Molecular dynamics simulation of landslide with two infiltration time scales due to micro and macro pore soil structure

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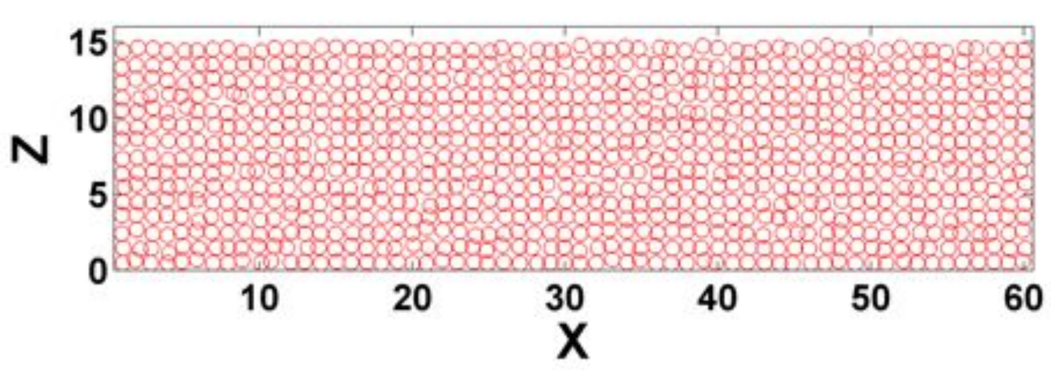
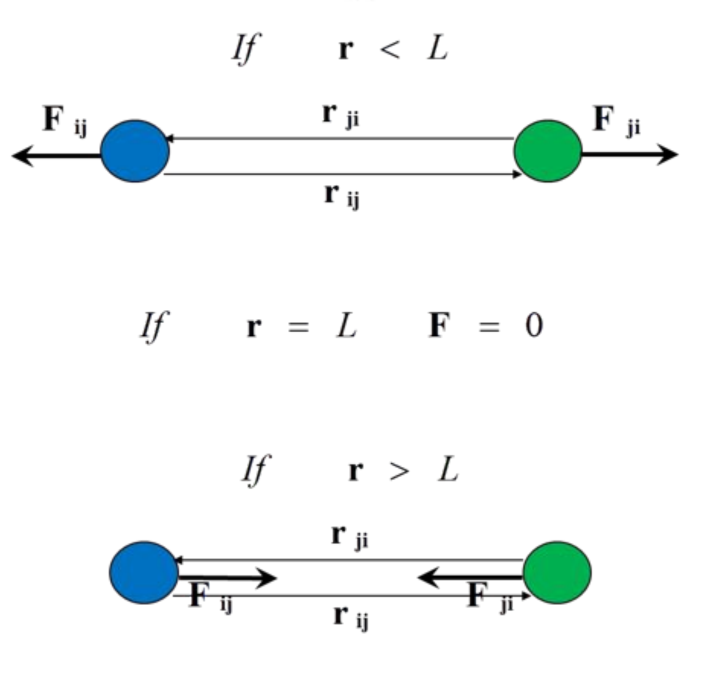
1) Introduction

