MATHEGRAM Newsletter

Issue No. 2 January 2021

Welcome to the 2nd issue of the MATHEGRAM newsletters! Firstly I would like to wish you all a happy new year and I hope we can regain normality in 2021. MATHEGRAM has just entered the second half of our project. In the past 24 months we have endured lots of unprecedented challenges due to the Covid-19 pandemic. I am very happy to see that our ESRs are still working very hard and overcome all sorts of difficulties in order to fulfill the objectives of their research projects.

Several ESRs engaged themselves in managing MATHEGRAM social network accounts, such as the Twitter account and LinkedIn, and co-organizing our monthly virtual seminars. The monthly virtual seminars were well received. I would like to take this opportunity to thank you for your endeavor to disseminate MATHEGRAM to wider audience.

MATHEGRAM Interim Check Meeting was held successfully in October 2020. We received positive feedbacks from the project officer at REA, including "They are a united team where communication between groups (Coordinator, supervisors and fellows) is open and fruitful"; "This is a very active consortium"; "The collaboration between supervisors appears strong, well complemented with the practicality of the Industrial Beneficiaries".

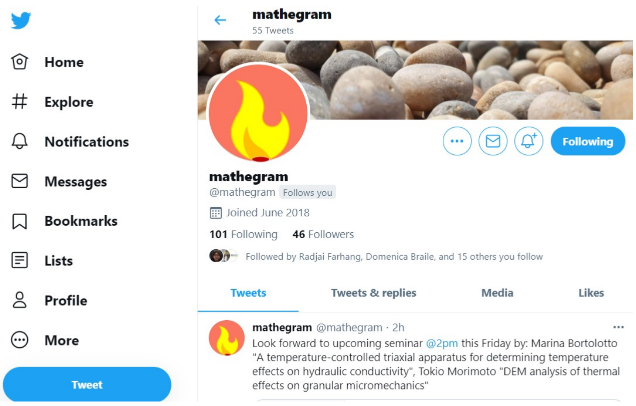
During past 24 months we held two consortium training events: ATC1 (The first advanced training course) and TS1 (the first Training School). TS1 on "Research Methods and Science Communication" is reported in this issue. We look forward for our next training event ATC2 that will be organised by CNRS-SIMAP in Grenoble, France.

Finally let us **stay safe, stay connected and stay positive**!

— Prof. Charley Wu, MATHEGRAM coordinator

Inside this issue

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



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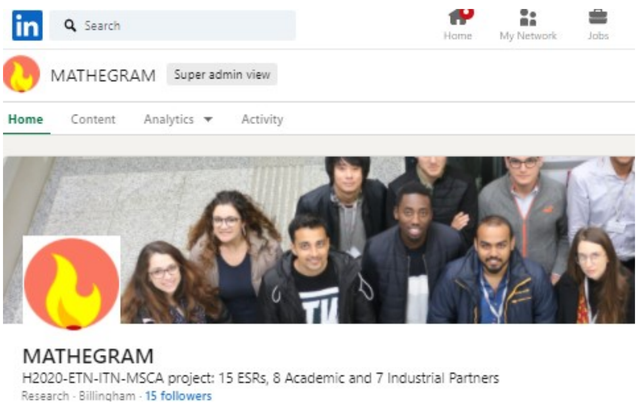
Look forward to upcoming seminar @2pm this Friday by: Marina Bortolotto "A temperature-controlled triaxial apparatus for determining temperature effects on hydraulic conductivity", Tokio Morimoto "DEM analysis of thermal effects on granular micromechanics"

MATHEGRAM Twitter account: @Mathegram



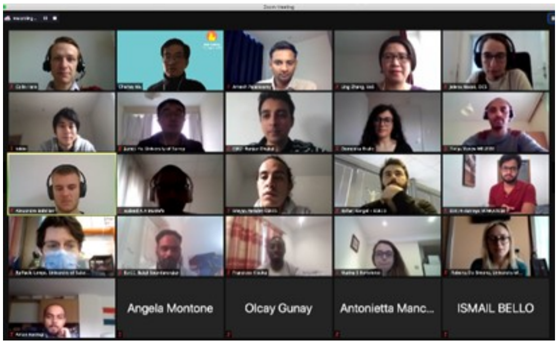
MATHEGRAM
H2020-ETN-ITN-MSCA project: 15 ESRs, 8 Academic and 7 Industrial Partners
Research · Billingham · 15 followers

MATHEGRAM LinkedIn account

The First MATHEGRAM Training School (TS1)

