MATHEGRAM Newsletter

Issue No. 4 March 2022

After the Interim report period MATHEGRAM has entered the last phase of the project. Over the last two years Covid pandemic caused enormous difficulties to both research and management aspects of MAHEGRAM project. Nevertheless, I am glad to learn from the third-year progress reports submitted by all the ESRs that exciting research results have been produced and some ESRs have managed to carry out their secondments at host institutes physically. All of them have found the secondment is a valuable experience and enjoyed the challenges and new opportunities created when performing research in a different lab and a different country. As Domenica comments: “I truly believe that spending some time in a foreign country is life changing because the exposure to a different culture and the experience you get will always be a part of you. “ (see Page 4 for more information). These secondment also enables our ESRs to ultilise the start-of-art research facilities in other labs to advance our scientific understanding of granular materials. For example, our ESR, Aatreya, has been using the 4th generation nano X-Ray tomography at ESRF to explore the sintering of granular materials at high temperatures in-situ (see Page 5). I hope you will enjoy reading the articles on ESRs‘ secondment experience and research progress in this Newsletter. I am also very pleased to see more and more research results being published in scientific journals and conference proceedings.

In the past few months, we successfully organized the Second Training School (TS2) on “Regulation, Legislation, Innovation & Collaboration” and the Third MATHEGRAM Training School (TS3) on “Entrepreneurship, career and research skills” virtually. TS2 and TS3 are both reported in this issue by the ESRs from the host institutes. Both training events were well received by ESRs, as ESrs comment, for example, “The best part about this training school that I learned well was preparing resumes. ” and “As the ESRs are approaching the end of their research, the sessions provided necessary guidelines on future career related possibilities and prospects”.

Our next network event will be the Special Interest Symposium on thermomechanical behaviour of granular materials that will be run in conjunction with the upcoming CHOPS 2022 conference in Salerno this summer. I hope this event will be a great opportunity to showcase MATHEGRAM consortium to a wider international audience. Watch this space!

Prof. Charley Wu
MATHEGRAM coordinator

Inside this issue

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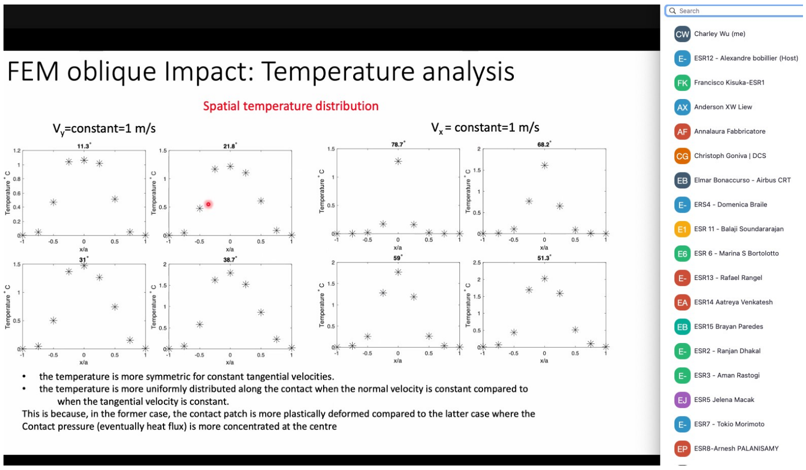
The Second MATHEGRAM Training School (TS2)

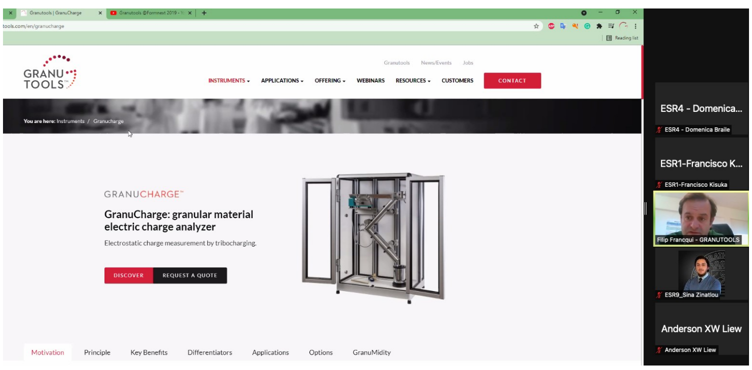
by Alexandre Bobillier (ESR12, Airbus)

The MATHEGRAM Training School 2 (TS2) on “Regulation, Legislation, Innovation and Collaboration” was virtually held in the second week of October 2021 . This new way of learning, adopted to cope with Covid-19 pandemic, is now the norm for the collaborative work in the MATHEGRAM network. The event organised by Airbus Central R&T was successful.

