

Issue No. 1 September 2020

Welcome to the 1st issue of the MATHEGRAM newsletters! MATHEGRAM is a research and training consortium funded by European Commission (EC) through the Marie Skłodowska-Curie Innovative Training Network. MATHEGRAM consists of 10 partners from 6 European countries, and trains 15 Early Stage Researchers (i.e. MATHEGRAM fellows). Each fellow works on a specific research projects.

MATHEGRAM uses a systematic approach to investigate the fundamental mechanisms of heat generation and transfer in granular materials; to analyse the effect of temperature on micromechanics, microstructure, flowability and mechanical properties of granular materials and to explore emerging applications involving granular materials at a wide range of temperatures.

MATHEGRAM was officially started in January 2019. I am so glad that we have successfully recruited 14 fellows who started their research projects. In addition, our 1st advanced training course (i.e. ATC1) on “Modelling and Characterisation of Granular Materials” was a great success, as it provided not only well structured training to MATHEGRAM fellows but also excellent opportunities for our fellows to start working as a team. I am extremely grateful to TU Graz for organizing ATC1, we all had an enjoyable and fruitful time in Graz, Austria!

— Prof. Charley Wu, MATHEGRAM coordinator

Inside this issue

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This project has received funding from the European Commission's Marie Skłodowska-Curie innovative training Network under grant agreement No. 813202.



MATHEGRAM Supervisors at the kick-off meeting in Guildford



MATHEGRAMers at the ATC1 in TU Graz

First MATHEGRAM Advance Training Course (ATC1)



The first MATHEGRAM advanced training course (ATC 1) on “Modelling and Characterisation of Granular Materials & Basic Coding” was successfully held at Technische Universitaet Graz, Austria, on 17th – 22nd November 2019. The MATHEGRAM ATC 1 proved an in-depth training on computational approaches and characterisation related to granular materials, including Python programming and Discrete Element modelling with LIGGGHTS.



The ATC1 consisted of lectures and hands-on sessions, which were delivered by MATHEGRAM supervisors and partners. The attendees also had the opportunity to visit the particle technology laboratory at TU Graz. Albeit it is an intensive training week, ESRs found the training was very useful. Most importantly, the ATC1 brought all MATHEGRAM ESRs together for the first time, from which exciting team work started!



Heat Generation and Transfer in Granular Materials at High Stresses

by Ranjan Dhakal (ESR2)

1. Introduction

During manufacturing, analysis of powder compaction plays an important role, for example in particle size enlargement process in the pharmaceutical industry, in tablet production, as well as in powder metallurgical applications.

During such a compaction process, temperature rise in the compressed powder can cause thermal degradation, which are critical to the change in crystallinity and can affect, for example, the physiochemical properties of the pharmaceutical powder. In this way, it is of practical significance to study the material properties of the powder and understand its thermal response during compaction. Being able to describe the thermal response during compaction of granular materials allows us to systematically optimize process conditions. Therefore, the aim of the present research is to investigate the thermo-mechanical behaviour of granular materials. Specifically, we here introduce a sub-grain-scale mathematical model that allows us to quantify heat generated by plastic deformation and friction in a particle ensemble directly.

2. Simulation Results

Numerical simulation are very common in recent years due to the availability of computing power. In the field of powder simulations, the discrete element method (DEM) and the finite element method (FEM) are quite common approaches. In a DEM model, a contact force is computed as a function of the (theoretical) overlap between two particles. Despite this, the deformation of particles cannot be considered effectively in DEM as the existing contact laws do not reproduce all the physical phenomena involved in the densification of granular media. In contrast to DEM, FEM simulations consider the powder as a continuum. However, classically the individual particles are not considered, but the powder is assumed to have field properties which are distributed continuously, e.g., density, stress and strain.

In order to resolve the detailed mechanical response that counts for the individual grain deformation, we are using "foam-extend" (an extended version of OpenFOAM which uses the finite volume method). This will not only allow us to predict particle deformation, but also thermal stresses

and heat generation due to friction and plastic deformation.

