



Where's the Maths?

Welcome

From SAMBa



#WherestheMaths



SAMBa: Statistical Applied Maths at Bath

- 160+ PhD students over 13 years
- MRes + PhD
- Fusion of stochastics, statistics, (numerical) analysis, computation, and applied mathematics, preparing students to work in academia or outside
- Funded by EPSRC and University of Bath
- 27 external partners and good links with departments across campus
- Integrative Think Tanks are flagship event, twice a year
- Lot of joint activities: events, grant proposals, PhDs
- **Students choose and scope their own PhD projects**
 - 12 students in current year 1 cohort
- Key people: Paul Milewski, Andreas Kyprianou, Alex Cox, Melina Freitag, Tim Rogers, Jess Ohren, Susie Douglas
- More at www.bath.ac.uk/samba

Here's the Maths

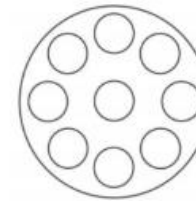
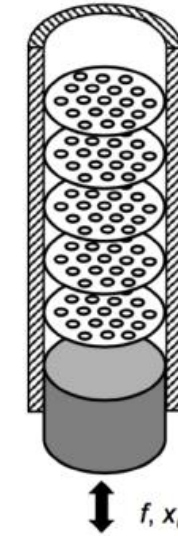
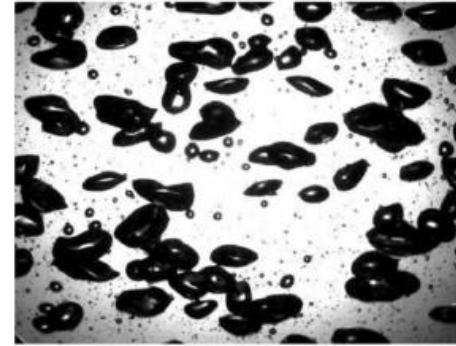
Oscillating Bubble Column Reactors & Fragmentation-Coalescence processes

Nuno Reis (Chemical Engineering)

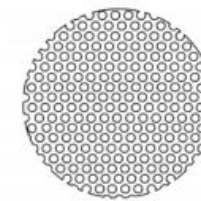
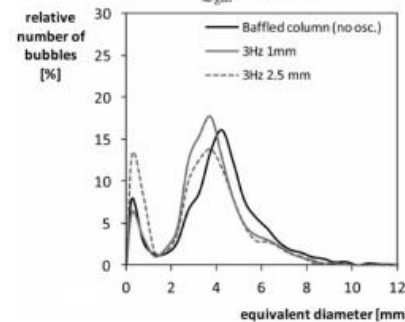
Tim Rogers (Mathematical Sciences)

Oscillating Bubble Column Reactors

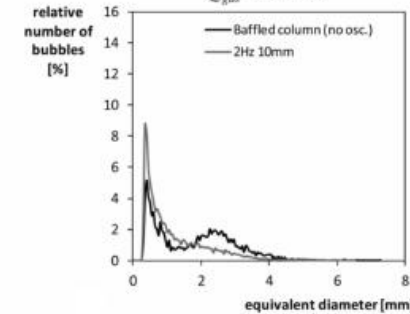
- Bubble column reactors used for gas-air reactions
- New idea: speed up reactions by oscillating the bubble column
- Efficiency of reactor linked to distribution of bubble sizes
- Need mathematical model to predict bubble sizes and optimise design



$Q_{gas} = 0.01$ vvm



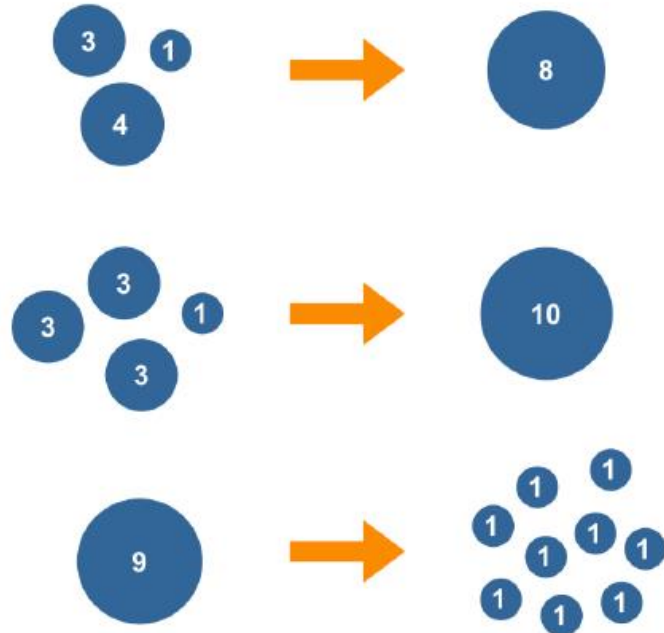
$Q_{gas} = 0.04$ vvm



Fragmentation-Coalescence processes

Theorem 2. *If α satisfies (6) and m is the smallest integer such that $\alpha(m) > 0$, then the stationary cluster size distribution exists and is unique. In particular, the limit of this stationary distribution as $\lambda \rightarrow 0$ exists and obeys*

$$\lim_{\lambda \searrow 0} p_k = \begin{cases} \frac{1}{k} \left(\frac{m-1}{m}\right)^k \left(\frac{1}{m}\right)^{\frac{k-1}{m-1}} \binom{m \left(\frac{k-1}{m-1}\right)}{\frac{k-1}{m-1}} & \text{if } m-1 \text{ divides } k-1 \\ 0 & \text{otherwise.} \end{cases}$$



EPSRC proposal

Part II: Pathways to impact (2 pages)

Positioning of the project: The research proposed is in the field of applied probability, but it is underpinned by theoretical results that are relevant to applications in the real world. As discussed earlier, there is a vast array of disciplines within the applied sciences, engineering, economics and social science for which fragmentation-coalescence are relevant. On this point it is worth repeating on the genesis of the proposed research, which has emerged naturally from the submission of a series of unusual scientific crossovers. Following a confidential invitation to the Home Office several years ago, Iyengar learned about the use of fragmentation-coalescence processes in the modelling of terrorist cells (see e.g. [8]), and the mathematical challenges of developing a rigorous theory for these processes. This led to the co-supervision of a PhD student between Iyengar and Rogers, culminating in the paper [17, 18]. These two works have opened up a number of natural questions which we address in the proposal, but have also raised the prospect of connections with the theory of genetic diversity as well as with population models with competition (see e.g. [19, 23, 25]). Later, at an intensive research workshop supported by the Royal Society EPSRC Centre for Doctoral Training SAMBA, the unexpected connection was made with the work of biophysicist Nuno Reis (Reader in Chemical Engineering at the University of Bath). Discussions with Dr Reis have highlighted the exciting possibility of an experimental realisation of known fragmentation-coalescence processes that could, in time, provide a pathway from the theoretical research we propose here to real impact in industrial chemistry.

Application to chemical engineering:

Fragmentation-coalescence processes, and particularly their spatial extensions, are not just fascinating and deep mathematical constructs: they in fact have an experimental realisation in the field of chemical engineering. A Bubble Column Reactor (BCR) is a device designed to control gas-liquid chemical reactions, for example in the manufacture of synthetic fuels, or the treatment of wastewater. The principle is simple: gas is injected continuously into a vertical chamber of liquid reactant, forming bubbles which rise and coalesce. Dr Reis and his team are developing new design of high-performance reactor in which the system is agitated by an oscillating pump, driving rapid fragmentation of large bubbles as they are forced through perpendicular baffles (see Figure 2(a)). The accelerated speed of reaction in this Oscillating Bubble Column Reactor (OBCR) depends on the size and spatial distribution of the bubbles formed, depending on the design of the baffles, and the gas injection dynamics; different stationary bubble size profiles are obtained (see Figure 2(c)). Control over the distribution of bubble sizes allows the reaction to be controlled and optimised in respect to yield and cost. For example, in [2] Dr Reis and his team demonstrated 100% oxidation (i.e. zero levels in soot) degradation of a pollutant, achieved by tuning the conditions of bubble fragmentation-coalescence. Understanding in general the mix from reactor design to bubble size distribution is, however, a considerable theoretical and technical challenge that is currently limiting the rate of development of this promising new technology.

A key activity in our pathway to impact will be to explore application of our probabilistic models to a range of gas-liquid reactions in this new reactor design. The work will have two phases:

- Impact investigation: Oscillating Bubble Column Reactors as FFC processes**
[C.6] Explore the potential of OBCR technology as a novel experimental realisation for out-of-equilibrium FFC processes. In Work Package [B.6], we propose to study the role of external drivers such as emigration (the continuous addition of new progenitor blocks) and extinction (the removal of mass from the system) in holding FFC processes far from equilibrium. It appears that these processes map naturally onto the mechanical operation of OBCR; Dr Reis and his team will adapt the existing setup to create an experimental realisation of a driven FFC process. As a first step the team will design and construct an experimental rig in which coalescence and fragmentation events can be observed in data



Figure 2: Example of image capture in bubble column reactor [2].

