KU LEUVEN

Faculty of Science

DRAFT

To remove, add 'final' to class options

Numerical Modelling of Sediment Generation

Bram Paredis

Supervisor:
Prof. dr. G. J. Weltje

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

August 2020

Numerical Modelling of Sediment Generation

Bram PAREDIS

Examination committee:
Prof. dr. ir. The Chairman, chair
Prof. dr. G. J. Weltje, supervisor
Prof. dr. J. Elsen
Prof. dr. G. Verstraeten
Prof. dr. P. Vermeesch
(University College London, UK)
dr. W. A. Heins
(Getech, USA)

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

August 2020

© 2020 KU Leuven – Faculty of Science
Uitgegeven in eigen beheer, Bram Paredis, Celestijnenlaan 200E box 2410, B-3001 Leuven (Belgium)

Alle rechten voorbehouden. Niets uit deze uitgave mag worden vermenigvuldigd en/of openbaar gemaakt worden door middel van druk, fotokopie, microfilm, elektronisch of op welke andere wijze ook zonder voorafgaande schriftelijke toestemming van de uitgever.

All rights reserved. No part of the publication may be reproduced in any form by print, photoprint, microfilm, electronic or any other means without written permission from the publisher.

Preface

This PhD gave me the opportunity to venture into the exciting world of programming and establish a strong foothold in Python. Combined with my geology knowledge it served this topic well.

Bram Paredis
Herent, August 2020

Instructies van de faculteit:

In het voorwoord wordt de algemene doelstelling van het werk samengevat in enkele regels en worden personen, diensten of firma's bedankt voor hun medewerking bij het tot stand komen van het werk.

De naam van firma's en personen uit deze firma's mogen slechts worden vermeld mits hun uitdrukkelijke toelating én na overleg met de supervisor(en)! Steeds wordt de supervisor(en) vermeld, de verantwoordelijke en eventueel de personen die rechtstreeks geholpen hebben bv. door het ter beschikking stelling van meetresultaten, faciliteiten. Ook de instantie die eventueel een doctoraatsbeurs heeft toegekend wordt bedankt (bv. FWO, IWT, ...).

Abstract

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

Instructies van de faculteit:

In een beknopte tekst van maximum 2 pagina's worden de belangrijkste doelstellingen en besluiten geformuleerd, zowel in het Nederlands als in het Engels. Zulke samenvattingen kunnen worden gebruikt in wetenschappelijke verslagen van het departement of de faculteit. Het Engels moet vlekkeloos zijn.

Beknopte samenvatting

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

Instructies van de faculteit:

In een beknopte tekst van maximum 2 pagina's worden de belangrijkste doelstellingen en besluiten geformuleerd, zowel in het Nederlands als in het Engels. Zulke samenvattingen kunnen worden gebruikt in wetenschappelijke verslagen van het departement of de faculteit. Het Engels moet vlekkeloos zijn.

List of Abbreviations

GGD Generalized Griffiths Descriptor. 5

Contents

Abstract iii

Beknopte samenvatting v

List of Abbreviations vii

List of Symbols ix

Contents ix

List of Figures xv

List of Tables xvii

1 Introduction 3

1.1 General introduction 3

1.2 Parent rock characterization 4

1.3 Model architecture 5

1.3.1 Main 5
1.3.2 Input & pre-processing 5
1.3.3 Mineral properties 5
1.3.4 Boundary conditions 6
1.3.5 Mechanical weathering 6
1.3.6 Chemical weathering & precipitation 7
1.3.7 Mass balance 7
1.3.8 Output 7
1.3.9 Post-processing 8
1.4 Objectives 8
1.5 Structure of this thesis 8

I Input **9**

2 Dataset **10**
2.1 Chapter contents 10
2.2 Data from literature 10
2.2.1 Data from Heins (1992) 10
2.2.2 Additional data sources 11
2.3 Own data 11

3 Modal mineralogy **13**
3.1 Chapter contents 13
3.2 First building block / fundamental property 13
3.3 Spatial variation of modal mineralogy 13

4 Crystal boundary interfaces **15**
4.1 Chapter contents 15

4.2 Second building block / fundamental property 15
4.3 15

5 Crystal size distributions 17
5.1 Chapter contents 17
5.2 Simulation of cutting spheres to circles 17
5.3 Digital image analysis 17
5.4 Truncation 17

6 Parent rock characterization and initialization 19
6.1 Chapter contents 19
6.2 19

7 Input based on modified GGD 21
7.1 Chapter contents 21
7.2 Griffiths' descriptor 22
7.2.1 Griffiths' descriptor for sediments 22
7.2.2 Generalized Griffiths' descriptor (for parent rocks) . . . 22
7.2.3 Fundamental properties of composition, texture and size 22
7.2.4 Remark on fundamental properties of shape and orientation 22