As a stepping stone, the foremost step is to verify our numerical simulations against an analytical solution. It is necessary for us to understand and predict the precision of our simulation. For this, we performed some simulations in "Foam-Extend-4.0" of two particles in contact as represented by two contacting spheres (shown in Fig. 1)

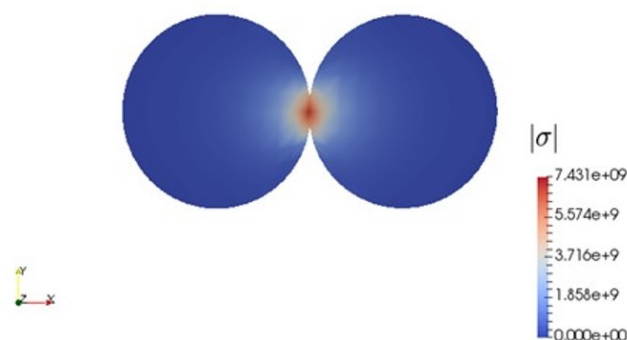


Fig 1: Stress distribution of two particles in contact

We compare our simulation results for the normal stress σ_{xx} with the Hertz solution as highlighted in the Fig. 2. The evaluation is made through the axial direction of the motion of particles in contact (i.e. along the x-direction in this case). It is clearly evident that the stress data from the simulation closely matches at the contact free region of the sphere and so does it in the region of contact. Note that the edge of the sphere that is free from contact is located at the 'x*=0' position in Fig. 2.

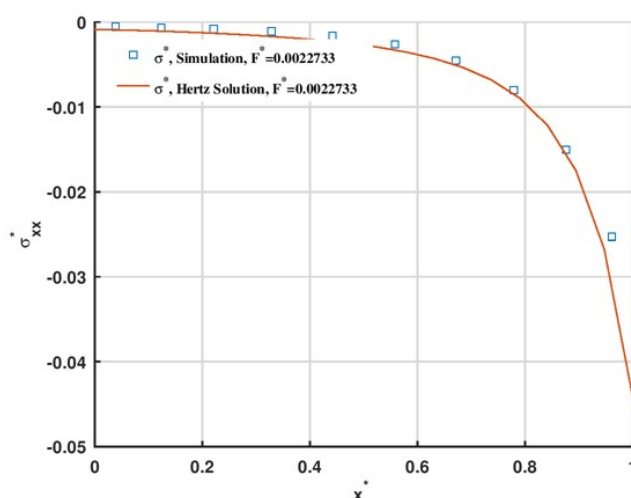


Fig 2: Stress plot along the axial direction

An experimental analysis of thermal effects on micromechanics of packed granular beds

by Marina Schnaider-Bortolotto (ESR6)

Materials and structures submitted to variations in temperature are a common issue for most engineers. These variations can be originated either from natural phenomena or human-made structures. From a geotechnics perspective, natural phenomena can range from mild weather changes to frost penetration in the ground. Human-made structures imposing variation in temperature can include nuclear waste repositories and also buried pipelines and power cables. Other practical applications of the understanding of thermal effects on materials are highway pavements and even slope stability.

Therefore, models to predict the behaviour of such materials under thermal loads are necessary and, consequently, experimental data are required in order to calibrate and validate these models. Most of the current studies (from both experimental and computational perspectives) focus on the finest portion of soils: clays. Therefore, there is still a lack of models and experimental data for coarser portions of soils in the literature, such as sands and gravels.

This project's research focuses on a geotechnical approach to the mentioned phenomena related to variations in temperature and, especially, on the understanding of the fundamental behaviour of granular materials subjected to thermal loads. Granular materials can be understood as the largest part of the particle size range of soils.

An important feature of porous materials is the hydraulic permeability, which can be understood as the characteristic of the material that determines the velocity at which a given fluid can flow through it. As a result, this property controls problems such as abstraction of water, losses of water under dams and spreading of contaminants in groundwater. For granular materials at ambient temperature, the hydraulic conductivity is directly related to their density and, consequently, their pores. Therefore, if the internal arrangement of particles is changed, the hydraulic permeability will be affected. A rise in temperature causes expansion of individual granular particles, which leads to a rearrangement of particles and potentially to changes in hydraulic conductivity. Moreover, temperature changes affect the viscosity of the fluid, which also has an impact on the hydraulic conductivity.

Given the importance of this property of granular media, hydraulic conductivity tests are being carried out in a bespoke apparatus that can mimic conditions of pressure that a soil element would be subjected to in field conditions. Also, the apparatus was specially developed to apply thermal loads from 5°C to 85°C. The effect of temperature on the hydraulic conductivity of a natural sand has been investigated. Beyond the determination of this property, it is hoped that measured changes in hydraulic conductivity will be an indirect way of assessing how thermal loads affect the internal arrangement of particles. This indirect measurement is particularly interesting because measuring deformations in porous media is challenging when working with temperatures higher than room temperature.

Currently, only the behaviour of samples as a whole has been characterised – instead of the ideal combination of bulk and micro responses. With the future addition of a second granular material (glass beads), it is expected to achieve a better understanding of the micromechanical behaviour of the tested samples, as glass beads can provide more input about the distribution of contacts among particles due to their homogeneity. Such outcomes are expected to be presented at international conferences to gather feedback from researchers in soil mechanics, energy geotechnics and granular media.

