IPROCOM Newsletter

Issue No. 5 July 2016

Welcome to the 5th issue of the IPROCOM newsletters! As ever, this edition has news about our fellows and the events IPROCOMers attended over the last 6 months. We are most grateful for the involvement of everyone in promoting IPROCOM to the wide range of audience around world.

IPROCOM conference was held successfully in conjunction with PARTEC 2016 in Nuremberg, Germany on 19-21st April 2016. Each fellow had a chance to present their work at this well-established international conference. In this issue, you will read a few splendid fellows' reports on their experience in attending this conference.

The Joint IFPRI and UK Particle Technology Forum (IFPRI-UKPTF) was held at the University of Surrey, 15-16th June. IPROCOM fellows Miss Serena Schiano and Mr Simone Loreti attended the Forum. Most excitingly Serena won the **3rd prize** in the Young Researcher Award oral presentation competition at this event. Well done, Serena!

I am delighted to inform you that Mr. Hossam M Zawbaa successfully defended his PhD thesis in June and passed his PhD viva. He is now officially Dr. Zawbaa. Many congratulations, Hossam!

My book entitled "*Particle Technology and Engineering*" has just been published by Elsevier. Any comments and suggestions on this book will be gratefully welcome.

I am also pleased to announce that an IPROCOM special issue on the **Powder Technology** journal has been arranged, we are now soliciting high quality contribution in the broad areas related to the IPROCOM project.

I wish you have a splendid summer break!

Yours Sincerely,

Prof. Charley Wu
IPROCOM coordinator

Inside this issue

This project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No. 316555.

Predictive Modeling Software

Varun Ojha

As part of IPROCOM research activities, Mr. Varun Kumar Ojha from VSB-Technical University of Ostrava has developed a software for predictive modeling and is available at http://dap.vsb.cz/aat/ [1]. The developed software tool called "Function approximation and feature selection" is particularly useful in modeling real-world application problems, such as pharmaceutical drug manufacturing and drug dissolution [2,3,4]. In a broad sense, the developed tool identifies appropriate functions for the data that has an input-output relationship. Another aspect of the developed software tool is its ability to identify significant features that help in identifying critical process variables for a manufacturing process. This helps reducing industrial manufacturing cost by eliminating insignificant variables from the production process. Some screen captures of the tool are illustrated in Figures 1 and 2. The efficiency of the trained model can be examined from the training output window that has statistical goodness measure values and by examining the agreement between actual test data and model predicted data. Therefore a post-processing module is also embedded in the software, as illustrated in Figure 3. Another useful feature is that an efficient module is implemented to save the trained models that can be used for prediction using new datasets.

