

EPSRC Centre for Doctoral Training in Cross-Disciplinary Approaches to Non-Equilibrium Systems (CANES)

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Outline

- 1 Non-equilibrium systems & the CANES mission
- 2 Vision for CANES training programme
- 3 London hub and partners
- 4 MSc programme
- 5 Transferable skills

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Equilibrium vs non-equilibrium

Equilibrium systems

- **Movie** of the system would look the same backwards
- **Time-reversible**
- General framework (statistical physics) for analysis and control
- Good understanding of **emergence of collective behaviour**
- For both **classical** and **quantum** systems

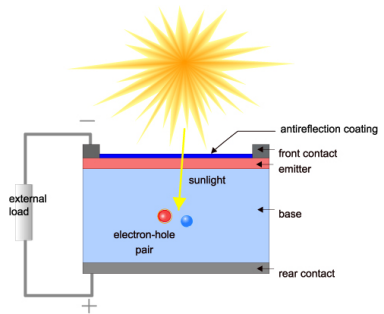
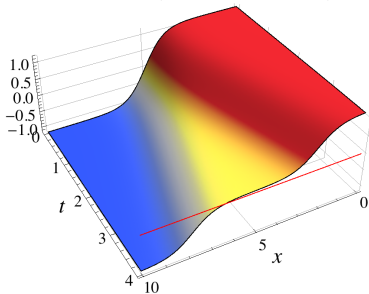
Non-equilibrium systems

- Typically **time-irreversible**
- May **age**
- Or be **driven**: dissipate energy input
- Can exhibit **cascades of failure**, extreme events
- No general framework

Non-equilibrium challenges

Materials science

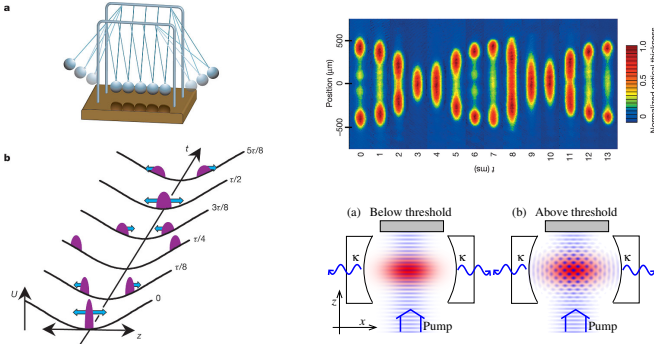
$$T^{\text{tt}} - T_s^{\text{tt}}(T_L = 2, T_R = 1.9)$$



- Transport in nanoscale devices
- Fundamental: many open problems
- Impact: next-generation solar cells

Non-equilibrium challenges

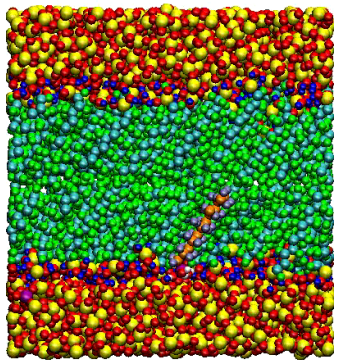
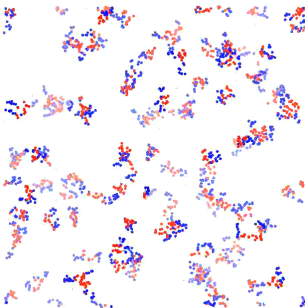
Cold atoms, matter-light systems



- Cold atomic gases manipulated using light
- Fundamental: quantum Newton's cradle, cold atoms in optical cavities
- Impact: superconducting qubits in cavities, quantum computation

Non-equilibrium challenges

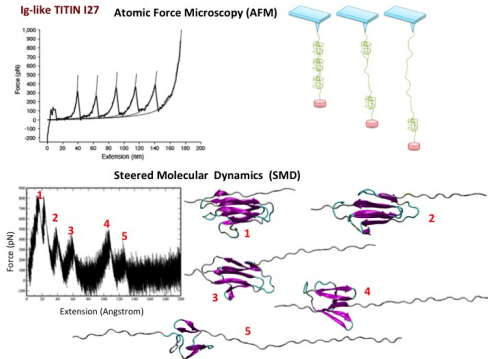
Molecular self-assembly



- Fundamental: simulation, predicting and controlling efficiency
- Impact: bottom-up design of smart materials, molecular filters, polymeric fuel cells