Theoretical analysis on thermal stresses of regular packings by Tokio Morimoto (ESR7)

Thermal stresses, which are stresses induced due to heating of materials, can be significant even if the change in the temperature of the material is small. In a one-dimensional case, a thermal stress can be calculated using Young's modulus (E), linear thermal expansion coefficient (α), and the change in temperature (ΔT);

$$\sigma_{thermal} = E\alpha\Delta T \quad (1)$$

Take an example of steel, a change in the temperature of 10 [K] leads to a thermal stress of 200 MPa. Transport networks have suffered bent rails due to a thermal stress caused by a seasonal temperature change. However, there has been little discussion on thermal-induced stresses in granular materials. This short article presents results of a theoretical analysis on thermal stresses of regularly packed spheres.

There are several tricky points when considering thermally-induced stresses in granular materials. One of them is that granular materials consist of a number of solid particles. The properties of granular materials can change if the arrangement of the particles changes even if material properties of solid particles do not change. In this article, two regular packings, simple cubic packing (SC) and face centered cubic packing (FCC) (**Fig. 1**) are considered to reflect this aspect.

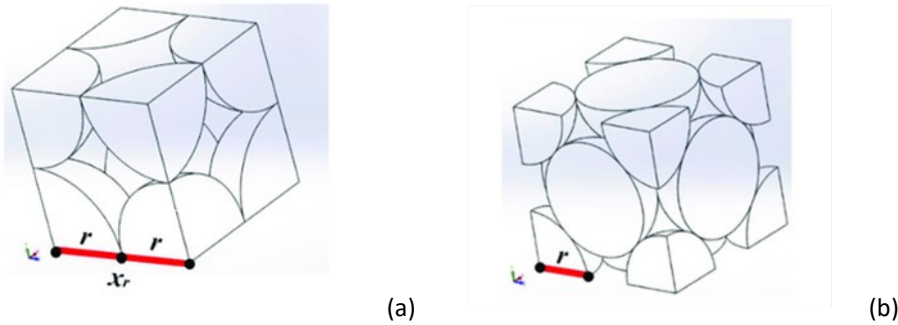


Fig 1: Schematic illustrations of (a) SC and (b) FCC packings

In addition, the effective stiffness at the contact between two particles is not constant but increases with an increase in the contact area according to Hertz's theory (Hertz, 1882). If two spheres with the same material properties (radius R , shear modulus G , Poisson ratio ν) are in contact, the simplified Hertzian contact model (Itasca, 2007) calculates the contact force at the contact point;

$$F_n = \left(\frac{2G\sqrt{2R}}{3(1-\nu)} \right) \delta_n^{\frac{3}{2}} \quad (2)$$

$$\text{where } \delta_n = 2R - d \quad (3)$$

where d is the distance between the two particles. Employing simplified Hertzian contact model, an isotropic stress of SC and FCC packings (P_{SC} and P_{FCC} , respectively) can be calculated from the material properties of the particles and the overlaps between the particles taking advantage of the symmetry of these packings;

$$P_{SC} = \frac{\sqrt{2}}{6} \frac{G}{1-\nu} \left(\frac{\delta_n}{R} \right)^{\frac{3}{2}} \quad (4)$$

$$P_{FCC} = \frac{2}{3} \frac{G}{1-\nu} \left(\frac{\delta_n}{R} \right)^{\frac{3}{2}} \quad (5)$$

Now supposing that the temperature of the particles increased by ΔT and the particles expand, the radius of the particles ($R^{\Delta T}$) and overlaps ($\delta_n^{\Delta T}$) between the particles increase according to the linear thermal expansion coefficient of the particles (α) as following;

$$R^{\Delta T} = R(1 + \alpha\Delta T) \quad (6)$$

$$\delta_n^{\Delta T} = \delta_n + 2R\alpha\Delta T \quad (7)$$

Supposing that both SC and FCC packing has an initial isotropic stress P_{ini} before the temperature change, thermal stresses of SC and FCC packings ($p_{SC}^{\Delta T}$ and $p_{FCC}^{\Delta T}$, respectively) read;

$$p_{SC}^{\Delta T} = \frac{\sqrt{2}}{6} \frac{G}{1-\nu} \left(\frac{\left(3\sqrt{2} \frac{1-\nu}{G} p_{ini} \right)^{\frac{2}{3}} + 2\alpha\Delta T}{1 + \alpha\Delta T} \right)^{\frac{3}{2}} \quad (8)$$

$$p_{FCC}^{\Delta T} = \frac{2}{3} \frac{G}{1-\nu} \left(\frac{\left(\frac{3}{2} \frac{1-\nu}{G} p_{ini} \right)^{\frac{2}{3}} + 2\alpha\Delta T}{(1 + \alpha\Delta T)} \right)^{\frac{3}{2}} \quad (9)$$

These equations are independent from R and δ_n .

