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Numerical Modelling of Sediment Generation

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Dissertation presented in partial fulfillment of the requirements for the degree of Doctor of Science (PhD): Geology

August 2020

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Preface

"Closing the gap in source-to-sink modelling" sounded as a real challenge to achieve in just four years of a PhD. Now, five and half years later, I can honestly say that couldn't be less true. Although the challenge is not yet complete, a first pioneering move into making this preposition sound has been made. This move is explained and discussed throughout this thesis alongside with the documentation of the resulting software package.

It was a quantitative approach to sediment generation modelling that was needed to close this aforementioned gap. Although there have been some pioneers before me, there are few, and we had basically to start from scratch, were it not for Gert Jan's research proposals with pseudo code. Coupled will all of the experience of Gert Jan and my own acquired programming skills I was able to develop a Python package called *SedGen*.

Allow me to convey how Gert Jan convinced to take on this challenge: He told me that we could probably not say a lot of absolute measures about our results of the sediment generation modelling because we would use relative properties to start with as input. Nevertheless, relative things can already allow one to say something about the outcome. He illustrated this with an example I still remember vividly: Say it's Easter day and there is a certain amount of eggs hidden in the garden. You do not know the exact number of eggs, nor do you know where they were hidden. Imagine that there are two children that will try to find and collect the eggs. One of them is four years old and the other is eight. Asked with how many eggs each of the children will be able to find,

you cannot possibly give the correct answer, except for mere coincidence. But if you are asked, which of the children will probably be able to collect most of the eggs, things get interesting. You could take their age in consideration and base your answer on that, or you could try to gain more information about the physical traits of the children in advance. All to say that by taking certain properties into consideration, you will be able to give a probabilistic answer to a relative question rather than a guess to a absolute question.

This PhD gave me the opportunity to venture into the exciting world of programming and establish a strong foothold in Python.

I would like to thank my colleagues and friends from the Geo-institute. Nick for the good times we had organizing the PhD Midweek, Geology BBQ and acting as Sinterklass and Easter bunny. Strangely enough driving to the supermarket with 6000+ RPM at ten minutes before closing time to basically 'rob' the store's meat supply to make sure enough meat can be put on the barbecue is one of my fondest memories. Aside from that I also enjoyed all the discussions about Python and data science we had, and big thanks for helping me getting around in the first year of my PhD. Bura and Alex for the friendship and many talks. Niels, Dominique, Jeroen, Hannes, Rieko, Sofie, Bura, and Alex for the numerous table tennis occasions. Alex, Michaël, Dominque, Wei Wei, Sander W., Fernando, Anneleen, Rik, Sander M., Wei Wang, Ward, Nick, Johanna, Hannes, Dongyu, Niels, Sreçko, Thomas, Wouter and many others that joined only once or twice for one or more of the fifteen LAN parties you joined each time I organized one. Michaël, Johanna, Sander, Monika for the summers filled with games of Kubb. Satur for her advice in the later stages of my PhD and the nice talks in our office.

Bram Paredis
Herent, August 2021

Abstract

Sediment generation is one the major challenges still remaining in sedimentary petrology.

Beknopte samenvatting

De vorming van sediment is een nog ondermaats onderzochte tak binnen de sedimentpetrologie.

List of Abbreviations

GGD Generalized Griffiths Descriptor. 5, 15, 17

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CHAPTER **1**

Introduction

1.1 General introduction

Sediment generation is the research field which studies the processes of how parent rock generates sediment along a specific pathway.

Parent rock is the rock from which the entire sediment generation process starts from. The properties of such a parent rock already confine the possible outcomes of the final sediment. Therefore, a proper way of characterizing the parent rock and thus its properties should be applied.

The **pathway** looks at by which processes sediment generation occurs, and along with it to which degree each process affects the outcome. Mechanical and chemical weathering are the major two groups with regard to the outlook of a pathway.

The properties of the resulting **sediment** is also of major interest as it will define its usefulness towards certain applications. Such applications for the

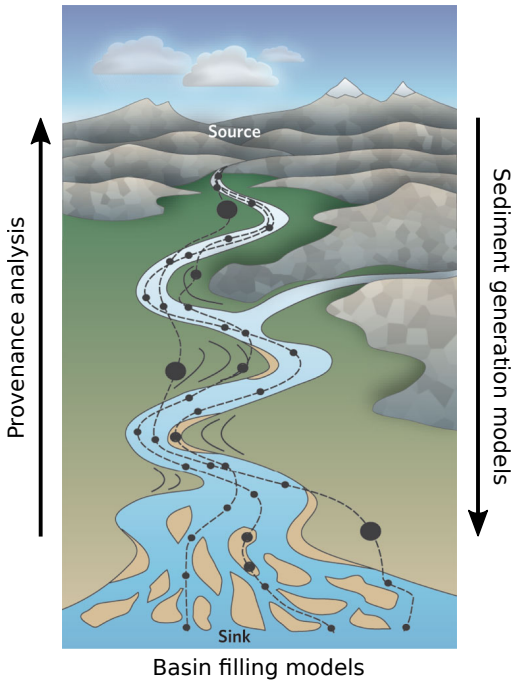

Figure 1.1: Source to sink representation with possible pathways indicated as lines and intermediate sinks as circles. Sediment generation models studying the way from source to sink, whilst provenance analysis does the opposite. At the sink, basin filling modelling takes place. All models combined will form source-to-sink modelling. Modified from Allen (2008)