In this work we integrate existing soil infiltration modeling with particle based methods in order to simulate landslides triggered by rainfall. In literature, usually, the infiltration models are based on continuum schemes (e.g. Eulerian approach) by means of which it is possible to define the field of the pore pressure within a soil. Differently, the particle based method implements a Lagrangian scheme which allows to follow the trajectory of the particles and their dynamical properties. In order to simulate the triggering mechanism, we test the classical and fractional Richards equations adapted to the molecular dynamics approach using the failure criterion of Mohr-Coulomb. In our scheme the local positive pure pressures are simply interpreted as a perturbation of the rest state of each grain, i.e., the pore pressure function can be interpreted as a time-space dependent scalar field acting on the particles. To initialize the system we generate, using a molecular dynamics based algorithm, a mechanically stable sphere packing simulating a consolidate soil. In this way we obtain the input structure of our "fictitious" soil to model landslides, considering the infiltration processes caused by rainfall. Moreover, in our scheme, the particles are porous and therefore we take into consideration the micro pore structure at intra-particle level, while the macro pore structure is due to inter-particle interstices. In this way we have two different infiltration time scales, as observed experimentally. The inter-particle interactions are modeled through a force which, in the absence of suitable experimental data and due to the arbitrariness of the grain dimension, is derived from a Lennard-Jones like potential. For the prediction of the particle positions, after and during a rainfall, we use a standard molecular dynamics approach. We analyze the sensitivity of the models by varying some parameters (hydraulic conductivity, cohesion, slope and friction angle, soil depth, variation of random properties, fractional order of the generalized infiltration model, etc.) and considering both regular and random configuration of the particles. The outcome of the simulations is quite satisfactory and therefore, we can claim that this is a promising new method to simulate landslides triggered by rainfall.

2) Granular packing

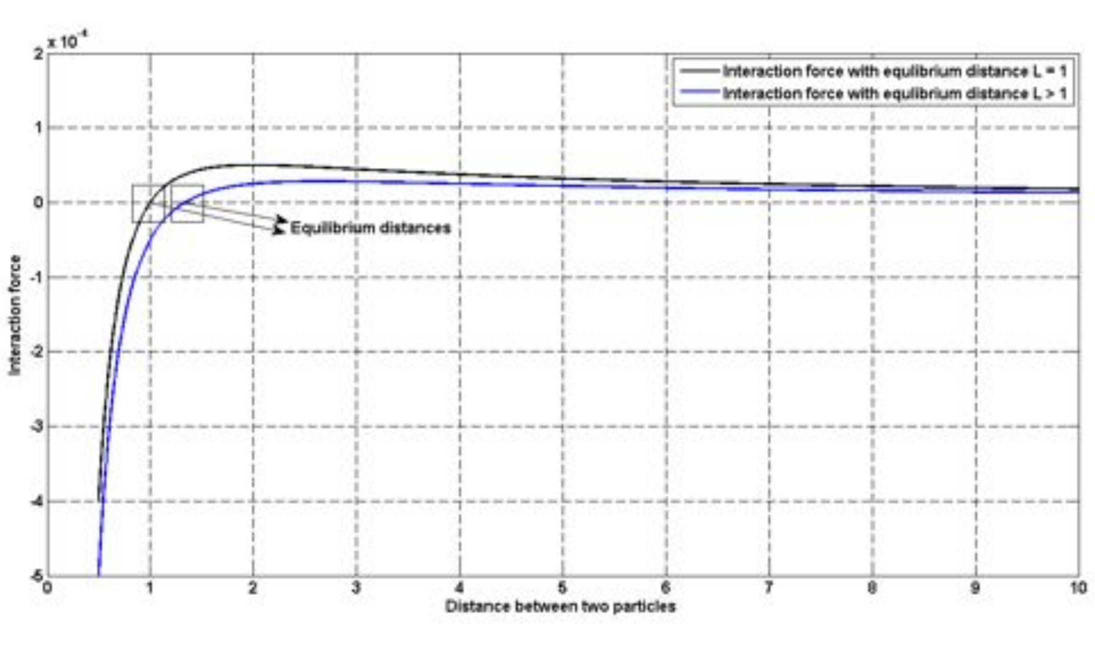
Using a molecular dynamics algorithm, based on sedimentation under the force of gravity and Lennard-Jones like potential, we obtain a mechanically stable sphere packing (with overlapping) simulating a consolidate soil.





$$\mathbf{F_{ij}} = -\mathbf{F_{ji}} = -\left[k_1 \cdot \left(\frac{r}{L}\right)^{-2} - k_2 \cdot \left(\frac{r}{L}\right)^{-1}\right] \cdot \hat{\mathbf{r}}$$

$$r = |\mathbf{r_{ij}}| = \sqrt{(x_j - x_i)^2 + (z_j - z_i)^2}$$



Acknowledgements:

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3) The anomalous infiltration process

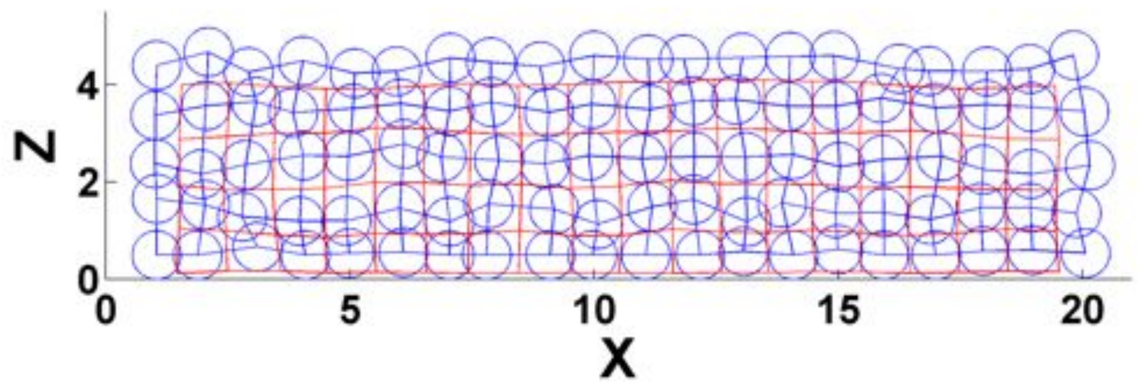
The hydrological scheme, due to rainfall input, is modeled by means of diffusion equation. Therefore, we take into account the normal diffusion at inter-particles level (macro pore structure) considering the water content θ_n and anomalous diffusion at intra-particle level (micro pore structure) considering the water content θ. Then we consider the stochastic term η due to arbitrariness of the soil structure.

$$\frac{\partial \theta_n(z,t)}{\partial t} = K_n \cdot \frac{\partial \theta_n^2(z,t)}{\partial z^2} + \eta_n(z,t) \qquad \frac{\partial \theta^\alpha(z,t)}{\partial t^\alpha} = K \cdot \frac{\partial^\beta \theta(z,t)}{\partial z^\beta} + \eta(z,t)$$

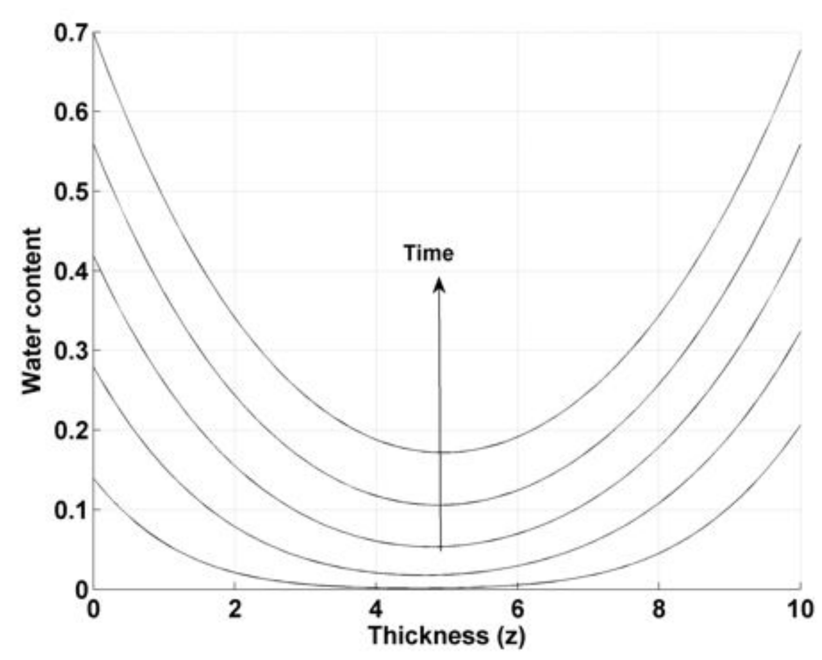
From water content to the pore pressure response p over space and time depending on the particle mass m, gravity acceleration g and elevation z (k is a random function depending on x):