If the material properties of the particles are known, equations (8) and (9) are functions of P_0 and ΔT . Supposing that the particles are made from glass, the following plots (**Fig. 2** and **Fig. 3**) can be created for a value p_0 of 100 kPa. **Fig. 2**

and **Fig. 3** show the values of $p_{SC}^{\Delta T}$ and $p_{FCC}^{\Delta T}$ and the ratio of $p_{FCC}^{\Delta T}$ to $p_{SC}^{\Delta T}$ for a wide range of ΔT , respectively. It is obvious that the FCC packing experiences a larger temperature-induced stress than the SC packing. According to

Fig. 3, the difference between $p_{SC}^{\Delta T}$ and $p_{FCC}^{\Delta T}$ is larger for a larger ΔT . In **Fig. 2**, if $\Delta T = 50K$, the stress after heating reaches 500 kPa for the SC packing and 1000 kPa for the FCC packing, which are significant stresses considering that the initial isotropic stress is 100 kPa. In engineering practice denser soils are associated with higher strengths and stiffnesses, interestingly, this result indicates that a denser packing may suffer from a larger thermal-induced stress. In the SC packing and the FCC packing, the solid particles occupy 52 % and 74 % of the total spaces, respectively.

In conclusion, this article presented the theoretical analysis on thermal-induced stress of SC and FCC packings using the simplified Hertzian contact model. Equations calculating the thermal-induced stress for SC and FCC packings as functions of the material properties, the initial isotropic stress, and the change in the temperature have been derived. The analysis showed that the FCC packing suffers from a higher thermal-induced stress than the SC packing. In future, analyses considering temperature-induced stresses in random packings will be carried out using the discrete element method.

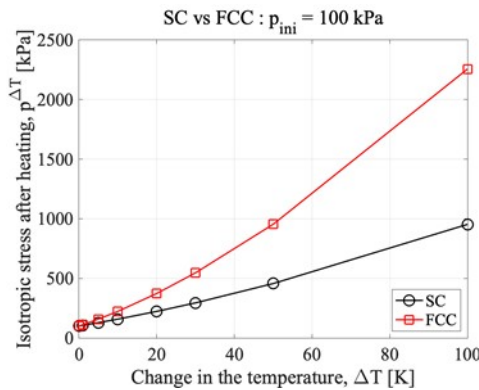


Fig 2: $p_{SC}^{\Delta T}$ and $p_{FCC}^{\Delta T}$ over various values of ΔT

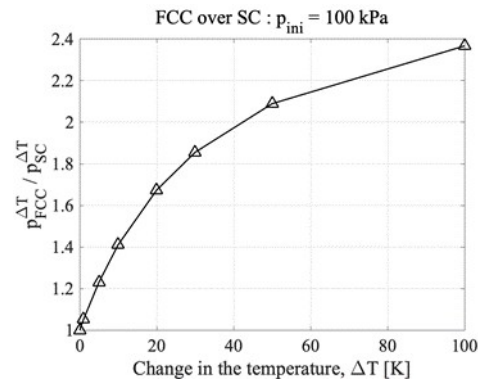


Fig 3: $p_{SC}^{\Delta T} / p_{FCC}^{\Delta T}$ over various values of ΔT

Reference

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- 2) Itasca Consulting Group, (2007). PFC3D version 4.0 user manual, Minneapolis, MN, USA.
- 3) De Moraes, D. A., & Czekanski, A. (2018). Parametric thermal FE analysis on the laser power input and powder effective thermal conductivity during selective laser melting of SS304L. Journal of Manufacturing and Materials Processing, 2(3), 47.

