Final report on

NKFIH grant 119245
(November 2016.- October 2021.)

The geometry of equilibrium and the evolution of shape

1. Summary

The main result of this project is that we established, both theoretically, computationally and experimentally, a new class of shape descriptors for rock particles. The evolution of these new descriptors, called *mechanical descriptors* is, unlike the evolution of *classical descriptors*, monotonic under natural abrasion, thus the study of the mechanical descriptors yields direct information on the provenance of rocks of various sizes (e.g. asteroids, bedrock, pebbles, sand grains) based solely on their shape. We distinguish between *first order* mechanical descriptors (represented by pairs of integers, defining *first-order mechanical classification* based on the number and type of static balance points) and *higher* (second and third) *order* mechanical descriptors (represented by graphs), defining *higher* (second and third) *order mechanical classifications.*

In particular, we were able to determine the evolution of first order mechanical descriptors under a broad class of evolution models, called *distance-driven flows,* the study of which was initiated by Aristotle. These models appear to be the key to describe frictional abrasion, characteristic both in fluvial and coastal environments. Of particular interest appears to be our model, incorporating distance-driven components, describing the shape evolution of ooids, which are rounded, sand-sized particles of calcium carbonate which –like trees– record their own growth history, so they are a the key to study geophysical processes of the past.

So far, only the evolution of first-order mechanical descriptors has been investigated, both theoretically and experimentally. While the existence of higher order descriptors was known and observations indicated that their evolution could be highly interesting from the geophysical point of view, still, the mathematical framework was lacking to study their

evolution under abrasion models. We made the first step in this direction by establishing, purely on geometric grounds, the mathematical existence of generic evolution paths, connecting second-order and third-order mechanical classes. This study could lead to a more complete understanding of this intriguing phenomenon.

Whether and to what extent our abrasion models offer a universal picture on earth surface and planetary processes was unclear. We conducted a broad study, establishing curvature-driven flows as universal component of abrasion models not only for coastal and fluvial environments, but also for sand-sized sedimentary particles. One key argument for the universality of the model was the evolution of first-order mechanical descriptors. We established the volcanic origins of microscopic grains recorded in a Martian meteorite and used our models to offer a simple, natural explanation for the curios, strongly elongated, cigar-like shape of the first-ever observed interstellar asteroid ‘Oumuamua.

By using large-scale discrete element simulations as models of collisional abrasion, we were able to identify several transitions between energy phases, delineating the energy range where curvature-driven flows may be applied as mean-field approximations of natural abrasion processes. Our study is a response to a call by Richard Hamilton, who was first to suggest that curvature-driven flows may be used as abrasion models and offered a stunning mathematical result which predicted (for cuboid initial conditions) the spontaneous emergence of two *geometric phases*. By identifying these two geometric phases in a large-scale discrete element computer simulation and coupling them with a well-defined energy phase, we established the missing link between partial differential equations as models and the physical process.

While mechanical descriptors offer obvious conceptual advantages, their recording is far from trivial. The shape of sedimentary particles can be captured by 3D scans, which result in multi-faceted, simplicial (triangulated) polyhedra as computational models. We studied the evolution of mechanical descriptors for this special class of polyhedra where we discovered a metric in which these discrete objects, no matter how finer the discretization is, do not converge to their smooth counterparts. We developed and implemented algorithms, targeting these special features, for the efficient extraction of mechanical descriptors from 3D images of evolving surfaces.

The initial conditions for the evolution of sedimentary particles are natural fragments the best geometric approximation of which are convex polyhedra. To achieve a full understanding how first order mechanical descriptors evolve in time, it is of crucial importance to understand the initial condition. We made the first steps in this direction by achieving a full classification of convex polyhedra based on their static balance points and we investigated how such polyhedral (as models of fragmented rock) may form space-filling patterns.

2. Detailed results

In this report, we will quote verbatim the research goals from the proposal and after each research goal we summarize the *relevant results* and list the *main corresponding publications*.