Theoretical results of this package will then be used to generate predictions about OBCR performance that can be tested in experiments.

As we stressed above, the purpose of this proposal is to design a deeper mathematical understanding of FFC processes. The application to OBCR technology is very promising, and we expect that the pathway to impact identified here will be extended beyond the end of the project, via an applied proposal more directly focussed on explicit detailed modelling of OBCR dynamics.

Outreach: We will take the opportunity to align existing funding with this project and ensure that the topic of fragmentation-coalescence is represented at an existing LMS workshop: Theoretical Structures from the Discrete to the Continuous that we currently have funding for at the very start of the project. At the end of second year of the research programme we will run a workshop on 'Fragmentation-Coalescence Processes in the Real World'. The workshop is limited carefully to showcase our results and, ideally, the physical realisation of FFC developed in [C.6], and to maximise the chances of eventual non-academic impact for the research undertaken in this project. In this workshop we will bring together industrial experts in the field, along with potential industrial partners and scientists from a range of application areas with an interest in fragmentation-coalescence models, including wastewater treatment, multiphase reactions and fermentation processes including biobubble production. This will provide an opportunity for dissemination and for making new connections between mathematical theory and out-world applications.

Training opportunities: A secondary route to impact for the project will be through the training provided to the PDRA, who will gain valuable skills and experience in mathematical modelling and analysis much needed by industry and academia alike. All parts of the project will be run in collaboration with a PDRA who, through this project, will receive excellent training in one of the UK's most vibrant mathematical departments with around 100 PhD students and approximately 20 postdocs, many of whom are working at the interface of probability, statistics and applied analysis. The PDRA will have the benefit of the training in future. In addition, the PDRA will be engaged in a variety of extra-curricular activities beyond their immediate research interests (seminars, workshop attendance and organization, reading groups, etc.). This LDRD based a large number of students each semester and junior members of the laboratory are strongly encouraged to interact with them. Through the project's collaboration with Chemical Engineering, there will additionally be opportunities to engage with training and dissemination activities at Chemical Sustainable Technologies and Water Infrastructure CDTs.

- [1] P. FERRER, F.M. SORSA, D.Z. AYIYI, M.M. MOGRI, M.D. BIRN, A.M. (2020) dissolution and design aspects of a multi-phase oscillatory baffled column. *Industrial and Engineering Chemistry Research* (2014), 53(44), pp. 17303
- [2] LUCAS, M.D., FERRE, M.M., LI, PING, G. (2019) Modelling of coalescence processes in a novel, novel, multi-phase oscillatory baffled column. *Chemical Engineering Journal* (2019) 296, pp. 308
- [3] FERREIRA, A., FERREIRA, D., THOMAS, J.A., ROCHA, F. (2016) Stochastic and nonlinear wave propagation in disordered hydrocolloids and foams trapped in a bubble column. *Chemical Engineering Journal* (2012) 181, pp. 216



Where's the Maths?

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Where's the Maths?

Where's the Maths



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Where's the Maths?

Paul Shepherd

Architecture and Civil Engineering

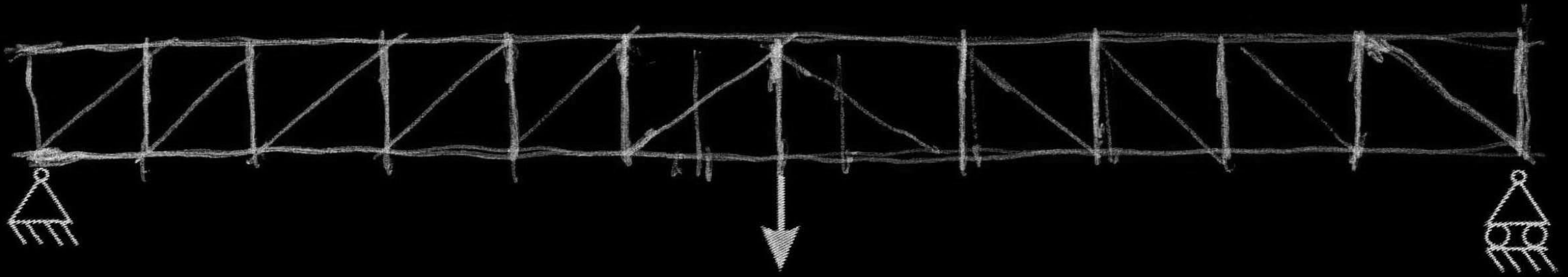


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Clustering of Hand Sketches for Structural Analysis

Paul Shepherd

Architecture & Civil Eng & IMI





Where's the Maths?

Anton Souslov

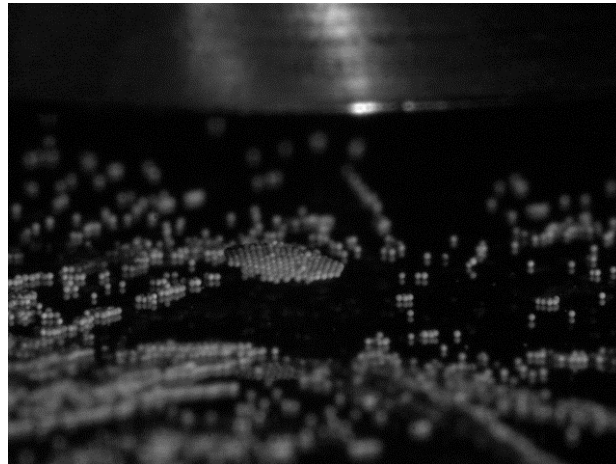
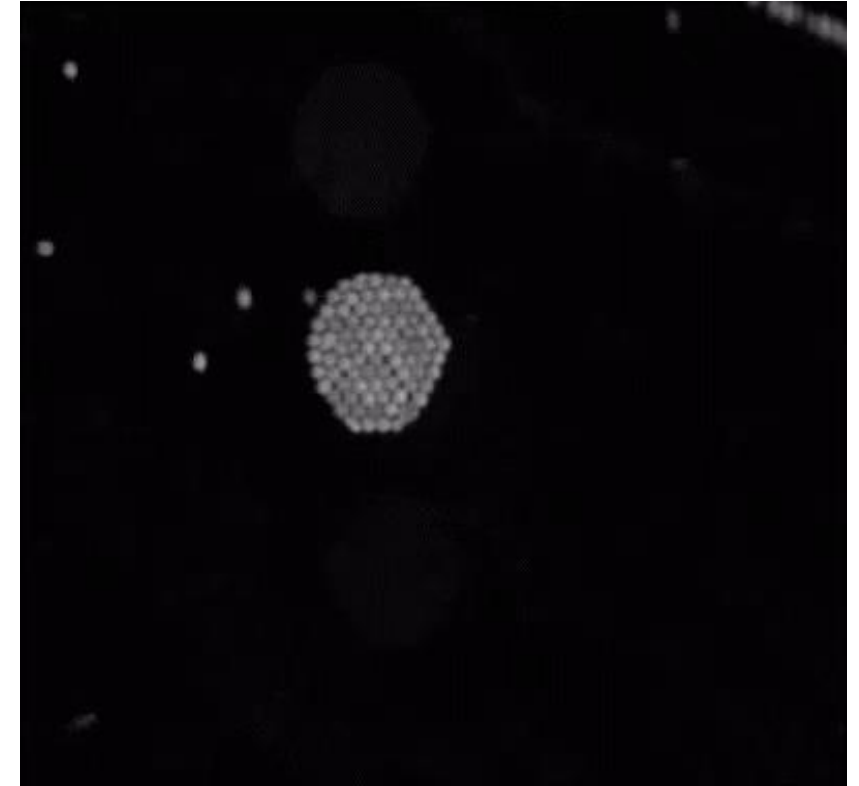
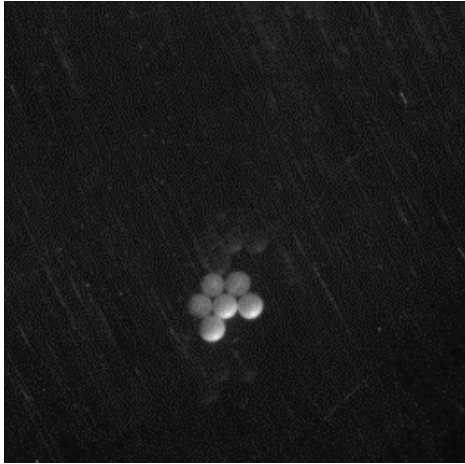
Physics



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Why do acoustically levitated clusters spin?