Heat transfer in Selective Laser Sintering (Additive manufacturing)

by Balaji Soundararajan (ESR11)

Selective Laser Sintering (SLS) is an Additive Manufacturing (AM) technique (also called as 3D printing) which uses Laser as a heat source to selectively sinter a powder bed layer by layer in order to build a 3D component. Figure 1 shows the working principle of SLS process. Firstly, the Computer Aided Design (CAD) file of the part to be printed is converted into Stereolithography format (STL) and is fed into the Laser scanning mechanism of the SLS machine. A powder spreading mechanism prepares the powder bed by spreading the powder into the build platform. Each layer is typically in micrometer range and the laser scans through the layer thereby sintering/melting the particles and fusing them. Once the layer is sintered or melted as per the part dimensions, the powder spreading mechanism prepares the powder bed for the next layer to be fused, thereby building the whole component. It is one of the latest manufacturing techniques which has a lot of advantages like design freedom, reduced wastage and ability to build complex and light weight parts which is not possible through conventional manufacturing methods. Because of these reasons, AM parts are ideal for low volume, high value manufacturing such as aerospace, automotive and medical applications. Despite continuous technological advancements in the field of AM, the lack of process repeatability and stability represents a barrier for the industrial breakthrough. SLS process is a complex phenomena which involves Laser heat absorption, high thermal gradients in powder bed, local melting and solidification of particles and phase change which are not fully understood. Because of these reasons, AM parts have quality issues such as volume shrinkage, delamination of layers, crack propagation, improper solidification and voids formation.

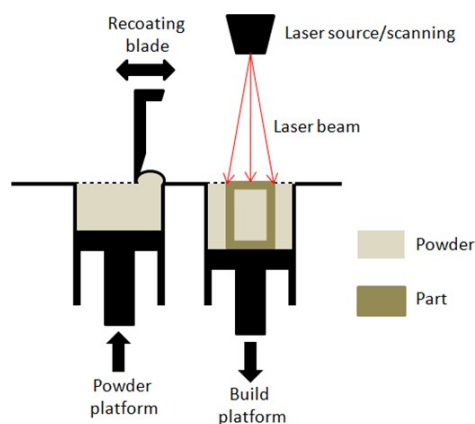


Fig 1: Working principle of Laser based Powder Bed Fusion process (SLS)

Therefore, the main objective of my research is to optimize the input process parameters such as Laser power and speed, scan strategy, powder bed thickness, and particle size distribution in order to get the ideal output. At the end of the project we expect to have a clearer picture of the relative weight of the different phenomena playing a role in the laser heating process. An attempt will be made to define simplified expression of the main heat generation and heat conduction terms appearing in the process as well as of the size of the volume interested by the effective laser sintering process, both in terms of the affected depth and the widths of the sintered material after a single laser pass. To achieve this, an experimental set-up with an infrared camera will be built to visualize the heat flow during the heating process. The thermal camera will be positioned on top to visualize the layer surface temperature and melt pool and also positioned below the powder bed and viewed through glasses transparent to infrared radiation to visualize the thermal profile inside the powder bed. A numerical heat transfer model will also be developed which in turn will be compared with experimental results and calibrated.

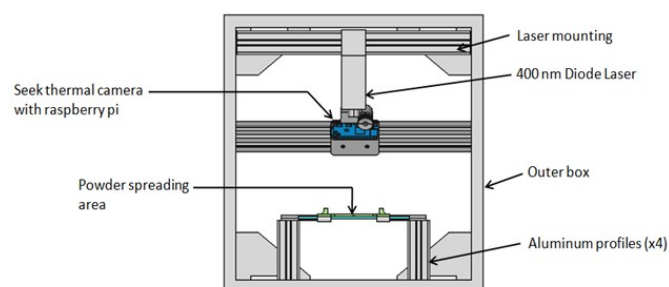


Fig 2: CAD model (top) and actual build of the experimental set-up (bottom)

Francisco Kisuka - ESR1



I am a Tanzanian male currently at the University of Surrey as ESR 1 working on a MATHEGRAM project entitled 'DEM modelling of heat generation induced by friction at low stresses'. Before becoming a MATHEGRAM fellow, I was at the University of Grenoble Alpes doing a master's degree in Geomechanics, Civil engineering and Risks. A year now, since I became a MATHEGRAM fellow, it has been nothing short of good experience from working with supportive supervisors, office colleagues, fellow ESRs. Moreover, the best part has been the birth of my beautiful twin babies (Heri and Zuri) who seem to be very much a part of this journey. Coincidentally, I found out that I was going to be a MATHEGRAM fellow and a father. The separate events relayed the same feeling, excitement and nervousness. Though far from me, my babies have been my powerhouse, especially during the sudden change of work environment due to Covid-19 lockdowns. During that period, I have explored in depth the literature related to my project, ran simulations remotely with the success of generating interesting results and with a degree of confidence I feel happy as I am writing my confirmation report. "I connect best with my babies through this work", I would tell myself that on every seemingly tricky morning amidst these challenging times.