2.1 Evolution of shape descriptors under distance-driven flows. While the theoretical aspects of collisional abrasion are more-or-less understood by the application of curvature-driven flows, next to nothing is known about the geometry of frictional abrasion. Based on the box model introduced in [Domokos and Gibbons 2012] it appears that distance-driven flows of type (1), beyond describing aristotelean shape evolution, may also be good candidate models for friction. Here we pose the following research questions:

2.1.1. What can be established on the time evolutions of classical geophysical shape descriptors and equilibrium classes under the action of not curvature driven (e.g. distance-driven) flows? How can these results be justified by laboratory experiments?

2.1.2. What can be established on shape descriptors evolving under Aristotle's famous model?

Relevant results:
We proved monotonicity (in a weak sense) for first order mechanical descriptors and proved semi-concave (non-monotonic) behavior for a classical descriptor under parallel distance-driven flows [1]. We constructed a general abrasion model, formulated as a partial differential equation, including distance-driven flows [2]. We constructed a hybrid evolution model for ooid growth which also contains a distance-driven flows a a component [3]. We studied a related evolution model, also based on affine transformations [4].

[1] G. Domokos, Z. Lángi: Evolution of geophyiscal shape descriptors under distance-driven flows. Math. Geosciences April 2018, Volume 50, Issue 3, pp 337–363.

[2] Domokos, G., Gibbons, G.: The geometry of abrasion. G. Ambrus et al. (eds.), New Trends in Intuitive Geometry, Bolyai Society (2019).

[3] Sipos, A. Á.: Ooid Growth: Uniqueness of Time-invariant, Smooth Shapes in 2D, European Journal of Applied Mathematics, doi:10.1017/S0956792519000019 (2019).

[4] G. Domokos, Z. Lángi, Mezei M.: A shape evolution model under affine transformations. Mediterr. J. Math. (2017) 14:210, doi 10.1007/s00009-017-1008.

2.2. Evolution of the secondary and tertiary equilibrium classes under the action of abrasion
In OTKA 104601 we introduced secondary and tertiary equilibrium classes [Domokos et al 2015], [Kápolnai et al 2012] and proved that there are no empty secondary and tertiary classes. From the point of view of shape evolution it would be crucial to know whether *generic* transition between these classes is possible. Preliminary measurements indicate that the vast majority of these classes is not present among pebbles: for $N<20$ total equilibrium points we found pebbles in ~20% of all primary classes and ~0.02% of all tertiary classes. The first ratio could be explained by the results in [Domokos 2015] (cf. research goal 2.4.3), however, so far there is not the faintest clue for the much more significant second ratio. We pose the following research goals:
2.2.1. Is it possible to establish the dynamical completeness of secondary and tertiary classification in the sense that generic transitions between these classes exist among convex bodies?
2.2.2. Is there a geometric theory, which would account for the absence of the majority of secondary and tertiary classes in field data?

Relevant results:
We established the generic paths connection secondary and tertiary mechanical classes [5]. This result provides a general template for the evolution of these classes under geometric evolution models.