sediment can be found in oil and gas exploration, geothermal energy, CO_2 capture and storage etc.

To this day, sediment generation remains to be fully understood, most notably in a quantitative way. That is where this PhD project comes into play, as it gives a first quantitative response to the long-standing questions of sediment generation. Assumptions and compromises had to be made along the way, of course, to keep the complexity of the model tangible while also limiting the requirements for running the model. Nevertheless, the value of a sediment generation model cannot be underestimated, as it will serve the purpose of closing the gap in source-to-sink models.

1.2 Parent rock characterization

A general approach to the characterization of parent rocks should be established if one wants a sediment generation model to be applicable to multiple input conditions. Therefore, the descriptor as proposed by Griffiths 1952, 1961 was extended to apply to parent rocks. The Generalized Griffiths Descriptor (GGD) is designed with the five fundamental properties of a parent rock in mind, be it:

- Composition
- Texture
- Size
- Shape
- Orientation

.

1.3 SedGen model

1.3.1 Main

The main code block runs the entire model. It can access all the global parameters and functions. When the model is run, input data will be requested to be provided. This can be done by pointing to a path or opening the file via the GUI. Next these data will be pre-processed to be in a format suitable for further analysis. The mechanical weathering module is then run, which will retrieve data from the input module as well as from the mineral properties and boundary conditions modules. As soon as grains and rock fragments become available, the chemical weathering module starts and with it the precipitation module. The mass balance module is already taken everything into account and bookkeeping all grains and rock fragments over different grains size classes and mineralogical classes. The user may specify at which time steps an output of the data is requested. The output data can then be post-processed to be presented as graphs and figures.

1.3.2 Input & pre-processing

Necessary user input data consists of three parts: modal mineralogy, relative interface frequencies and crystal size distribution. (i) The modal mineralogy contains the volume proportions of the minerals present in the source rock. (ii) The relative interface frequencies contain the fractions of all present mineral interface occurrences. See chapter 4. (iii) The crystal size distribution (CSD) provides information on the 3D aspects of the present minerals. See chapter 5. When the CSD data is in 1D, it will be transformed to 2D and then to 3D. When the CSD data is in 2D, it will be transformed to 3D (using CSD corrections Higgins 2010). A fourth, optional input is the chemical composition of the source rock. This can be in element or oxide form and may contain only the bulk or mineral chemical compositions as well. In the latter case, the modal mineralogy can be retrieved from the chemical composition data.

1.3.3 Mineral properties

The properties of all input minerals and possible output minerals will be stored here. It consists of chemical properties, physical properties and inter-mineral properties. (i) The chemical properties include molar volume, molar mass, mineral formula and weathering rates. All except the latter are fixed properties, meaning that they will be retrieved from literature and will not change during running the model. The weathering rate of a mineral may be influenced by pH, temperature and relief (see boundary conditions). (ii) The physical properties are a mineral's strength and its density. The former plays a role in intra-crystal breakage (see mechanical weathering). (iii) The 'inter-crystal properties' have been separated from the previous 'intra-crystal properties' because they relate to properties between different crystals (of possible different mineralogy). Interface strength is the main property here, and will play a role in the inter-crystal breakage during mechanical weathering.

The intra- and inter-crystal strengths may be dependent on many factors such as anisotropies in crystal structure changes due to changes in temperature or pressure. A detailed approach to estimate the absolute strengths may be considered as building a model on its own and will thus be estimated here for time-efficiency reasons. The data of Heins (1992) may prove valuable here for estimating relative inter-crystal strengths while intra-crystal strengths may be gathered from literature. Notwithstanding these data, a more detailed approach could be argued here, and may be incorporated in the future. The modular architecture of SedGen will allow for such an adaptation.

See chapter 8.

1.3.4 Boundary conditions

The boundary conditions cover climate and physiography. (i) Climate governs temperature, pH and precipitation, all of which have an influence on chemical weathering rates. A general water availability model could also be incorporated in future work to better assess these influences. (ii) Physiography consist of the relief (in source area) and plays a role in both weathering processes. The general trend here is thus 'time' vs. intensity.

See chapter 9.