Anton Souslov



Cluster formation by acoustic forces and active fluctuations in levitated granular matter
Melody Lim, AS, Vincenzo Vitelli, Heinrich Jaeger. *in press, Nature Physics* (2019) [arXiv:1808.03862](https://arxiv.org/abs/1808.03862)

Department of
Physics





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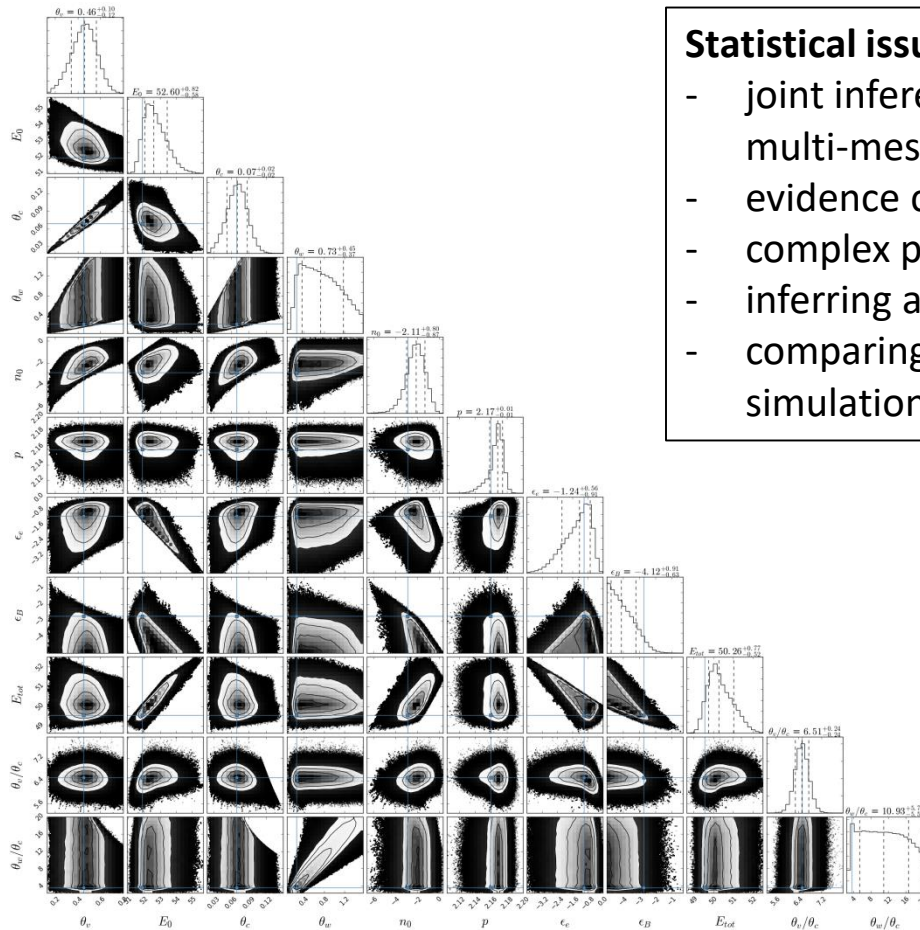
Hendrik Van Eerten

Physics



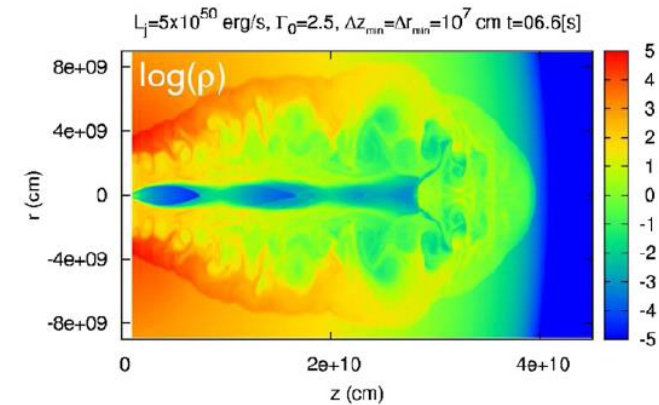
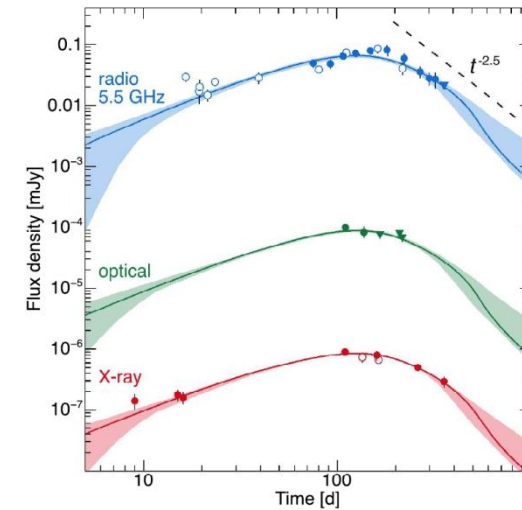
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The statistics of inferring the physics underlying cosmic explosions from comparing computational models to electro-magnetic and gravitational wave observations



Statistical issues:

- joint inferences from multi-messenger data sources
- evidence comparison models
- complex priors
- inferring at larger sample level
- comparing noisy numerical simulations to noisy data



Hendrik van Eerten, lecturer in astrophysics, Physics Dept.



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Carolyn Villforth

Physics

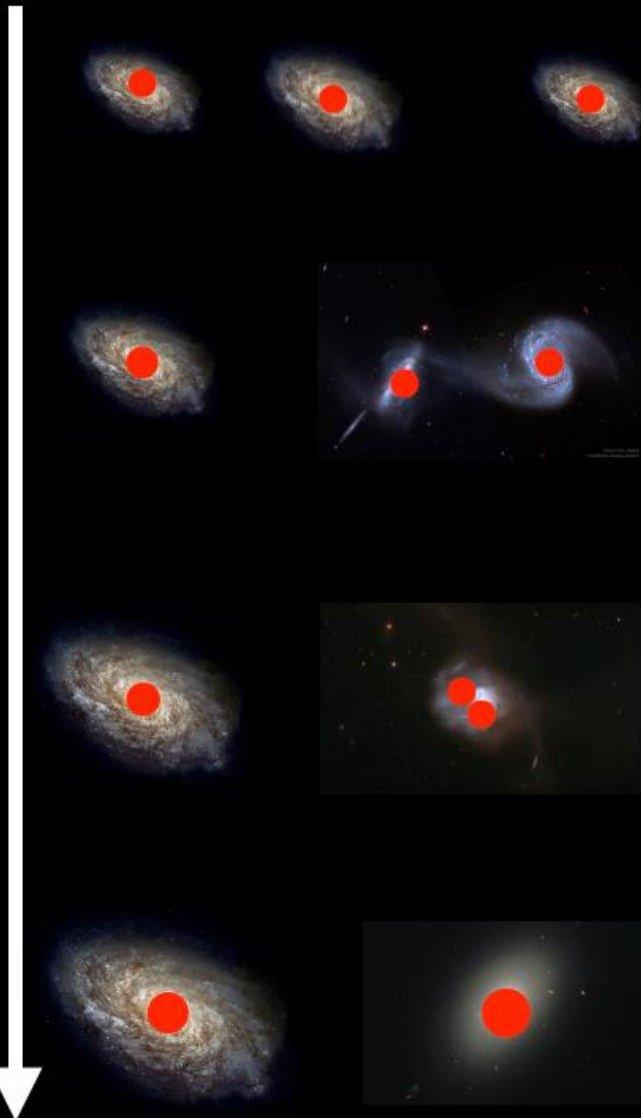


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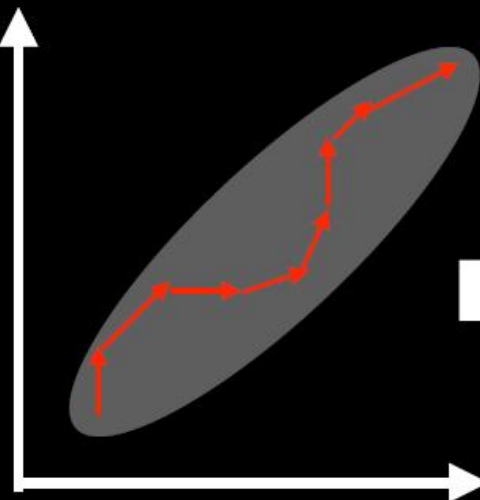
Connecting the growth of supermassive black holes and galaxies

Carolin Villforth (Physics)

time



log(Black Hole Mass)



log(Galaxy Mass)

Modelling of
observed data

With Beate Erhardt (IMI)

- M1: $\log(L_{60}) \sim \log(M) + \log(L_x) + z + \text{Fields}$
 - M2: $\log(L_{60}) \sim \log(M) + z + \text{Fields}$
 - M3: $\log(L_{60}) \sim z + \text{Fields}$
- Model comparison

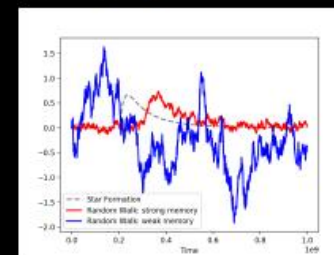
Res.Df	RSS	Df	Sum of Sq	F	Pr[>F]
230	18.29314	NA	NA	NA	NA
231	18.30965	-1	-0.0165099	0.2075798	0.6491008
232	18.70553	-1	-0.3958773	4.9773730	0.0266460

Creating Stochastic Models of BH growth

With Beate Erhardt (IMI)

$$dL(t) = N(\mu(t), \sigma)$$

$$\mu(t) = -\alpha(L(t-1) - \beta(\text{SFR}(t-\delta)))$$



How can we recover the physically interesting coevolution on short timescales?
(Given only sample properties and limited sampling in time)