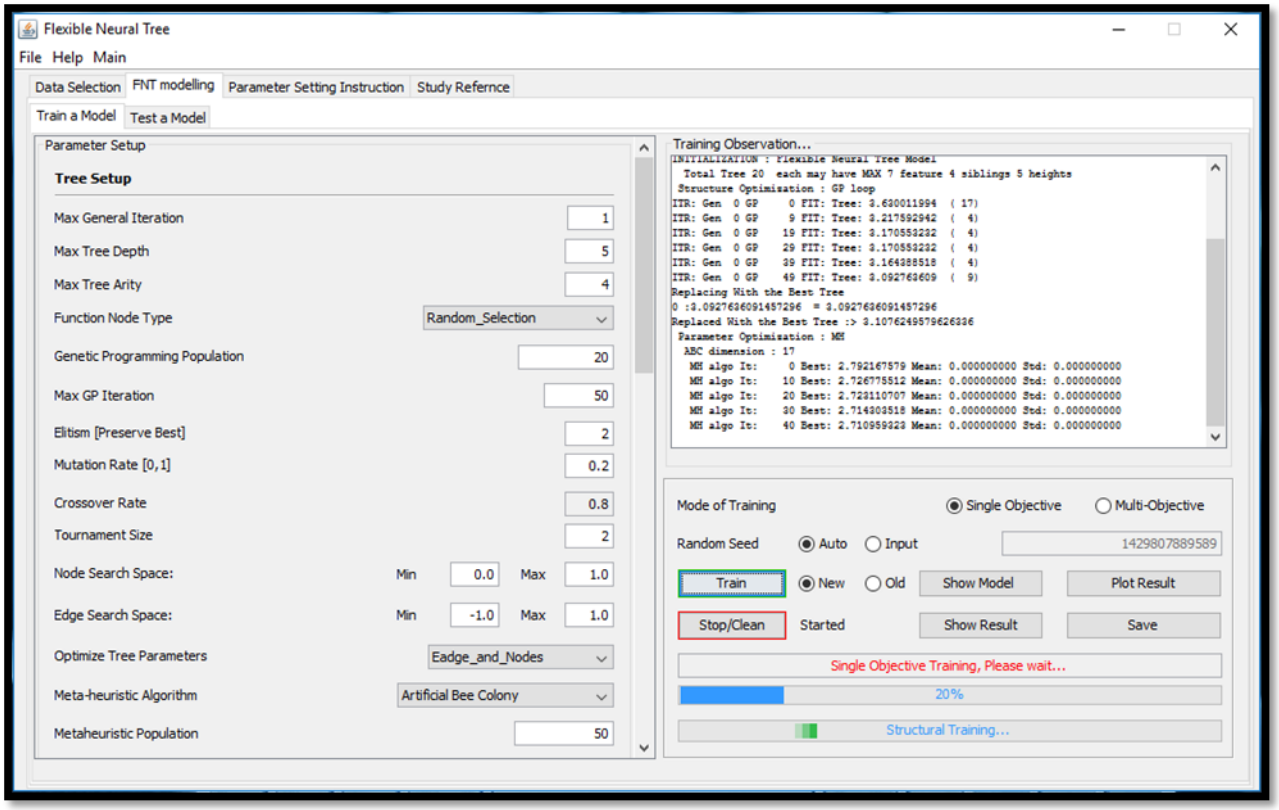

Figure 1: GUI for the function approximation and feature selection tool

Predictive Modeling Software

Varun Ojha

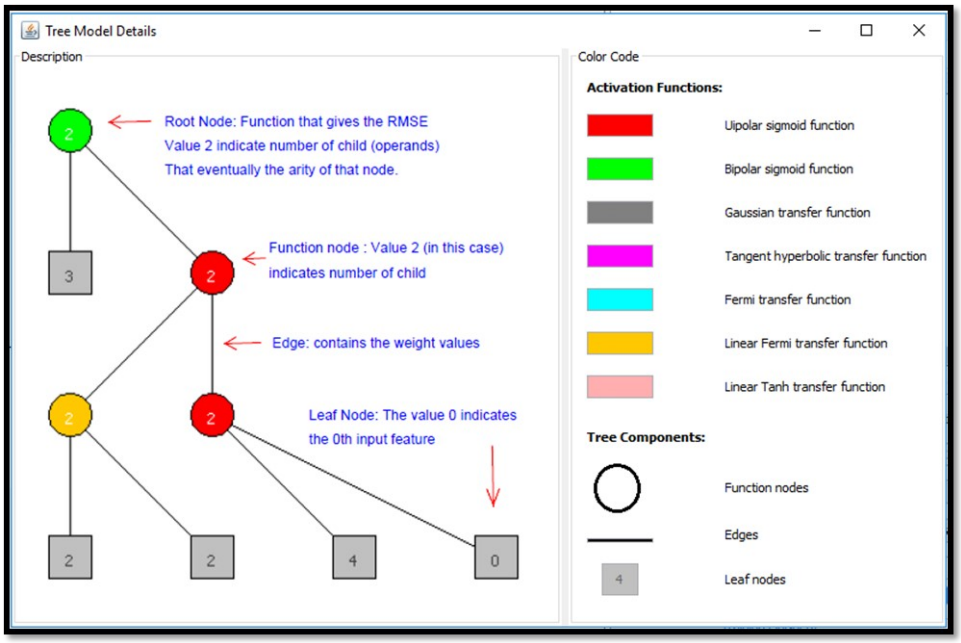

Figure 2: A typical tree-like prediction model

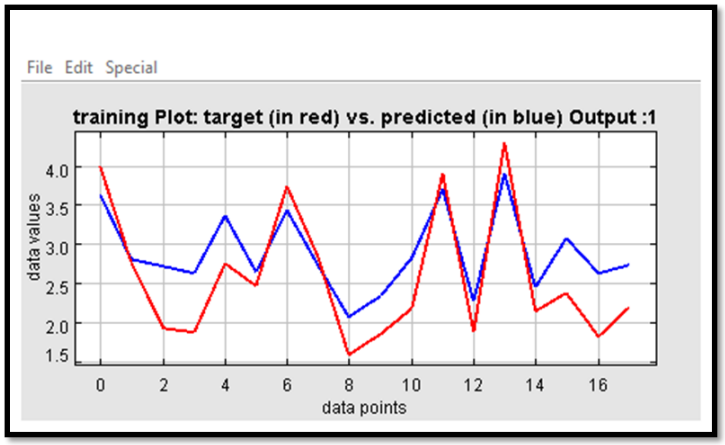

Figure 3: Target versus predicted values

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[1] Ojha, V. K, (2016), MOGP-FNT: Multiobjective Flexible Neural Tree Tool, http://dap.vsb.cz/aat/

[2] Ojha, V. K., Abraham, A., Snasel V., Ensemble of Heterogeneous Flexible Neural Trees Using Multiobjective Genetic Programming, Applied Soft Computing.

[3] Ojha, V.K., Abraham, A., Snasel, V., Ensemble of heterogeneous flexible neural tree for the approximation and feature-selection of Poly (lactic-co-glycolic acid) micro- and nanoparticle, Advances in Intelligent Systems and Computing, 427, 2016 pp. 155-165. (Scopus, Springer)

[4] Abdelwahab, S., Ojha, V.K., Abraham, A., Ensemble of flexible neural trees for predicting risk in grid computing environment, Advances in Intelligent Systems and Computing, 427, 2016 pp. 155-165. (Scopus, Springer)

IPROCOM sessions at PARTEC 2016

