

SAMBa ITT5: Chemical Dispersion and Effectiveness
30th January - 3rd February 2017

BRLSI, Bath



Participants with resident dinosaur on day 2 of ITT4

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1 Introduction to SAMBa

SAMBa is the EPSRC Centre for Doctoral Training in Statistical Applied Mathematics at the University of Bath. It is funded by EPSRC and aims to support 50+ PhD students over 8 years. There will be 5 intakes (in September each year) of around 10 students. 2014 was the first intake of students to SAMBa.

Students undertake a 1+3 model PhD, with taught courses in their first year, leading to an MRes qualification, and then 3 years of research funding, leading to a PhD. Throughout their time in SAMBa, and in addition to their PhD research, students will be exposed to a range of mathematical problems, faced by non-academics, and academics in non-mathematics departments, as well as those at the forefront of mathematical research. Central to this goal are the Integrative Think Tanks (ITTs).

Integrative Think Tanks bring together students, academics and external partners over a week. Problems are presented and students, with support from academic attendees from the Department of Mathematical Sciences, are expected to *formulate* research solutions, defining the routes to solving the problems, rather than solving them outright. It is hoped that discussions at ITTs will form the basis of PhD projects for some SAMBa students, hopefully a number of these will be co-funded by external partners. However, ITTs generate a range of problems that can be tackled in different ways by experts in the department through short- or long-term research projects, funded through a variety of mechanisms.

In short, ITTs provide a vibrant working environment, leading to a high volume of quality research with impact.

2 Theme and Participants

The major theme of this ITT will be *chemical dispersion and effectiveness*. The partner organisations attending are Roche (<https://www.roche.co.uk/>) and Syngenta (<http://www4.syngenta.com/>).

Roche is a Swiss multinational health-care company that operates worldwide. **Syngenta** is a global Swiss agribusiness that produces agrochemicals and seeds. Over the last few months, we have been working with them on scoping a variety of statistical applied mathematics driven problems including dynamical systems, modelling and prediction of chemical environments, and data-driven decision making. These subjects will be expanded further through discussion at ITT5.

The ITT is part of the SAMBa students' training programme and as such, all students who are in their first year will attend. We also welcome students who are in the later years of SAMBa, additional PhD students from across the department, and students from the Quantum Technologies Centre for Doctoral Training at the University of Bristol. Non-SAMBa students will not be expected to present or write up a report, as the SAMBa students are, but will of course be welcome to do so if they would like to.

Many academics from the Department of Mathematical Sciences will participate in the ITT, alongside academics from the departments of Pharmacy and Pharmacology and Management. These are both academics who have worked with the partners attending, and those who have had no interaction with them.

It is expected that all participants of the ITT commit to attend for the full week and that they are fully engaged on each day. There will be plenty of flexibility in the planning so if we find that something is not working, we will be able to change the format (within reason) as we go along. The timings have deliberately been kept flexible to allow this to happen. The Friday of the ITT will be an Observation Day where people interested in future ITTs, or other ways to engage with SAMBa, will be present to see what has come out of the week.

3 List of Participants

Students and postdocs

- Aoibheann Brady (SAMBa 2015)
- Thomas Burnett (PhD, Bath)
- Federico Cornalba (SAMBa 2015)
- Gianluca Detommaso (SAMBa 2015)
- Emiko Dupont (SAMBa 2016)
- John Fernley (SAMBa 2016)
- Uziel González (SAMBa 2016)
- Elizabeth Gray (SAMBa 2016)
- Emma Horton (PhD, Bath)
- Marcus Kaiser (SAMBa 2014)
- Nadeen Khaleel (SAMBa 2016)
- Matthias Klar (SAMBa 2016)
- Amélie Klein (SAMBa 2016)
- Matt Lee (SAMBa 2016)
- Andrea Lelli (SAMBa 2015)
- Alice Maciel Tabosa (PhD, Bath)
- Kgomotso Morupisi (PhD, Bath)
- Ellen Murphy (CRA, Bath)
- Daniel Ng (SAMBa 2016)
- Sandra Palau Calderón (Postdoc, Bath)
- Sam Pallister (Quantum Tech CDT)
- Robbie Peck (SAMBa 2015)
- Tom Pennington (SAMBa 2016)
- Lizzi Pitt (SAMBa 2016)
- Ben Robinson (SAMBa 2015)
- Malena Sabate Landman (SAMBa 2016)
- Tsoogii Saizmaa (SAMBa 2016)
- Cameron Smith (SAMBa 2016)
- Stasja Stanisic (Quantum Tech CDT)