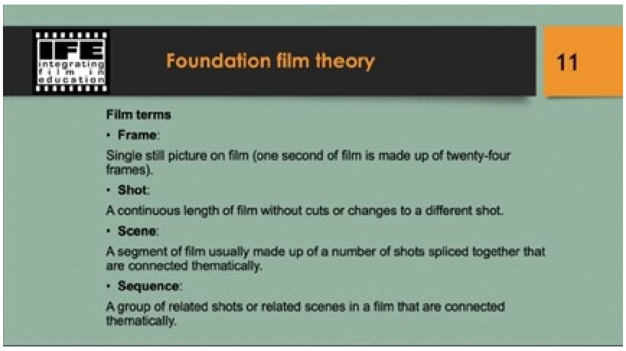
by Francisco Kisuka (ESR1,UoS) & Domenica Braile (ESR4, UoS)

The MATHEGRAM training school 1 (TS1) on “Research Methods and Science Communication” was held in the first week of November 2020 on a virtual modality, the new way of learning adopted to cope with Covid-19 pandemic. Even though it was the first time that we engaged in virtual training, the event organised by the University of Surrey was successful.



TS1 covered a wide range of exciting topics, including scientific writing and public engagement. Learning research methods and communicating one’s research through scientific papers is basal for any researcher. The lectures given by Prof. Charley Wu and Dr Colin Hare provided profound knowledge in those areas. Useful workshops and classes about IP and commercialisation, data management and public engagement were given by the University of Surrey staff.

The centrepiece of TS1 was the workshop on “Using digital media for science communication” given by Dr Eirini Konstantinidou and Robin King. This fascinating course, which filled the afternoons of the entire week, introduced ESRs to their first film production experience. Albeit intensive, it was fun! ESRs enjoyed practising taking pictures of random objects inside their house and listening to Eirini’s opinion on how to improve their shots. However, a world free of the Covid-19 pandemic would have allowed the physical interaction among fellows, making this training even more enjoyable and helpful.



Foundation film theory

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Film terms

- **Frame**:

Single still picture on film (one second of film is made up of twenty-four frames).

- **Shot**:

A continuous length of film without cuts or changes to a different shot.

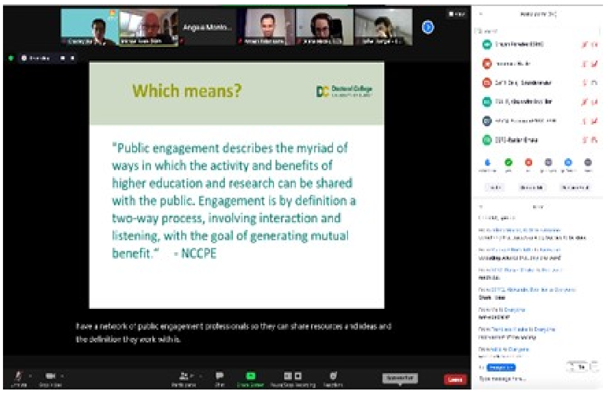
- **Scene**:

A segment of film usually made up of a number of shots spliced together that are connected thematically.

- **Sequence**:

A group of related shots or related scenes in a film that are connected thematically.

In the end, the virtual modality was a surprise for everyone because of its advantages. First of all, it was less expensive to organise, and it allowed us to reach a high number of attendees. Indeed, most lectures were also attended by a good number of external particiapnts! Moreover, most ESRs found the materials presented in training to be handy and in line with their individual projects’ status. It was then reasonable to conduct the training virtually rather than waiting for the uncertain time when the physical meeting would be possible.



Which means?

"Public engagement describes the myriad of ways in which the activity and benefits of higher education and research can be shared with the public. Engagement is by definition a two-way process, involving interaction and listening, with the goal of generating mutual benefit." - NCCPE

have a network of public engagement professionals so they can share resources and ideas and the definition they work with is.

Overall, the first MATHEGRAM virtual training was a success, but if someone asked the ESRs to choose between a virtual or a traditional course, many of them would still prefer the traditional one. Even though virtual events possess some benefits as highlighted above, holding events in person remains fundamental for building networks between attendees, which is an essential aspect of research. Not by chance, MATHEGRAM encourages meetings and social events among ESRs during these challenging times to keep connected.