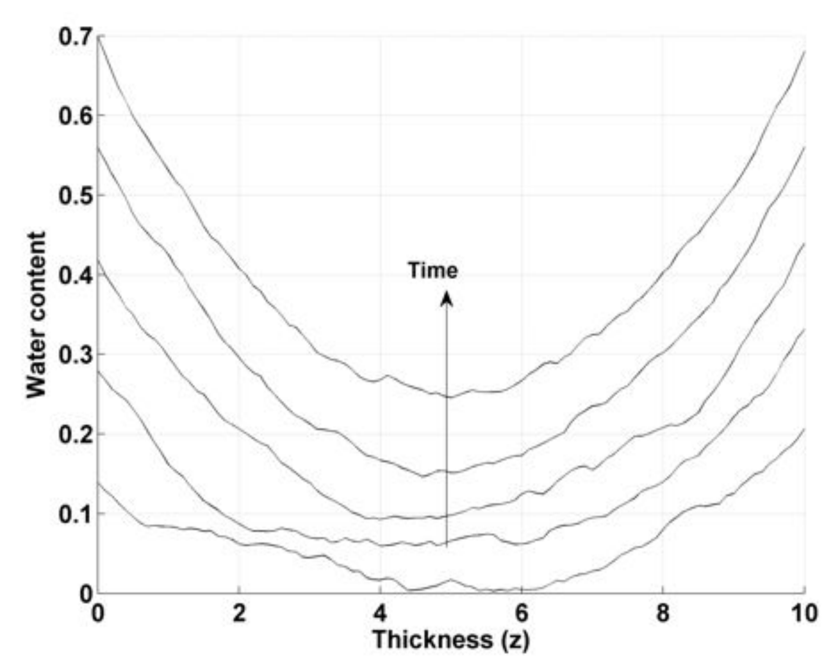
$$\theta(x,z,t) = k(x) \cdot \theta(z,t)$$
$$p(x,z,t) = \theta(x,z,t) \cdot m(x,z) \cdot g \cdot z$$

In the figure below in evidence the schemes for the numerical integration of diffusion equation (the blue grid for the numerical integration of anomalous diffusion and the red grid for the normal one).