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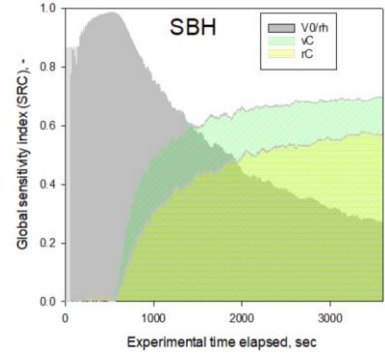
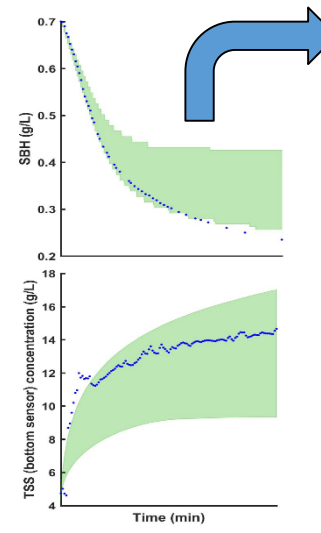
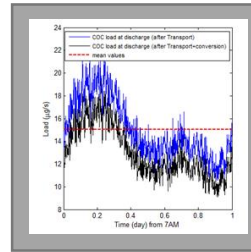
Benedek Plosz

Chemical Engineering

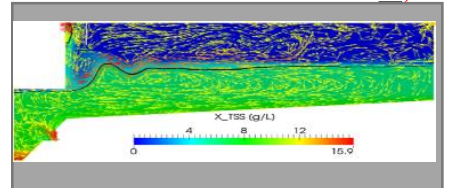
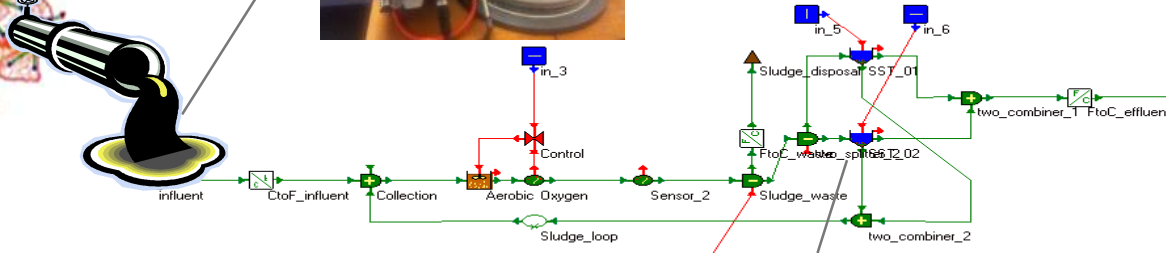
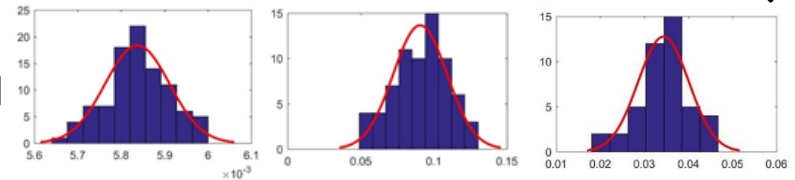


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Data handling, model identification and parameter estimation for climate change adaptation in urban water treatment



$$v_s = \begin{cases} v_H = v_0 e^{-r_H X_{TSS,i}}, & X_{TSS,i} \leq X_{TSS,c} \\ v_H \left(1 - \frac{\rho_s}{(\rho_s - \rho_f)g} \cdot X_{TSS,i} \frac{\partial \tau}{\partial X_{TSS,i}} \frac{\partial X_{TSS,i}}{\partial z} \right), & X_{TSS,i} > X_{TSS,c} \end{cases}$$





Where's the Maths?

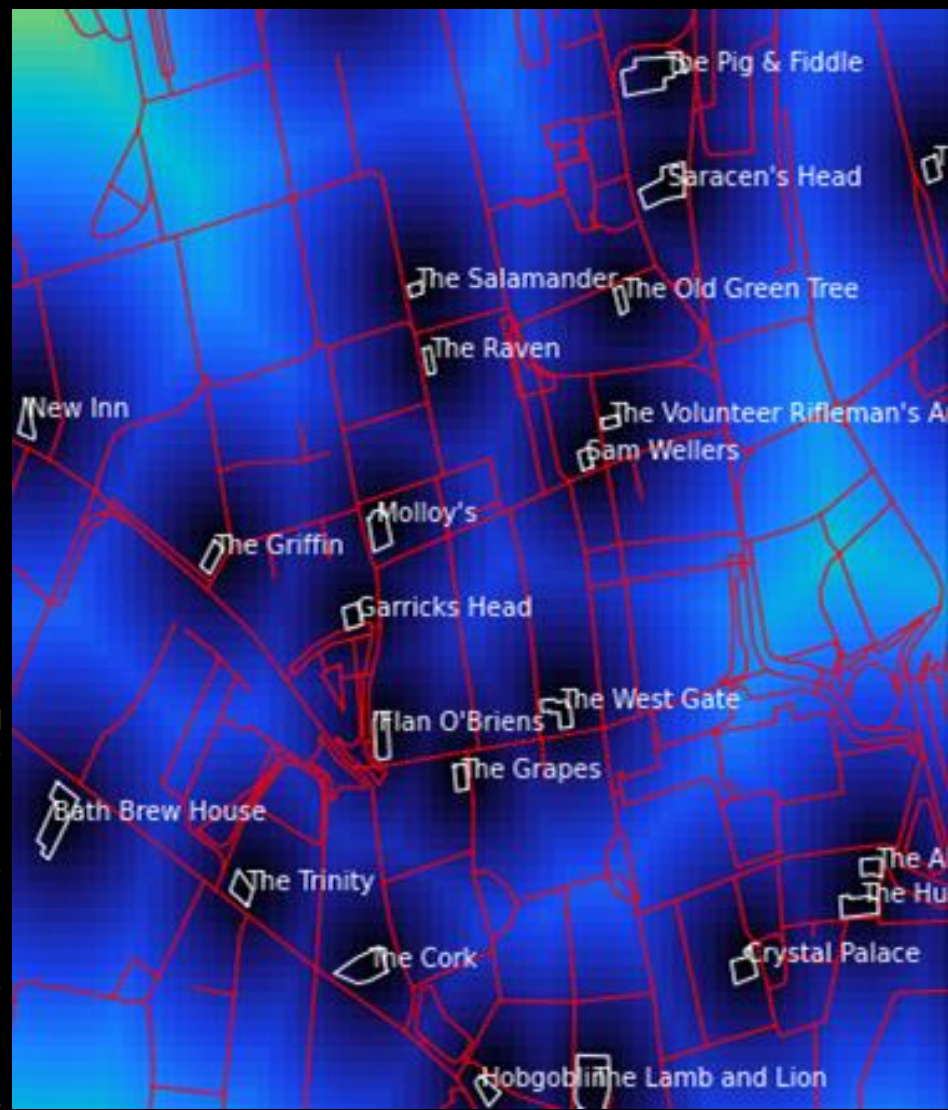
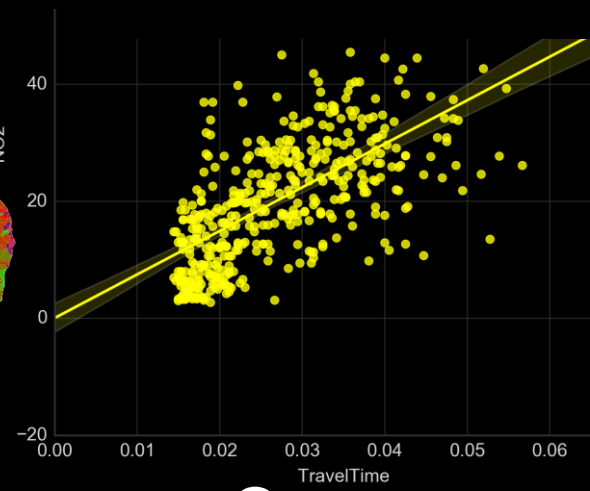
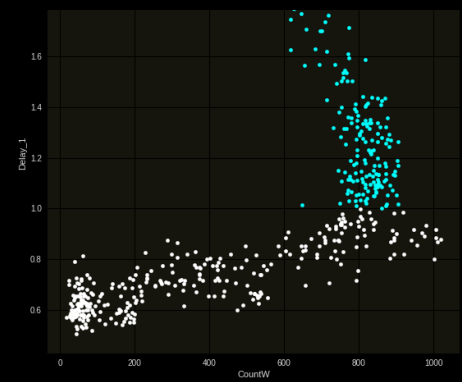
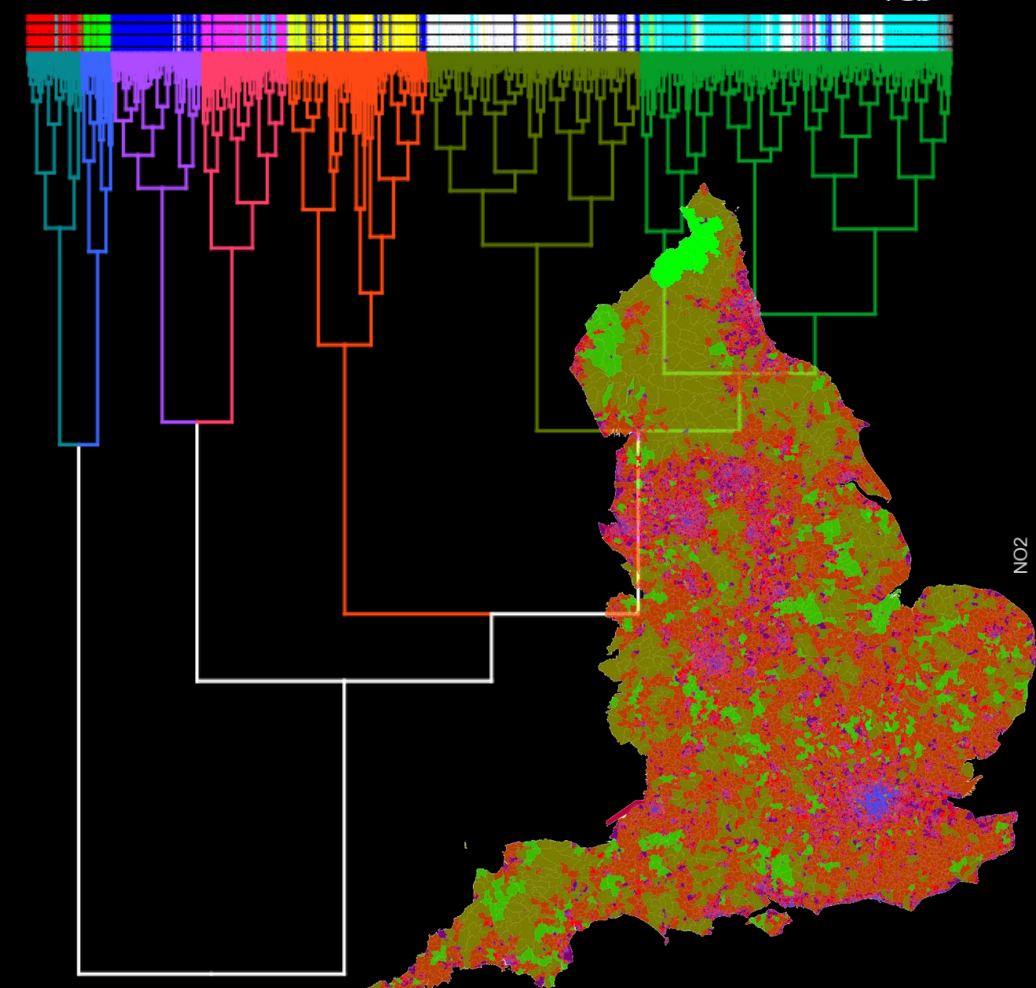
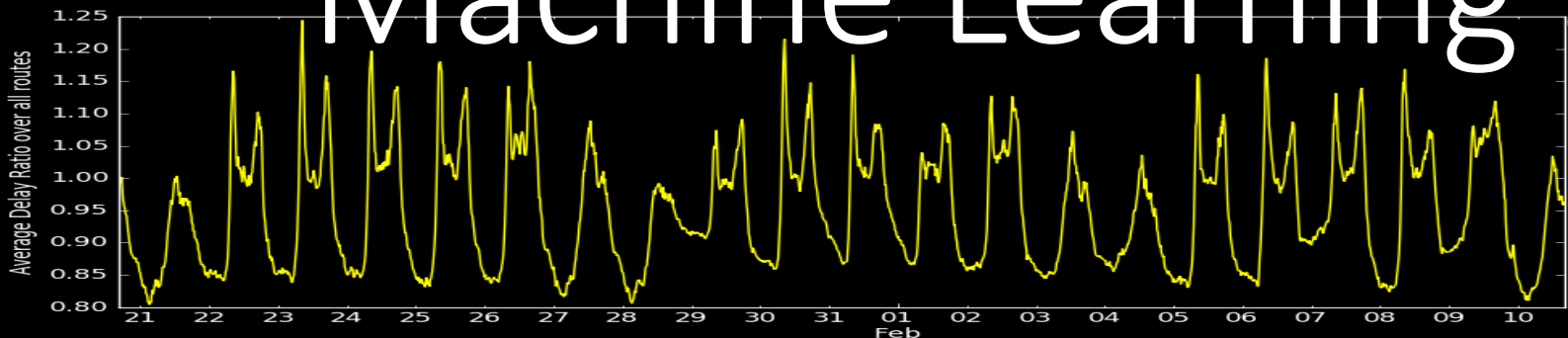
Nick McCullen