IPROCOM conference in conjunction with PARTEC 2016 was held in Nuremberg, Germany on 19-21st April 2016. On Monday 19th April 2016, dedicated IPROCOM sessions took place to showcase our fellows' collaborative work. Eight oral presentations were given by our fellows in pairs. The sessions were well attended and well received. Please find fellows' report on PARTEC conference in the following pages.

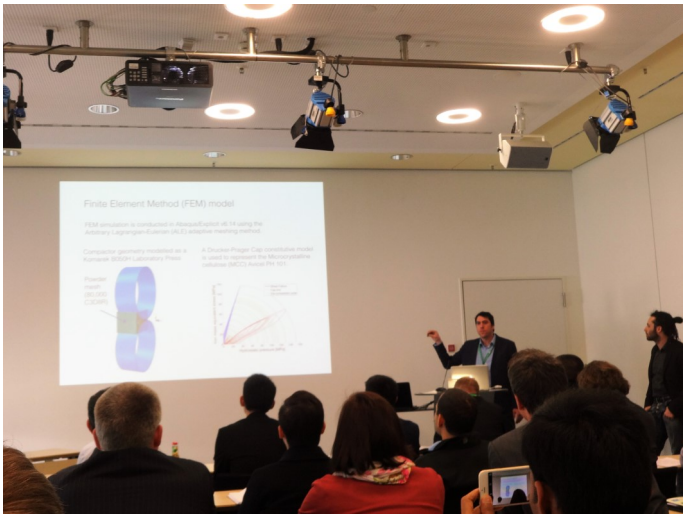
During the project management meeting, the coordinator professor Charley Wu was thrilled to receive a thank-you hamper prepared by all the IPROCOMers. It was a marvelous occasion showcasing our strong collaboration and corporation.

A combined DEM & FEM modelling of powder flow & compaction during Roll pressing

Reported by Alon Mazor

The international particle technology congress PARTEC is held every three years and is combined with the powder processing trade fair, POWTECH. At PARTEC 2016, beside the regular multiple sessions, two extra IPROCOM sessions were added. These sessions provided the opportunity for both the scientific and industrial community to discover the fine collaborative work done in IPROCOM.