1.3.5 Mechanical weathering

The pre-processed input data are combined with the mineral properties and boundary conditions during the calculations of the mechanical weathering (as they will with the chemical weathering and clay formation modules). First, the source rock is broken into large rock fragments during 'intra-rock breakage'. A detailed mass balance is not accounted for these fragments, only their number and size. This can be argued because their compositions will be very similar to the initial conditions. When a large fragment, upon further abrasion, gets below a certain fractionation limit threshold, the detailed mechanical weathering kicks in. If a rock fragment is to be broken, inter-crystal breakage will be applied while if it concerns a (mono-mineralic) grain, intra-crystal breakage will be triggered. Bookkeeping by the mass balance of all grains and rock fragments becomes very important now for further developments of the system (see mass balance module).

See chapter 11.

1.3.6 Chemical weathering & precipitation

Grains and rock fragments resulting from mechanical weathering will be available for chemical weathering and thus will be dissolved. These solutes may remain in this state or may precipitate as authigenic minerals such as oxides or clays. Clay minerals can again be chemically weathered and re-enter the system in doing so.

See chapter 12.

1.3.7 Mass balance

The mass balance keeps track of all mono crystalline grains, poly crystalline grains (rock fragments), solutes and clay/oxides. The poly crystalline grains are further subdivided in mono mineralic and poly mineralic rock fragments. The accounting is done according to a Lagrangian framework, meaning that where the parts are present in the system is not relevant, only how many (and in which form) of each part is. For the mono crystalline grains a matrix of grain size classes and number frequencies per mineral is sufficient. For the polycrystalline grains a same matrix with number frequencies and grain size classes is combined with a separate matrix with rock fragment sizes.

1.3.8 Output

Output data consists of grains size distributions, mineralogy and grain number frequencies in the form of the accounting done in the mass balance module. The output of data can be requested (at any time?) by the user to zoom in on output at a specific time step.

1.3.9 Post-processing

Output data may be post-processed to generate time-evolution figures such as trajectories on ternary diagrams e.g.

1.4 Objectives

1.5 Structure of this thesis

- In all relevant chapters parts of the SedGen model classes/functions/objects/constructs/ scripts may be included in the text or referenced as in appendix or online.
- Always note what we are and what we are not implementing into the model ⇒ Things can always be improved later on due to SedGen's modularity.

Part I

Input

CHAPTER **2**

Datasets

2.1 Introduction

For the model to be put to use, data has to be provided. This data can be gathered from legacy datasets, newly acquired or be a combination of both. Suggested ways and formats for data to be collected in will be discussed in later chapters. The main dataset used in this research will be discussed in this chapter alongside with some additional datasets. As this dataset missed some data required for the model, the efforts made to collect this complementary data will also be established.

2.2 Legacy data

2.2.1 Data from Heins (1992)

The PhD thesis of Heins (1992) was the main source for data of this project. Since it holds detailed data on the mineralogical composition and texture of six granitoid plutons it was very suited to serve as the starting point for this

Table 2.1: Details of plutons from dataset collected by Heins (1992) with coordinates and number of samples for parent rock (P) and sediment (C: coarse; M: medium; F: fine). Abbreviation codes will be used throughout the thesis.

Pluton	**Location**	**Coordinates**	**Code**	**# samples**	
				P	C, M, F
Granite Wash Mountains	West-central Arizona, USA	33.708N, 113.639W	AZ	15	8
Kinney Lakes Granodiorite	Sierra Nevada, California, USA	38.568N, 119.852W	CA-EW	6	9
Kinney Lakes Granodiorite	Sierra Nevada, California, USA	38.568N, 119.852W	CA-NS	5	9
Ocotito Granitoid Complex	Sierra Madre del Sur, Guerrero, Mexico	17.148N, 99.541W	GR	10	6
McCartney Mountain Stock	Southwestern Montana, USA	45.508N, 112.647W	MT	8	8
Mt. Stuart Batholith	Cascades, Washington, USA	47.479N, 120.805W	WA	4	6

PhD. Later on, the available data would be extended by means of own data collection (see next section).

Granitoid plutons

Six granitoid plutons were sampled by Heins (1992) which resulted in ca. 50 thin sections of parent rock and ca. 150 sediment samples across three size fractions (see Table 2.1). Five of the six plutons are situated in the US: Arizona (AZ), California (CA-NS for northern and southern drainage basins and CA-EW for eastern and western drainage basins), Montana (MT), Washington (WA). The sixth pluton is located in Guerrero (GR), Mexico.

2.2.2 Additional data sources

Throughout the PhD, other sources for data of various forms have also been used. References to those may be found in the relevant chapters. One worth noting here is the Vistelius et al. (1983) which was used for both the spatial variability of modal mineralogy and textural information studies.

2.3 New data

Additional data was gathered to elaborate the dataset already collected by Heins (1992). The main addition was the digital image analysis carried out over a period of four months. During this analysis, data on crystal size was collected of all available thin sections from Heins (1992).