University of Bath academics

- Karim Anaya-Izquierdo (Maths)
- Nicole Augustin (Maths)
- Chris Budd (Maths)
- Alex Cox (Maths)
- Begoña Delgado-Charro (P & P)
- Evangelos Evangelou (Maths)
- Julian Faraway (Maths)
- Silvia Gazzola (Maths)
- James Hook (Maths)
- Antal Járαι (Maths)

- Chris Jennison (Maths)
- Marcel Ortgiese (Maths)
- Dimitris Paraskevopoulos (Management)
- Tiago Peixoto (Maths)
- Ilaria Prosdocimi (Maths)
- Matt Roberts (Maths)
- Tim Rogers (Maths)
- Theresa Smith (Maths)
- Jane White (Maths)
- Kit Yates (Maths)

Partners

- Alun Bedding (Roche)
- Federica Cattani (Syngenta)
- Chris Harbron (Roche)
- Francois Mercier (Roche)
- Kim Travis (Syngenta)

SAMBa team

- Susie Douglas (Manager)
- Andreas Kyprianou (Co-Director)
- Paul Milewski (Co-Director)
- Jess Ohren (Administrator)
- Fran Staples (BIRD)

Observer Day attendees

- Nick Brook (Dean of Science)
- Jon Dawes (Maths)
- Tina Düren (Chemical Engineering)
- Richard Guy (P & P)
- Darrell Patterson (Chemical Engineering)
- Can Evren Yarman (Schlumberger)

4 Summary of ITT5

Start time: 9:30 End time: before 17:30	Monday	Tuesday	Wednesday	Thursday	Friday OBSERVATION DAY
	Coffee				
Morning (before 12:30)	<ul style="list-style-type: none"> • Introduction to ITT • Presentations of problems 	<ul style="list-style-type: none"> • Presentations of problems • Group discussion 	<ul style="list-style-type: none"> • Team work with roving academics 	<ul style="list-style-type: none"> • Team work with roving academics 	<ul style="list-style-type: none"> • Consolidation of ideas/briefing • Student presentations
	Lunch				
Early afternoon (before 15:30)	<ul style="list-style-type: none"> • Group discussion 	<ul style="list-style-type: none"> • Group discussion • Form working teams 	<ul style="list-style-type: none"> • Team work with roving academics 	<ul style="list-style-type: none"> • Team work with roving academics 	<ul style="list-style-type: none"> • Student presentations • Summing up
	Coffee				
Late afternoon (before 17:30)	<ul style="list-style-type: none"> • Further background presentations 	<ul style="list-style-type: none"> • Consolidation 	<ul style="list-style-type: none"> • Student presentations • Review progress 	<ul style="list-style-type: none"> • Team work with roving academics 	<ul style="list-style-type: none"> • Informal discussion and refreshments
	Break				
Evening	<ul style="list-style-type: none"> • Informal discussion with drinks 	<ul style="list-style-type: none"> • Participant dinner 	<ul style="list-style-type: none"> • Optional late working with pizza 		

Summary of programme for ITT5

5 Structure of ITT5

5.1 Monday 30th January, 9:30 - 17:30

Aim of the day:

To gain a full understanding of high-level non-academic problems, through presentations and group discussions, and to determine the direction further discussions should take during the rest of the week.

Introduction and welcome, 30 minutes

Andreas Kyprianou, Paul Milewski, and Susie Douglas, of SAMBa will welcome everyone to the ITT and explain the format of the week. This will augment the information provided in this booklet.

Presentation of problems and discussion

The first two days will be devoted primarily to understanding the nature of the problems that Roche and Syngenta have, and distilling them into mathematical language. It is important at this stage that the ITT participants fully understand the context of the problems that they are being presented with. Therefore, this session should be seen as a very open and supportive one, with no question being judged as trivial or stupid.

There will be a number of presentations from non-academic and academic participants who have experience of working on the sorts of problems being presented. Whilst non-academic representatives will present high level problems that their organisations are facing, the academics will give a flavour of the approaches that can be used to work on these sorts of problems. It is not expected that the approaches described will necessarily be the ones that are taken forward during the rest of the ITT, where the focus is primarily on developing new areas of research, and exploring a range of different routes to do this.