All Early Stage Researchers have shown excellent work and a fruitful collaboration within the IPROCOM consortium. It is amazing to see how the researchers evolve during the last couple of years, resulting in a significant collaborative work, leading to the success of the IPROCOM consortium.



Mr. Mazor (ESR6) and Mr. Orefice (ESR5) presented their work on "A combined DEM & FEM modeling of powder flow and compaction during roll pressing". This work presents an innovative approach to combine the strength of both the Discrete Elements Method (DEM) and the Finite Element Method (FEM) in order to model a complex process, such as roll compaction.

Moreover, Mr. Mazor also presented his work "The effect of roll compactor sealing system design: a finite element analysis" in the Modelling and Simulation session. In this work, a 3D Finite Element Method (FEM) modelling was performed to analyze the roll compaction process and the effect of sealing system designs. The results demonstrate the capability of FEM modelling to provide insight and help achieving a better understanding of the roll compaction process. At the end of his presentation, the audience asked several interesting questions, which were gladly answered.

It is fair to say that the international particle technology congress PARTEC 2016 was a huge success for the IPROCOM consortium, disseminating the fine collaborative work of the entire research team to a wide scientific and industrial community.

Roll Compaction: The impact of system design and Scale up

Reported by Ana Pérez Gago

The International Congress on Particle Technology (PARTEC) takes place every 3 years in Nuremberg (Germany) together with the Trade Fair for Processing, Analysis and Handling of Powder and Bulk Solids also known as POWTECH. This time, PARTEC and POWTECH were held during 19 – 21st April 2016, and more than 500 participants attended PARTEC alone. Therefore, it was a fantastic opportunity and a great privilege for the IPROCOM members to celebrate our achievements in this congress. This gave us the chance to disseminate our work in front of significantly wider audience and to promote the interest and outcome of our project. Due to these important facts, all early stage researchers of the IPROCOM project attended this event and the fellows presented some of our results during a special session: the IPROCOM Conference. In general, the venue for the IPROCOM conference was full of attendees, what implies the impact and attractiveness that our project has.

My presentation named as "Roll Compaction: The Impact of System Design and Scale-up" was given together with my colleague Kitti Csordás. We both presented our work and discussed the difficulties we face when transferring the roll compaction process between compactors of different designs (Kitti) or scales (myself). Apart from the stimulating discussions which took place after the presentation, the congress is also divided into 7 parallel sessions providing the opportunity to attend to very interesting presentations. Furthermore, PARTEC was great opportunity to meet new or old friends, as well as a good occasion for us to enjoy our IPROCOM network one more time as IPROCOM members.

Reported by Kitti Csordás

In April 2016, PARTEC (International Congress on Particle Technology) was held in Nuremberg, Germany. At the same time, POWTECH 2016, the leading fair for the processing, analyses and handling of powder and bulk solids at the Nuremberg Exhibition Centre took place.

Since PARTEC and POWTECH is one of the biggest meeting and knowledge exchange platform between scientists from the pharmaceutical and other industrial fields, it was a fantastic opportunity for us to showcase our research achievement and to update research progress. Thus, all IPROCOM fellows presented their results collaboratively. Fruitful discussion with the audience immediately after the presentations and during the breaks showed the success of the IPROCOM project. Not only the Partec congress, but also the POWTECH 2016 was a huge experience for all fellows, because we could have conversation in live with experts from different field. Several roll compactor suppliers, e.g. Gerteis Maschinen + Processengineering AG, Howokawa Alpine AG etc. were present and gave the possibility for idea exchange about the roll compaction process. I found the participation on the PARTEC 2016 one of my best experience in my PhD, especially I receive many constructive feedbacks on my research topic.

Machine learning tools for modelling of powder mixing

Reported by Varun Ojha

PARTEC 2016 was an existing experience, particularly due to the facilities, the networking opportunity, and programme. The presentations in the IPROCOM sessions were attended by many PARTEC participants that made the presentation more enjoyable than the presentation I delivered elsewhere. The collaborative presentations was the first experience and the synchronization with my counterpart enhanced the presentation session. I had opportunity to attend many other PARTEC sessions that were of my interest to gain knowledge in some additional powder technology topics, such as powder mixing and its quality identification using color hue. I also establish a new collaboration with the presenter and to offer computational intelligence perspective to the presenter (Kahilil Desai, Monash University, Australia. Title: Understanding Pharmaceutical Dry Powder Blending Using the Iron Oxide Tracer Method).