Architecture and Civil Engineering



#WherestheMaths

Machine Learning and Cities



Contact: n.j.mccullen@bath.ac.uk



Where's the Maths?

Elizaveta Suturina

Chemistry



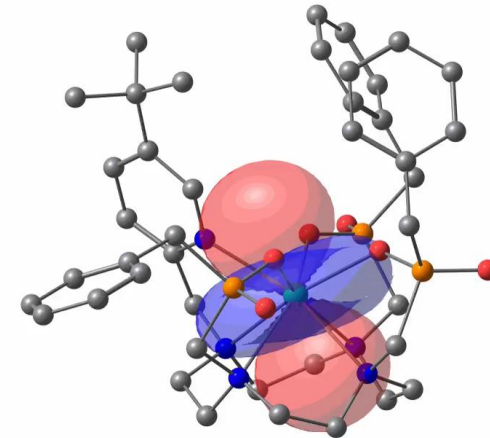
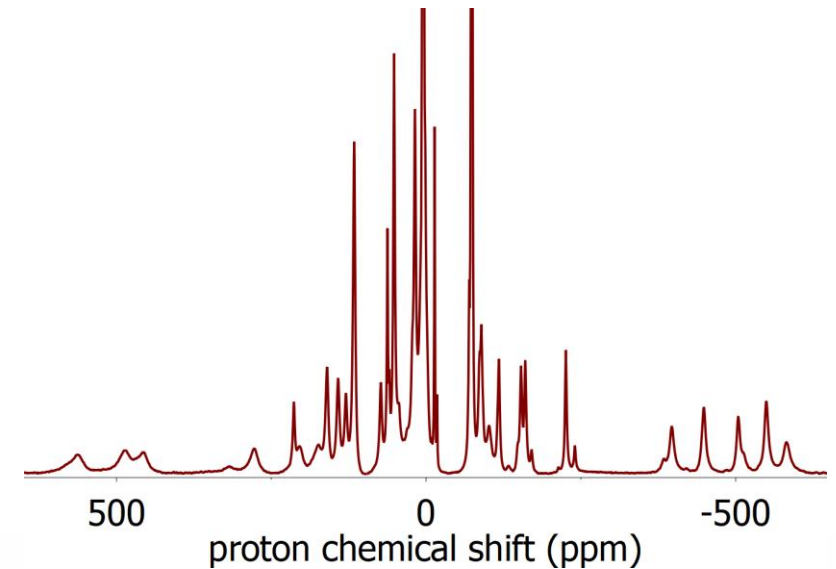
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Paramagnetic NMR assignment

- Position of the NMR signal depends on the structure of the molecule and magnetic properties of the paramagnetic center
- Lanthanide induced shift can be written as a linear combination of second rank spherical harmonics

$$\sigma^{\text{point}} = \frac{1}{4\pi r^3} \sum_{m=-2}^2 \chi_m Y_2^m(\hat{\mathbf{r}})$$

- For which arrangement of atoms (protons) we can uniquely define 5 parameters (χ) of magnetic susceptibility ?
- Is it possible to make an unambiguous linear scaling assignment protocol?