CFD-DEM Simulation of Compressible Flow in Packed Beds

by Jelena Macak (ESR5, DCS)

Introduction

While every fluid is inherently compressible, we use variable density only in certain calculations: for flow through a long, thermally insulated pipe with friction; for flow through a pipe with a variable cross-section; for flow through a pipe that is cooled or heated. Flows through columns packed with particles are usually calculated as incompressible. We question the incompressibility assumption, by studying compressible flow through a packed bed: 1) with significant particle drag; 2) with variable solid fraction; 3) with particle-fluid heat transfer. For the first time, we determine conditions that require a compressible model. Here, we present some of the findings related to adiabatic flow with significant particle drag, i.e. the frictional flow regime.

Model Formulation

To study compressibility in particle-fluid systems, we use numerical and analytical methods. Our numerical model uses combined computational fluid dynamics and discrete element method (CFD-DEM). The solution algorithm is as follows. Firstly, position and forces are calculated for every particle. The discrete particle data is then averaged and mapped onto continuous fluid field. In this step, forces from particles to fluid, such as drag, are calculated and added to fluid equations. Fluid fields are calculated using a pressure-based algorithm. We implemented our model in CFDEMCoupling (1), (2).

To isolate the effect of particle drag on fluid compressibility we derived a set of one-dimensional governing equations for adiabatic flow in a packed bed (Figure 1). We assume constant solid fraction and friction co-efficient along the bed length. The resulting equations are equivalent to those of Fanno's flow regime (3).

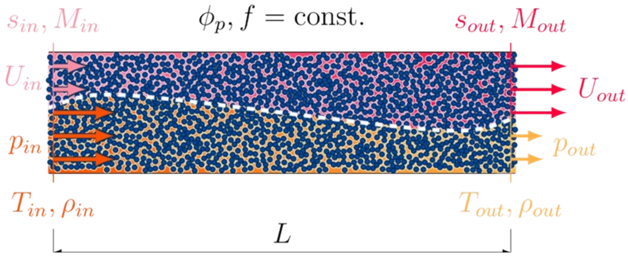


Fig 1: One-dimensional adiabatic flow in a packed bed with constant packing and friction coefficient

To achieve constant mass flow through a packed bed, fluid needs to overcome friction exerted by particles. This results in a pressure drop between inlet and outlet. Models that estimate the pressure drop, for example that of Ergun (4), assume incompressible flow, leading to constant velocity profile, and a linear pressure decline along the bed length. Allowing density to change, leads to following trends as illustrated in Figure 1: between the inlet and outlet, velocity , entropy and Mach number will rise, while pressure , temperature and density will drop.

Model Verification

To verify the CFD-DEM implementation we tested it against analytical solutions for frictional regime. We impose a range of boundary conditions given in Table 1 onto a geometry setup depicted in Figure 2.

Table 1 *Boundary conditions for CFD-DEM simulations*

Simulation	P_{out} [Pa]	U_{in} [m/s]	L/d_p [-]
1	10,000	10	200
2	100,000	10	200
3	10,000	1	1,000
4	10,000	0.01	10,000
5	100	0.01	1,000

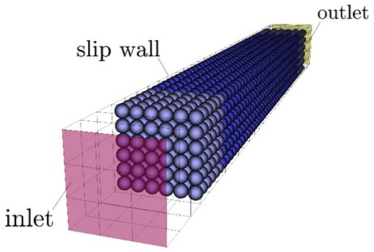


Fig 2:CFD-DEM test case

For all simulation setups, average disagreement between analytical and CFD-DEM solutions stayed below 1%. Figure 3 shows results for simulation setup 3. We see pressure, and density dropping, while velocity and Mach number rise. Pressure decline is not linear as it would be under incompressible conditions.

Only qualitative deviation from the analytically predicted trends is experienced by temperature, for which simulation predicts a slight rise towards the outlet. However, maximum disagreement between the temperature solutions is small,. Compared to changes of other properties, the drop in temperature is negligibly small-in fact its order of magnitude approaches CFD precision. Hence this deviation does not affect the overall accuracy.