The additional aspect of IPROCOM final meeting and discussion was a necessary and important event, though it was a very brief meeting. However, the overall programme was beneficial to learn and gain experience.

DEM modelling of powder flow & powder-filling during die compaction

Reported by Raphael Schubert

This having been my first attendance at a major conference, I was slightly nervous about my presentation, especially with some big names in the field also scheduled to speak later. But as always, most of the worries were unnecessary. The IPROCOM sessions were very well attended and well received by an interested audience. Luckily, they were also among the first sessions, so I could really enjoy the conference and the exhibition.

A particular pleasure was the meeting with Prof. Hans Herrmann again, who advised me on my master's thesis, and to attend his interesting keynote, which he delivered with the same enthusiasm I remembered from his lectures.

The conference was also the last opportunity for all the IPROCOM fellows together to have some interesting discussions with a lot of fun, beer and excitements.

Multiscale modelling of ribbon Milling: a DEM-PBM framework

Reported by Simone Loreti

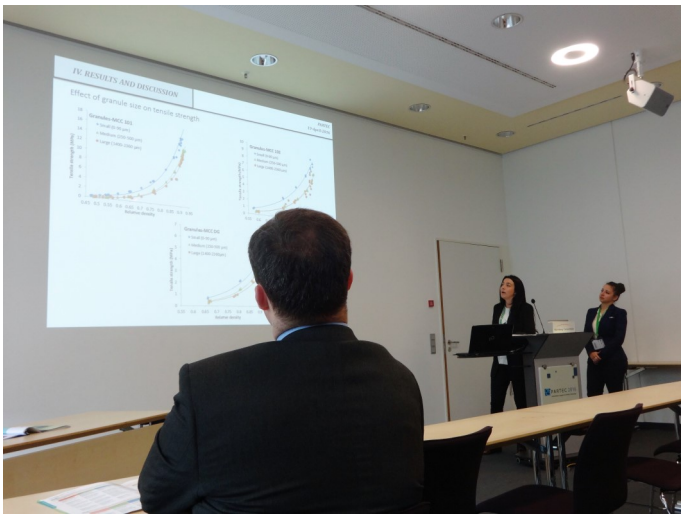
The PARTEC conference is one of the most important international scientific events in particle and powder technology and it was held on 19-21st April 2016 in Nuremberg. The Surrey Team attended the conference with a four people delegation composed by Prof. Chuan-Yu Wu, Dr. Alexander Krok, Mr. Simone Loreti and Ms. Serena Schiano.

A part of the PARTEC conference was entirely dedicated to the European multidisciplinary and inter-sectoral project IPROCOM, with eight oral presentations delivered collaboratively by the fellows. Each presentation was performed jointly by two fellows showcasing their scientific collaborations. For example, Ms. Schiano presented "Machine learning tools for modelling of powder mixing" with Varun Kumar Ojha, "Feature selection techniques for roll compaction" by Hossam Zawbaa and Lucia Perez Gandarillas, "The impact of roll compaction process on die filling and die compaction" with Lucia Perez Gandarillas. I presented "Multiscale modelling of ribbon milling: a DEM-PBM framework", a collaborative work with Dr. Andreja Mirtic.

The impact of roll compaction process on die filling and die compaction

Reported by Lucía Pérez Gandarillas

From 19 to 21 April 2016, IPROCOM fellows had the opportunity to meet international experts on particle technology, from both research and industry.



On the first day of the conference, the IPROCOM sessions took place and all the fellows presented their collaborative works. I was impressed for the great efforts and the progress of the fellows over the recent months. We presented a wide range of topics without much overlap.

