A MECHANICS-BASED PEBBLE SHAPE CLASSIFICATION SYSTEM AND THE NUMERICAL SIMULATION OF THE COLLECTIVE SHAPE EVOLUTION OF PEBBLES

A brief summary of the dissertation submitted to the
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INTRODUCTION

Beginning with Aristotle (*Krynine 1960*), illustrious scientists have been interested in the geometry and abrasion processes of pebbles (*Leonardo da Vinci: Codex Leicester – Richter 1939; Lord Rayleigh 1942, 1944a,b*). A recent series of articles published in *Nature* (*Ashcroft 1990; Lorang and Komar 1990; Yazawa 1990*) indicates that the great diversity of pebble shapes also attracts considerable attention nowadays, because investigation of natural shapes formed by abrasion processes (e.g. landforms, asteroids or pebbles) helps understand abrasion processes itself. Pebble shapes carry important information on the history of sediment transport and deposition, helping to differentiate facies. The significance of pebble shape investigations can be clearly illustrated by the latest discovery of NASA: photos by the Curiosity Rover at Link rock outcrop show well-rounded, abraded pebbles on the surface of Mars (Figure 1). Solely based on the pebble shapes, NASA scientists concluded that these pebbles must have been transported by flowing water, so Curiosity's discovery is the first time scientist have identified an ancient streambed on Mars.

Despite the long time elapsed since Aristotle, both describing the morphology and modeling the shape evolution of pebbles still pose scientific puzzles. The aim of the dissertation is twofold. Firstly, we apply a new, mechanics-oriented classification system (*Várkonyi and Domokos 2006a*) to describe pebble shapes and investigate the practical applicability and the mathematical/mechanical background of this system. Secondly, we present a new numerical model describing the collective shape evolution of large pebble populations, based on a recent theoretical result called the *box equations* (*Domokos and Gibbons 2012*). We apply the numerical model to the Williams River located in the Hunter Valley, Australia. Next we outline these two research goals and our results.

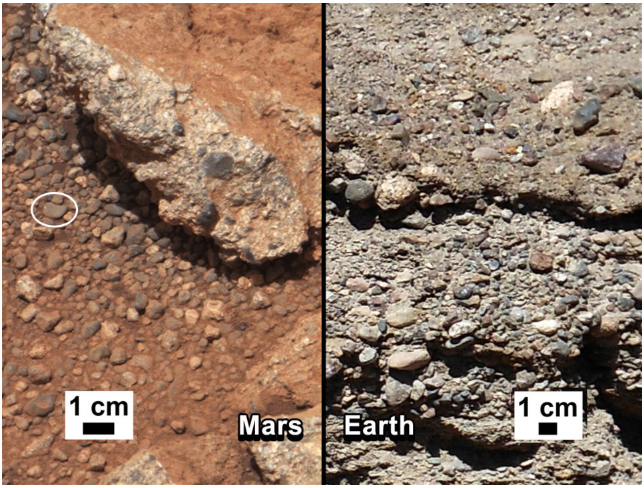

Figure 1. Left: Ancient streambed on Mars, imaged by the Curiosity Rover on Sept. 2, 2012. Right: A similar fluvial conglomerate on Earth. Photo: NASA/JPL-Caltech/MSSS and PSI, PIA16189.

A MECHANICS-BASED PEBBLE SHAPE CLASSIFICATION SYSTEM

Background

A variety of shape indices and diagrammatical presentations of pebble shape have been proposed in the past (e.g. *Wentworth 1922; Zingg 1935; Krumbein 1941; Sneed and Folk 1958; Dobkins and Folk 1970; Blott and Pye 2008*). These classical methods rely on length measurements, the simplest and most widespread classification system was set up by *Zingg* (*1935*) who proposed approximating pebbles with a three-axial ellipsoid with axis lengths $a>b>c$ and classified shapes based on the axis ratios c/b and b/a (Figure 2). While these classical systems have undoubtedly proved to be useful tools, their application inevitably requires ambiguous measurements, and the classification involves the introduction of arbitrarily chosen constants. The Zingg system uses an axis ratio value of 2/3 to discriminate the four classes. Instead of assuming a universally optimal constant, the classical Zingg system can be unified if an internal parameter $0 \le p \le 1$ is introduced which separates classes from each other.