8 Mineral properties 23
8.1 Chapter contents 23

9 Boundary conditions 25
9.1 Chapter contents 25
9.2 Climate 25
9.3 Physiography 25
9.4 Weathering rate 26

II Calculations/Implications/Algorithms 27

10 SedGen: design and architecture 28

10.1 Introduction 28

10.2 Python 28

10.3 SedGen's initialization 29

10.4 Binning 31

10.5 Crystals 31

10.6 Grain representation 31

10.7 Weathering modules 33

10.7.1 Mechanical weathering 33

10.7.2 Chemical weathering 33

10.8 Chapter contents 34

11 Mechanical weathering 35

11.1 Chapter contents 35

12 Chemical weathering 37

12.1 Chapter contents 37

III Applications 39

13 Calibration 40

13.1 Chapter contents 40

14 Applications 41

14.1 Chapter contents 41

15 Discussion 43

15.1 Chapter contents 43
15.2 Future updates to SedGen 43
15.2.1 Fundamental property of shape 43
15.2.2 Texture representation in 2D/3D 44
15.2.3 Fundamental property of orientation 44

16 Conclusions **45**
16.1 Chapter contents 45

A Appendix **49**
A.1 Chapter contents 49

Curriculum **53**

List of Figures

10.1 Representation of empty mcg 3D matrix 32

List of Tables

2.1 Number of samples collected by Heins (1992) for parent rock (P) and sediment (C: coarse; M: medium; F: fine) 11

Instructies van de faculteit:

De hoofdstukken: Elk hoofdstuk is ingelast met een bepaald doel voor ogen. Dit doel wordt vermeld in de eerste paragraaf van elk hoofdstuk. Naargelang de aard van de tekst (experiment, uitvoering, theoretische ontwikkeling, ...) volgen de paragrafen elkaar op. Beweringen worden altijd gestaafd, hetzij door eigen experimenten, hetzij door een theoretische afleiding, hetzij door verwijzingen naar de literatuur. Elk hoofdstuk eindigt met een kort samenvattend besluit waarbij nagegaan wordt in hoeverre de doelstelling van het betrokken hoofdstuk verwezenlijkt is. De deelbesluiten moeten de lezer automatisch leiden naar het algemeen besluit aan het einde van het werk.

CHAPTER **1**

Introduction

Instructies van de faculteit:

De inleiding situeert de problematiek, beschrijft de stand van de huidige kennis terzake, omschrijft de voornaamste doelstelligen van het werk, samen met de beperkende randvoorwaarden en de ter beschikking gestelde middelen en poneert de belangrijkste stellingen.

1.1 General introduction

Sediment generation is the research field which studies the processes 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 limit 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 effects 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.

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 tries to give 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 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 to be the input of 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 build upon five fundamental properties of a parent rock, be it:

- Composition
- Texture
- Size
- Shape
- Orientation

.

1.3 Model architecture

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**

Dataset

2.1 Chapter contents

- Introduction to main data set of Heins (1992): Geological setting of different plutons, number and identity of samples, etc. .
- Introduction to three main 'building blocks' of modal mineralogy, relative crystal interfaces and CSD

2.2 Data from literature

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

Table 2.1: Number of samples collected by Heins (1992) for parent rock (P) and sediment (C: coarse; M: medium; F: fine)

	P	C	M	F
AZ	15			
CA-NS	5			
CA-EW	6			
GR	10			
MT	8			
WA	4			

Granitoid plutons

Six 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).

2.2.2 Additional data sources

Throughout the PhD, other sources for data of various forms have also been used. 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. References to those may be found in the relevant chapters.

2.3 Own 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).

CHAPTER **3**

Modal mineralogy[1]

3.1 Chapter contents

- Modal mineralogy as one of the building blocks for SedGen
- Spatial variation of modal mineralogy (Ordinary Kriging of PCA) based on Weltje et al. 2020

3.2 First building block / fundamental property

3.3 Spatial variation of modal mineralogy

[1]this chapter is in part based on G. J. Weltje 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 **4**

Crystal boundary interfaces

4.1 Chapter contents

- Based on Weltje et al. 2018 publication

4.2 Second building block / fundamental property

4.3

CHAPTER **5**

Crystal size distributions

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 **Paredis_et_al_2020**

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} to 2^{5}. 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 of two or more crystals. Although a crystal might consist of sub-crystals these are not considered in SedGen.

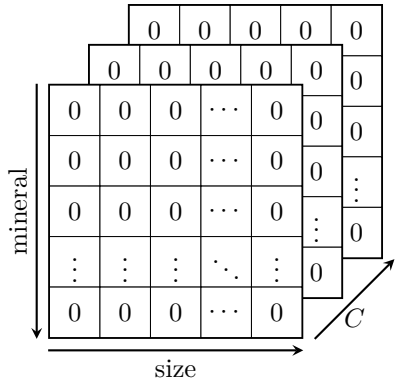

Figure 10.1: Representation of empty mcg 3D matrix

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.