As ESR4, I participated in two presentations together with ESR1 and ESR10:

-" The impact of roll compaction process on die filling and die compaction", S.Schiano/L.Perez-Gandarillas

- "Feature selection techniques for Roll Compaction", H. Zawbaa, S.Schiano/L.Perez-Gandarillas

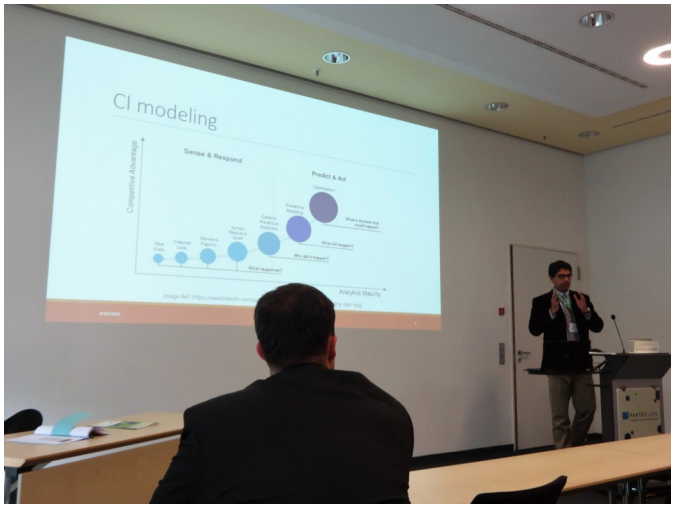
I found the tandem presentations an interesting activity, to create more links between fellows and possible future publications.

In general, the experience in PARTEC was good. Good organization, comfortable conference rooms and the possibility to attend the exhibition, where I had the opportunity to discuss with some roll compactor suppliers.

CI for solid dosage forms: modeling milling and die compaction processes

Reported by Hassan Khalid

PARTEC: The conference included presentation on many useful topics on the theme of particle technology. Symposia particularly of my interest were modelling and simulation methods and applications, Life and food science, and pharmaceutical particles. Poster sessions were great as I got a chance to talk to people from different research groups about their work. Posters from the Ghadiri group in Leeds were particularly interesting.



Works on Applications of computational intelligence (CI) tools to powder technology was represented by very few talks and posters.

IPROCOM Session: This was a great session with large interest from general attendees as well. Our talks were well received and it felt good to be part of a large, recognized team. The session was integrated very well in the conference.

Social/Networking events: Visit to the science museum was nice. In my opinion, IPROCOM social events are better (no offense to PARTEC organizers) – my opinion could be biased partly because we can joke around freely with each other.

Feature selection techniques for roll compaction

Reported by Serena Schiano

PARTEC is one of the largest international conferences focus on particle and powder technology. The main topics are particle formation processes, particle characterisation, measurement methods and their equipment. Furthermore, in this conference, industrial processes in powder technology, such as agglomeration, compaction, die filling, coating, formulation and product quality, were as well discussed.

This conference has been a great experience for several reasons. It was my first time to have a group presentation in a conference together with other colleagues, more precisely I had 2 presentations: the first one entitled “The impact pf roll compaction on die filling and die compaction” in collaboration with the CNRS in Albi and a second presentation on “Predictive Modelling of Die Filling of the Pharmaceutical Granules Using the Flexible Neural Tree” in collaboration with the University of Ostrava in Czech Republic. These group presentations helped me a lot in the improvement of my collaboration and presentation skills. Moreover, I had the opportunity to show my scientific work to a very wide range of experts from companies to universities, which gave me constructive advices and opinions. Also it was very interesting to visit the large exhibitions with many industrial instruments from different sectors (pharmaceutical to navy).

Nuremberg is a lovely and sunny city with several interesting historical places that are worth the visit!

10th World Meeting on Pharmaceutics, Biopharmaceutics & Pharmaceutical Technology

Ana Pérez Gago

The World Meeting on Pharmaceutics, Biopharmaceutics and Pharmaceutical Technology (also known as PBP World Meeting) takes place every two years. It was the 10th meeting this year and held in Glasgow (UK) during 4-7th April 2016. More than 1,200 attendees coming from more than 50 countries from the 5 continents participated this conference. Therefore, it was a great opportunity to disseminate our work and have interesting discussions with other experts in our field.