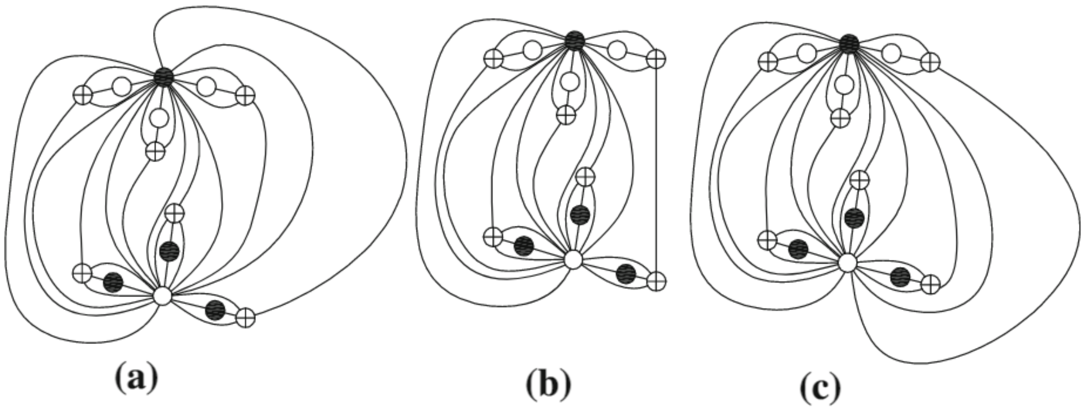


Fig 1: Topology graphs **a** and **c** corresponding to two vertices of $\mathcal{G}$ in primary equilibrium class {4, 4} and the tertiary edge (**b**) connecting them. Graphs are shown in the triangulated representation of graph class $\mathcal{T}^3$. Note the saddle–saddle connection on (**b**), and that **a** and **c** are isomorphic as abstract graphs, but not homeomorphic as embedded graphs on $\mathbb{S}^2$

[5] Domokos, G., Lángi, Z., Holmes, P.J.: A geneaology of convex bodies via local and global bifurcations of gradient vector fields. *Journal of Nonlinear Science* 26(6), 1789-1815, DOI 10.1007/s00332-016-9319-4, public acces: http://rdcu.be/tLQA

2.3. Universality for the evolution of classical (individual and statistical) geophysical shape descriptors. Our laboratory and field measurements as well as some theoretical results indicate that several classical geophysical shape descriptors may have a universal time-evolution. We are particularly interested in the evolution of the isoperimetric ratio of individual particles as well as the evolution of the relative sizes of particles in a co-evolving population of particles. We address the following research questions:

2.3.1. Is it possible to establish universal features for the time evolution of any of the classical geophysical shape descriptors based on mathematical models?

2.3.2. Is it possible to demonstrate experimentally and numerically that the time evolution of any classical geophysical shape descriptor shows universal features?

Relevant results:
Whether and to what extent our abrasion models offer a universal picture on earth surface and planetary processes was unclear. We conducted a broad study [6], establishing curvature-driven flows as universal component of abrasion models not only for coastal and fluvial environments, but also for sand-sized sedimentary particles. One key argument for the universality of the model was the evolution of first-order mechanical descriptors. We also proved another universal feature: the monotonicity of the isoperimetric ratio under the Eikonal abrasion model [7].

