (\vartheta) \\
y_{r, \vartheta}^{(i)} & =y_{r, \vartheta}^{(0)}+i \cdot s_{r} \sin (\vartheta), \quad i=1, \ldots, n_{r_{\max }},
\end{aligned}
$$

where $n_{r_{\text {max }}}$ is the maximum number of grid points in this new system (see Figure 3). Naturally, it may happen that the nodes such created exceed the limits of the DEM or are more than the maximum flow runout away from the vent, in which cases the grid construction is stopped.
Then, for each point of the new grid, we determine the "pixel" of the initial DEM it is in. In this way, we can find the elevation $z_{r, \vartheta}^{(i)}$ of the $i$-th node, $i=0, \ldots, n_{r_{\text {max }}}$.

The procedure just designed is implemented in the Python subroutine dem_section, in which $\mathbf{x}_{r, \vartheta}, \mathbf{y}_{r, \vartheta}, \mathbf{z}_{r, \vartheta}, n_{r_{\text {max }}}$ and $s_{r}$ are respectively labeled $\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathrm{nmax}$ and d. As we can see from the code, when looking for the "pixel" containing a certain node, we distinguish between four cases, according to the quadrant the angle $\vartheta$ terminates in.

### 4.3 Numerical integration

The set of equations (4)-(6) (or (7)-(9)) is numerically integrated by using RungeKutta 3(2) method (below, also RK3(2)).

## Explicit $s$-stages Runge-Kutta methods

Let us consider the problem of numerically solving the first order system of Ordinary Differential Equations (ODEs)

$$
\left\{\begin{array}{l}
\dot{\mathbf{y}}(t)=\mathbf{f}(t, \mathbf{y}(t)), \quad t \in\left(t_{0}, t_{\max }\right]  \tag{10}\\
\mathbf{y}\left(t_{0}\right)=\mathbf{y}_{0}
\end{array}\right.
$$

where $\mathbf{y}(t) \in \mathbb{R}^{m}, t \in\left[t_{0}, t_{\text {max }}\right]$, and $\mathbf{f}: \mathbb{R} \times \mathbb{R}^{m} \rightarrow \mathbb{R}^{m} .{ }^{4}$
Recall that, in the most general form, all the explicit s-stages Runge-Kutta methods for the numerical solution of the initial value problem (below, IVP) (10) can be written as (Dormand and Prince, 1980; Atkinson, 1989; Lambert, 1992; Gautschi, 1997)

$$
\begin{equation*}
\mathbf{y}_{n+1}=\mathbf{y}_{n}+(\Delta t)_{n} \mathbf{F}\left(t_{n}, \mathbf{y}_{n},(\Delta t)_{n} ; \mathbf{f}\right), \quad n=0, \ldots, N_{\max }-1, \tag{11}
\end{equation*}
$$

where, once constructed a discrete mesh $\left\{t_{i}\right\}_{i=0, \ldots, N_{\max }}$ in the interval $\left[t_{0}, t_{\text {max }}\right], \mathbf{y}_{n}$ represents an approximation to the values $\mathbf{y}\left(t_{n}\right)$ of the solution at the grid points, i.e., $\mathbf{y}_{n} \approx \mathbf{y}\left(t_{n}\right)$. Furthermore, $(\Delta t)_{n}$ is the current time step, that is, $t_{n+1}=t_{n}+(\Delta t)_{n}$, and $\mathbf{F}$ is a function defined as follows:
$\mathbf{F}\left(t_{n}, \mathbf{y}_{n},(\Delta t)_{n} ; \mathbf{f}\right)=\sum_{i=1}^{s} \gamma_{i} \mathbf{V}_{i}, \mathbf{V}_{i}=\left\{\begin{array}{l}\mathbf{f}\left(t_{n}, \mathbf{y}_{n}\right), i=1, \\ \mathbf{f}\left(t_{n}+\alpha_{i}(\Delta t)_{n}, \mathbf{y}_{n}+(\Delta t)_{n} \sum_{j=1}^{i-1} \beta_{i j} \mathbf{V}_{j}\right), i>1 .\end{array}\right.$
Coefficients $\left\{\beta_{i j}\right\},\left\{\alpha_{i}\right\}$ and $\left\{\gamma_{i}\right\}$ completely characterize a Runge-Kutta method and are arranged in the so-called Butcher tableau

$$
\begin{array}{c|c}
\boldsymbol{\alpha} & \beta \\
\hline & \boldsymbol{\gamma}^{t}
\end{array}
$$