For more information contact

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David Tsang

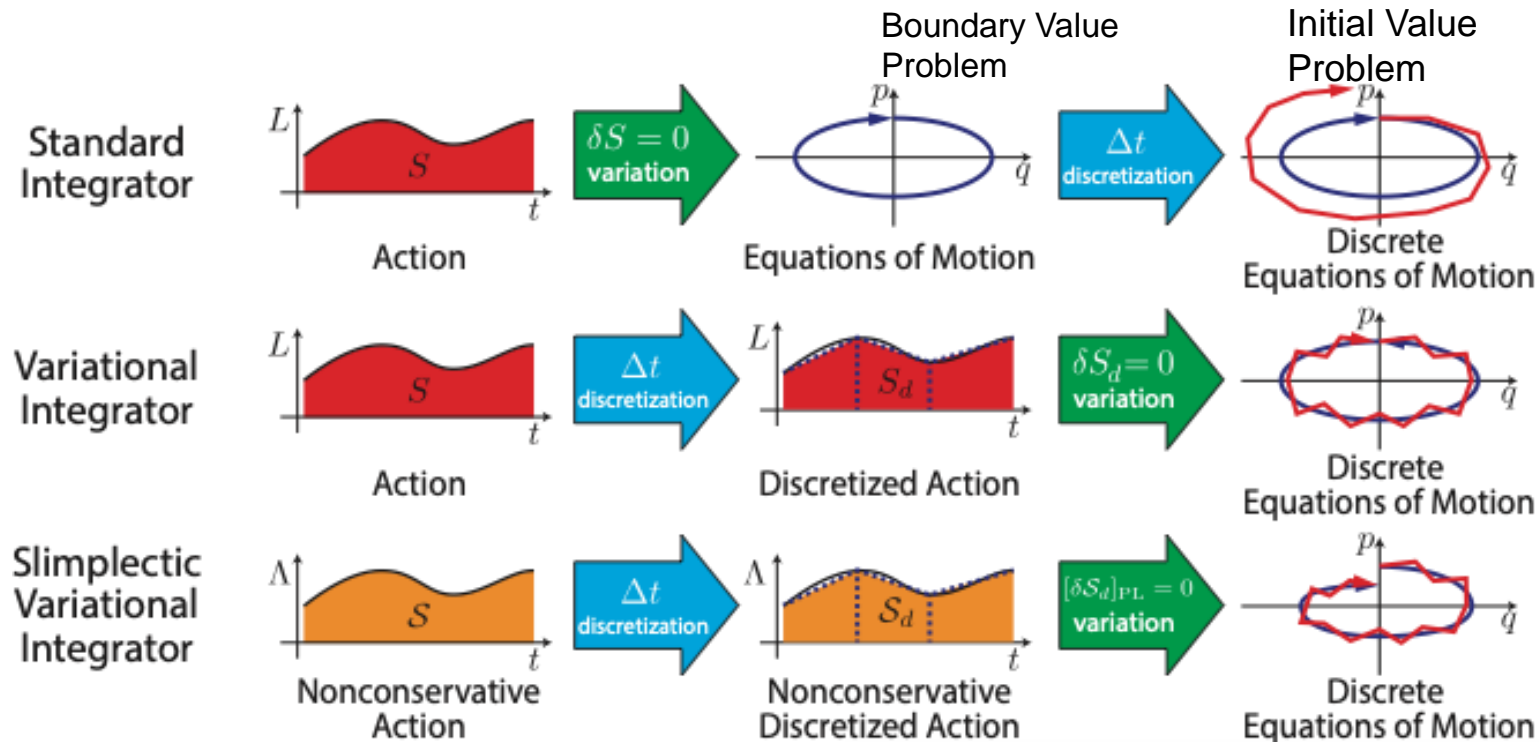
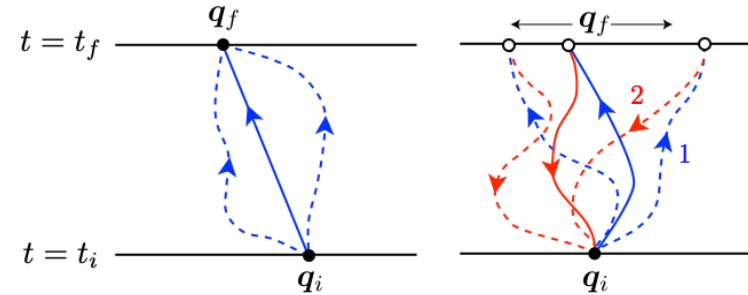
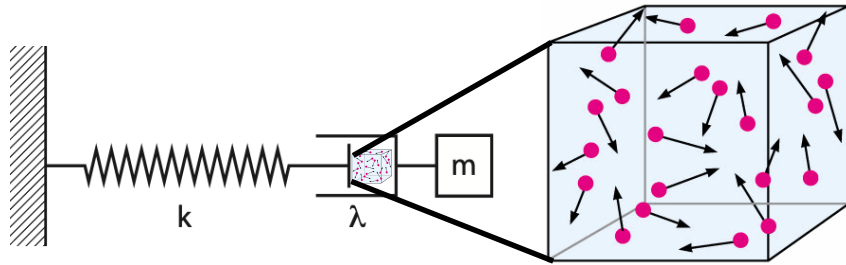
Physics



#WherestheMaths

Non-Hamiltonian Action Principles: Numerical and Physical Applications

David Tsang
Dept of Physics
D.Tsang@bath.ac.uk





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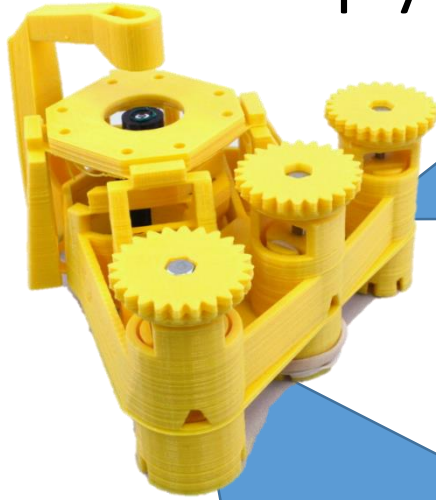
Richard Bowman
&
Neill Campbell

Physics & Computer Science

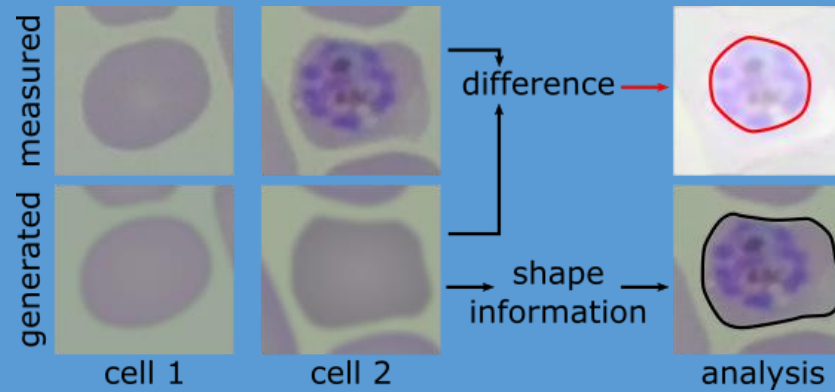


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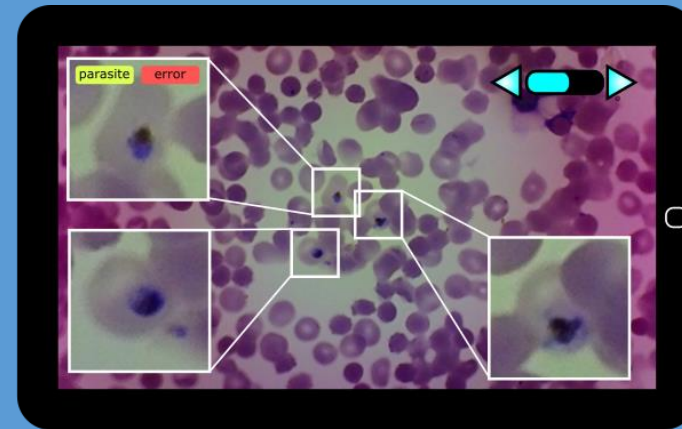
Spotting malaria with smart microscopy



Generative models of blood & parasites



- Locally made hardware
- Open source designs
- Computer vision to spot parasites
- Trials with users in Tanzania and Kenya
- Clinical work in Bagamoyo & Cambridge





Where's the Maths?

Mauro Carnevale

Mechanical Engineering



#WherestheMaths

Background

- Numerical techniques such as **Computational Fluid Dynamics (CFD)** simulations are essential to develop new technologies for aero-engines and aerospace applications. (not only)

PhD: High order CFD of secondary air systems

- Development of the state of the art in CFD techniques (LES-DES) to investigate cavity flows: **unsteady flows**