Domenica Braille - ESR4



I am a Marie Curie fellow on the framework of MATHEGRAM programme. I graduated from the University of Calabria in Italy with a bachelor's in chemical engineering in 2016 and, subsequently, went on to get my master's degree from the same university in December 2019.

Towards the end of my master studies, I got a chance to participate in the Erasmus+ Exchange project where I spent eight months in another tertiary educational institution in the European Union to complete my master research project. During that period, I had the opportunity to work at the University of Leeds in the United Kingdom, on a project about the triboelectric charging of particulate solids.

The time I spent working on my master research project ignited in me a passion to carry out research and that is when I decided that I want to embark on a research career. Therefore, I decided to apply for the Early Stage Researcher position with MATHEGRAM at the University of Surrey.

In December 2019, I began with my MATHEGRAM research project under the supervision of Prof. Charley Wu and Dr. Colin Hare. In this framework, I am now working on developing and validating a model of swelling of grains due to water absorption, which can be implemented into a DEM code.

In the second stage of my research project, I will spend six months in France, where I am expecting to complete my secondment, under the supervision of Dr. Marco Ramaioli at the Institute National de la Recherche Agronomique (INRA), where I will carry out some experiments to investigate the effect of environmental conditions and material properties on sintering of food.

During the course of the PhD, so far, I have learnt that the journey of research is not always smooth sailing and it's very challenging to obtain meaningful results. However, I am enjoying the challenge and feeling a sense of accomplishment in contributing to science.

Aman Rastogi - ESR3



I am a MATHEGRAM ESR working at Johnson Matthey, Billingham, one of the largest chemicals company in the UK. My research focus as part of MATHEGRAM is on heat generation and transfer in reactive granular materials. I use computational tools such as the discrete element method and computational fluid dynamics to investigate multi-phase systems in high temperature processes.

I was born in India and completed my bachelor's in Chemical Engineering from BITS Pilani, Rajasthan. Before joining Johnson Matthey, I was a research assistant at Rutgers Catalyst Manufacturing Consortium where I was part of the Catalyst impregnation focus group. I have also served as a part-time lecturer in physics at Rutgers University, New Jersey, USA where I finished my master's in Chemical and Biochemical Engineering. My research thesis was aimed at investigating the dry catalyst impregnation process and optimizing the vessel geometry for the process.

In my free time, I like to play badminton, hike and sketch. I can be reached at aman.rastogi@matthey.com and invites connections at <https://uk.linkedin.com/in/amanr7>.

Alexandre Bobillier - ESR12



I was born in France and grew up in Lyon where I graduated from the Institut National des Sciences Appliquées de Lyon (INSA Lyon) with a major in Materials Science and Materials Engineering in 2018. During my first year of Master, I conducted a research project on thin glass plates in order to avoid catastrophic failure in X-ray detectors by doing micro-mechanical tests of glass plates coated with semiconductors from various suppliers. This project has kindled my interest in research. Therefore, I completed my end of study project at Airbus Central Research & Technology in the Aerodynamic Efficient Surface Technologies' team led by Dr. Elmar Bonaccorso, in Munich. I mainly worked on anti-contamination coatings on laminar flow controlled surfaces. Thrilled by my experience at Airbus Central Research & Technology, I had the opportunity to join the team as an Early Stage Researcher within the MATHEGRAM ITN, supervised by Dr. Elmar Bonaccorso (Airbus Central R&T) and Prof. Charley Wu (University of Surrey) to work on "Ultra-thin powder coatings at temperature suitable for aerospace applications".

Powder coatings are a promising alternative to traditional liquid coatings in the aerospace industry. For instance, powder coating processes have a significantly smaller environmental impact as no solvent is involved and there is considerably less waste as the overspray can be recycled. However, in order to fulfil the very selective requirements for the aerospace industry, it is mandatory to improve these processes by reducing the curing temperature of the coatings while keeping small thicknesses. My work at Airbus Central R&T consists of understanding the thermomechanical behaviour of polymeric particles by combining the fundamental understanding of physics of film formation with small particles ($<30 \mu\text{m}$) and numerical investigations with the finite element method.

To conduct my research, I have a lab-scale powder coating cabin available as well as an ensemble of testing devices to analyse the coatings I am able to produce. Also, I can count on a partnership with a powder manufacturer to work with the most advanced powders for coating applications. Finally, I benefit from a cooperation with my fellow ESRs from the University of Surrey through a bi-monthly meeting supervised by Prof. Charley Wu and Dr. Colin Hare to develop the finite element model.