We impose the conditions (Gautschi, 1997)

$$
\sum_{i=1}^{s} \gamma_{i}=1 \quad \text { and } \quad \alpha_{i}=\sum_{j=1}^{i-1} \beta_{i j}, i=2, \ldots, s
$$

We also recall that an explicit $s$-stages Runge-Kutta method cannot have order of accuracy greater than $s .{ }^{5}$ Moreover, we remark that a Runge-Kutta method of order $s$ for a

[^2]scalar IVP may have order less than $s$ when applied to solve a system of ODEs (Lambert, 1992).

Herein, we do not deal with the stability analysis of explicit Runge-Kutta schemes. It is worth mentioning that explicit A-stable Runge-Kutta methods do not exist, although the stability regions become larger, as the order increases (Lambert, 1992).

## Embedded Runge-Kutta methods

Since Runge-Kutta methods are one-step, they are particularly suitable for changing step size, as long as we are provided with an acceptable estimator of the local truncation error (12), introduced in the single integration step.
This aim can be achieved by taking two $s$-stages Runge-Kutta methods of orders $p$ and $q, q>p$ (usually $q=p+1$ ), and applying them simultaneously to the same problem. Moreover, in order to cut down the computational effort, we impose that the two schemes share the same function evaluations (i.e., have same coefficients $\alpha_{i}, \beta_{i j}$ ).
So, at each step, we can express the two approximations for the solution as

$$
\begin{aligned}
& \mathbf{y}_{n+1}=\mathbf{y}_{n}+(\Delta t)_{n} \sum_{i=1}^{s} \gamma_{i} \mathbf{V}_{i} \\
& \overline{\mathbf{y}}_{n+1}=\mathbf{y}_{n}+(\Delta t)_{n} \sum_{i=1}^{s} \bar{\gamma}_{i} \mathbf{V}_{i}
\end{aligned}
$$

and the Butcher tableau can be summarized as


By definition (see note 6), we have that

$$
\begin{aligned}
& \boldsymbol{\tau}_{n+1}=\mathbf{y}\left(t_{n+1}\right)-\mathbf{y}_{n+1}=\mathcal{O}\left((\Delta t)_{n}^{p+1}\right) \\
& \overline{\boldsymbol{\tau}}_{n+1}=\mathbf{y}\left(t_{n+1}\right)-\overline{\mathbf{y}}_{n+1}=\mathcal{O}\left((\Delta t)_{n}^{q+1}\right)
\end{aligned}
$$

hence, by subtracting the two above relationships, we get

$$
\boldsymbol{\tau}_{n+1} \approx \boldsymbol{\omega}_{n+1} \stackrel{\text { def }}{=} \overline{\mathbf{y}}_{n+1}-\mathbf{y}_{n+1}=(\Delta t)_{n} \sum_{i=1}^{s}\left(\bar{\gamma}_{i}-\gamma_{i}\right) \mathbf{V}_{i} \stackrel{\text { def }}{=}(\Delta t)_{n} \sum_{i=1}^{s} c_{i} \mathbf{V}_{i}
$$

Step control. Now, the idea is the following: if the two numerical solutions are in close agreement, the approximation $\mathbf{y}_{n+1}$ is accepted, whereas, if their difference exceeds a specified accuracy, the step size is reduced. In particular, we impose that (Atkinson, 1989)

$$
\left\|\boldsymbol{\tau}_{n+1}\right\|_{\infty} \leq \text { tol }_{\mathrm{a}}+\left\|\mathbf{y}_{n}\right\|_{\infty} \mathrm{tol}_{\mathrm{r}} \stackrel{\text { def }}{=} \varepsilon_{n+1}
$$