From the IPROCOM project attended were Prof. Charley Wu (together with his team members, Alexander Krok and Jianyi Zhang) from the University of Surrey; Prof. Peter Kleinebudde, Kitti Csordás and Ana Pérez Gago from the Heinrich Heine University, and Pezhman Kazemi and Hassan Khalid from the Jagiellonian University in Cracow, Poland. The fellows presented their work during the poster session besides attending to the different presentations structured in 4 parallel sessions. This meeting was also a fantastic opportunity to meet old friends as well as make new contacts.

IFPRI Robert Pfeffer Symposium & UK Particle Technology Forum 2016

Serena Schiano

The International Fine Particle Research Institute, IFPRI, is an organisation with members from global companies with active research programmes in particle science and technology. It is a non-profit organization where some of the world's largest manufacturing industries specialised in pharmaceuticals, minerals, chemicals, coating, detergent and food are able to collaborate and discuss. This year the IFPRI symposium has been combined with the UK Particle Technology forum, which provided a platform to facilitate the interaction of researchers, especially young researchers, active in all aspects of particle technology in the UK.

This conference was held at the University of Surrey and I had the opportunity to be part of the local organising committee, helping in the reception for almost 200 participants. I also have been selected to participate at the UK PTF Young Researcher Award with an oral presentation where I could share the outcome of my work based on "A Novel Use of Friability Testing for Characterising Ribbon Milling Behaviour". This experience has been of great impact for me as it promoted many interesting discussions with numerous companies. Furthermore I was delighted to win the **3rd prize as Young researcher Award,** a very rewarding experience to me .

My Journey through IPROCOM

Hossam M. Zawbaa

During my undergraduate studies in the Faculty of Computers and Information, Cairo University, Egypt, I have established my personal goal to become a successful professor and researcher in computer science field. As well, I have a Lecturer position at Information Technology Department, Faculty of Computers and Information, Beni-Suef University, Egypt. I have defended my PhD thesis in June 2016 from Babes-Bolyai University, Cluj-Napoca, Romania. My PhD thesis titled "Computational Intelligence Modelling of Pharmaceutical Roll Compaction", through working in Marie Curie - IPROCOM project (European Union's Seventh Framework Programme FP7).

My research interests are in the area of Computational Intelligence, Machine Learning, Image Processing, and Pattern Recognition. They include both theoretical and algorithmic improvement as well as applications for various problems, such as classification, regression, clustering, and data mining. Through my professional experiences, I have decided to participate in multi-disciplinary projects that have to employ in developing a better life for the humanity. For sure, the idea of "*The development of in silico process models for roll compaction (IPROCOM)*" is one of the best projects that satisfy this objective.

It is obvious that starting with IPROCOM project, the quantity and quality of my research publications have been grown. Before I have joined this project, I had **18** publications with **4** **h-index**, **1** **i10-index**, and **0** **impact factor**. In the mid of 2014 (after 6 months), I decided to improve even more the publication's quality and research collaboration before finishing the IPROCOM project. Now (in mid of 2016), I have authored/co-authored **50** publications in peer-reviewed reputed journals and international conference proceedings (**32** scientific papers published and accepted through IPROCOM project as shown in Fig 1). As per Google Scholar, I have **229** **citations**, **10** **h-index**, and **10** **i10-index** as well. As per ResearchGate, I have more than **16** **impact points** and more than **3800** **readings**. Now, almost at the end of the project, I can say that I am fully satisfied with the evolution of my research contributions during IPROCOM fellowship.

Thanks to IPROCOM to give me this opportunity to develop myself and continue my research work even more successfully and established collaborations within IPROCOM network. Every day I commit myself to work towards my personal goal as is evident by the academic accomplishments and publications record.