Presentation of procedure problems 2 hours

The session will be chaired by **Andreas Kyprianou** and presenters are:

- Chris Harbron (Biomarkers and Personalised Healthcare)
- Alun Bedding (The Design of First in Human Clinical Trials)
- Kim Travis (Ranking based on Heterogeneous Data)
- Kim Travis (Formulation Toxicity)
- Evangelos Evangelou (Statistical problems from Syngenta)

Group discussions on procedure problems 2 hours

Following the presentations, there will be a chance to discuss the information presented in a plenary session. The participants will then split into small, pre-determined **groups** and work together to identify 3 or 4 key mathematical questions that have arisen from the information so far and that they feel warrant further discussion during the week. Each of these groups has been assigned an academic chair, who is responsible for ensuring that discussions stay on track and that everyone contributes.

After the group discussion, there will be a further plenary session where the groups will share the questions that they have identified and these will be clustered into potential areas for further work during the week.

Further presentations *1 hour*

The day will end with some background presentations that may come in useful during the remainder of the week.

- Chris Jennison (Interim Monitoring of Clinical Trials)
- Tom Burnett (Adaptive Enrichment Designs for Clinical Trials)

Informal discussion

There is the opportunity to stay on after day 1 to meet more of the participants, drinks will be provided at the BRLSI.

5.2 Tuesday 31st January, 9:30 - 17:30

Aim of the day:

To gain a full understanding of high-level non-academic problems, through presentations and group discussions, to determine the direction further discussions should take during the rest of the week, and to form teams for working on problem formulation for the rest of the week.

Presentation of *model problems* 2 hours

The session will be chaired by **Paul Milewski** and the day 2 presenters are:

- Federica Cattani (What does shaking do to a bag of seeds? Predicting collisional mass exchange)
- Kim Travis (Dermal Absorption)
- Francois Mercier (Challenges and opportunities in the statistical modelling of tumour size time dynamics in oncology clinical trials)
- Jane White (Dermal Absorption)

Group discussions on *methods problems* 2 hours

Initially there will be a review and discussion of the information presented during a plenary session. The participants will then split into small, pre-determined **groups** and work together to identify 3 or 4 key mathematical questions that have arisen from the information so far and that they feel warrant further discussion during the week. Each of these groups has been assigned an academic chair, who is responsible for ensuring that discussions stay on track and that everyone contributes.

After the group discussion, there will be a further plenary session where the groups will share the questions that they have identified and these will be clustered into potential areas for further work during the week.

Review material and form working teams 1 hour

At the end of the two group discussions, there should be a fair number of problems (5-10) that have been identified for further work during the week. The next step is to determine which of these problems will be pursued and who will be part of the associated **teams** working on them.

There will be an initial discussion between the student participants and the SAMBa management to determine what problems the students are keen to pursue and ensure that there are a quorum of 2-3 students per team. These teams and problems will then be presented briefly to the rest of the participants. It is expected that some participants will immediately identify with one problem and will therefore commit to that team for the rest of the week. This is particularly the case for non-academic attendees whose expertise will be essential during the team work, but it is also hoped that a small number of academics will join each team.

Some of the academics may feel that they have interests across more than one problem, some expertise that underpins a large amount of the mathematics being discussed, or an area of research that they would like to pursue independently of the teams that have been formed. All of these situations are acceptable and indeed welcome. Academics may choose to:

- *Float* between teams, sharing the outputs of discussion where relevant
- *Tutor* teams in a mathematical concept fundamental to the discussion by running short tutorials that participants can attend
- *Splinter*, forming an academic discussion team on a different topic

Although some indication of the role each participant will play should be given during day 2, it will be possible to change teams and roles during the course of the week. Student participation is fixed for the whole week.

Consolidation of information and team planning *1 hour*

There will be a chance during the afternoon of day 2 to begin working on the problems that have been identified. Teams may choose to start working together immediately but this is also the chance for individuals to have some time to review what they have been presented with, and pursue further reading and investigation should they wish to do so. There is no prescribed way of working through the information and every approach is acceptable. However, it is important that from the beginning of day 3, the team is ready to start working intensively together.

On the evening of day 2, there will be a participant dinner held at Hall and Woodhouse. This will be a chance for further discussion on what has been covered during the first 2 days and other opportunities.

5.3 Wednesday 1st February, 9:30 - 17:30

Aim of the day:

To begin developing problem formulation. Students to present (*for assessment*) on early approaches being taken.

Team work *5 hours*

Teams focus on the problems, considering how they could develop a challenging and quality research project from it. Those participants not in teams will *float*, *tutor* or *splinter*, or a combination of the three.

Student presentations *1.5 hours*

At least one student member of each team presents for *10 minutes* on the approach that is being discussed. SAMBa students are expected to present at least once during the week, and will be assessed on this but, time permitting, other students are also encouraged to present.