In practice, starting from an initial guess $(\Delta t)_{0}$, we compute $\mathbf{y}_{1}, \overline{\mathbf{y}}_{1}$ and hence the estimator $\boldsymbol{\omega}_{1}$ for $\boldsymbol{\tau}_{1}$. Suppose the aforementioned test has not passed, so we have to reduce $(\Delta t)_{0}\left((\Delta t)_{n}\right.$, for the generic step). How this can be done?
Assume that the local truncation error can be written as

$$
\boldsymbol{\tau}_{n+1}=\mathbf{T}\left(t_{n}, \mathbf{y}\left(t_{n}\right)\right)(\Delta t)_{n}^{p+1}+\mathcal{O}\left((\Delta t)_{n}^{p+2}\right)
$$

where the function $\mathbf{T}(t, \mathbf{y}(t))$ is called the principal error function.
Thus, considering a smaller step size, i.e., $(\Delta t)_{n} \rightarrow(\Delta t)_{n}^{\text {new }}=\zeta(\Delta t)_{n}, \zeta<1$, we have

$$
\boldsymbol{\tau}_{n+1}^{\mathrm{new}} \approx \mathbf{T}\left(t_{n}, \mathbf{y}\left(t_{n}\right)\right) \zeta^{p+1}(\Delta t)_{n}^{p+1}=\zeta^{p+1} \boldsymbol{\omega}_{n+1}^{\mathrm{old}}
$$

and we force

$$
\left\|\zeta^{p+1} \boldsymbol{\omega}_{n+1}^{\mathrm{old}}\right\|_{\infty} \leq \varepsilon_{n+1} \Rightarrow \zeta \leq\left(\frac{\varepsilon_{n+1}}{\| \boldsymbol{\omega}_{n+1}^{\mathrm{old} \|_{\infty}}}\right)^{\frac{1}{p+1}}<1
$$

Set a safety factor $\mu \in(0,1),{ }^{6}$ we estimate $(\Delta t)_{n}^{\text {new }}$ as

$$
(\Delta t)_{n}^{\text {new }}:=(\Delta t)_{n}=\mu\left(\frac{\varepsilon_{n+1}}{\left\|\boldsymbol{\omega}_{n+1}^{\mathrm{old}}\right\|_{\infty}}\right)^{\frac{1}{p+1}}(\Delta t)_{n}
$$

and accept the solution $\mathbf{y}_{n+1}^{\text {new }}$ (obtained with this new time step) as $\mathbf{y}_{n+1}$. It is recommended to control whether or not the requested accuracy has actually been reached, anyway.
Once admitted the time step $(\Delta t)_{n}$, since $\left\|\boldsymbol{\omega}_{n+1}\right\|_{\infty}<\varepsilon_{n+1}$, we can try to estimate $(\Delta t)_{n+1}$ as

$$
(\Delta t)_{n+1}=\underbrace{\left(\frac{\varepsilon_{n+1}}{\left\|\boldsymbol{\omega}_{n+1}\right\|_{\infty}}\right)^{\frac{1}{p+1}}}_{>1}(\Delta t)_{n}
$$

i.e., the step size is increased, and we repeat, for the current time, the tests above described for the previous one.

## Runge-Kutta-Fehlberg method

A widely used scheme is Runge-Kutta-Fehlberg method (below also RKF45), that embeds Runge-Kutta formulas of order 4 and 5: it controls the local truncation errors assuming accuracy of the fourth-order method and taking the steps with the fifth-order accurate scheme.
RKF45 Butcher tableau, according to one of the Dormand-Prince formulas, ${ }^{7}$ is shown below (Dormand and Prince, 1980): ${ }^{8}$