2.3.1 Digital image analysis

The only information on the CSPDs of minerals in the parent rocks (property 3) is given by the arithmetic averages of the lengths of crystal intercepts (1-D apparent diameter) obtained from the parent-rock interface tallies of Heins (1992). Therefore, the original thin sections of the parent rocks were revisited to estimate crystal-size distributions of the minerals in each pluton. The thin sections were digitized by taking ca. 200 pictures per thin section in circularly polarized light (CPL) Higgins (2010). The pictures were stitched together using the software package PTGui. CPL is very useful for the purpose of tracing crystal boundaries. It highlights texture because all crystals will show their maximum birefringence colour for their respective cross-section independently of their orientation with regard to the polarizers. This allows identification of the majority of crystals from the images without the need for a microscope. Flatbed scan images of the thin sections in plane- and cross-polarized light were used for verification purposes throughout the process.

The following was carried out for each of the six mineral classes in each of the thin sections: A predetermined number of crystals (25, 50 or 100) was randomly selected in Adobe Photoshop. Random selection consists of assigning a uniform probability distribution to all points falling within the limits of the digitized specimen (rectangular thin section). A crystal is selected if the pair of random coordinates (generated from a uniform distribution) falls within its limits, and the crystal falls entirely within the bounds of the specimen. Crystals larger than 25 µm could be reliably identified. By using the 'quick selection tool' in Photoshop the crystals were converted to paths in vector format and given a corresponding mineral-class colour. All in all, about 14,000 crystals were digitized. The images were exported and loaded into the JMicrovision software for segmentation and data acquisition of 16 features including length, width, area, perimeter, and equivalent circular diameter. The equivalent circular diameter (D2) was chosen as the feature for further data analysis, in accordance with the assumption that crystals are spherical. The distributions of equivalent circular diameter (D2) were subsequently converted to 3-D and fused with the 1-D intercept data of Heins (1992) under the assumption of a lognormal

frequency distribution of crystal size. The lower limit on crystal size in the data of Heins (1992) is 10 µm. The upper limit on crystal size is given by the smallest dimension of the rectangular specimens, i.e., ca. 25 mm. The stereological method used to estimate the crystal-size distributions is discussed in detail in Appendix A.

Unfortunately, the data set of the sediments does not include measurements of property 3, so we cannot compare directly CSPDs of parent rocks and sediments. We will, therefore, limit ourselves to presenting the two parameters of the best-fit lognormal distributions (mean and standard deviation) of each mineral in each of the thin sections of the parent rocks separately, as well as the average values for the minerals in each pluton. All distributions will be compared against the observations by means of four statistical goodness-of-fit tests: Anderson-Darling, Pearson's Chi-squared, Kolmogorov-Smirnov, and Shapiro-Wilk (e.g., Stephens, 1974; Davis, 2002 and references therein).

CHAPTER 3

Modal mineralogy[1]

Modal mineralogy, also known as the volumetric proportions of minerals, within a parent rock is used as the measure for the first fundamental property of composition according to the GGD. It defines the amount of each mineral that is present within the parent rock as a volumetric proportion. The modal mineralogy can be estimated through optical microscopy and is hence a straightforward property to establish.

What might be less straightforward is how representative the modal mineralogy of a certain sample (i.e., thin section) is for the entire pluton. To answer that question, part of the research conducted in this PhD, looked at the variability of the modal mineralogy within plutons. This may not only help us to assess the variability with regards to the proposed research question but might also aid in a better error-propagation calculation of the final SedGen model.

[1]This chapter is in part based on G. J. Weltje and B. Paredis (2020). "Geostatistical modelling of compositional variability across granitoid complexes: Its relevance to petrogenetic interpretations and specification of parent-rock properties in sediment-generation models". In: *Earth-Science Reviews* 208

3.1 First building block / fundamental property

3.2 Spatial variation of modal mineralogy

CHAPTER **4**

Interfacial composition[1]

The second property of the GGD is that of texture which thus tells something about the spatial relations between elements (i.e., minerals) of an aggregate (i.e., parent rock). The measure used during this PhD to characterize this property was the interfacial composition which looks at the volumetric proportions of element contacts/interfaces between the specified classes. In our case these elements consist of crystals while the classes are the different mineral classes but it can also match other elements/classes as is discussed in Le Pera and Morrone (2020).