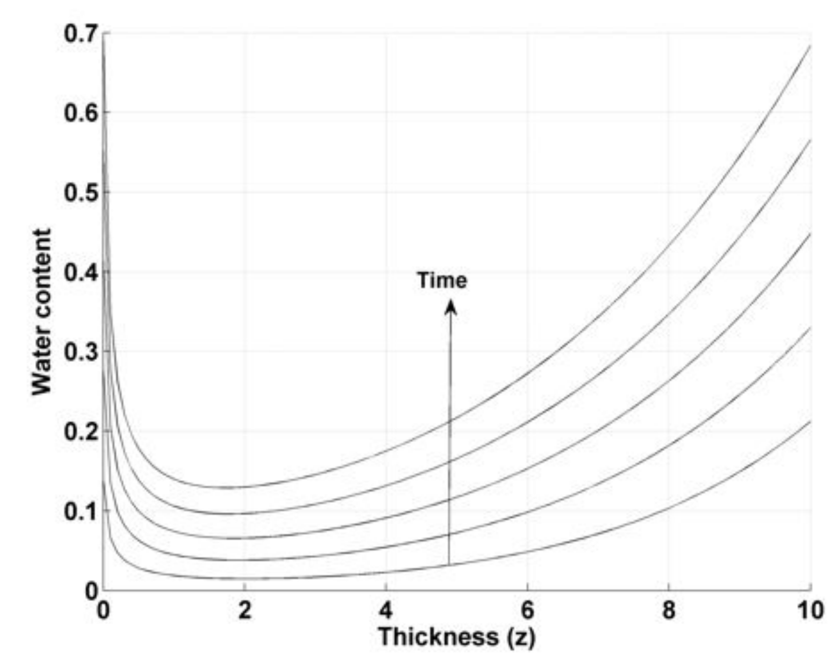


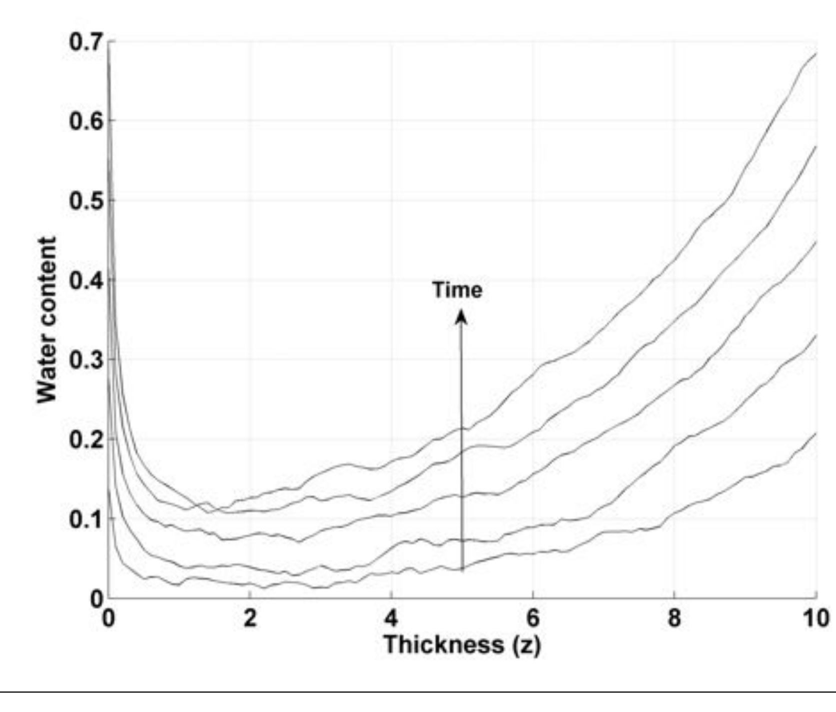
In the two figure below we show the water content vs. thickness of the soil (simulating the rainfall input response in the soil) in case of normal diffusion without and with stochastic term.





In the two figure below we show the water content vs. thickness of the soil (simulating the rainfall input response in the soil) in case of sub-diffusion without and with stochastic term ($2\alpha<\beta$, α=0.5 and β=1.5).