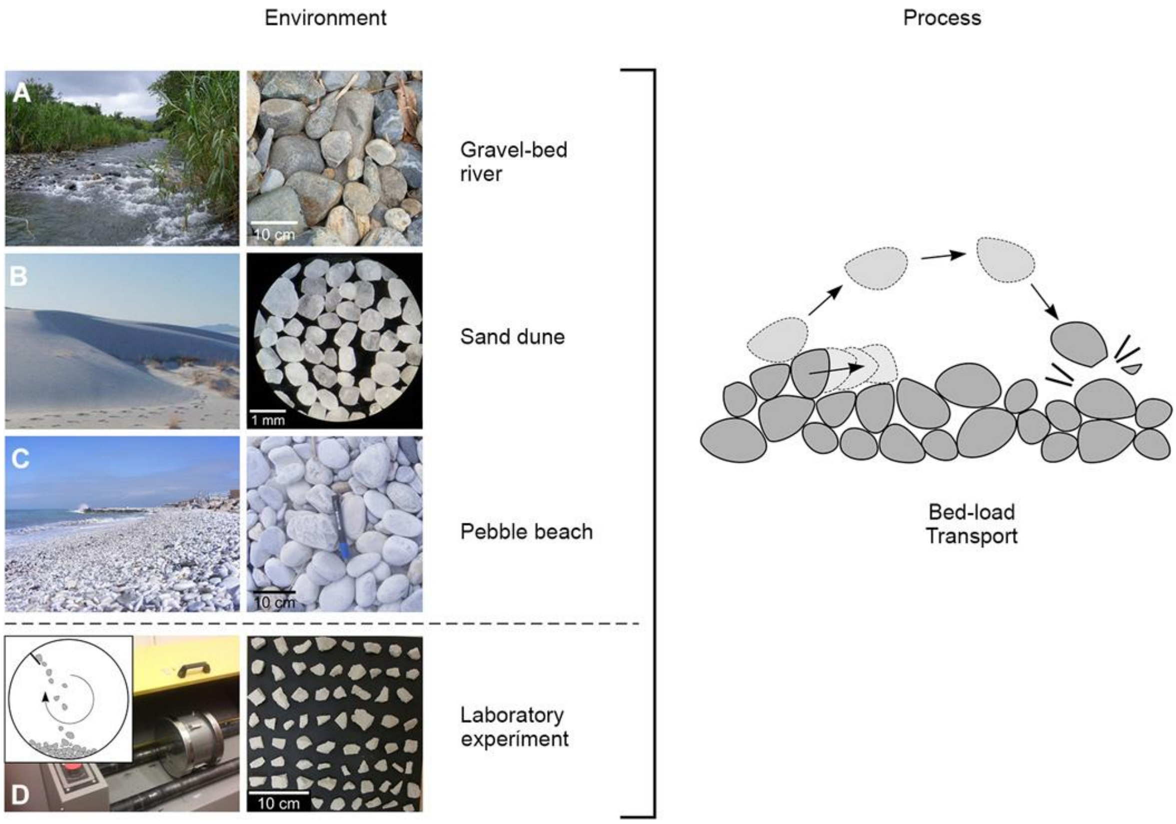


Fig. 2 Environments and sediments examined in this study.
Field data were collected from different environments: (**A**) gravel-bed river in Puerto Rico, (**B**) gypsum dune field in New Mexico, (**C**) pebble beach in Marina di Pisa, and (**D**) experiment in a rotating drum. All illustrated environments select for the conditions of bed-load transport (right side) where impacts from saltation drive chipping.

[6] Novák-Szabó, Z., Sipos, A.Á,., Shaw, S., Bertoni, D., Pozzebon, A., Grottoli, E., Sarti, G., Ciavola, P., Domokos, G. and Jerolmack, D.J.: Universal characteristics of particle shape evolution by bed-load chipping. Science Advances Vol. 4, no. 3, eaao4946
DOI: 10.1126/sciadv.aao4946

[7] Domokos, G., Lángi, Z.: The isoperimetric quotient of a convex body decreases monotonically under the Eikonal abrasion model. Mathematika 65 (2019) 119-129, doi:10.1112/S0025579318000347

2.4. Monotonicity of spatial critical points evolving under curvature-driven flows. The results in [Domokos 2015] predict that under curvature-driven abrasion the expected number *N* number of static balance point will decrease. The experimental and numerical verification of the results in [Domokos 2015] is still lacking, partly because the construction of a suitable numerical code poses considerable difficulties. As demonstrated in [Domokos et al. 2011], on the convex hull of pebbles equilibria exist on two scales and the separation of these scales is a delicate mathematical problem. Since the theoretical predictions in [Domokos 2015] are of stochastic character, the code should be capable to produce statistical samples of suitable size. Here we formulate the following research goals:

2.4.1. Is it possible to rigorously define global equilibria on finely discretized curves and surfaces? If yes, what are the characteristic features of the co-evolution for the number *n* of local equilibria and the number *N* of global equilibria?

2.4.2. Is it possible to build a code based on the previous definition that is so efficient that it can track the time evolution of spatial equilibria on many pebbles in a reasonable amount of time to produce a meaningful statistical sample?

2.4.3. Is it possible to find a good match between numerical results of the aforementioned code to laboratory and field data?