4.1 Second building block / fundamental property

4.2

[1]This chapter is in part based on G. J. Weltje, B. Paredis, et al. (2018). "Quantitative analysis of crystal-interface frequencies in granitoids: Implications for modelling of parent-rock texture and its influence on the properties of plutoniclastic sands". In: *Sedimentary Geology* 375, pp. 72–85

CHAPTER **5**

Crystal size distributions[1]

5.1 Chapter contents

- Based on Paredis et al. 2020 publication
- 2D/3D CSD data
- Ways to transform and correct legacy data from 1D to 3D

5.2 Simulation of cutting spheres to circles

5.3 Digital image analysis

5.4 Truncation

[1] This chapter is in part based on B. Paredis et al. (2020). "Quantitative analysis of the joint variability of rock texture and composition in thin section: The Generalized Griffiths Descriptor and its application to sediment generation from granitoids". In: *Earth-Science Reviews* 205

CHAPTER **6**

Parent rock characterization and initialization

6.1 Chapter contents

- Based on Paredis et al. 2019a publication
- Determination of texture in granitoids
- Interaction of the three building blocks discussed by Heins' (1992) dataset as a way to initialize and characterize parent rocks for SedGen
- Characterization of all plutons from Heins (1992) separately

6.2

CHAPTER **7**

Input based on modified GGD

7.1 Chapter contents

- Griffiths' descriptor for sediments
- Our translation of Griffiths' description for granitoids and parent rocks in general (discussion): i) modal mineralogy, ii) relative crystal interfaces, iii) crystal size distributions
- Mention the fact that we leave out orientation and shape properties but that these could be included in future versions of SedGen (part of discussion)

7.2 Griffiths' descriptor

7.2.1 Griffiths' descriptor for sediments

7.2.2 Generalized Griffiths' descriptor (for parent rocks)

7.2.3 Fundamental properties of composition, texture and size

Composition - modal mineralogy

Texture - relative crystal interfaces

Size - Crystal size distributions

7.2.4 Remark on fundamental properties of shape and orientation

CHAPTER **8**

Mineral properties

8.1 Chapter contents

- Overview of physical and chemical properties of minerals
- Partly based on Weltje et al. 2020 with regard to relative interface strengths (inter-crystal properties)

CHAPTER **9**

Boundary conditions

9.1 Chapter contents

- Climate (temperature, pH, precipitation)
- Physiography (relief)
- Weathering rates (time vs intensity) → Alex Blum (reference)

9.2 Climate

Climatic conditions also have a role to play in the sediment generation process. **Temperature** and **precipitation** are the two most obvious factors. The **pH** of water can also be of importance when chemical weathering is the main form of weathering (e.g. solubility of K-feldspar).

9.3 Physiography

The **relief** of the terrain in which the sediment generation is occurring must also be taken into consideration. Along with the present **vegetation**, both will have an effect on mechanical and chemical weathering.

9.4 Weathering rate

All the factors mentioned in the above sections boil down to have a combined effect on the **rate of weathering**, be it mechanical or chemical.

Part II

Calculations/Implications/Algorithms

CHAPTER **10**

SedGen: design and architecture

10.1 Introduction

SedGen was written in Python, a popular, easy-to-use, programming language. The code base has been tracked through Git as version control system (VCS) with an online version available on GitHub (see link). This makes sure SedGen can be easily maintained in the future as well as receive updates. It was opted to write the different functions of SedGen into various modules thus resulting in a modular structure. As long as the input and output formats cohere to the expected formats, any function can be implemented to modify the rock along its way to sediment. How meaningful such operations might be, however, is totally dependent on the understanding of the function's creator.

10.2 Python

Python has been developed by Guido van Rossem in 1991 to overcome problems of available programming languages at the time. It has been written as a dynamic language, meaning that the user does not need to specify things such as data types, memory usage etc. . Since then it has grown a large community base, resulting in popularity among various fields such as general programming,

data science, web development, etc. . Although, in the past Python 2 had the largest use cases, after its deprecation in 2020 Python 3 is now the way forward. Therefore, SedGen was also implemented in Python 3 with a vision towards future-proofing it.

Aside from Python's standard library of packages some additional third party packages were used, including:

- *Numpy* for linear algebra and mathematical operations in general.
- *Numba* to compile Numpy functions before actually running SedGen, thus making Python behave as a static language resulting in significant execution time speed-ups.
- *Scipy* to use mathematical distributions and various additions to Numpy's library.
- *Pandas* to handle all tabular format data and handling input/output operations from/to spreadsheets.
- *Matplotlib* and *Seaborn* to plot and 'prettify' results.

All of these packages are widely used throughout the scientific community, of which a nice example is their use to take the first images of a black hole (ref).

10.3 SedGen's initialization

The user is expected to provide the following model properties as a necessity:

- Modal mineralogy to specify which minerals are present in the rock as well as their volumetric proportions.
- Mean and standard deviation of each mineral's crystal size distribution, which, as discussed in section ..., is assumed to be derived from a (truncated) log-normal distribution.