Arnesh Palanisamy - ESR8

I am a PhD student at AgroParisTech since April 2019. I graduated with masters in chemical engineering at Indian Institute of Technology Madras in 2016. Later, I joined Dr Reddy's laboratories working as a process engineer in the modelling and simulation group responsible for scale-up and robust process development of complex pharmaceutical compounds. My current research topic is thermal effects on starch granule suspension (which means I investigate how to optimally cook your food, fancy!).

Starch is a carbohydrate and main source of energy for millions of people all over the globe. Yes, It is all starch whether you eat rice like me (I am a south Indian) or baguettes like the French or any other tasty combinations of the grains such as corn, millets, etc. People who have visited the kitchen floor and tried their luck in learning to feed themselves (If you are the other kind like me a couple of years ago, This is the sole mantra you need to feed yourselves on a deserted island), know that starch when heated in presence of water swell. This process is called gelatinization. During this process, the viscosity (the effort or force required to move your spoon through your delicious starch and water) increases. Most starches after swelling burst and ooze out a liquid called amylose. However, I don't like things which burst (remembering childhood balloon bursts :(). So, I chose a kind maize starch which in the first place contain very little of this "Amylose" (less than 1%) and also is chemically-modified by our magician wizards (read scientists) to ensure it does not burst. Great, but do we use these kinds of chemically-modified maize starch in food ever? Yes, Of course, it is used in making some industrially produced ice-cream.

In an industrial setting (call it the ice-cream factory), this starch cooking is carried out in quantities of tonnes per day. This cooking is carried out in a so-called tubular reactor (nothing but a pipe with water + starch flowing inside this pipe and heat applied on the surface). During this process, it is difficult to predict what is happening inside this tube (For example -At what length of the pipe the starch is completely cooked). Nobody likes burnt starch (*screams inside in Gordon Ramsay's voice). Hence, My project entails predicting this phenomenon in a tubular reactor (pipe) accurately using CFD (i.e. using computers to tell you how water flows in your tap) coupled with DEM (using computers to tell how grains, sands and powders flow) so that you don't end up with a burnt dessert and spend less money on your next dessert.

Outreach and publications:

I attended FOODSIM2020 conference online held in KU leuven university, Ghent, Belgium on 07-09-2020. I presented a talk and submitted an extended paper titled –

"Transient DEM Simulation of starch granule suspension undergoing thermal treatment". It was an interesting conference with a lot of presentations on the control systems in food processing industries. It also gave a lot of exposure to various challenging unit operations and processing equipment design in the same arena.

I also published an article titled "Kinetic modelling of individual starch granules swelling" in the Food-Structure Journal. <https://doi.org/10.1016/j.foostr.2020.100150>.



Aatreya Manjulagiri Venkatesh - ESR14

Growing up in India, imbibing the eternal ideologies of Sanatana Dharma, which propounds that, there is smaller than the smallest and larger than the largest, and that Infinity is reflected in the tiniest of finite things while the finite-ness is also a part of infinity..., it feels fascinating now to be of service, however minute, in trying to unlock the secrets of matter - deep down at the nano-meter scale!

I am Aatreya Manjulagiri VENKATESH. By educational qualification, I am a mechanical engineer, with a strong affinity towards materials science.

Banking on my inclination towards applied science and a decent academic record, I got into one of the premier engineering institutions in my state in India, and chose to go and get a Bachelor's degree in Mechanical Engineering.

During my graduation, my interests became specific and focused, which inspired me to fly out of India and pursue a Master's degree in Computational Mechanics from the University of Stuttgart, Germany.

Also, after bachelor's, I was fortunate enough to get recruited by Larsen & Toubro, the bellwether of India's Engineering and Construction sector, who though, made me fly and work miles away from home, but nevertheless, I managed to get some hands-on experience and a taste of the real world.

Subsequently, after master's, I worked for some time at the corporate research division of Robert Bosch, Stuttgart, Germany, before I managed to now secure the Marie Curie research fellowship, to be part of the MATHEGRAM innovative training network.

And... So, in this context, I flew out again and I am now based in Grenoble, France, working for the French National Centre for Scientific Research, CNRS.

During the course of my PhD research here, I am expecting to take advantage of the outstanding features of the upgraded synchrotron, ESRF, in Grenoble, to find out more about a powder processing technique called sintering. The plan is to bombard some powerful X-rays onto some of my ceramic powders, and get to know what really happens deep inside them during sintering - at the nanometer scale, while being in-situ as well, i.e. throughout the entire process, in real time!

On the non-professional front, I have been trying to explore the roots of Yoga as a way of life for some years now.

Plus, I like to travel and explore. I travelled so extensively during my master's that I had planned on reducing it by some extent during the PhD, but looks like Covid-19 has had better (worse) plans for me!