TS2 covered a wide range of exciting topics, including a collaboration and innovation lecture. This lecture given by Jamie Cleaver provided information about the conditions to collaborate in a group and the ways of working in order to create a sound collaborative environment. In fact, this lecture was very useful since it highlighted what our team was doing well to develop an innovative and collaborative working environment. Indeed, the MATHEGRAM consortium is made of 14 ESRs and their advisors, making a team composed of different personalities with various interests working towards one goal: understanding and modelling the thermomechanical properties of granular materials.



The second day of TS2 was focusing on regulations and legislations in two different industries: the pharmaceutical and fine chemical industry, and the aerospace industry. Dr. Bart Nitert provided insights and details about the very specific requirements of the regulations and legislations in the pharmaceutical and fine chemical industries. Dr. Jürgen Wehr has given a workshop about the REACH regulations, the perspectives and the compliances with a special eye on the aerospace industry.



On the last day of the TS2, a very unusual workshop was given by Pablo M. Navarro Bullock on “How to Think Wrong?”. During this workshop, the ESRs could learn about one methodology that is used to enhance the innovation capability of a person, a team of researchers, or on a larger scale a company. To conclude the TS2, Filip Francqui held a discussion with the ESRs showcasing his example on how to go from a research idea to a business.

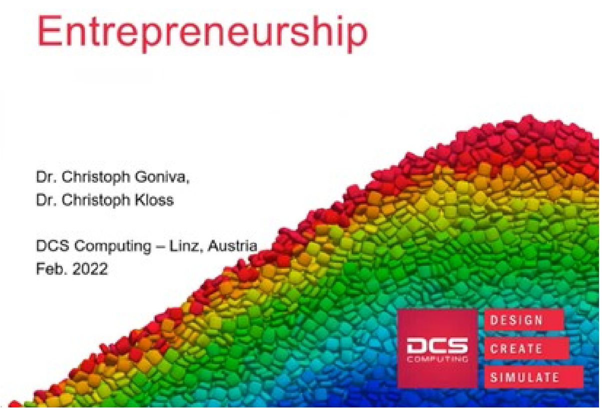
Overall, the second MATHEGRAM virtual training was a success. Just as it was the case at the end of the TS1, the ESRs would still prefer the training schools to be held in person. But being able to adapt our ways of working and collaborate within the MATHEGRAM consortium is an outstanding aspect that the ESRs and their advisors have shown during these challenging times.

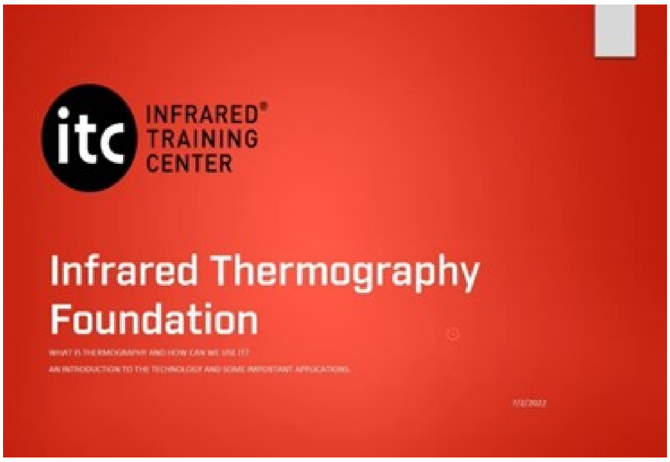
The Third MATHEGRAM Training School (TS3)

by Arnesh PALANISAMY (ESR8, INRAe)

MATHEGRAM Training School 3 (TS3) on "Entrepreneurship, Career and Research Skills" was held from 04-Feb-2022 to 10-Feb-2022 virtually. TS3 covered a wide range of topics containing both technical presentations and soft skill trainings. This was the first event organised by MATHEGRAM that incorporated the attendees' needs. Indeed, a poll was conducted a priori among ESRs to know about what skills or training session they would like to have and was used to design the programme.