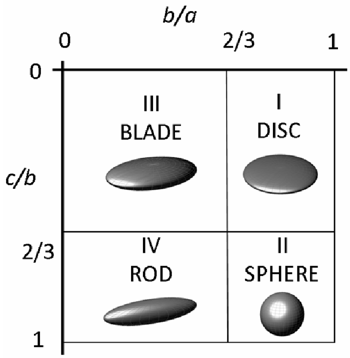

Figure 2. Zingg classes. *a*>*b*>*c* denote the side lengths of the bounding box of the pebble.

In the dissertation we apply a completely different classification scheme for pebble shapes which does not rely on length measurements and shape indices; rather, it involves *counting static equilibria*, i.e. points of the surface where the pebble is at rest when placed on a horizontal, frictionless support surface. Typical 3D bodies may have three types of equilibrium points: stable equilibria and two types of unstable equilibria, namely unstable maxima and saddle points; unstable maxima will be simply called unstable equilibria. Based on the number of stable (*S*) and unstable (*U*) equilibria, every homogeneous, convex body can be classified unambiguously into the class (*S*,*U*) (*Várkonyi and Domokos 2006a*). (*S*,*U*) is called the *primary equilibrium class* of the body (Figure 3). For example, the cube belongs to class (6,8) with 6 stable points (faces) and 8 unstable points (vertices). The *Gömböc* (*Várkonyi and Domokos 2006b*) belongs to class (1,1).

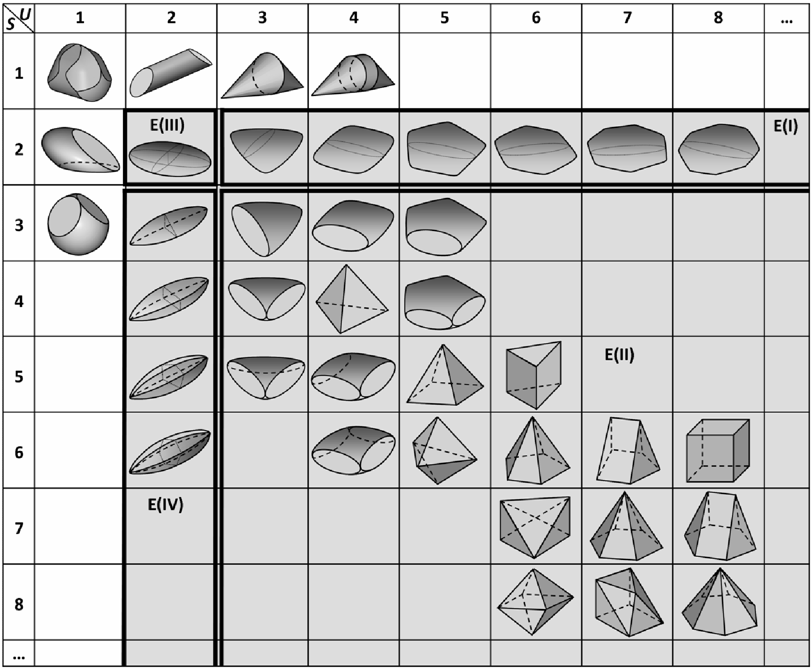

Figure 3. Primary equilibrium classes. Rows (*S*) denote the number of stable equilibria, columns (*U*) the number of unstable equilibria. The 4 simplified equilibrium classes (*E-classes*) are shaded.

Research goals and results

In the first part of the dissertation we apply the equilibrium-based classification scheme to categorize pebble shapes. We address three main questions:

(1) Do primary equilibrium classes carry any important information on the geometry of pebbles?
(2) Can primary equilibrium classes be reliably determined on pebbles using hand experiments?
(3) Can primary equilibrium classes be refined to obtain a detailed taxonomy on the shapes of homogeneous, convex bodies?

We answer question (1) in Principal Result 1. We propose a simplified classification scheme called *E-classification* (Figure 3) and demonstrate that the new method is practically applicable: simple hand experiments are suitable and easy to use to determine primary equilibrium classes and E-classes (Figure 4). (The reliability of these hand experiments is addressed separately in question (2)). The new approach does not contain any arbitrarily introduced constants or directions (like classical shape measurements) since it involves *integer* numbers by counting static equilibria. Based on detailed statistical data of 1200 pebbles from several different geological locations, we demonstrate that E-classes are closely related to the geometric shape of pebbles i.e. equilibrium class is a natural property which describes pebble geometry well. We compare E-classes to the classical Zingg classes, and show that most of the information contained in the Zingg classification can be extracted from E-classification. However, the new system provides more detailed data and it may shed light on special shape features not discovered so far. We also present an interesting logarithmic relationship between the flatness of pebbles and the average number of stable points, which also indicates a close connection between classical shape categories and the new classification system.