As optional properties the following may be provided during the initialization:

- Interfacial composition to specify the texture of the parent rock. If this property is not specified, the alpha factor can be specified to determine the interfacial composition after the number frequencies of the parent rock have been calculated. In the event when the alpha factor is also not

given, a default alpha factor of 1 will be used thus resulting in a random texture or a pre-specified factor for a certain rock type with a certain texture based on literature included into SedGen beforehand; (e.g., 1.05 for granite).

- Parent rock volume to specify the initial volume of rock to be weathered. By default this is set to $1\,m^3$ of parent rock.
- Boundary conditions such as climate, including temperature and precipitation, and vegetation might be given or be chosen from a pre-specified list of options. Another possibility exists in providing an option per time step in the model, thus altering the ratio between mechanical and chemical weathering throughout the model's runtime.

These initial parameters are then passed to a constructor instance of the SedGen class. The initialization of an instance takes about 10 s (for 10 million crystals initially). After assigning the initial parameters as attributes of the instance, new attributes are calculated based on them. Firstly the binning occurs, in which the crystal sizes are discretizized for computational benefits. Secondly, the mineral occurrences are simulated based on the modal mineralogy and the crystal-size distribution data. This is performed in a separate function in which the parent rock volume is filled up with crystals until it is filled. This is done per mineral class by taking the product of the modal mineralogy and parent rock volume as the mineral class' volume. By initializing a log-normal distribution based on the csd mean and std, crystal sizes might be generated from it. A 'learning-rate' parameter is passed to the function to determine how many crystals are requested from the log-normal distribution during every iteration of the while loop. The while loop continues until the sum of the volume of generated crystals reaches the mineral class' volume. By tweaking the learning rate the resulting simulated mineral class' volume might better approximate the true mineral class' volume. Once the required volume has been filled, the array of generated crystal volumes is binned according to the already initialized volume bin array.

At this point, the crystal size/volume array has been initialized. The number of crystals per mineral class is also known at this point. These numbers might be used later on to request new material to be generated to enter the model at a later timestep. This generation of material can then occur without the need of filling up a volume via a learning-curve but might be performed by just requesting N crystals from the log-normal crystal size distribution.

10.4 Binning

Since SedGen was developed for use on personal computers, trade-offs between accuracy and performance had to be made. One such trade-off is the use of bins to represent crystal sizes. By default, the model works with 1500 crystal size classes in a geometric series of 2^{-10} mm to 2^{5} mm. This translates to a minimal crystal size of ca. 1 µm and a maximal crystal size of 30 mm.

In most of the model's functions, however, volume classes are used for calculations. This is done to establish a 'volume-balance' cfr. mass-balance practices. The size bins are converted to volume bins under the assumption that all crystal are spheres. Hence:

$$bins_V = \frac{4}{3}\pi \; bins_S^3 \tag{10.1}$$

The bins are represented by bin labels ranging from 0 up to 1500 in the default case. For ease of use, the median of each bin is used during calculations.

$$bins_{S,med} = median(bins_S) \tag{10.2}$$

$$bins_{V,med} = median(bins_V) \tag{10.3}$$

10.5 Crystals

The base unit of the model is the crystal which represents a single entity of a mineral class. Its boundaries thus lie in the crystallographic characteristics of the mineral class to which it belongs. A distinction between so-called sub-crystals is not made within the model even though crystals may split in two during intra-crystal breakage. If such a splitting happens the crystal (or mono-crystalline grain at this point) is merely assigned to two new crystals of the same mineral class, be it of a smaller size/volume of course. A mineral class can represent one mineral or several ones, e.g. for accessory minerals, within the parent rock that is being studied. This should be borne in mind when certain physical or chemical properties are set for these 'combined mineral classes'.

10.6 Grain representation

SedGen makes a distinction between mono- and poly-crystalline grains. The former is a grain consisting out of one crystal while the latter may consist out

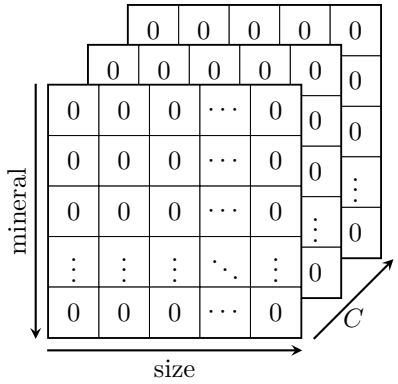

Figure 10.1: Representation of empty mcg 3D matrix

of two or more crystals. Although a crystal might consist of sub-crystals these are not considered in SedGen.

The poly-crystalline grains are represented by a list of arrays in which each array represents one pcg.

$$pcgs = [pcg_1, pcg_2, \ldots, pcg_p] \tag{10.4}$$

The mono-crystalline grains are represented by a n x m x d matrix in which the values represent the number of mcgs (of a specific chemical weathering state, mineral class and size) present in the model.