The first day started with an interesting lecture on dimensional analysis given by Dr. Guillaume Delaplace, in which he provided a systematic procedure to follow and the session was very well designed with case studies from industrial food processing. Later in the afternoon Dr. Christoph Goniva shared with us his journey on entrepreneurship. This gave an overview of different dimensions one has to think about as an entrepreneur.

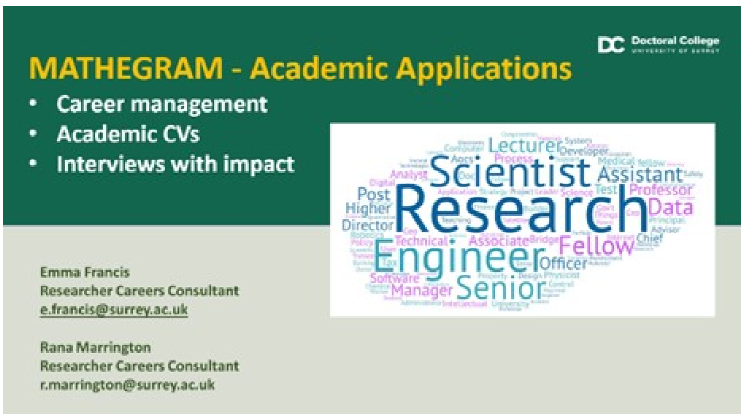




Sylvain Telmi introduced the audience to the basics of thermography and showcased some applications using case studies. This had immediate impacts in the projects of some of the ESRs. Véronique Köstlin, from Airbus, presented behind the scene process that is carried out by human resources personnel during candidate selection in the private sector.

Oliver Pitois presented his interesting and novel research on physics of foams and stabilising role of particles.

TS3 ended with a session from the Doctoral College of the University of Surrey about how to prepare and apply for academic positions in United Kingdom. This workshop was, indeed, interesting for all the attendees, as it provided a complementary view of academia compared to private research.



Secondment experience

My secondment experience at INRAe

by Domenica Braile (ESR4, UoS)

Despite the challenging times, I was lucky and glad to be offered the opportunity to carry out my secondment in person at the “Institut National de Recherche pour l’Agriculture, l’alimentation et l’Environnement” (INRAe) in Massy, France.

Hence, in mid-September, I joined the research group headed by Marco Ramaioli, who is also in charge of my secondment supervision. Their research activities range from analysing the swallowing using an artificial tongue to the analysis of the rheological behaviour and dynamics of multiple fluids, for pharmaceutical and food applications. Therefore, I had the opportunity to interact with research projects different from mine and learn from researchers coming from different backgrounds. Indeed, carrying out part of research in another institution offers several opportunities in terms of expanding knowledge in our own and other fields, learning new skills and mostly “networking”. During this experience, I also had the chance to carry out outreach activities in the hosting institution, i.e. I was offered the opportunity to present my research at the “Journée du Doctorat 2021”, which stands for “PhD student’s day”, during which I engaged with a large scientific audience.

Prior to reaching INRA, my research project at the University of Surrey has been mainly modelling because of the Covid-19 disruption, while my research activities during my secondment were predominantly experimental investigation in the lab. The research objectives included the analysis of sintering dynamics of two chocolate spheres as affected by heat transfer and sphere dimensions. We faced many challenges to design the right experimental set-up and such circumstances made me capture the way of problem solving as taught by all my supervisors. Surely, in these months my experimental skills improved considerably.

I truly believe that spending some time in a foreign country is life changing because the exposure to a different culture and the experience you get will always be a part of you. On the other hand, ever since I was little, I wanted to visit Paris and luckily enough this city is about half an hour by train from the town where I lived during my secondment, hence, I had the opportunity to spend almost all my weekends in this beautiful European city. Needless to say, it did not take long to fall in love with Paris and the French culture and in the blink of an eye, I wish to have had more time to explore and get more from this country.

Sadly, time has flown by and my secondment in this research institution is almost over. I’m thankful to MATHEGRAM and all the people I’ve met in INRAe for such amazing experience. I’ve gained a lot in these months and will keep with me all the things they have taught me, and all the beautiful moments spent together.

To the times at the ESRF!