Jelena Macak - ESR5

I studied aeronautical engineering at Faculty of Mechanical Engineering and Naval Architecture in Zagreb, Croatia, and obtained a master's degree in 2018. Since 2019 I am based in Vienna, Austria, working as a research assistant at DCS Computing. I attend Doctoral School of Chemical and Process Engineering at Technical University Graz. My primary research interest is numerical modeling of heat transfer phenomena in particle-fluid systems, in particular, on the use of granular layers to regulate heat transfer and fluid flow.



Sina Zinatlou Ajabshir - ESR9

I am Sina, an Iranian guy, who is working on this amazing project and I am proud of myself for being a little member of the MATHEGRAM big family as ESR9 studying on the Effect of temperature on the powder flow properties and their dispersion in SLS processes.

I have a master degree in materials science and engineering, and before joining this incredible MATHEGRAM family, I was a researcher at Sharif University of Technology, investigating on additive manufacturing and welding. Over the last year since I joined the group, I have been experiencing excellent time in Italy with my supportive and kind supervisors as a part of our welcoming team, although we have been through some challenging days due to COVID-19 which drastically affected our work.

I hope everything goes well again and we could come back to our laboratories where I consider as my second home. However, lockdown and isolation impacted my routine life and project, but I have been preparing a review paper, a little bit getting experience in simulation, and joined some online courses such as “Italian language and powder technology” which both were super useful especially for improving my Italian language skill.



Brayan Marcelo Paredes - ESR15

I am a MATHEGRAM Early Stage Researcher at SIMAP, CNRS|Université Grenoble Alpes. I specialize in mathematical modeling and computational simulation of processes involving mass and heat transfer. I enjoy contributing to solve real problems using maths. I graduated from Federal University of Santa Catarina in Brazil with a Bachelor's Degree on Chemical Engineering. At the same institution, I obtained a Master's Degree studying some neurophysiological processes using a chemical approach and numerical methods. In parallel, I worked in a software company solving industrial problems using CAE (Computer-aided engineering) and teaching numerical methods. It has been a nomad journey, growing up in Ecuador, living in Brazil, Colombia, Mexico and now France.

During my PhD project I am developing a DEM model of constrained powder sintering, which appears in industrial process but its mechanisms are not yet fully understood. Two main avenues of development will be adopted: the implementation of a realistic model for grain growth and, as we do not deal with spherical cows in a vacuum, the introduction of non-spherical particles using the level-set method. In addition, this project will integrate the microstructures obtained using nanotomography (from another MATHEGRAM ESR) into DEM simulations.

At this point of the research, we are finalizing the grain growth model with satisfactory comparison to experimental data. A paper is being written and it will be ready by the end of this year. At the same time, we just started the second part of the PhD, that is, the implementation of real particle shapes in our sintering model.

Finally let's welcome new fellow Rafael Rangel who joined MATHEGRAM consortium in August after sudden exit of Massimiliano Zecchetto. He has quickly adapted himself into MATHEGRAM family. Please read his short biography below.



Rafael López Rangel - ESR13

I was born in 1992 in Rio de Janeiro, Brazil, and has both the Brazilian and the Spanish nationalities. I obtained his Bachelor's degree in Civil Engineering from the Pontifical Catholic University of Rio de Janeiro (PUC-Rio) in 2016. During my senior year studies, I became an enthusiastic of computational mechanics and decided to start my postgraduate studies in the department of Civil / Structural Engineering at the same institution. I completed my Master's degree in 2019 by carrying out a research on nonlinear analysis of frame structures while working as a member of the Tecgraf Institute of Technical-Scientific Software Development of PUC-Rio. During that period, I also attended several congress and conferences to present my work, and served as teaching assistant in some undergraduate level courses, which made me very interested in educational activities for engineering. I currently lives in Barcelona, Spain, where I started my Ph.D. in Civil Engineering at the Polytechnic University of Catalonia, in the second semester of 2020. I conducts my research at the International Center for Numerical Methods in Engineering (CIMNE), working in the framework of the MATHEGRAM project, in which my focus is on performing a numerical study on the use of granular layers to regulate heat transfer and fluid flow.

For more information please contact

Dr Ling Zhang
MATHEGRAM Project Manager
Department of Chemical and Process Engineering
Faculty of Engineering and Physical Sciences
University of Surrey
Guildford, GU2 7XH, UK
Email: ling.zhang@surrey.ac.uk
Tel: 0044(0)1483 68 3003
http: www.MATHEGRAM.eu

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This issue was edited by Dr. Ling Zhang with contributions from following 14 ESRs:

- Francisco Kisuka
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