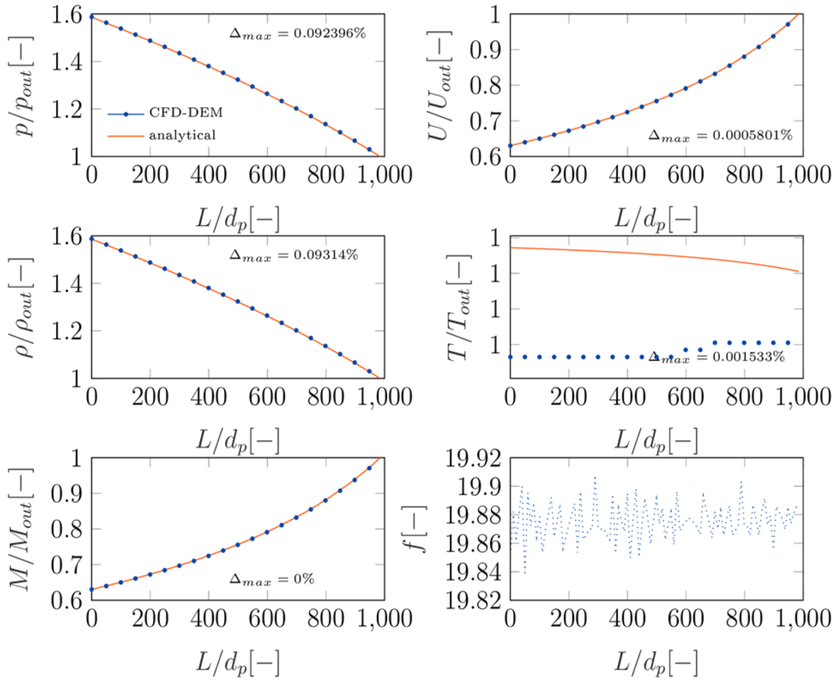


Fig 3. Comparison of CFD-DEM and analytical solutions for simulation setup 3

Conclusion

To study compressibility in particle-fluid systems, we use numerical CFD-DEM model and an analytically derived model for one-dimensional adiabatic flow in a packed bed. We tested the two against each other achieving good agreement under a wide range of conditions.

Reference

1. Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations. Goniva, C, et al. 5, 2012, Particuology, Vol. 10, pp. 582--591.

2. CFDEMcoupling open source CFD-DEM framework. [Online] [Cited: 01 15, 2021.] https://www.cfdem.com/cfdemrcoupling-open-source-cfd-dem-framework.

3. Zucker, R. D and Biblarz, O. Fundamentls of Gas Dynamics. s.l.: John Wailey & Sons, 2002.

4. Fluid flow through packed columns. Ergun, S. 1952, Chem. Engr. Prog., Vol. 48, pp. 89--94.

The Particle Finite Element Method for Simulating Heat Transfer & Fluid Flow

by Rafael Rangel (ESR13, CIMNE)

Granular materials play an important role in regulating heat transfer in some industrial applications, especially when dealing with connected fluid zones that need to have their thermal characteristics kept under control. An immersed layer of a granular material can provide an efficient mechanism of heat exchange regulation and flow convection control. However, the characteristics of the granular layer that optimise the regulation of heat and fluid fluxes, simultaneously, are not well established.

This project aims to fill this gap, by identifying innovative solutions for regulating heat transfer using packed granular layers. This is being done mainly from a numerical perspective. The adopted strategy is to explore the continuum and discrete approaches at the same time. Therefore, a coupled method between the Particle Finite Element Method (PFEM) and the Discrete Element Method (DEM), taking into account the thermal effects, is being developed. The first step, which is presented here, was to couple the PFEM for fluid dynamics with a convection-diffusion analysis for the thermal problem.

The PFEM is numerical tool for multiphysics simulations, suitable for problems with severe changes of topology. It exploits the Lagrangian description of motion, so that the mesh nodes are treated as particles, transporting their physical properties as they move according to the equations of motion. As the mesh deforms, a remeshing procedure is performed via an efficient combination of the Delaunay triangulation and the Alpha Shape method to identify the boundaries (figure 1). After the mesh is generated for a new configuration, the governing equations are solved with the standard FEM, which characterizes this method as being continuous. When applied to fluid dynamics, the momentum and mass conservation equations are solved for the velocities and pressure, respectively, in a nonlinear iteration loop within each time step.