Relevant results:

While mechanical descriptors offer obvious conceptual advantages, their recording is far from trivial. The shape of sedimentary particles can be captured by 3D scans, which result in multi-faceted, simplicial (triangulated) polyhedra as computational models. We studied [8] the evolution of mechanical descriptors for this special class of polyhedra where we discovered a metric in which these discrete objects, no matter how finer the discretization is, do not converge to their smooth counterparts. We developed and implemented algorithms [9], targeting these special features, for the efficient extraction of mechanical descriptors from 3D images of evolving surfaces. We described how the monotonic evolution of mechanical descriptors offers conceptual advantages in the understanding of natural abrasion processes [10].

Polyhedra appear not just as approximations of scanned surfaces: the initial conditions for the evolution under abrasion are natural fragments, the best geometric approximation of which are convex polyhedra. To achieve a full understanding how first order mechanical descriptors evolve in time, it is of crucial importance to understand their initial condition. We made the first steps in this direction by achieving a full classification of convex polyhedra [11] based on their static balance points. We also investigated how such polyhedral (as models of fragmented rock) may form space-filling patterns [12,13], thus coupling the shape of fragments with global patterns. These finding led to deeper mathematical results, connecting the geometry of polyhedra with their first order mechanical classes [14,15,16].

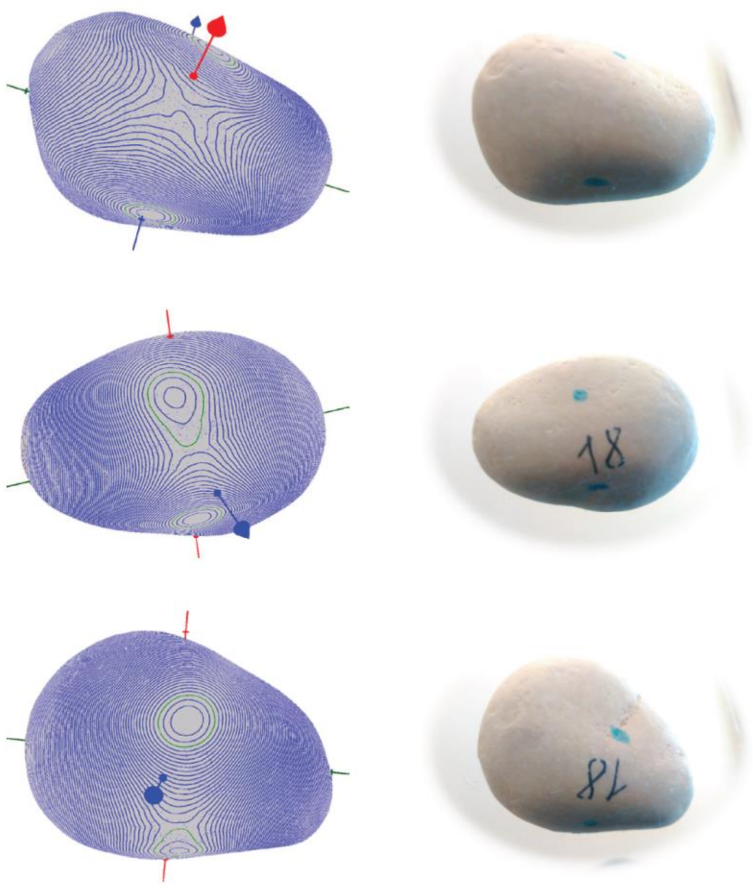


Fig. 3: Experimental verification of global equilibria. Right panel: pebble exhibiting 3 global stable equilibria, marked with dots on the surface of the pebble. Three different views are displayed below each other. Left panel: 3D scanned image of the pebble. Regular contour lines appear in blue color while global equilibria are surrounded by green contour line. Same three views displayed as in right panel.

[8] Domokos, G., Lángi, Z. and Sipos, A.Á.: Tracking critical points on evolving curves and surfaces. Experimental Mathematics DOI 10.1080/10586458.2018.1556136 (2019).