[^3]| $\frac{1}{5}$ | $\frac{1}{5}$ |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :--- |
| $\frac{3}{10}$ | $\frac{3}{40}$ | $\frac{9}{40}$ |  |  |  |  |  |
| $\frac{4}{5}$ | $\frac{44}{45}$ | $-\frac{56}{15}$ | $\frac{32}{9}$ |  |  |  |  |
| $\frac{8}{9}$ | $\frac{19372}{6561}$ | $-\frac{25360}{2187}$ | $\frac{64448}{6561}$ | $-\frac{212}{729}$ |  |  |  |
| 1 | $-\frac{9017}{3168}$ | $-\frac{355}{33}$ | $\frac{46732}{5247}$ | $\frac{49}{176}$ | $-\frac{5103}{18656}$ |  |  |
| 1 | $\frac{35}{384}$ | 0 | $\frac{500}{1113}$ | $\frac{125}{192}$ | $-\frac{2187}{6784}$ | $\frac{11}{84}$ |  |
| $\frac{0}{384}$ | 0 | $\frac{500}{1113}$ | $\frac{125}{192}$ | $-\frac{2187}{6784}$ | $\frac{11}{84}$ | 0 |  |
| $\frac{5179}{57600}$ | 0 | $\frac{7571}{16695}$ | $\frac{393}{640}$ | $-\frac{92097}{339200}$ | $\frac{187}{2100}$ | $\frac{1}{40}$ |  |

## RK3(2)

As already said, we perform our numerical integrations with RK3(2), which controls the local truncation error assuming accuracy of the second-order method, but takes the steps by means of the third-order accurate formula. Here the scheme proposed by Bogacki and Shampine (1989), i.e., the so called Bogacki-Shampine pair of formulas, is used, whose Butcher tableau is

| $\frac{1}{2}$ | $\frac{1}{2}$ |  |  |  |
| :--- | :--- | :--- | :--- | :--- |
| $\frac{3}{4}$ | 0 | $\frac{3}{4}$ |  |  |
|  | $\frac{2}{9}$ | $\frac{1}{3}$ | $\frac{4}{9}$ | 0 |
| $\frac{7}{24}$ | $\frac{1}{4}$ | $\frac{1}{3}$ | $\frac{1}{8}$ |  |

With respect to RKF45, this approach is preferred because RKF45 does not succeed in preserving the monotonicity of the settling solid fractions.
Following the notation from this subsection, we have to apply RK3(2) to numerically
solve Eqns. (4)-(6) or (7)-(9), with

$$
\mathbf{f}(t, \mathbf{y})=\left(\begin{array}{c}
\operatorname{Fr} \sqrt{g^{\prime}\left(y_{2}, \ldots, y_{N+1}\right) \frac{V_{0}}{y_{1}}} \\
-\frac{w_{s, 1} y_{2} y_{1}}{V_{0}} \\
\vdots \\
-\frac{w_{s, N} y_{N+1} y_{1}}{V_{0}}
\end{array}\right) \quad \text { or } \quad \mathbf{f}(t, \mathbf{y})=\left(\begin{array}{c}
\operatorname{Fr} \sqrt{g^{\prime}\left(y_{2}, \ldots, y_{N+1}\right) \frac{V_{0}}{\xi \pi}} \frac{1}{y_{1}} \\
-\frac{\xi \pi w_{s, 1} y_{2} y_{1}^{2}}{V_{0}} \\
\vdots \\
-\frac{\xi \pi w_{s, N} y_{N+1} y_{1}^{2}}{V_{0}}
\end{array}\right),
$$

depending on whether flag_coords is greater than zero or not. In the code, we define proper subroutines for computing these terms and call them fun_cartesian and fun_cylindrical, respectively.

Python function scipy.integrate.solve_IVP. We solve the box model equations with the already existing function scipy.integrate.solve_IVP, available in Python$3 . x,{ }^{9}$ which makes use of the Bogacki-Shampine pair of formulas (Bogacki and Shampine, 1989).