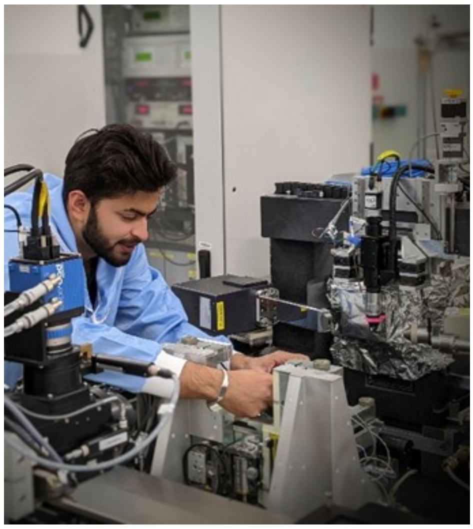
by Aatreya Manjulagiri VENKATESH (ESR14, CNRS – SIMaP)

One of the highlights of my research project has been the opportunity to carry out a secondment at the European Synchrotron Research Facility, ESRF.

Fortunately for me, the fact that the ESRF is situated in Grenoble, which happens to be my workplace (at SIMaP/CNRS) as well, made my secondment really flexible. So I could plan my experiments way ahead and do my secondment in turns rather than having to complete it in one go. Also, thanks to my supervisors at the synchrotron, I even got myself a Visiting Researcher's tag, which has given me 24*7 access to the ESRF for the past 2 years.

The thought that the ESRF hosts the world's brightest X-ray source is in itself exciting enough; however, the opportunity to access the ESRF facility so often and perform experiments at the nano-beamline is something else altogether!

The purpose of my secondment in fact was to explore the recently upgraded facilities at this 4th gen synchrotron and perform nano-tomography experiments in-situ to track ceramic sintering at the particle scale, which obviously has never been done before, owing to the complexities of the ceramic particles, as well as the super high resolution required, in addition to several other constraints.



In this regard, as a standard procedure, we submitted a scientific proposal to the ESRF explaining what we would like to do and we in turn got ourselves a 24h hour beamtime to perform our experiments in late 2020. Needless to say, we failed in our very first attempt. We in fact even broke one of the furnaces while we were working with it. We then went back to SIMaP, tried to inspect where we went wrong and came back to the ESRF for our next available beamtime several months later in 2021. 48 hours non-stop this time - We failed yet again and had to be content with a few ex-situ analyses, which, although novel were not what we desired. There was no other way than to build the furnace on our own. We re-submitted one more proposal and devoted the next 6 months to come up with a compact furnace which could go up to 1500 degrees; coupled with an efficient cooling system, so that the temperature just outside the furnace inside the synchrotron hutch would remain stable at less than 20 degrees. A lot of preliminary trials in the lab, 72 continuous hours of beamtime, and 2 sleepless nights later, as the saying goes, we got third time lucky - we managed to successfully perform nano-tomography at a brilliant resolution of 25nm, providing us with complete 3d in-situ images of ceramic sintering - at the nano-scale - for the first time!

The anxiety, the anticipation and the resolve were all worth it! We are now in the process of trying to decipher what we see in these images and further expand the scope of this research by performing some more in-situ experiments. Of course, this adventure would not have been possible without the guidance and support of my supervisors, engineers and technicians both here at SIMaP and at the ESRF.

And above all, a big shout out to *MATHEGRAM!*

Rotary Kiln Modelling: Challenges and Opportunities

by Aman Rastogi Arnesh Palanisamy (ESR3, JM)

Thermal processing is a necessary step in many granular materials manufacturing processes. Thermal treatment may be used to induce physical, chemical or phase transformation. The critical quality attributes for such processes depend strongly on the duration, intensity and uniformity of the heat received by the material.

The equipment for thermal processing can be chosen from a variety of furnaces available in all shapes and sizes, direct or indirect heating, batch or continuous operation, depending on the type of treatment desired and the material. Among them, rotary kilns are one of the most widely used equipment for thermal treatment of granular materials because of their versatile utility and simple operation. In a crude sense, a rotary kiln could be described as a long rotating cylinder inclined at an angle with a heated wall or internal heating through combustion of gases. It could include a gas flow along the length of the cylinder which can be against or along the direction of flow of solids. The solid flow can be in either transverse or axial direction. The rotating wall drives the transverse flow whereas the axial flow mainly derives from gravity.