[9]B. Ludmány, G. Domokos: Identification of Primary Shape Descriptors on 3D Scanned Particles. Periodica Polytechnica Electrical Engineering, https://doi.org/10.3311/PPee.12313 (2018).

[10] Domokos, G.: Natural Numbers, Natural Shapes. Axiomathes https://doi.org/10.1007/s10516-018-9411-5 (2019).

[11] G. Domokos, F. Kovács, Z. Lángi, K. Regős, Z. Varga: Balancing polyhedra. ARS MATHEMATICA CONTEMPORANEA, [S.l.], june 2020. ISSN 1855-3974. https://amc journal.eu/index.php/amc/article/view/2120

[12] G. Domokos, Z. Lángi: Plato' error and a mean field formula for convex mosaics Axiomathes DOI:10.1007/s10516-019-09455-w (2019)

[13] G. Domokos, Z. Lángi: On some average properties of convex mosaics. Experimental Mathematics DOI:10.1080/10586458.2019.1691090 (2020)

[14] Z. Lángi, A solution to some problems of Conway and Guy on monostable polyhedra, arXiv:2008.02090, accepted in Bull. Lond. Math. Soc.

[15] K. Bezdek and Z. Lángi, Volumetric Discrete Geometry, Discrete Mathematics and Its Applications, CRC Press, Taylor & Francis Group, 2019, 286 pages

[16] Z. Lángi: Centering Koebe polyhedra via Möbius transformations, Groups Geom. Dyn., Volume 15, Issue 1, 197-221 (2021).

2.5. Application to geophysical data. Related to item (D) on the task list we propose to conduct a broad range of case studies on geophysically particularly interesting shape evolution phenomena. Among others, we seek to address questions like the following ones:

2.5.1 Is it possible to identify geophyisical scenarios where the combined action of surface growth and abrasion produce time-invariant shapes?

2.5.2 Is it possible to extract information from particle contours in meteorites?

Relevant results:

We measured the abrasion rates on marble pebbles and found that these rates are so substantial that, beyond transport, abrasion needs to be considered as a major factor when describing shape distributions for coastal pebbles [17]. We established [18] the volcanic origins of microscopic grains recorded in a Martian meteorite and used our models to offer [19] a simple, natural explanation for the curios, strongly elongated, cigar-like shape of the first-ever observed interstellar asteroid 'Oumuamua. We gave a physically motivated geometric model for the shape evolution of ooids [20].

[17] Bertoni, D., Sarti, G., Grottoli, E., Pozzebon, A. Domokos, G., Szabó-Novák, T.: Impressive abrasion rates of marked pebbles on a coarse-clastic beach within a 13-month timespan. *Marine Geology* Volume 381, 1 November 2016, Pages 175-180

[18] McCubbin, F., Boyce, J.W., Novák-Szabó, T.,A.R. Santos, Tartèse, R., Muttik, N., Domokos, G., Vazquesz, J., Keller, L.P., Moser, D.E., Jerolmack, D.J., Shearer, C.K., Steele, A., Elardo, S.M., Rahman, Z., Anand, M., Delhaye, T., Agee, C.B.: Geologic history of Martian regolith breccia Northwest Africa 7034: Evidence for hydrothermal activity and lithologic diversity in the Martian crust. Jounal of Geophysical Research/Planets Volume 121, Issue 10 October 2016 Pages 2120–2149. DOI: 10.1002/2014JF003156

[19]G. Domokos, A.Á.Sipos, G. Szabó, P.L. Várkonyi: Explaining the Elongated Shape of 'Oumuamua by the Eikonal Abrasion Model. Research Notes of the AAS Vol 1, No. 1,