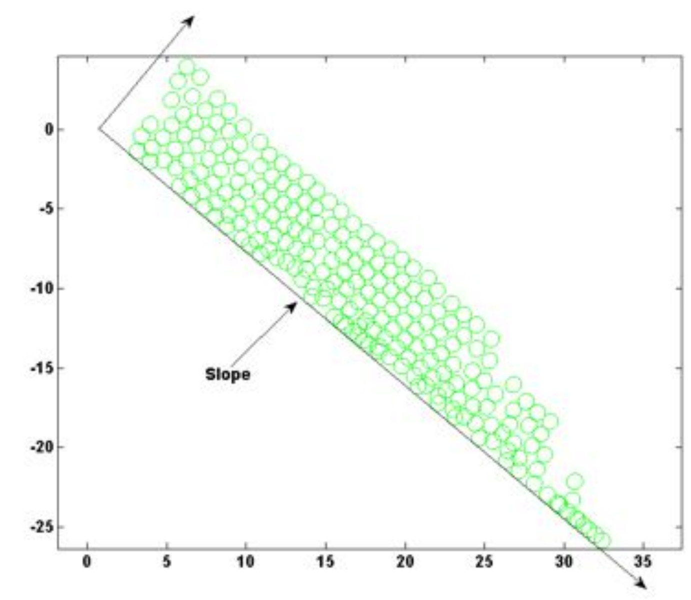




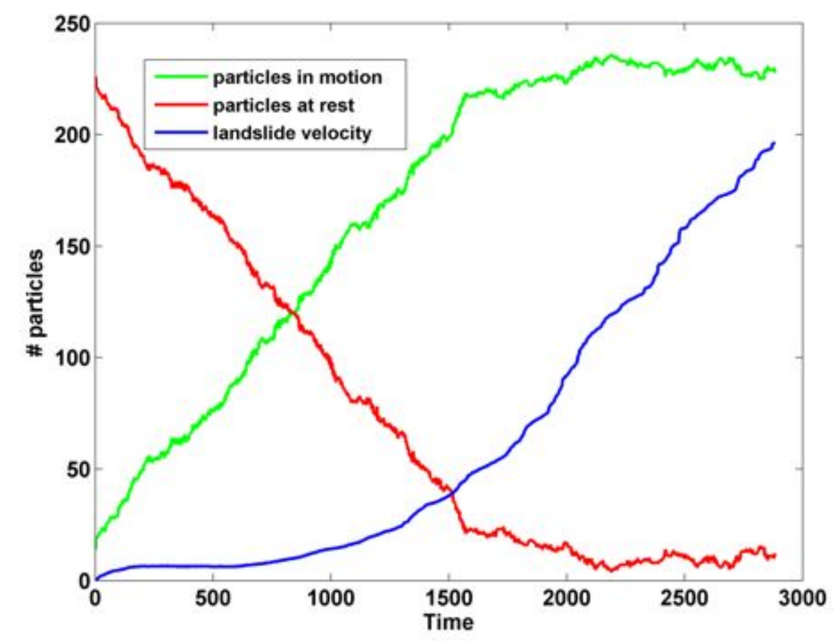
4) Landslide dynamics

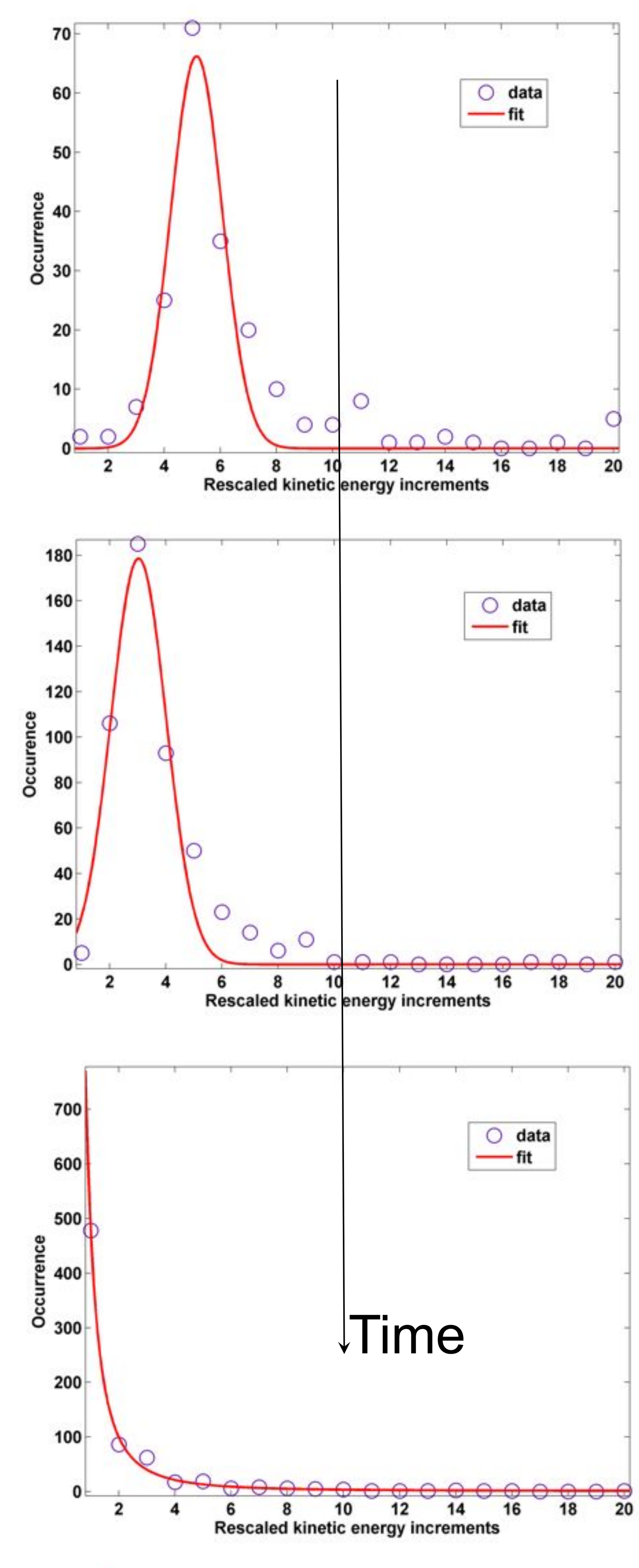
In this 2D model the output of hydrological model is integrated in the Mohr-Coulomb criterion. Therefore the triggering mechanism is based on static and velocity threshold condition. For the updating of positions we use a standard molecular dynamics scheme based on the Verlet algorithm.