Challenge in Math

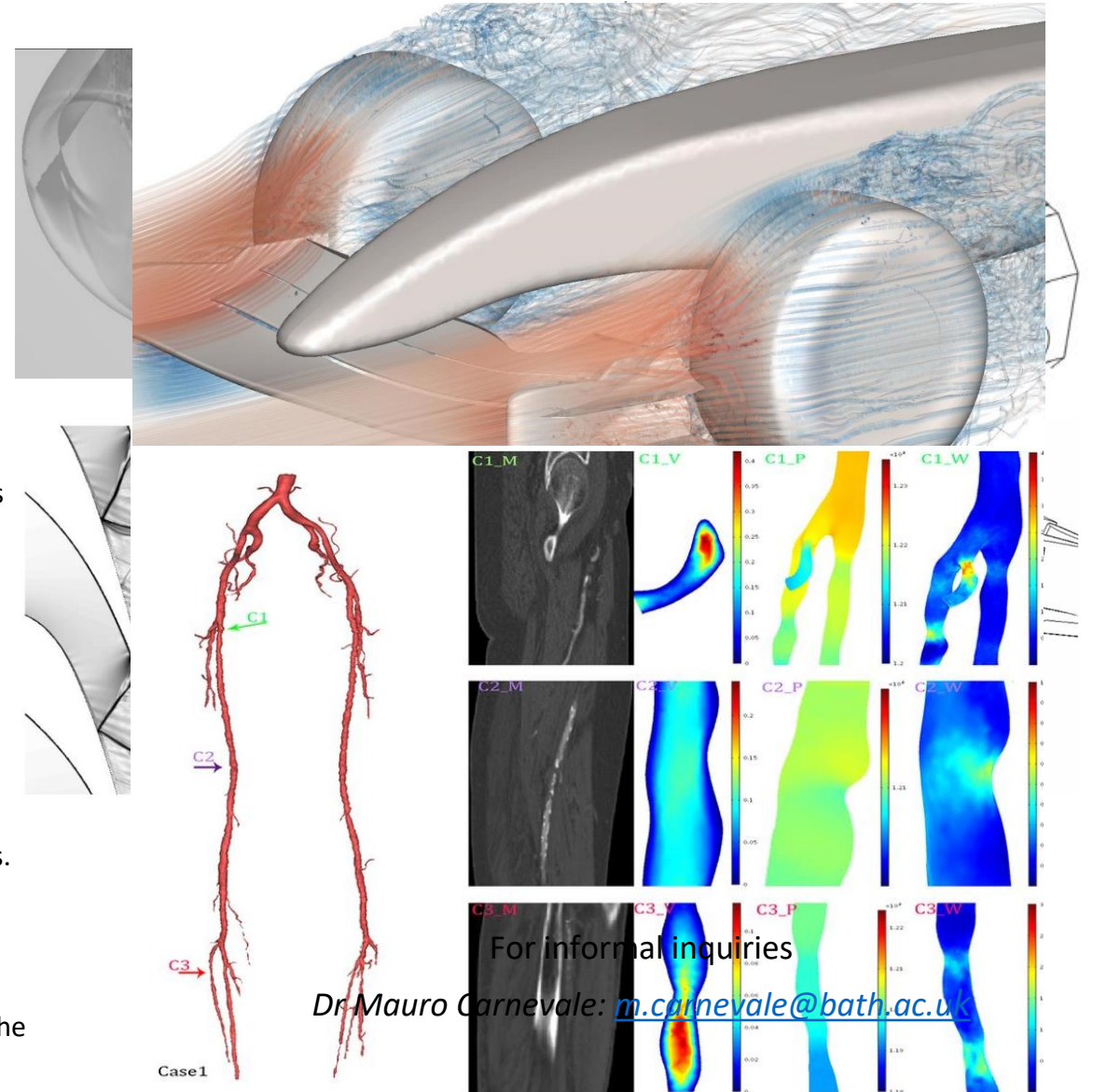
- High order CFD is characterised by the capability in catching stochastic phenomena such as turbulence $\mathbf{u}(t) = \bar{\mathbf{u}} + \mathbf{u}'$
- Turbulence is identified by Reynolds Stresses $= \overline{u'_i u'_j} = \sum_k \phi_{u_i}^k \phi_{u_j}^k$
- Proper Orthogonal Decomposition POD:**
Any instantaneous flow property h'_{tn} can be evaluated by projecting on a suitable orthogonal basis

$$\phi_{u_t}^k = \sum_{n=1}^N \chi_n^{(k)} h'_{tn}$$

- This new procedure will allow to identify the nature and the source of the unsteady effects.

Impact

- The aim is to investigate flow structures in turbine cavities and their interaction with the main flow in turbine stage.
- Results will be disseminated in international journals and conferences.





Where's the Maths?

Richard Guy

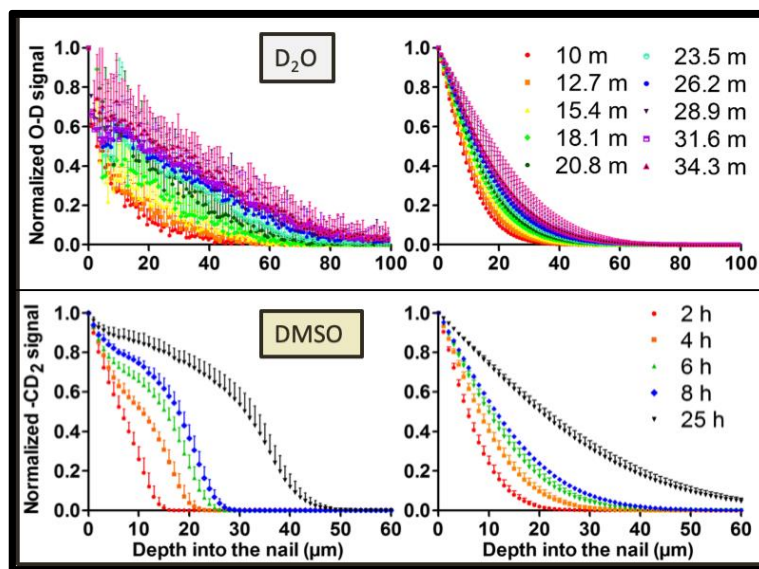
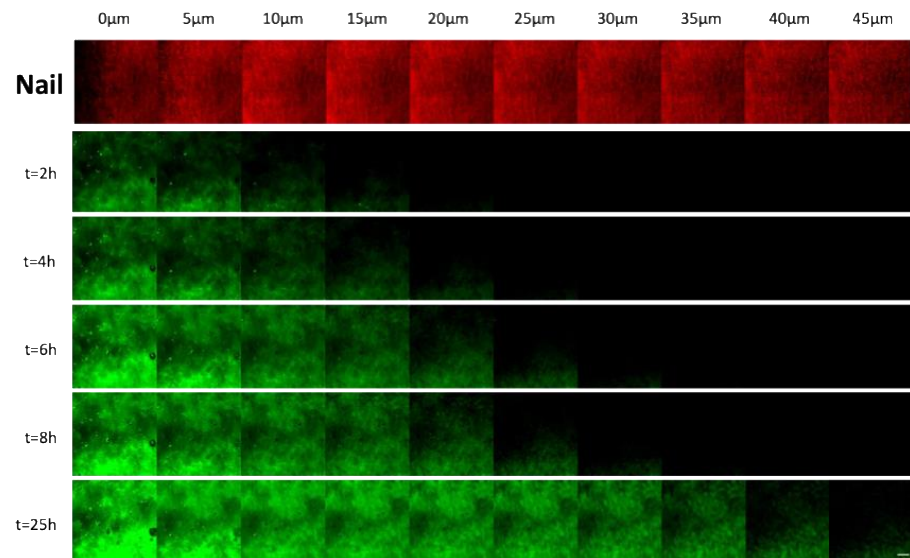
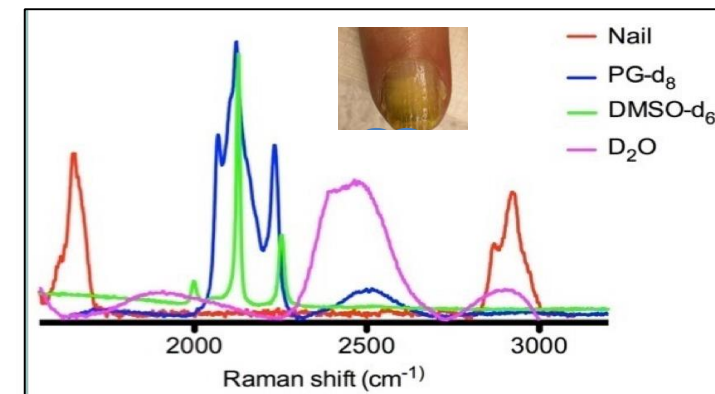
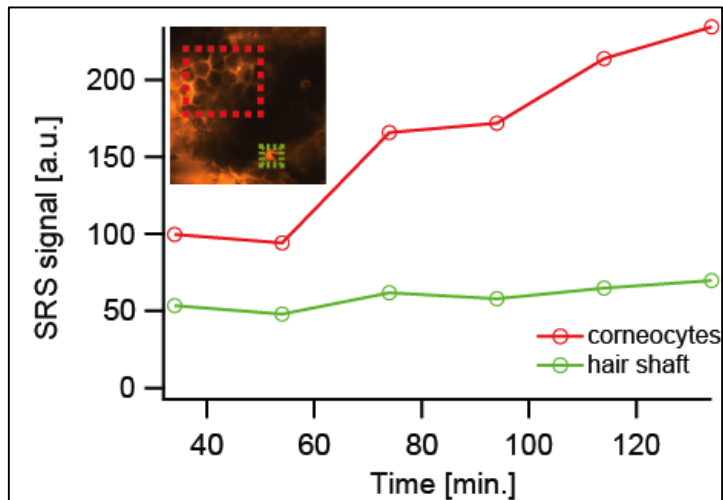
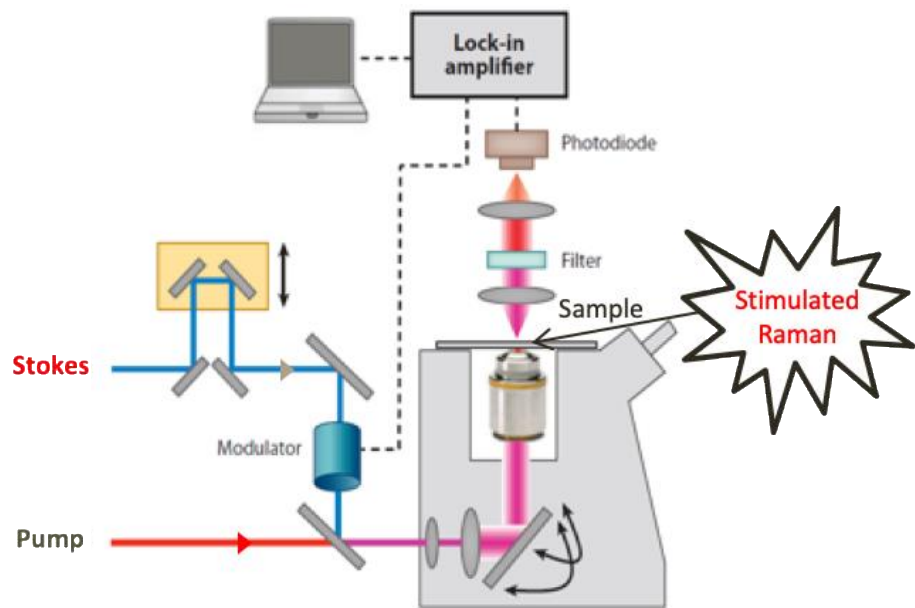
Pharmacy and Pharmacology