This is a chance to obtain feedback and further expertise on the problems, and it is not expected that what teams present here will be their final approach to the problem.

More team work

Those who would like to stay late on Wednesday should let us know by lunch time and we will order pizza to help the thought process. There is only one of the smaller rooms available so there will not be room for everyone to stay.

5.4 Thursday 2nd February, 9:30 - 17:30

Aim of the day:

To formulate a research problem that can be taken forward into a future project.

Team work *all day*

Teams will work together, utilising the resources around them and interacting where necessary. There will be the chance to come back together into plenary, if requested by the participants.

5.5 Friday 3rd February, 9:30 - 15:00

Aim of the day:

To consolidate and summarise the problem formulation via *assessed student presentations*. To identify outputs, determine next steps and share feedback.

Observer Briefing *1.5 hours - in parallel*

Invited observers will meet with SAMBa management who summarise the week. There is then the chance to network with ITT participants.

Consolidation of ideas *1.5 hours - in parallel*

A chance for teams to finalise their problem formulation and consider the future work which could ensue.

Student presentations *2 hours*

At least one student member of each team presents for *15 minutes* on the final formulation of the problem that they have discussed. SAMBa students will be assessed on this (and *must* present if they have not earlier in the week) but other students are also encouraged to present, time permitting.

Summing up *1 hour*

This session will be led by the SAMBa Management and will summarise the outputs of the week, and outline the next steps. Feedback in writing is also requested after the event.

Informal discussion

There will be a chance to interact with all participants less formally, reflecting on the achievements and hard work of the week. Refreshments will be provided.

5.6 After the ITT

There will be a number of activities that will be pursued post-ITT

SAMBa student proposals

SAMBa students must each write a proposal for a project, based on the formulation that was developed during the ITT week. The aim of this is to give students a chance to develop their skills in developing a route to pursue research. A document, based on the style of an EPSRC call for proposals, outlining the expected structure and content of the ITT proposal, is included as an annex. The proposals submitted will be assessed by the SAMBa Management team and other participants where deemed appropriate.

Future projects

Non-academic partners will discuss the potential projects that have been identified, with the SAMBa Management team, determining the routes to how they could be supported. This could take a number of routes:

- Student PhD projects, wholly or partially supported by partners
- Student PhD projects, with influence from partners
- Short-term, focussed, application-motivated projects (led by Bath IMI)
- Development of a proposal to a funder, such as EPSRC, to explore fundamental mathematical concepts with associated financial support
- Further discussion and contemplation of an idea with additional expertise from the Department, University, IMI or further afield

Developing future ITTs

ITT6 takes place in June 2017 and the experience and feedback from ITT5 will be essential in planning for this and future ITTs. Please complete your feedback forms to make sure that we can keep improving the experience.

6 Annex 2: Call for ITT proposals

Submission deadline: 24th February 2017

As part of the SAMBa training programme, students are expected to learn about and experience the process of writing grant proposals.

6.1 Writing a research proposal

All academics in the UK fund their research through a mixture of sources. This funding pays for the time of permanently based academics on the project (typically one of which will be formally applying for funding), as well paying for temporary research costs, such as a PhD studentship, 2-3 years of a postdoctoral researcher's salary, scientific equipment, travel, networking meetings and much more.

There are a number of major funders supporting Mathematics research in the UK and they all have different schemes and routes to funding.

These are:

- **Engineering and Physical Sciences Research Council (EPSRC):** a Government agency which is part of Research Councils UK (RCUK) and funds 200M GBP of Mathematical Sciences research in the UK. RCUK also consists of BBSRC (Biotechnology and Bio Sciences Research Council), NERC (Natural Environment Research Council), STFC (Science and Technology Facilities Council), AHRC (Arts and Humanities Research Council), ESRC (Economic and Social Science Research Council). All of these Councils also fund Mathematics research where it has an impact on their research areas.
- **European Commission:** this includes a large number of different schemes and mechanisms including the Marie Skłodowska-Curie programme, the European Research Council and Horizon 2020. All areas of research and training are funded and the impact of the research is as important as quality.
- **Leverhulme Trust:** a charitable body which supports research in all areas. They are particularly keen on research which has a benefit to society.
- **Royal Society:** a learned society, which funds primarily fellowships and networking activities in science, engineering and medicine.
- **London Mathematical Society:** a learned society which awards a variety of small grants for internships, travel, conference attendance and networking, amongst other things.
- **Institute of Mathematics and its Applications:** funds small grants and networking activities across Universities and schools.