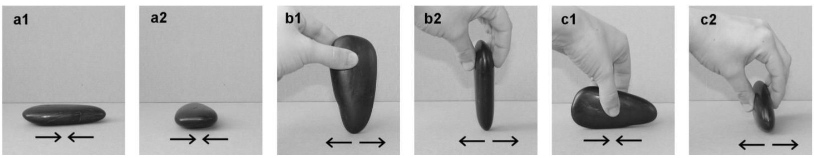

Figure 4. Counting equilibrium points in hand experiments. a) Stable point. b) Unstable point. c) Saddle point.

Question (2) is addressed in Principal Result 2. We demonstrate that equilibria typically appear on two well-separated scales on many faceted polyhedra like on the convex hull of pebbles: *microscopic* equilibria occur in highly localized groups (*flocks*), the number of the latter can be reliably determined by hand experiments since the experimenter only perceives these flocks as *macroscopic* equilibrium points (Figure 5). We verify this phenomenon by analyzing the high-precision 3D scans of 300 pebbles, identifying all micro-equilibria by computer. Based on the algorithm presented in (*Domokos, Sipos and Szabó 2012*), we compare the results of computer experiments to our hand experiments by introducing a scalar parameter measuring the accuracy of the experimenting person (i.e. the error that a human experimenter cannot distinguish between micro-equilibria). Results verify that hand experiments are consistent and reliable because for the *same* experimenter we measured parameter values in a narrow range, also, the parameter value (and so the number of equilibria) change only slightly *between* different experimenting persons. This result validates the practical applicability of the new, equilibrium-based shape classification system.

Figure 5. Six stable micro-equilibria on a pebble forming one macro-equilibrium (flock).

Finally, we answer question (3) in Principal Result 3. We show that primary equilibrium classes can be divided into *secondary equilibrium classes*, based on the topology of the so called *Morse-Smale complex* which can be represented by a graph embedded in the pebble's surface (Figure 6). Equilibrium points are the vertices of this graph, edges represent the adjacency relationships between equilibrium points. We prove that all secondary equilibrium classes are non-empty in the sense that for every, combinatorially possible Morse-Smale complex embedded in the 2-sphere, there exists a corresponding smooth, homogeneous, rigid, convex solid (*Domokos, Lángi and Szabó 2013*). Thus, in theory, any of these graphs can appear in nature among pebble shapes.

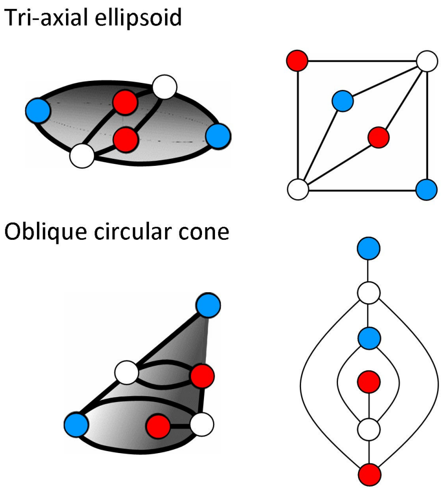

Figure 6. The two secondary equilibrium classes in primary class (*S*,*U*)=(2,2).

THE NUMERICAL SIMULATION OF THE COLLECTIVE SHAPE EVOLUTION OF PEBBLES

Background

While the first part of the dissertation discusses how to *describe* the morphology of pebbles, in the second part we deal with the *evolution* of these shapes during abrasion processes. Throughout these investigations, we rely on the classical shape description of pebbles, based on length measurements. In this way, our results are readily comparable to previous results in the literature. Our main goal is to track the *collective* shape evolution of large pebble *populations* in natural environments. For this aim, a suitable tool is the recently published theoretical result called the *box equations* by

Domokos and Gibbons (*2012*). Box equations are able to follow up the evolution of the *shape and size* distributions of large particle populations as the cumulative effect of collisions between particles, frictional abrasion and size-selective sorting. Therefore, it is an appropriate tool to model abrasion processes in various sedimentary environments, e.g. in fluvial or coastal settings.

The dissertation focuses on fluvial environments by complementing the original box equations, implementing them (and some other features) in Matlab and applying this framework to simulate numerically the downstream evolution in shape and size along the *Williams River* located in the Hunter Valley, Australia. However, the framework implemented for fluvial environments can be readily applied to other sedimentary environments as well, and in fact, it is among our future plans to do so.