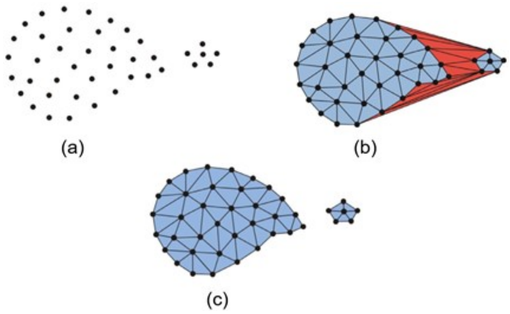


Fig 1: (a) Cloud of nodes in a new configuration; (b) Mesh obtained with the Delaunay triangulation; (c) Mesh with identified boundaries after applying the α-Shape method

The coupling between the fluid dynamics PFEM and the thermal convection-diffusion was done according to Figure 2, which shows the scheme of a single time step. The solution of the mechanical problem corresponds to the velocities and new nodal positions, computed with the PFEM as described above, keeping a constant temperature. Then, based on the new configuration, the temperature field is calculated using a convection-diffusion FEM solver. This strategy belongs to a class of staggered schemes because the mechanical and heat problems are solved in two different linear systems. Particularly, it is called external staggered scheme because the heat problem is solved after the convergence of the mechanical one, in contrast to an internal staggered scheme when both problems are solved together in the same iteration loop.

The result is a thermally coupled PFEM application that provides the possibilities to apply different thermal boundary conditions, such as prescribed temperature and heat flux, and heat transfer by convection and radiation, including the free surface. In addition, temperature dependency can be set to the material properties. Newtonian and non-Newtonian constitutive laws were also implemented for the fluid elements. Figure 3 shows an example with free surface flow and natural convection.

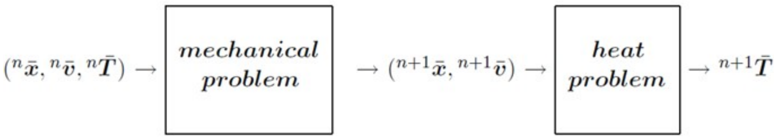


Fig 2: Scheme of a time step for an external staggered coupling between PFEM and the heat problem

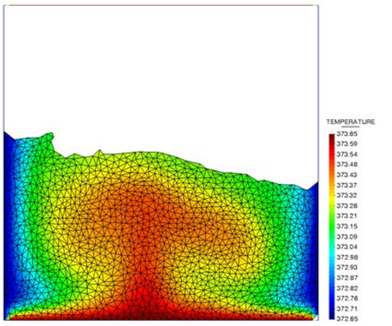


Fig 3: Temperature field in a sloshing of a fluid in the presence of natural convection

Marina Bortolotto - ESR6, Imperial College

Marina Bortolotto is a PhD student in Geotechnics and a Research Assistant at Imperial College London. Her research aims to investigate the thermal behaviour of granular materials as part of MATHEGRAM, a Marie Skłodowska-Curie Innovative Training Network (MSCA-ITN), funded by the EU. She earned her MSc degree in Geotechnics from the Federal University of Rio Grande do Sul (UFRGS), and Bachelor degree in Civil Engineering from the State University of Maringa (UEM) both in Brazil. During her Bachelor course, she spent 1.5 years in Australia, where she developed her Final Year Thesis (FYT) at the University of Western Australia (UWA).

The fellowship in Australia was sponsored by the Brazilian Government through the Science Without Borders Programme, after a highly competitive selection process. Her FYT was conducted at the Centre for Offshore Foundation Systems (COFS) - UWA, where she conducted research using a recently acquired equipment (resonant column) for the assessment of stiffness degradation and damping ratio of silica and carbonate sands. Despite the difficulties in operating a brand-new equipment, she achieved a distinction mark for her FYT. Results were then published in an international symposium in Oslo, Norway.

After earning her Bachelor degree, she was awarded with a scholarship for one of the best Masters programme in Geotechnics in Brazil. During the first year, additionally to core units focused on the fundaments of Geotechnics, Marina collaborated with MSc and PhD colleagues, which led to later publications of two articles in journals. The following 1.5 years were dedicated to her dissertation work, during which she developed a Bender Elements (BE) system for triaxial and bench tests from scratch. A Matlab® script was also especially developed for signal analysis in the time domain. The stiffnesses of artificially cemented sands were successfully measured, resulting in her Master Thesis, which was presented to an international panel of lecturers during her Viva.

Before joining the Geotechnics section at Imperial College London, she worked as a Research Fellow (Technological and Industrial Development Scholarship) in UFRGS. During this period, she developed a bench cubical apparatus for bender elements to investigate anisotropy of artificially cemented cubical specimens. Nonetheless, Marina was also invited to join the reviewer panel of two international journals (Geotechnical and Geological Engineering Journal, Springer International Publishing and Ground Improvement Journal, ICE Publishing) after reviewing papers from an international conference, and she remains as a reviewer since then.