For the numerical solution of the generic problem (10), the basic syntax is sol = scipy. integrate.solve_IVP(fun, tspan, y0, method, events, rtol, atol), where fun is the r.h.s. of the system, tspan and y0 are respectively the interval of integration ${ }^{10}$ and the initial condition, method indicates the integration scheme ('RK23', ${ }^{11}$ in our case), while the event entry allows to stop the integration process if a specific condition occurs. Finally, tolerances tol ${ }_{r}$ and tol $_{a}$ (above referred to as rtol and atol) are respectively set to rtol $=10^{-13}$ and a_tol value, specified as input by the user.

Restart procedure It may happen that, when solving the problem numerically, the computed solid fractions fall below zero. This case is not acceptable since errors may be magnified leading to inexact solutions.
We can avoid these situations by interrupting the integration process whenever (at least)

[^4]depending on whether a buoyant interstitial gas is present or not, as follows by equating $\rho_{\mathrm{c}}$ and $\rho_{\mathrm{atm}}$ (since, when $g^{\prime}$ falls below zero, the flow stops). In order to obtain the estimates above, in the equations (6), (9) we have replaced the ratios $\frac{w_{i}^{s}}{h(t)}$ with the (lower) quantities $\frac{\min _{i=1, \ldots, N} w_{i}^{s}}{h_{0}}$, leading to an overestimation of the effective $t_{\text {max }}$.
${ }^{11}$ 'RK45', that is, RKF45, is employed by default.
one solid fraction becomes lower than zero (or extremely small) ${ }^{12}$ and restarting it with a new initial value, obtained by setting to zero such fractions.

Thus, in our case, the integration process is blocked (and then restarted) when a solid volume fraction becomes extremely small and it is permanently interrupted when the reduced gravity $g^{\prime}$ falls below zero, regardless of the values of the solid fractions.

### 4.4 Subroutines for computing physical quantities

## Computing density of a polydisperse mixture

As we can see in the Python code, we enable the possibility of considering polydisperse mixtures.
In particular, in the subroutine polydisperse_density, we compute the density of the polydisperse current, according to (1).

## Computing reduced gravity of a polydisperse mixture

Similarly, referring to (2), we determine the reduced gravity of the polydisperse mixture by means of the polydisperse_rg subroutine. In the code, we respectively call rg and phi [i] the quantities

$$
\frac{\rho_{\mathrm{g}}-\rho_{\mathrm{atm}}}{\rho_{\mathrm{atm}}} \quad \text { and } \quad \frac{\rho_{i}^{s}-\rho_{\mathrm{g}}}{\rho_{\mathrm{atm}}} .
$$

## Estimating terminal velocities

We determine each particle class terminal velocity with the settling subroutine. In particular, once denoted the grain-size class diameters by $d_{s, i}, i=1, \ldots, N$, the asymptotic, stationary settling velocities are calculated by means of the Newton's impact formula (Dellino et al., 2005; Dioguardi et al., 2018)

$$
\begin{equation*}
w_{i}^{s}=\sqrt{\frac{4 d_{s, i} \rho_{i}^{s}}{3 C_{\mathrm{D}_{i}} \rho_{\mathrm{g}}}} g, \quad i=1, \ldots, N \tag{13}
\end{equation*}
$$

where the gas-particle drag coefficient $C_{\mathrm{D}_{i}}$ is defined, as a function of the relative gasparticle Reynolds number $\operatorname{Re}_{r_{i}}, \operatorname{Re}_{r_{i}}=\frac{\rho_{\mathrm{g}} d_{s, i} w_{i}^{s}}{\mu_{g}}, \mu_{g}$ being the interstitial fluid dynamic

[^5]viscosity, ${ }^{13}$ by the following expression
\[

C_{\mathrm{D}_{i}}= $$
\begin{cases}\frac{24}{\operatorname{Re}_{r_{i}}}\left(1+0.15 \cdot \operatorname{Re}_{r_{i}}^{0.687}\right) & \text { if } \mathrm{Re}_{r_{i}}<1000 \\ 1 & \text { otherwise }\end{cases}
$$
\]

We have therefore used the Schiller-Naumann correlation (Crowe et al., 2011), which accurately describes the drag force acting on a sphere up to $\operatorname{Re}_{r_{i}} \simeq 1000$, whereas, for $\operatorname{Re}_{r_{i}} \geq 1000$, we have set $C_{\mathrm{D}_{i}}=1$, according to Woods and Bursik (1991).