A controversial question in fluvial geomorphology is connected to the size diminution of pebbles observed along numerous gravel-bed rivers, a phenomenon called *downstream fining*. This phenomenon has been attributed to two main processes: abrasion and size-selective transport. While the previous process explains the observed size diminution by the erosion of particles during their downstream transport, the latter means the preferential transport of small particles which can also result in a downstream decrease in size. There is a long-standing debate on the relative importance of these two processes (e.g. *Lewin and Brewer 2002; Surian 2002*), most of the authors have emphasized sorting by size-selective transport as the dominant fining mechanism (e.g. *Bradley et al. 1972; Ferguson et al. 1996; Seal and Paola 1995*). In addition, there are surprisingly few field studies which examine the evolution of grain size *and* shape simultaneously in a natural stream (e.g. *Bradley et al. 1972; Mikos 1994*), although possible downstream variation in shape can clearly indicate the relative importance of abrasion. Also, none of the models in the literature (e.g. *Le Bouteiller et al. 2011;*

Parker 1991a; Ferguson et al. 1996) describes the changes in both the shape and size distributions of the particles during abrasion; they only deal with the size of the particles and mostly focus on size-selective transport.

Research goals and results

We performed a field study along the Williams River in which we collected and measured basalt particles at 12 sampling sites. The main question which we address and answer connected to this field study is the strongly debated problem presented above:

(4) The downstream fining observed in the Williams River is dominantly caused by abrasion or by size-selective transport?

We answer question (4) in Principal Result 4. Compared to other natural streams, the small downstream fining rate observed in the river strongly indicates that abrasion plays a key role (*Surian 2002*). In addition, we demonstrate that pebbles get flatter and thinner along the river, also, so-called *aquafacts* (*Kuenen 1947*) i.e. pebbles having sharp edges and planar faces emerge in the downstream reaches (Figure 7). These are especially rare pebble shapes similar to ventifact-shapes (specifically, to *ein-*, *zwei-* and *dreikanters*, *Greeley et al. 2002*). Based on the predictions of the box equations, these phenomena reflect that collisional abrasion by small abraders („*sandblasting*") is important in the downstream reaches (*Domokos and Gibbons 2012; Domokos et al. 2009*). We apply the implemented framework to simulate numerically the downstream evolution along the river. By introducing two scalar parameters based on physical considerations and field observations, we reproduce the evolution of both the shape and size distributions downstream. Results suggest that abrasion is sufficient to produce the desirable exponential downstream fining for small diminution rates. The simulation allows tracking the shape and size evolution of the *individual* particles as well, revealing an interesting phenomenon on how particle size controls shape evolution.

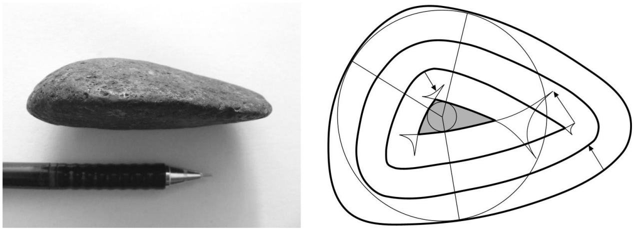

Figure 7. Aquafact shape found in the Williams River and the formation of sharp edges (*Domokos et al. 2009*).

PRINCIPAL RESULTS

Throughout my principal results, statistical data of 3 pebble sample collections will be referred. These are:

1. *The 24 European pebble samples*
   24 pebble samples collected from 11 European locations, each sample consists of 50 pebbles, meaning 1200 pebbles altogether. Samples correspond to different geological settings, so they represent various sedimentary environments, abrasion and transport processes and pebble lithology. I measured the axis lengths $a>b>c$ on the pebbles and counted the stable and unstable equilibrium points.

2. *The 300 scanned pebbles*
   300 pebbles from the 24 European samples, scanned with a 3D laser scanner.

3. *The 12 Australian pebble samples*
   12 pebble samples collected along the Williams River, Hunter Valley, Australia. Altogether 1626 basalt pebbles were sampled, average sample size is around 140. I measured the axis lengths $a>b>c$ on the pebbles.

PRINCIPAL RESULT 1

(*Domokos et al. 2010; Szabó and Domokos 2010; Domokos, Sipos and Szabó 2012*)

Based on the *primary equilibrium classes* (*Várkonyi and Domokos 2006a*), I proposed a *simplified* classification (*E-classification*) to categorize pebble shapes. Relying on the statistical results of the 24 European pebble samples, I compared E-classes to the classical Zingg classes so that I generalized the Zingg system by introducing a parameter *p* separating the classes from each other. Based on the statistical results, the following statements can be made:

1.1. The optimal choice of *p*, at which the agreement between the two classifications is the largest, is not universal: for well-rounded pebbles it is higher (between 0.75 and 0.89), for angular shapes it is smaller (between 0.55 and 0.75).