In-situ X-ray tomographic analysis of sintering: current understanding

by Aatreya Manjulagiri Venkatesh (ESR14, SIMAP)

Sintering and the associated microstructural evolution is inarguably one of the most essential steps in powder processing of metals and ceramics. In this process, a powder or a powder compact, when subjected to thermal energy, below the melting point of its main constituent, is transformed into a bulk material of controlled density. In essence, the objective is to produce a coherent bulk body from the initial compact. As a result of this, the final product is not only densified but is most often accompanied by an increase in the size of the individual grains.

Over the years, extensive investigations carried out to understand the thermodynamics and kinetics of these two phenomena of densification and grain growth, have led to various theories on microstructural evolution, modeling and analyses to predict the path of microstructural development and its dependence on controllable parameters.

The experimental studies, in comparison with the theoretical research and numerical simulation, have been picking up speed in the recent years, thanks to the usage of non-conventional characterization techniques, like X-ray tomography.

Fig 1: Dilatometer set-up for preliminary sintering experiments

However, even though considerable progress has been achieved with regard to metallic powders, the experimental work has not yet attained a satisfactory level with ceramics, and numerous questions remain unanswered – while it has to be noted that high temperature sintering is the main fabrication process for ceramic materials.

Hence, researching the internal microstructural evolution and studies on the microstructure improvement of the ceramic materials are essential for enhancing the production process as well as for improving the overall material properties.

Indeed, as a consequence of their small size, ceramic particles most often form agglomerates and therefore, all of the experimental studies that have been attempted at the same are concerned with agglomerates. Owing to the complex and fine architecture of the individual ceramic grains, no in-situ tomography of sintering, in the real sense, has been performed so far!

The objective of the proposed project therefore is to take advantage of the outstanding features of the upgraded synchrotron at ESRF to investigate free and constrained sintering of ceramic powders by in-situ nanotomography and answer unsolved questions, thereby improving existing sintering theories and models.

Nevertheless, the analysis is bound to be delicate and challenging because of the higher temperatures needed (>1500°C), setting up of a suitable furnace, and the extremely higher and precise spatial (~50nm) and temporal (1min) resolutions required at the beamline.

However, if successful, these experiments will provide, as far as we know, the first 3D images obtained by in-situ nanotomography with real ceramic powders! And, simply viewing the image sequences would be greatly gratifying and will be of utmost importance in understanding the sintering process better for powder processing enthusiasts!

Project introduction

Additive manufacturing in simple words

by Sina Zinatlou Ajabshir (ESR9, UNISA)

Additive Manufacturing, or more commonly 3D printing, is one of the most frequent terms that we can see everywhere these days, but what it really is? Why is it important, and how it can change our lives? In a simple word, we can define additive manufacturing as a transition from analog to digital, which means that with the help of digital commands from computers, a high technological device can create any object even with complex geometry or in any materials from metals to ceramics and polymers, faster than all traditional manufacturing methods. Therefore, AM can revolutionize the manufacturing industries by bringing the flexibility and time efficiency.

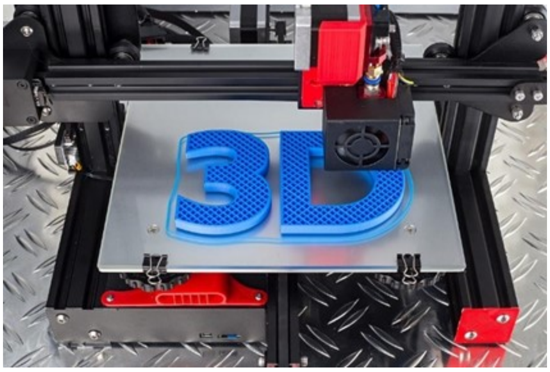


Fig 1: Fused deposition modeling (FDM) device: one type of 3D printing

The process is mainly based on adding materials layer by layer to create a three-dimensional object. It could be categorized into various processes depending on the type and intensity of energy source, the way of the deposition, or the kind of base material.

A wide variety of materials can be used in AM technology to fabricate the final object, whether it is a turbine blade made of superalloys or a sweet candy for children, due to the flexibility of this process. Although all industries can benefit from the advantages of 3D printing technology, it has mostly influenced on aerospace, automotive, machinery, and medical industries to increase the production rate, efficiency, speed, decrease wasting time and materials, and more importantly, help to improve reliability and strength of final products with any shapes and geometries.

In the last word, 3-D printing manufacturing plays an important role in the industries today and due to its undeniable advantages, it is not unlikely that all the traditional manufacturing methods will be replaced by AM in the near future.

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- Aatreya Venkatesh