The different mineral classes are assigned a number from 0 to m, with m being the total number of mineral classes. An array of numbers from 0 to m in SedGen not only represents the mineral occurrences (number frequencies) but also the interfacial composition. The interfacial composition is represented by the order of the crystals in an array in which the array represents one poly-crystalline grain. It should be noted that at the start of a SedGen initialization there is thus only one poly-crystalline 'grain', the block of parent rock from which all other grains will derive. As weathering kicks in, the initial array will be split into arrays of smaller length and when this length becomes one, a mono-crystalline grain (mcg) is formed. When this happens, the mcg is transferred from the list of poly-crystalline grains (pcg) to a matrix of mcg with dimensions m x d where d is the number of grain size classes. The grain size representation is done in a similar way as the mineral occurrence/interface array, except for the fact that d numbers are used instead of m. Each number ranging from 0 to d thus represents a size/volume class.

When intra-crystal breakage kicks in, mcg formed during inter-crystal breakage,

will break. To restrict numerical operations for this to happen the number of ways a mcg might be broken is limited in relation to d, i.e. the amount of discretization of the model. Since a geometric series of grain size classes is used the ratio between neighbouring size classes is constant. This property might be exploited to determine a dictionary of size classes that 'belong together' during the initialization phase of SedGen.

10.7 Weathering modules

A distinction has to be made between mechanical and chemical weathering as to how they interact on the building blocks of the model. Mechanical weathering will operate on the interfaces of grains, or in the case of intra-crystal breakage of mcg, on its virtual interfaces. In the case of inter-crystal breakage, upon breakage along an interface, this interface is thus destroyed and removed from the model's interface counts matrix.

Chemical weathering will operate on the crystals themselves and this may result in two cases depending on the crystal's size and chemical weathering state.

1. When a crystal is chemically weathered and its size is still bigger than its chemical weathering state's residue threshold, it is kept in-place and only residue is formed due to weathering process.
2. When a crystal is chemically weathered and its size is smaller than its chemical weathering state's residue threshold, the crystal as a whole is dissolved and thus added to residue (of the corresponding mineral class).

10.7.1 Mechanical weathering

Inter-crystal breakage

Intra-crystal breakage

10.7.2 Chemical weathering

To accommodate the arithmetic nature of chemical weathering, a new approach to the binning was added since the binning consists of a geometric series. By using multiple arrays of bins with each array representing the initial geometric series of bins minus x times the chemical weathering, a new trade-off between accuracy and performance is obtained. This operation results in the expansion

of multiple matrices from 2D to 3D with the dimensions being n x m x d, where n is the number of iterations the model has gone through. As chemical weathering occurs once every time step, n immediately reflects the number of times chemical weathering has occurred on a certain grain. By thus shifting the grains to higher n arrays, chemical weathering is simulated. By requesting the corresponding bin array, the exact bin values for a specific chemical weathered grain may be retrieved.

Chemical weathering of mcg

Chemical weathering of pcg

Clay formation

10.8 Chapter contents

- General overview of how data should be formatted to be accepted by the model and the modules at work to clean, transform and calculate data in the case of legacy data.
- Types of weathering and their interaction
- Types of crystals/grains within SedGen (poly, mono, RF...)
- Discuss their implementation into the SedGen model and how they are tracked
- Different frameworks that are used in SedGen (e.g. Lagrangian framework, compositional space vs physical space)
- Discuss data that SedGen model can output and at what timesteps (GSD, mineralogy, grain number frequencies)

CHAPTER **11**

Mechanical weathering

11.1 Chapter contents

- Based on Paredis et al. 2019b publication in which state-of-the-art in mechanical weathering will be discussed
- Since this field is less discussed in the geological literature, literature from others research fields will be consulted
- Discuss the mechanical weathering module of SedGen
- Intra- & inter crystal breakage along with intra-rock breakage in early stages of simulation (fractionation limit)
- Rock fragments on-demand

CHAPTER **12**

Chemical weathering

12.1 Chapter contents

- State-of-the-art in chemical weathering and clay formation research
- Discuss sources from which information was implemented into the SedGen model
- Discuss the chemical weathering and clay formation modules of SedGen

Part III

Applications

CHAPTER **13**

Calibration

13.1 Chapter contents

- Discuss the validity of SedGen based on the calibration results of Heins (1992) and unseen test dataset

CHAPTER **14**

Applications

14.1 Chapter contents

- Provide a non-exhaustive list of possible applications of SedGen output data based on post-processed data (e.g. ternary diagrams, timestep based plots)

CHAPTER **15**

Discussion

15.1 Chapter contents

- Discuss the applicability of SedGen in general
- Possibilities to upgrade SedGen due to its modularity (e.g. of including shape and orientation properties to input)

15.2 Future updates to SedGen

15.2.1 Fundamental property of shape

Since SedGen rather makes use of a 'crystal volume distribution' (cvd) than the csd, this may be used to our benefit for including the fourth fundamental property of shape. Together with a crystal's size, its shape also determines its volume after all. Volume can thus be considered as a derived property of the fundamental properties of size and shape. Although the cvd will give information about the absolute occurences of volumes of a mineral class, relative proportions of mineral classes in unit volume of a rock still need to be provided by the modal mineralogy, i.e., the composition fundamental property.