As we can see, the computation of settling velocities requires an iterative procedure: in fact, the Newton's impact formula (13) must be solved together with the relationship for the Reynolds number and the correlation between $C_{\mathrm{D}_{i}}$ and $\mathrm{Re}_{r_{i}}$.
Hence, starting from an initial guess $w_{i}^{s(0)},{ }^{14}$ we determine the corresponding Reynolds number, which is further used to find settling velocity by (13); a new Reynolds number is then calculated and the process is continued until the solution converges ${ }^{15}$ or iterations exceed a maximum number, be it kmax.

## Computing deposits

For each particle class, we can compute the amount of mass loss by sedimentation, per unit area, per current time step, as

$$
m_{i}(t)=w_{i}^{s} \rho_{i}^{s} \epsilon_{i}(t) \Delta t, \quad i=1, \ldots, N
$$

$\Delta t$ being the current time step size. ${ }^{16}$
Thus, for a given time $\bar{t}$ and the corresponding current front position $l(\bar{t})$, we determine the total mass deposited by the PDC in that point as the sum of $m_{i}(t)$, for all $i$, for all time $t \in\left[\bar{t}, t_{\mathrm{max}}\right]$, where $t_{\max }$ is the final run time, as usual. ${ }^{17}$ Similarly, by keeping $i$, we can compute the deposited total mass of the $i-$ th particle class, hence the deposited mass fraction of that class, at distance $l(\bar{t})$.

[^6]At last, from the previous quantities, we deduce the thickness profile of the $i$-th class deposited layer as the ratio of the deposited total mass of that class to the $i$-th class solid density (multiplied by the packing fraction, above referred to as alpha, see 4.1). In the code, the vector $\mathbf{m}$ is called deposit, whereas the other quantities above introduced are named totalmass, mass, fract and thick, respectively.

### 4.5 Writing invasion maps

Before building invasion maps, we express $h_{\text {max }}$ in terms of $l$ : starting from the initial front position $l_{0}$, we thus determine the value of $h_{\max }$ corresponding to all the possible integer current lengths up to the maximum flow runout.
For this purpose, in the code we construct a proper vector named hmax_of_l, in which the evolution of $h_{\text {max }}$ as a (discrete) function of $l$ is recorded.

With a view to define invasion maps, we take each "pixel" of the original DEM and build a new DEM, in which "pixels" do not register elevation data but binary values, 1 or 0 , depending on whether the cell has been invaded or not by the current.

## Energy-conoid model: method 1

A first, simple way to construct invasion maps is described below.
We set a vent location, then we compute the distance dist between the vent and each point (xdem[i], ydem $[j]$ ) of the original DEM. So, we deduce the value of $h_{\max }$ corresponding to the nearest integer to dist and compare it with the elevation of the cell; we also compare dist with the maximum flow runout. If dist exceeds the maximum runout or the "pixel" elevation is greater than $h_{\max }$, that cell is assumed not to be invaded.

## Energy-conoid model: method 2

Nevertheless, the approach above described may lead to unphysical invasion regions in the lee of topographical barriers (see Fig. 4(a)).
For this reason, in order to improve hazard assessment, in the case of radially spreading currents, we can divide the 360 -azimuth volcanic area, centered on the vent, in a certain number of thin circular sectors, be it $N_{s}$ (typically, $N_{s}=360$, see subsection 4.2), and compute the energy-conoid solution along all the $N_{s}$ sectors.

Step 1. By using the function dem_section, defined in subsection 4.2, for each angle $\vartheta$ we determine the elevation of the grid points along the direction specified by $\vartheta$. Then, we check if their elevation is greater than the value of $h_{\text {max }}$ relative to the closest integer to the distance from the vent. As soon as this condition is satisfied, the flow is stopped in that direction and the maximum traveled distance is stored.