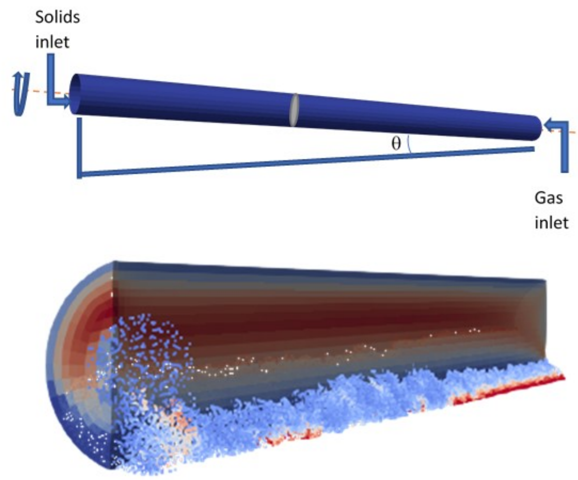


Figure 1. Rotary Kiln Schematic and corresponding unresolved CFD-DEM simulation

As any other process, rotary kilns suffer from a range of issues such as excessive entrainment, ring formation, poor uniformity. These problems can be disruptive to the continuous operation of the kiln and can even cause shutdown of the process, resulting in heavy losses. The process becomes more complicated when using powders. Powders are already a difficult material to deal with, having stress dependent behaviour, sensitivity to moisture, cohesion, wide particle size distribution. These mechanisms usually give rise to secondary phenomena such as agglomeration, breakage, entrainment and sintering, all of which can further be affected by high temperatures and may significantly affect the process output. Unfortunately, the mechanism by which these adverse phenomena occur are generally hardly understood, thus a more sophisticated model is needed that can help to predict and avoid their occurrence.

Modelling a process involving granular materials at high temperatures can be a very difficult task owing to the number of mechanisms to consider in a multiphase system as well as the variability in the operations and design of the equipment. The solid flow is usually not uniform and can be significantly affected by local conditions e.g. stress, temperature, moisture content. Heat transfer to the solid happens through conduction, convection and radiation. Adding to the complexity, the heat transfer, mass transfer and reaction mechanisms are highly interlinked and dependent on the mixing of the solids and gas flow. Inserts such as baffles, lifters and dams are also frequently used to control the solids flow.

Such a process cannot be modelled through simple analytical or empirical models, as they cannot capture the relevant physics which occurs at the granular level, or even risk misrepresenting reality due their oversimplified nature. Lately, DEM and CFD-DEM have been used widely to model multiphase systems. The ability to define complex models for particle-particle and particle-fluid interactions promises deeper insight into the mechanisms affecting the process. However, the computational cost scales exponentially with the number of particles and for systems with a very large number of discrete particles, coarse graining and calibration must be used to limit computational effort. It is therefore a challenge to reach the best possible compromise between feasibility and accuracy of the model.

A discrete element model of grain growth in sintering

by Brayan Paredes (ESR15, CNRS – SIMaP)

Sintering of a powder is a high temperature process (below the melting temperature) which aims to give strength to the compact, generally by decreasing its porosity. The fundamental driving force for sintering is the reduction of internal or interface surface energy. Diffusion processes will be activated by high temperatures. The reduction of energy will also give rise to a phenomenon called grain growth, which is simply the increase of the average grain size towards the end of sintering. Thus, it is observed that grain growth affects sintering kinetics.

Most grain growth models in the literature are empirical and define a mean grain size for the packing with its evolution with time given by a power law. On the other hand, some realistic models are described just for very small number of particles. The aim of this part of my PhD is to introduce a realistic grain growth model based on the interactions of individual particles. Also, the objective is to represent real packings (large number of particles), it will be reached by using a DEM approach.