Published	No.	IF	Accepted	No.	IF
Journals	5	10.80	Journals	2	5.63
Conferences	18	-	Conferences	7	-
Submitted	**No.**	**IF**	**Ready for submission**		**No.**
Journals	2	7.07	Journals		3
Conferences	3	-	Conferences		-

Fig 1 Statistics of the publications through IPROCOM

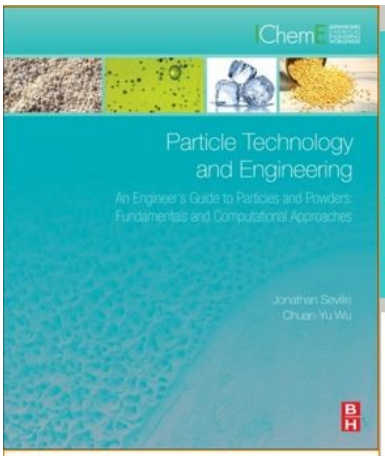
From Albi to Dusseldorf

Lucia Perez-Gandarillas

From 21st March until 24th March 2016, Dr. Abder Michrafy (Ecole de Mines d'Albi-CNRS) and fellow Lucia Perez-Gandarillas (ESR4) and Alon Mazor (ESR6) visited the Institute of Pharmaceutics and Biopharmaceutics of the University of Dusseldorf. They had the opportunity to meet Prof. Kleinebudde and fellows Kitti Csordas (ESR3) and Ana Perez-Gago (ESR4). During this visit, they had interesting discussions on how to collaborate together, mainly focusing on the scalability of the roll-compaction process. Also Abder Michrafy gave a lecture entitled "FEM Modeling of Compaction Process: Case Studies on Die and Roller Compaction" to the researchers of the Institute.

New Book: 'Particle Technology and Engineering'

Co-authored by Prof. Charley Wu



Particle Technology and Engineering

An Engineer's Guide to Particles and Powders: Fundamentals and Computational Approaches

Jonathan P.K. Seville and ***Chuan-Yu Wu***

Department of Chemical and Process Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, UK

B H

An essential guide for all engineers working with particles and powders, which make up over 50% of all chemical products

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Fellow of this issue

Hassan

Khalid is our ESR 12 in IPROCOM based at Jagiellonian University, Poland. He comes from Islamabad, Pakistan. He obtained his undergraduate degree in Bioinformatics from COMSATS Institute of Information Technology (CIIT), Pakistan and his Masters degree in Bioinformatics from Queen Mary University of London where he was also awarded a partial scholarship. As part of his graduate project he worked on computational analysis of intrinsically disordered proteins.

In 2009, Hassan joined CIIT as a lecturer in bioinformatics and helped supervise undergraduate research projects including phylogenetics study of HIV and miRNA analysis of MMTV. The Faculty Development Academy (FDA) at CIIT recruited Hassan to design and manage pre-service trainings for newly hired faculty members across seven CIIT campuses.

In 2012, Hassan co-founded Modus operandi Bioinformatics (MoB), a IT based initiative focused on finding Information Communications Technology (ICT) and data science solutions to health and agriculture problems in the developing world. Hassan deployed several development projects during this time. An electronic medical reporting and recording tool for tuberculosis was developed in partnership with the National TB program. A comprehensive weed database and weed image identification system was developed in collaboration with the Weed Science Society of Pakistan.

Hassan won a Marie Curie scholarship as an Early Stage Researcher at IPROCOM, an EU funded consortium of academia and industry aimed at creating in silico models for critical research and development processes within the pharmaceutical and chemical domains. His role in the project is to use computational intelligence tools to model powder flow and tableting processes. During his time with IPROCOM, Hassan has attended various specialized trainings and conferences, and spent time at Ecoles de Mines, Albi, France and Johnson Matthey, UK for his secondments. Hassan won the best paper award in Modeling and Simulation track at IEEE FIT' 15, Islamabad, Pakistan for his work titled "Transparent Computational Intelligence models for pharmaceutical tableting process".

Hassan is truly passionate about Data science and Predictive analytics. Currently, Hassan is enrolled in a Data Science Fellowship program conducted by The Data Incubator, a program that has a lower acceptance rate than Harvard. As part of the course Hassan is actively working on Data driven Geospatial Analysis of food insecurity across the globe.

In his free time, Hassan likes to go hiking and discover unexplored places and take part in data science competitions online.

Key Dates

December 2016 IPROCOM management meeting, Albi, France

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- Lucia Perez Gandarillas & Alon Mazor
- Varun Ojha
- Raphael Schubert