Some remarks to this: - Volume is also dependent on a mineral's density - What's the influence of modal mineralogy and interfacial composition on the cvd?

Since the assumption of all crystals inside SedGen being spheres eliminates the fundamental property of shape, some extra functionality to SedGen would have to be added to incorporate it. This can be easily done however by adding an additional list of arrays for the pcg, indicating in a qualitative way to which shape a crystal belongs. As with the mineral occurence array, '0' could stand for a spherical shape, '1' for a cubic shape and so on. For the mcg, an additional dimension to the currently 3D array would have to be added to keep track of the shape property in the same qualitative way as described above. When operations are done on crystals, be it from the pcg or mcg part, the shape indicator could act as a lookup value to activate corresponding formulas for calculating volumes, sizes etc. Rules for how shapes might change when a mcg is broken, will also have to be established. The way crystal shapes might occur due to breakage might be characterized in a similar way as with crystal interfaces. With a proportions 3D array the outcomes per mineral class might be provided: SS PP SP etc. Q S 0.25 0.2 0.3 C 0.1 0.6 0.1 P 0.05 0.2 0.3 P ...

Where Q and P stand for quartz and plagioclase and S, C, P stand for spherical, cubic and plate-like (i.e. planar).

For the pcgs, the consideration might be made to also keep track of the shape of an individual pcg, as this might be of interest to some people.

Although it is still quite a challenge to measure the shapes of crystals contained within a rock, it is not impossible. Nevertheless, an estimation or variation of shapes based on the mineral class might prove sufficient as input to SedGen or such estimations can build into the model beforehand.

15.2.2 Texture representation in 2D/3D

Currently, the texture representation in SedGen is done in a one-dimensional manner. Crystals in pcgs are represented by one-dimensional arrays in which their order also dictates the texture. Each crystal can thus only have two contacts at most and one at the least. If a crystal has no contacts, it is by definition a mono-crystalline grain as should have been moved from the pcg part to the mcg one.

15.2.3 Fundamental property of orientation

The fundamental property of orientation would only enter the picture once the shape fundamental property has been successfully incorporated into the SedGen model. This is true, since as long as all crystals would be spheres, orientation of crystals would not have a meaning. That is, as long as sub-crystals are not being considered, which is the case at the moment. Even when the shape property would have been incorporated, an upgrade of the texture representation in 1D to 2D or even to 3D would truly make the orientation property's importance to come to the foreground.

15.2.4 Integration of time

The time aspect of SedGen is quite abstract at the moment. In the future, an integration of time into the model might enable a better understanding of the processed and conditions present during a SedGen model. One such way of integrating this, might be by enable a 'flushing rate' in the model. This rate would define how much water is moving through the system in a certain time step (iteration of the model). By specifying this, the time steps could also be attributed a true time duration. Most prominently, the flushing rate would determine the balance between mechanical and chemical weathering.

CHAPTER **16**

Conclusions

16.1 Chapter contents

- General conclusion of the current version of SedGen

Appendices

APPENDIX **A**

Appendix

A.1 Chapter contents

- Additional figures
- Most important SedGen code snippets
- GitHub page reference for complete model code

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Curriculum

Bram Paredis was born in Neerpelt on July 6th, 1992. After completing his Latin-sciences studies at WICO Campus Sint-Hubertus in Neerpelt he started his academic studies at KU Leuven in 2010. There, he obtained his B.Sc. degree in Geology in 2013, followed by his M.Sc. degree in Geology in 2015. His M.Sc. thesis, which was supervised by Prof. Dr. Philippe Muchez, entitled 'Concentration and distribution of platinum group elements in sulfide ores: Musongati, Burundi' won the 'From Silex to Chip' prize awarded by the 'Beroepsvereniging Leuvense Geologen'. After receiving a negative advice for his application of a PhD grant to continue his petrology research, he made the switch to sediment petrology under the supervision of Prof. Dr. Gert Jan Weltje where he started a PhD. Since then he presented the results and outcomes of his PhD on numerous occasions. Bram has developed a strong interest for programming and data science in particular whilst putting these acquired skills already to use in his PhD.

Publications

Journal papers

Weltje, G.J. and **Paredis, B.**, 2020. Geostatistical modelling of compositional variability across granitoid complexes: Its relevance to petrogenetic interpretations and specification of parent-rock properties in sediment-generation models. Earth-Science Reviews 208, pp. xx-xx

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Miscellaneous

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