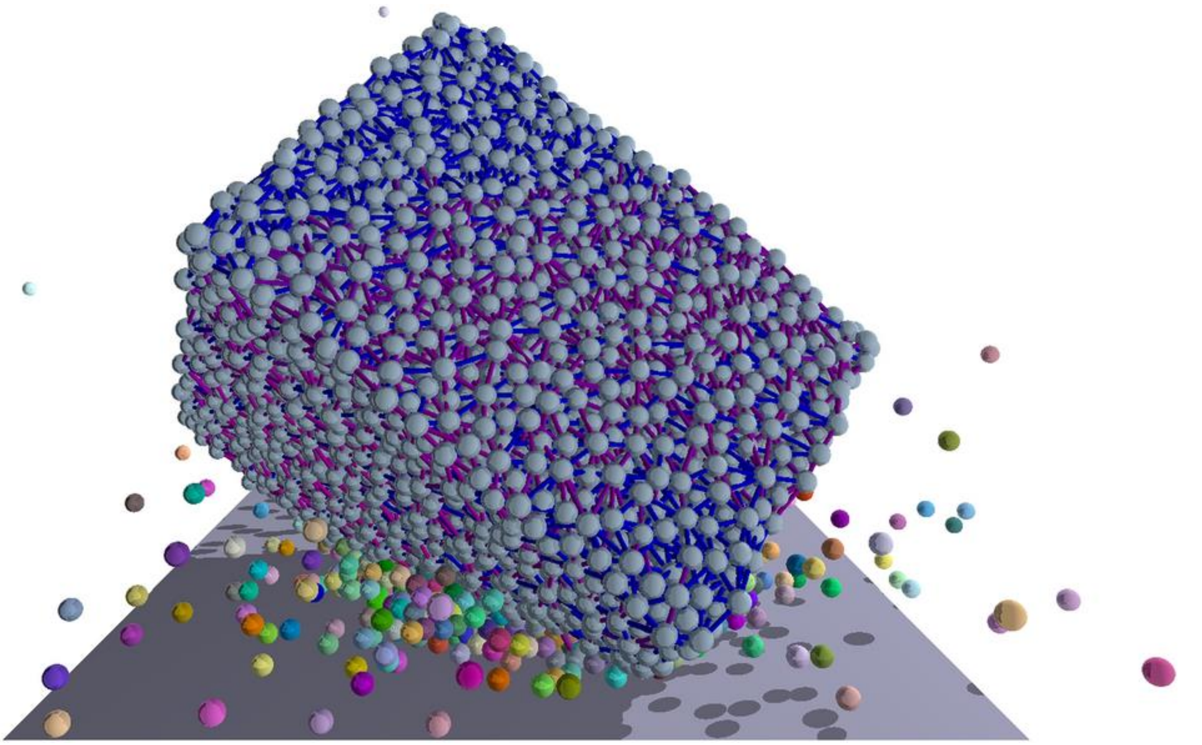
[20] A. Sipos, G. Domokos, D.J. Jerolmack: Shape evolution of ooids: a geometric model. Nature Scientific Reports 8, Article number: 1758, doi:10.1038/s41598-018-19152-0 (2018)

2.6. Realistic discrete element model running on supercomputer. Our theoretical framework is purely geometrical which has the advantage that it can be applied on a broad scale ranging from sand grains to asteroid shapes. Nevertheless, related to items (C) and (D) on the task list, it would be highly valuable to validate these geometric equations by computer simulations which consider inhomogeneous material models. Here we ask the following question:

2.6.1. Is it possible to verify the geometric models (1) and (2) based on a realistic, 3-dimensional discrete-element model which considers the heterogeneous micro-structure and dynamics of fracture of geomaterials?

Relevant results:

By using large-scale discrete element simulations as models of collisional abrasion [21], we were able to identify several phase-transitions, delineating the energy range where curvature-driven flows may be applied as mean-field approximations. Our study is a response to a call by Richard Hamilton to investigate curvature-driven flows as abrasion models and our results reaffirmed his ideas.



[21] Pál Gergő, Domokos Gábor, Kun Ferenc: Curvature flows, scaling laws and the geometry of attrition under impacts, SCIENTIFIC REPORTS 11: (1) 20661, 2021