In our approach it is necessary to ensure mass conservation at the particle level. The equation for the volume variation of a particle i in contact with a particle j writes:

$$\frac{dV_{i,j}}{dt} = 4\pi r_i^2 \frac{dr_i}{dt} = \sum_k J_k A_k = \sum_k -\frac{D_k}{k_b T} \nabla P_k A_k \Omega$$

where the volume exchanged for a given contact $dV_{i,j}$ is due to different mechanisms of grain growth k, each one represented by a flux of matter J_k crossing an area A_k. Grain boundary migration and surface diffusion are the considered mechanisms for a wide variety of ceramics and metals. Both mass fluxes can be represented by a generic form, where D_k is the diffusion coefficient of the mechanism, ∇P_k the local pressure gradient that causes mass transfer, k_b the Boltzmann constant, T the temperature and Ω is the atomic volume of the sintering species. Each mechanism has its necessary configurational conditions in order to be activated. Figure 1 shows these conditions and the possible scenarios for each pair of particles in contact, a_s is the current contact size and a_{eq} is the equilibrium contact size.

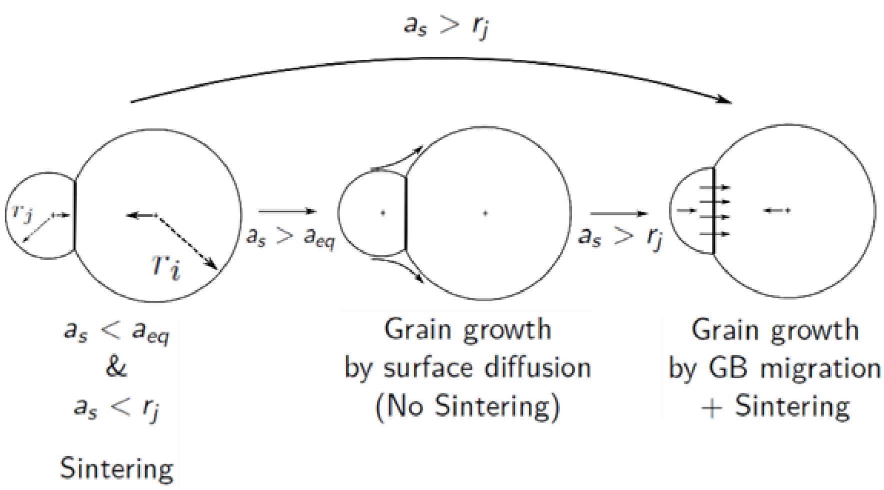


Fig 1: Different possible scenarios for sintering and grain growth

The developed grain growth model is included in our in-house DEM code dp3D where a sintering (densification) model already exists. Grain growth may be seen as a process in which small grains are eaten away by larger ones to decrease the total surface and grain boundary energy of the system. Figure 2 shows the evolution of a packing during sintering following our model. The validation of the model for two particles and for a packing is being performed.

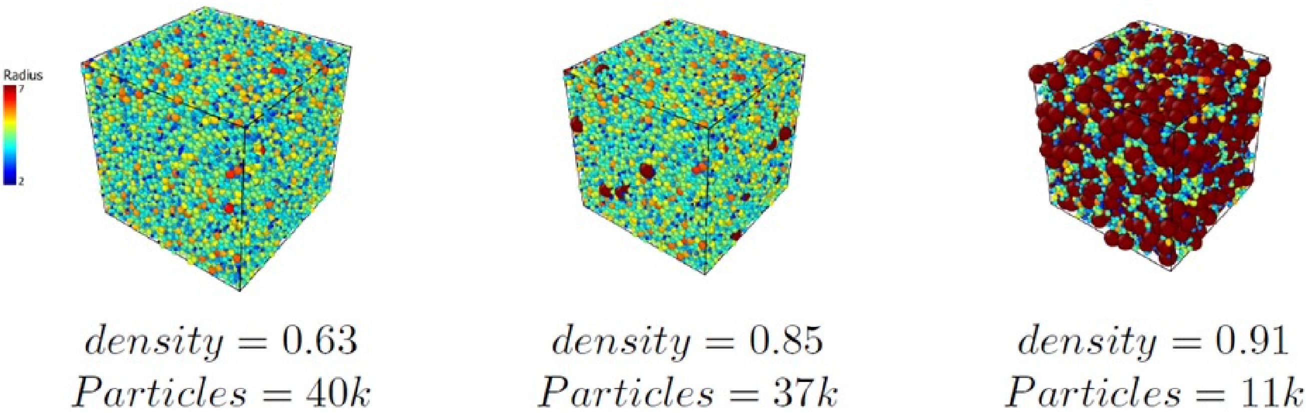


Fig 2: An illustrative packing evolution of our sintering model including densification and grain growth

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