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.

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.

CHAPTER **16**

Conclusions

16.1 Chapter contents

- General conclusion of the current version of SedGen

Instructies van de faculteit:

Algemene besluiten: Verwijzend naar de inleiding en naar de besluiten van de afzonderlijke hoofdstukken worden op het einde van het proefschrift de voornaamste besluiten gebundeld. Hier wordt de nadruk gelegd op de eigen inbreng, de verworven resultaten, de 'stellingen' van het proefschrift en de originele bijdragen tot het onderzoeksdomein. De onopgeloste problemen worden aangestipt en suggesties voor eventueel verder onderzoek worden gemaakt.

Appendices

APPENDIX **A**

Appendix

A.1 Chapter contents

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

Instructies van de faculteit:

De appendices: ze omvatten alle gedeelten uit de tekst die weliswaar essentieel zijn voor het proefschrift, maar waarvan de inlassing in de tekst de leesbaarheid ervan nadelig zouden beïnvloeden bv. omwille van hun lengte. Zo kunnen bv. de brute meetresultaten of een computerprogramma met zijn bron, commentaar en voorbeelden beter thuishoren in een appendix dan in de tekst zelf. De appendices kunnen desgevallend worden gebundeld in een apart boekdeel.

Bibliography

Griffiths, J. C. (1952). "Grain-size distribution and reservoir-rock characteristics". In: *AAPG Bulletin* 36, pp. 205–229.

– (1961). "Measurement of the properties of sediments". In: *The Journal of Geology* 69, pp. 487–498.

Heins, W. A. (1992). "The effect of climate and topography on the composition of modern plutoniclastic sand". PhD thesis. University of California, Los Angeles, 465 p.

Higgins, M. D. (2010). "Imaging birefringent minerals without extinction using circularly polarized light". In: *The Canadian Mineralogist* 48.1, pp. 231–235.

Vistelius, A. B., F. P. Agterberg, S. R. Divi, and D. D. Hogarth (1983). *A stochastic model for the crystallization and textural analysis of a fine grained granitic stock near Meech Lake, Gatineau Park, Quebec.* Tech. rep. Geological Survey of Canada, p. 67.

Weltje, G. J., B. Paredis, L. Caracciolo, and W. A. Heins (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.

Instructies van de faculteit:

De bibliografie. Departementale richtlijnen terzake te volgen.

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 the sediment petrology under supervision of Prof. Dr. Gert Jan Weltje where he started a PhD. Bram presented the results and outcomes of this PhD on numerous occasions. Bram has developed a strong interest for programming and data science in particular.

Instructies van de faculteit:

Beknopt CV van de doctorandus.

Publications

Journal papers

Weltje, G.J. and **Paredis, B.**, 2020. Spatial variability of modal mineralogy in granitoid plutons. Earth-Science Reviews xx, pp. xx-xx

Paredis, B. and Weltje, G.J., 2020. Generalized Griffiths Descriptor. Earth-Science Reviews xx, pp. xx-xx

Weltje, G.J., **Paredis, B.**, Caracciolo, L., Heins, W.A., 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. Sedimentary Geology 375, pp. 72–85

Conference proceedings and abstracts

Paredis, B. and Weltje, G.J., 2018. Numerical modelling of sediment generation: characterizing parent rock's properties by digital petrography. Oral presentation at the 6^{th} International Geologica Belgica Meeting. September 12-14, 2018. Leuven, Belgium.

Paredis, B. and Weltje, G.J., 2018. Numerical modelling of sediment generation: characterization of parent rock properties. Oral presentation at

20^{th} International Sedimentological Congress. August 12-17, 2018. Québec, Canada.

Paredis, B. and Weltje, G.J., 2018. Numerical modelling of sediment generation: characterisation of granitoid parent rocks. Oral presentation at 4^{th} meeting of the Working Group on Sediment Generation (WGSG). June 27-29, 2018. Dublin, Ireland.

Paredis, B. and Weltje, G.J., 2017. Numerical modelling of sediment generation: a modular approach. Oral presentation at the 33^{rd} International Meeting of Sedimentology. October 10-12, 2017. Toulouse, France.

Paredis, B. and Weltje, G.J., 2016. Numerical modelling of sediment generation. Poster presentation at 3^{rd} meeting of the Working Group on Sediment Generation (WGSG). July 4-6, 2016. Leuven, Belgium.

Miscellaneous

FACULTY OF SCIENCE
DEPARTMENT OF EARTH AND ENVIRONMENTAL SCIENCES
GEOLOGY
Celestijnenlaan 200E box 2410
B-3001 Leuven
balie.ees@kuleuven.be
http://www.aow.kuleuven.be