Research proposals for these agencies are peer reviewed. That is to say, leading academics in the field are asked to provide a commentary on the quality, novelty, impact and relevance of the proposed research. In many cases, and in order to guarantee a degree of uniformity, reviewers are asked to complete a standard form which asks them to address specific questions about the

proposal. These forms are collated and brought to a further panel of experts who finally decide which proposals will receive funding.

In industry, where scientific research is taking place in a large organisation, it is often the case that research groups or individuals must write cases for internal financial support following a similar pattern to the way academics obtain funding. The main difference in that case is that the awarding body is the company itself, and no public funds are involved. For this reason, the criteria used to assess proposals may be quite different from those of, for example, EPSRC. Nonetheless, it is an important part of the process that the applicant can demonstrate the relevance of the research against the criteria of the awarding body.

6.2 ITT proposal

Following the ITT, students are asked to prepare a report in the style of a research proposal (the **Case for Support**). The format of this proposal, outlined below, is styled on a real call document. The main difference, however, is that the proposal need not specify details concerning the financial costing of the proposed research.

6.2.1 Introduction

For the purposes of this exercise, this proposal should be written as if the project has every intention of being carried out. It is likely that some of the proposals will form the basis of thesis formulation reports but they will not be supported as proposed.

Proposals will be reviewed using forms mimicking that attached in **Annex 2**. In addition reviewers will be asked to assign a score to each section and an overall score out of 100.

6.2.2 Assessment Criteria

There are a number of criteria which proposals will be assessed against. These are:

- **Quality:** the novelty and timeliness of the research proposed, in the context of the research area more generally
- **Impact:** including how realistic the impact described is, what activities will be undertaken to realise it, and whether the right interested parties have been identified
- **Approach:** the methodology proposed, whether this is feasible and appropriate for the challenges described, and whether the routes to involve partners is appropriate

6.2.3 Case for Support

Description of proposed research and its context (max. 7 sides of A4)¹: Describe the proposed research and its context, to aid those reviewing your proposal in understanding what you plan to do and achieve, and where it fits into the current research activity. The document should include:

- **Background.** Introduce the proposal topic and explain its academic and applied context. To do this, you need to demonstrate understanding of related past and current work, explain the

¹Lists of references and illustrations should be included in the seven A4 page limit, and not be submitted as additional attachments or as an annex.

long term effects of the proposed research, how it contributes to the health of other research disciplines, current or future economic success, future development of emerging industries or addresses societal challenges.

- **Impact.** Describe how your research would benefit researchers in the field and related disciplines, and what will be done to ensure that they can benefit. Explain collaborations with other researchers and their role in the project. Describe who potential beneficiaries outside the academic research community might be, and how the research might impact them.
- **Research hypothesis and objectives.** Set out your research ideas or hypotheses. Explain why the proposed project is novel and timely, both from societal and academic viewpoints. Identify the overall aims of the project, and the measurable objectives the outcome of the work will be assessed against.
- **Programme and methodology.** Detail and justify research methodology. Describe the work programme, detailed for each member of the research team, indicating research to be undertaken and milestones that will be used to monitor its progress. Explain how the programme of research will be managed.

In a real proposal, the Case for Support is your opportunity to convince peer reviewers that your research should be funded. Therefore, it needs to be written in a clear, concise and jargon free style. Describe how potential benefits align with existing priorities; and how it complements other research activity in the field. Explain what is exciting about the research to your audience, in particular your reviewers. You need to convince experts in the relevant research field about the value of your project. Convince reviewers your proposal is original, and describe your objectives clearly and succinctly. In real life, proposals are not rejected just because others are doing similar work, but if you don't describe the novelty of your approach or the likelihood of success, the value of your proposal is uncertain. Don't leave it to the proposal assessor to ask questions. Show that you have thought the proposal through, and explain how it will succeed. Potential applications might be obvious to you, but leave no doubt in reviewers' minds.

7 Annex 3: Assessment form for ITT proposals

Assessment Criteria

- **Quality:** the novelty and timeliness of the research proposed, in the context of the research area more generally
- **Impact:** including how realistic the impact described is, what activities will be undertaken to realise it, and whether the right interested parties have been identified
- **Approach:** the methodology proposed, whether this is feasible and appropriate for the challenges described, and whether the routes to involve partners is appropriate

Quality

	/35
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Impact

	/30
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Approach

	/35
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Other comments

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Conclusions

	/100
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Notes

Notes