Step 2. Once done this, we compute the distance dist between the vent and each point (xdem[i], ydem[j]) of the original DEM. Then, we determine which direction (starting from the vent) the point is in, hence the angle corresponding to this direction.

Step 3. Since we consider currents spreading within a circular sector of central angle $\theta$, we take every DEM point lying in this sector and, if its distance from the vent is lower than the maximum runout in the corresponding direction (as determined above), the cell containing the point is assumed to be invaded.
It is worth noting that, for both the approaches, the model does not allow a partial block of the current: a cell cannot be partially invaded.

The difference between these two approaches is shown in Figure 4: under the same initial conditions, the invasion maps obtained via energy-conoid method 1 (a) and energyconoid method 2 (b) are extremely dissimilar.

## Currents spreading on slopes

When investigating the current flow on complex topographies, we have to take into account that the flow may start from positive elevation or encounter upward slopes after downward slopes. ${ }^{18}$ In this case, enabled by setting differential_topography input parameter to True, it is reasonable to compare $h_{\max }$ at a given distance from the vent not with the corresponding topographic elevation but with the difference in level experienced by the current between the previous and the present sampled positions.
Figure 5 compares a PDC propagation in the Mt. Vesuvius volcanic region (Italy), with differential_topography = True (a) and differential_topography = False (b). Note that in the first case the invaded area is greater: this is due to the fact that, in proximity to the vent, the $h_{\max }$ required to completely stop the current is higher than in the second case.

### 4.6 Visualizing invasion maps

Finally, we included a plotting tool in the code. ${ }^{19}$
In particular, after having found longitude and latitude coordinates of the DEM limits and the vent via Python module utm, we download the map of the corresponding zone from the Google Maps Static API. The Maps Static API service returns the map as an image we can display. Then, using salem module, ${ }^{20}$ we can reconstruct on the image such obtained the grid of the original DEM and hence add and plot our georeferenced data about the invasion.
Results of this process are shown in Figures 4 and 5, where each pixel of the original DEM

[^7](easily distinguishable from the rest of the region) is colored blue or yellow, depending on whether it is invaded or not. Moreover, the vent is marked as a red spot on the map.


Figure 4: Comparison between the two approaches, outlined in subsection 4.5, to obtain invasion maps, with regard to the numerical simulation of a PDC propagation at Campi Flegrei Caldera, Italy. In the second case, some topographical reliefs are able to completely shield the rear zones against the current.

(b)

Figure 5: Comparison of the invasion maps achieved with regard to the numerical simulation of a PDC propagation at Mt. Vesuvius area (Italy), by using the two boolean values allowable for differential_topography. Note the differences near the vent.

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[^0]:    ${ }^{1}$ The fraction refers to a constant volume of the mixture flow, not reduced by the deposition.

[^1]:    ${ }^{2}$ Not pixel!
    ${ }^{3}$ See subsection 4.5.

[^2]:    ${ }^{4}$ Here we suppose that all the hypotheses for the local existence and uniqueness of the solution hold.
    ${ }^{5}$ A numerical scheme for solving IVPs is said to be $p-t h$ order accurate if, once defined the local truncation error $\boldsymbol{\tau}_{n+1}$ of (11) as the residual

    $$
    \begin{equation*}
    \boldsymbol{\tau}_{n+1}=\mathbf{y}\left(t_{n+1}\right)-\mathbf{y}\left(t_{n}\right)-(\Delta t)_{n} \mathbf{F}\left(t_{n}, \mathbf{y}\left(t_{n}\right),(\Delta t)_{n} ; \mathbf{f}\right), \quad n=0, \ldots, N_{\max }-1 \tag{12}
    \end{equation*}
    $$

    $p$ is the largest integer such that $\boldsymbol{\tau}_{n+1}=\mathcal{O}\left((\Delta t)_{n}^{p+1}\right)$ (Dormand and Prince, 1980; Lambert, 1992; Brugnano and Trigiante, 1998).
    Otherwise said, $\boldsymbol{\tau}_{n+1}$ represents the error introduced in the single integration step, in the local hypothesis $\mathbf{y}_{n}=\mathbf{y}\left(t_{n}\right)$.