$$\begin{cases} \tau_f = F_s + c' \\ F_s = [M_i(z,t) \cdot g \cdot \cos(\alpha) - p(z,t)] \cdot \tan\phi' \end{cases} \qquad \begin{cases} |\mathbf{F_i}| < F_{si} + c'_i \\ |\mathbf{v_i}| < v_d \end{cases} \qquad \mathbf{F_i} = \mathbf{F_{gi}} + \sum_{\mathbf{j}=1}^{\mathbf{j}=n_k} \mathbf{F_{ij}}$$

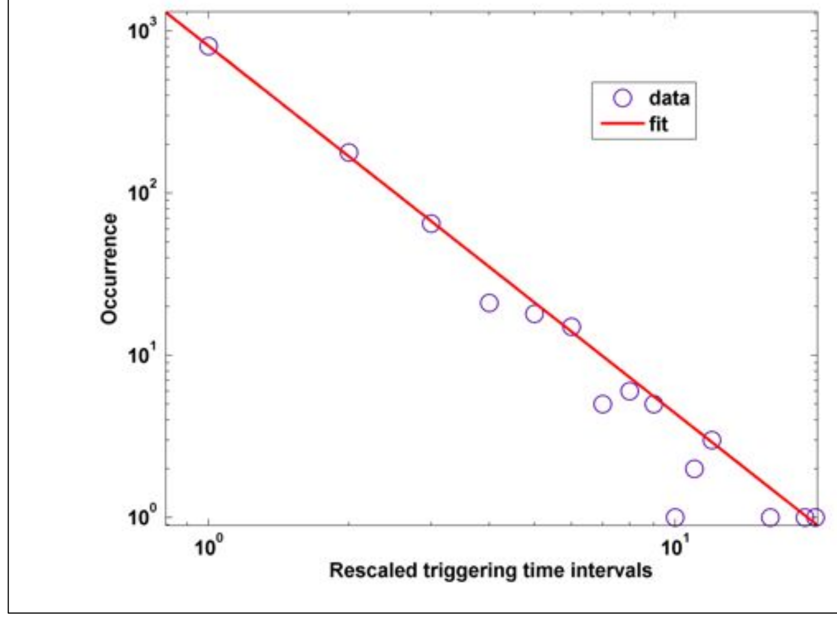


The simulated landslide in the coordinate system of the slope after triggering; in the figure below, the number of particles in motion (green curve) and at rest (red curve), and the landslide velocity (blue curve).





In the three figures on the left side we show the distributions of mean kinetic energy increments over time that exhibits a transition from Gaussian to power law due to the stick and slip phases.



The distribution of triggering time intervals between single particle movements exhibits a power law with exponent 2.26.