 @SAMBa_CDT

#WherestheMaths

Mathematical modelling of chemical permeation across biological barriers

Richard Guy (P&P) r.h.guy@bath.ac.uk



Stimulated Raman scattering
Chemical penetration through skin/nail
Non-Fickian diffusion profiles
Signal attenuation as $f(\text{depth})$
Mathematical modelling...
Prediction of drug uptake as $f(\text{time})$...

W.S. Chiu et al., P.N.A.S., USA, 112, 7725-7730, 2015



Where's the Maths?

Neil McHugh
Pharmacy and Pharmacology

 @SAMBa_CDT

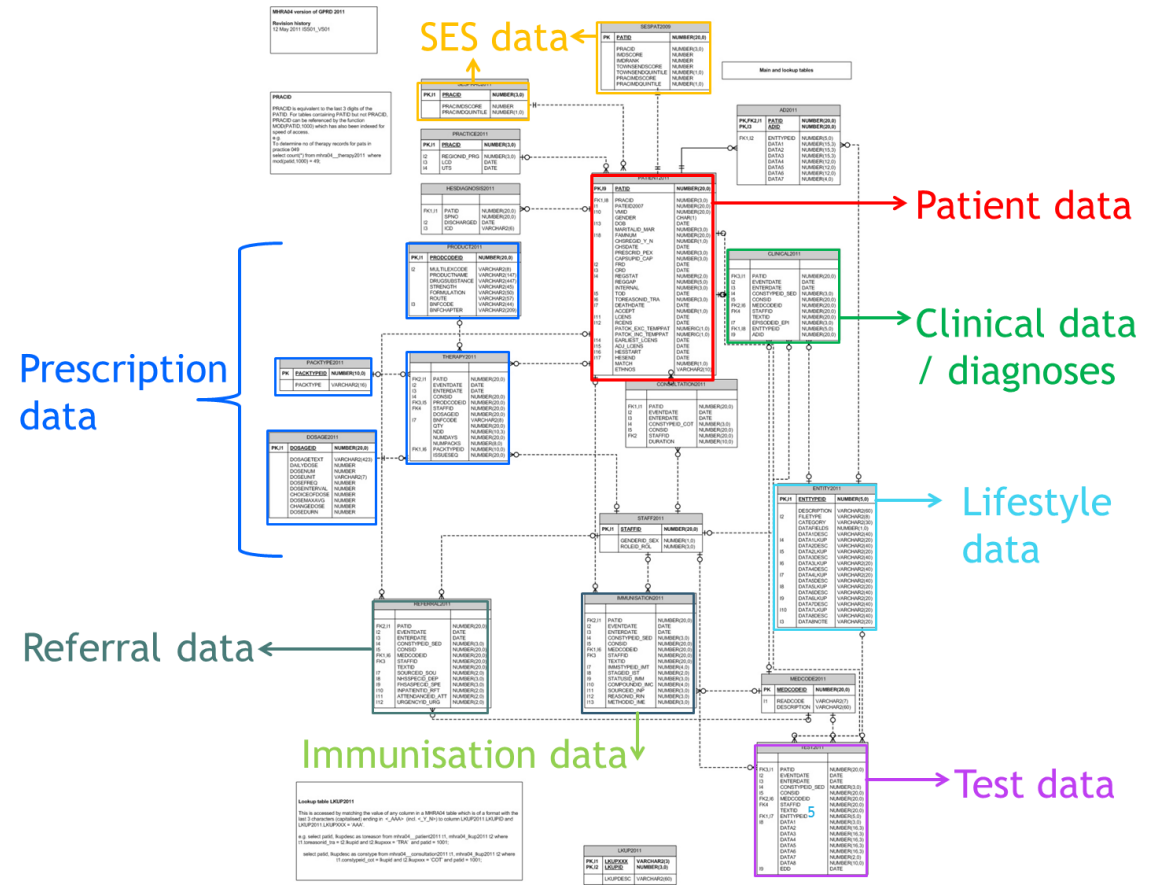
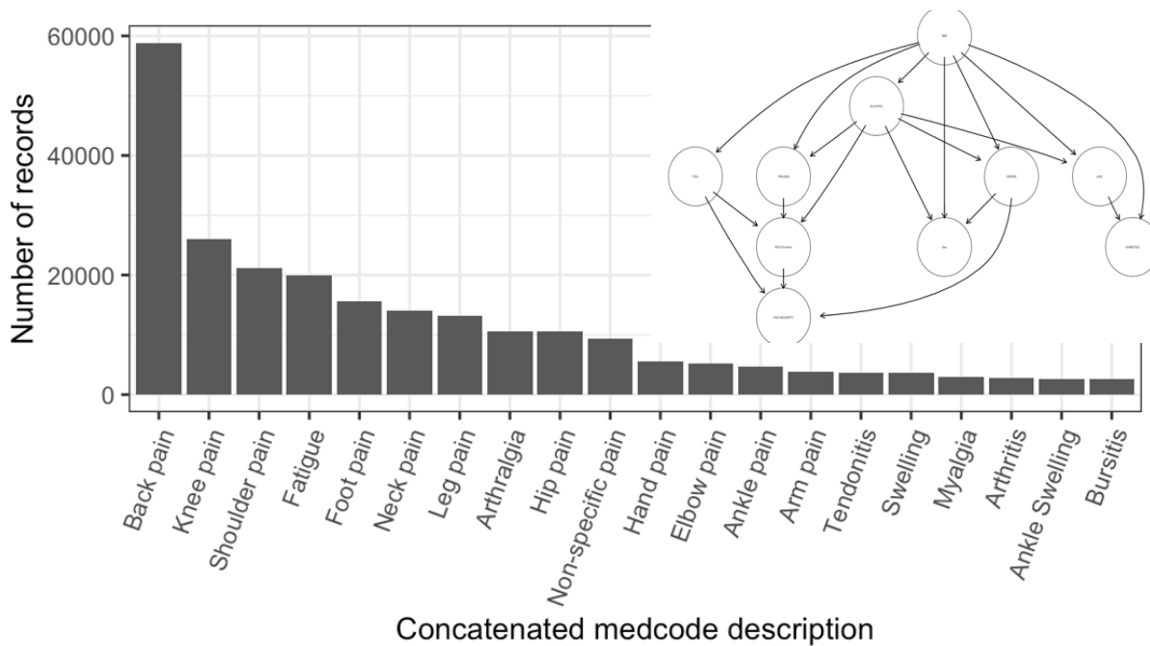
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The Clinical Practice Research Datalink

Anonymised primary care data for ~15 million people in the UK
 ‘Modelling primary care health codes to enable early diagnosis’



- One third of individuals with psoriasis develop arthritis
- Delay in diagnosis leads to worse outcome





Where's the Maths?

James Grant

High Performance Computing



#WherestheMaths

1.0 2.0 3.0

<real> <real> <real>

vector: 1.0 2.0 3.0

<key: vector> <real> <real> <real>

vector_follows

<key: vector_follows>

1.0 2.0 3.0

<real> <real> <real>

vectors_follow

<key: vectors_follow>

1.0

<real>

2.0

<real>

3.0

<real>

vectors_start

<loop>

1.0 2.0 3.0

- <start_key: vectors_start>

4.0 5.0 6.0

- <real> <real> <real>

7.0 8.0 9.0

- <stop_key: vectors_end>

vectors_end

```

'$content':
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    '$value': 'vector'
    '$type': '!split'
    '$unit': 'angstrom'
    '$label': 'data'
    '$types': [float]
    '$number': [3]

```

data: [1.0, 2.0, 3.0]

data: [[1.0, 2.0, 3.0],
[4.0, 5.0, 6.0],
[7.0, 8.0, 9.0]]



Where's the Maths?

The End

Thank you for listening



#WherestheMaths