[^3]:    ${ }^{6}$ We put it since our estimation of the local truncation error is not exact.
    ${ }^{7}$ Dormand-Prince formulas are a class of Runge-Kutta schemes of order 4 and 5 , first derived in Dormand and Prince (1980). Herein, we make use of one of these formulas.
    ${ }^{8}$ This scheme is quite similar to the RKF45 method implemented in Python function scipy.integrate.solve_IVP. Proper modifications with respect to the Butcher tableau here represented are introduced, in accordance with Shampine (1986).

[^4]:    ${ }^{9}$ Please refer to SciPy v1.2.1 Reference Guide (2019), available at https://docs.scipy.org/doc/ scipy/reference/index.html.
    ${ }^{10}$ The maximum run time $t_{\text {max }}$ is estimated as

    $$
    t_{\max }=-\frac{h_{0}}{\min _{i=1, \ldots, N} w_{i}^{s}} \log \left(\frac{\rho_{\mathrm{atm}}-\rho_{\mathrm{g}}}{\sum_{i=1}^{N} \epsilon_{0, i}\left(\rho_{i}^{s}-\rho_{\mathrm{g}}\right)}\right) \quad \text { or } \quad t_{\max }=-\frac{h_{0}}{\min _{i=1, \ldots, N} w_{i}^{s}} \log \left(\frac{\sum_{i=1}^{N} \epsilon_{0, i} \rho_{\mathrm{atm}}}{\sum_{i=1}^{N} \epsilon_{0, i} \rho_{i}^{s}}\right)
    $$

[^5]:    ${ }^{12}$ In the code we force the computation to stop when (at least) one solid fraction, be it $\epsilon_{\bar{i}}$, is $\epsilon_{\bar{i}} \leq$ $10^{-10} \sum_{i=1}^{N} \epsilon_{i}(0)$.

[^6]:    ${ }^{13}$ Dynamic viscosity as a function of temperature is computed according to Sutherland's law for ideal gases (Sutherland, 1893), which states that

    $$
    \mu(\vartheta)=\frac{C_{1} \vartheta^{\frac{3}{2}}}{\vartheta+C_{2}}
    $$

    $\vartheta$ being the absolute temperature of the gas, $C_{1}=1.458 \cdot 10^{-6} \mathrm{~kg} \cdot\left(\mathrm{~m} \cdot \mathrm{~s} \cdot \mathrm{~K}^{\frac{1}{2}}\right)^{-1}, C_{2}=110.4 \mathrm{~K}$.
    ${ }^{14}$ In the code, the initial guess is provided by the Stokes free-fall velocity formula, i.e.,

    $$
    w_{i}^{s}=\frac{d_{s, i} \rho_{i}^{s}}{18 \mu_{g}} g
    $$

    which has remarkable experimental confirmations within the regime $\operatorname{Re}_{r_{i}}<1$.
    ${ }^{15}$ We mean that the difference between two consecutive iterates is within a tol tolerance.
    ${ }^{16}$ From the discussion on the step control mechanism, recall that we use an adaptive time step technique, hence the vector of time output may not have any "regularity".
    ${ }^{17}$ This choice is due to the fact that, before $t=\bar{t}$, the current has not yet arrived to the position $l(\bar{t})$.

[^7]:    ${ }^{18}$ In calderas, where the mean topographic slope is about zero, we can make use of the procedure just described.
    ${ }^{19}$ Although both the previous approaches were present in the original version of the code, the first one has been removed, since we actually visualize invasion maps defined only by energy-conoid method 2 .
    ${ }^{20}$ See https://salem.readthedocs.io/en/v0.2.3/.

