

Report on the Workshop on Theory and Applications of Coagulation–Fragmentation Equations

September 6, 2005

The talks in the workshop dealt with a number of topics central to the area of coagulation– fragmentation processes. Applications of such processes were discussed by a number of speakers. Controlled nanoparticle manufacturing was covered by Pratsinis; Walde talked about transformations of fatty acid aggregates, presenting many fascinating aspects of micelle formation and evolution. Richardson showed exciting simulations of asteroid formation and breakage due to gravitational pull of celestial bodies. Only hours after NASA’s Deep Impact probe successfully collided with comet Tempel 1, he gave a brief overview of the initial results and their implications for our understanding of the internal structure of comets. All of these show how much more complicated than current models many coagulation-fragmentation events really are; the challenge to develop new realistic models which incorporate more effects remains.

Modelling aspects were discussed by Blythe, Coveney/Chin, Family, Fasano, Ford, Penrose, Rudnicki and Sharma. The applications modelled included, among others, a detailed thermodynamical description of nucleating clusters, in which each particle’s energy was analysed as a function of its distance from the centre of cluster. This careful modelling led to a more detailed description of the role of temperature in nucleation kinetics. Finite size effects were discussed by a number of speakers; most notably, Penrose presented the meeting with the challenge of describing solidification in alloys where anisotropic effects influenced the size, as well as the shape, of nucleating regions. Fasano discussed the ‘volume scattering’ model in which finite size effects are explicitly incorporated into the model equations. Family demonstrated how the coagulation–fragmentation framework can be used to understand island formation in molecular beam epitaxy. Intriguingly, his use of Voronoi cells to determine domains of attraction of atoms also arose in the description of dissipative particle dynamics included in the talk of Coveney/Chin. Blythe considered a simple spatially dependent model of particles moving by diffusion until they collided, showing that complex behaviour occurs even in microscopic models of coagulation.

Mathematical issues arising from coagulation–fragmentation equations were presented in the lectures of Babovsky, Banasiak, Canizo Rincon, Fournier, Kolokoltsov, Lushnikov, Leyvraz, Laurençot, Niethammer, Pego, van Roessel, Walker, Wagner, and Ziff. The speakers provided an excellent overview of the wealth and depth of mathematics involved in the analysis of coagulation–fragmentation equations. In particular, the interplay of stochastic and deterministic methods, and the close connection of coagulation equations with nonlinear conservation laws was stressed throughout. The insight provided by solvable kernels and the importance of self-similar solutions have been stressed throughout. Perhaps an important point to emerge from the theoretical discussions of the workshop is that a much deeper understanding of gelation in coagulation processes is needed, both in the description of asymptotics of gelation for general kernel systems and in the physical interpretation of results.

It is obvious that participants would disagree in their nominations for the highlight of the workshop. Several commented very favourably on the success of the workshop in bringing together a diverse range of specialists with shared interests in coagulation–fragmentation processes. It also provided some of them with an opportunity to meet for the first time prominent fellow workers in the field. A large number of the talks were very well received, among them, these of Ford, Family, Laurençot, Leyvraz, Pego, Pratsinis, Richardson, and Wagner garnering the most praise. The closing discussion session chaired by Lushnikov was certainly thought-inspiring. It is our feeling that the atmosphere at the workshop was very cordial and pleasant and that the social programme, the visit to Roslyn Chapel and the banquet at Howies’ were also memorable occasions.

In terms of the impact of the workshop on future research in the area, it is certainly too early to tell. From the responses of the participants, it is clear that the workshop provided them with food for thought and new directions for research. The special issue of *Physica D* on the themes of the workshop is in preparation. It will reflect the state of the art in the area and we expect it will become a major bibliographical resource for the coagulation–fragmentation community for years to come.

We are gratified to see a high level of satisfaction expressed by the participants in the questionnaires. All were very pleased with the content of the workshop and its organisation; perhaps the only persistent quibble was that Arden house is too far from Kings’ Building to manage without some form of transport in the mornings.

On a personal level, we found many of the talks fascinating and excellently prepared; the workshop exposed us to aspects of the topic we were not aware of and opened new venues of research, such as dynamics of bubble formation and growth, coagulation-fragmentation with ring formation, analysis of coagulation–fragmentation equations in “nonstandard” spaces, such as that of Borel-summable series, exploration of connections between gelation and parabolic blow-up, etc. etc.

We are grateful to the ICMS for making it possible to run the workshop, and to the ICMS staff for so effortlessly and professionally taking care of all administrative matters, and to both the ICMS and Centro e Análise Matemática, Geometria e Sistemas Dinâmicos of Instituto Superior Técnico, Lisbon, Portugal, for providing generous support for participants.

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