1.2. The best agreement between E-classes and the generalized Zingg classes is 80% on average (standard deviation: 10%), i.e. most of the information contained in the Zingg classification can be extracted from the simplified equilibrium classification.

1.3. I established a strong (R^2=0.85) logarithmic relationship between the mean number of stable equilibria and the flatness (mean value of axis ratio *c*/*b*) of pebbles. This relationship also verifies that the number of equilibrium points is closely connected to the overall shape of pebbles.

PRINCIPAL RESULT 2

(*Domokos, Sipos and Szabó 2012; Domokos, Lángi and Szabó 2012*)

Based on the algorithm identifying *micro*- and *macro-equilibria* (*Domokos, Sipos and Szabó 2012*) and data of the 300 scanned pebbles, I simulated the hand experiments on the BME Supercomputer, based on the hypothesis that the scalar parameter μ_0 introduced in the algorithm is a measure of the inaccuracy of the experimenting person during counting equilibrium points. By comparing the results of computer experiments to hand experiments, the following statements can be made, which verify the reliability of hand experiments:

2.1. Based on hand experiments of 9 different people, μ_0 values are typically higher for unstable equilibria (mean value: 0.0082) than for stable equilibria (mean value: 0.0016).

2.2. Parameter μ_0 varies in a narrow range for the *same* experimenter and also, the results of hand experiments can be modeled well (R^2=0.74–0.97) by $\overline{\mu}_0$ (the mean value of μ_0). Thus, hand experiments are *consistent* and $\overline{\mu}_0$ describes the inaccuracy of the experimenting person well.

2.3. Based on hand experiments of 9 different people, $\overline{\mu}_0$ changes only slightly *between* different experimenting persons (mean value: 0.0049, standard deviation: 0.0019). Therefore, the number of stable and unstable equilibria counted in hand experiments varies also only slightly among different people: the standard deviation is very small (0.02) for small number of equilibria (2.06) and is acceptable (0.46) for larger number of equilibria (3.49) as well.

PRINCIPAL RESULT 3

(*Domokos, Lángi and Szabó 2013*)

I refined the *primary equilibrium classification* (*Várkonyi and Domokos 2006a*) by defining *secondary* classes, based on the topology of the *Morse-Smale complex*. Every Morse-Smale complex associated with a homogeneous, convex, rigid body can be represented by a 2-colored plane quadrangulation (*Dong et al. 2006*), we denote this graph class by $\mathcal{Q}$. I showed that class $\mathcal{Q}$ can be generated inductively by a combinatorial operation called *vertex splitting* from the stem-graph P_2 (the path graph with 2 vertices). With this, I generalized the result of *Bagatelj* (*1989*) and *Negami and Nakamoto* (*1993*), who showed the same for *simple* plane quadrangulations *without* coloring. Also, this combinatorial result is a first building block in the proof of a more complex theorem (*Domokos, Lángi and Szabó 2013*). The theorem states that all secondary classes are non-empty, i.e. for every graph in $\mathcal{Q}$, there exists a corresponding homogeneous, rigid, convex solid.

PRINCIPAL RESULT 4

(*Szabó, Fityus and Domokos 2013*)

Based on the *box equations* (*Domokos and Gibbons 2012*), I developed a flexible numerical model for simulating the collective shape and size evolution of large particle populations in different sedimentary environments. Using this model with only two, physically-based parameters, I reproduced the downstream evolution of pebble shape and size distributions measured along the Williams River in the 12 Australian pebble samples. Based on this simulation, which was run on the BME Supercomputer, the following statements can be made:

4.1. I complemented the stochastic box equations (*Domokos and Gibbons 2012*) by considering fragment production during collisional abrasion. By adding the fragments to the particle population, the abrasive effect of sand-size particles, which turned out to be important in the Williams River, could be directly simulated.

4.2. While most researchers explain the well-known exponential downstream fining in grain size, observed in numerous gravel-bed rivers, by the effect of *size-selective transport*, through the example of the Williams River I demonstrated that *abrasion* is efficient enough to produce this size decrease for small diminution coefficients.

4.3. I verified that the phenomenon predicted analytically by *Domokos and Gibbons* (*2012*), in which a pebble that first moves away from the sphere, turns back and finally converges to the sphere, is demonstrable in a real sedimentary environment as well.

ACKNOWLEDGEMENTS

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