Non-equilibrium challenges

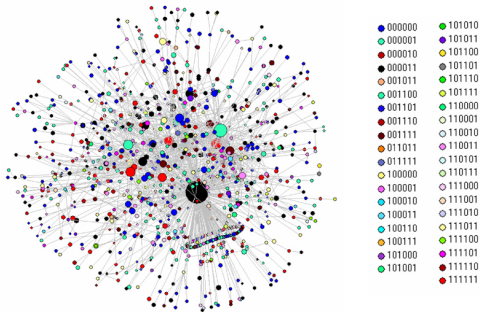
Biophysics



- Protein un/folding, e.g. using atomic force microscope
- Fundamental: development of dedicated simulation techniques, predicting rate constants of activated processes
- Impact: optimizing gene delivery from nanoparticles

Non-equilibrium challenges

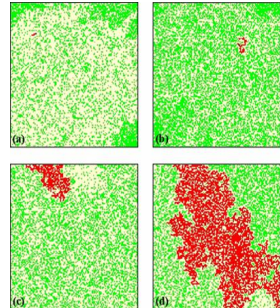
Systems biomedicine



- Dynamics of protein interaction networks, transcriptional regulation, metabolic networks
- Fundamental: partially observed networks, uncertain parameters, experimental biases
- Impact: understanding/control of genetic programmes

Non-equilibrium challenges

Environmental sciences



- Fundamental: characterizing and predicting extreme events, rare deviations, long-range persistence
- Impact: Prediction of natural hazards (wildfires, earthquakes, landslides, floods, tornadoes)

Interdisciplinarity



- Challenges **cross discipline boundaries**
- Many surprising connections:
 - string theory — condensed matter
 - epidemiology — infrastructure / financial networks
 - statistical physics of glasses — protein interaction networks

National and international context

- Emergence and physics far from equilibrium identified by EPSRC as **Grand Challenge**
- EPSRC NetworkPlus, to develop roadmap (**Tobias Galla's talk**)
- Similar initiatives in USA: Office of Science (Dept of Energy) grand challenge, Non-Equilibrium Energy Research Centre
- CANES will bring UK to forefront of this research agenda
- CANES is integrated into:
 - Thomas Young Centre (materials theory and simulation)
 - CoSyDy (complex systems dynamics) LMS network
 - European network NETADIS (statistical physics on / for networks)
 - CECAM-UK-JCMaxwell node (advanced computation)

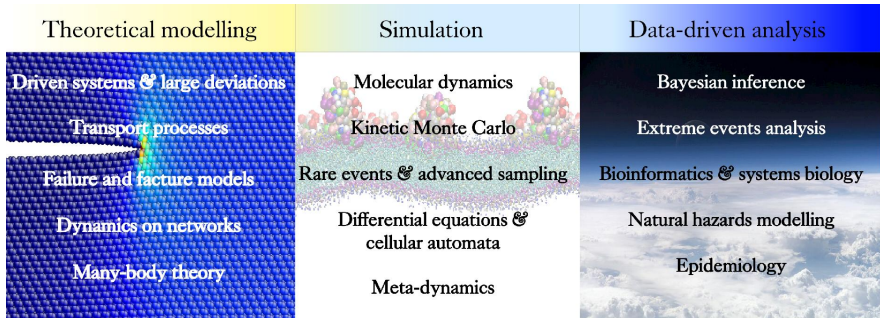
The CANES mission

The mission of CANES is to train future research leaders in the understanding, control and design of systems far from equilibrium, based on rigorous training in theoretical modelling, simulation and data-driven analysis, and a breadth of awareness of common themes across disciplines.

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Cohesive training in three strands



- Strands cut across disciplines
- Existing tools need to be applied to new areas
- Applications provide “driving questions” for new tools

Innovative 1+3-year programme

- Taught 1st year, cohort integration via group research projects
- Annual retreat
- Cross-disciplinary PhD projects
- Open questions sandpits
- Master classes, journal clubs, seminars
- Transferable skills, Creativity-at-home course
- Contributions to outreach, social media channels
- Careers sessions & fora
- Internships in year 3
- Biennial CONES conference

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Participating departments and universities

Departments at King's College London

- Mathematics, Physics, Informatics, Chemistry
- Geography
- Randall Division of Cell & Molecular Biophysics
Institute of Pharmaceutical Science
Centre of Human & Aerospace Physiological Sciences

Partners

- Computational Chemical Physics, Theoretical Physics (Imperial College)
- Condensed Matter and Materials Physics (UCL)
- London Centre for Nanotechnology
- Mathematical Sciences (Queen Mary London)

Industrial and international academic partners

Industry

- National Physical Laboratory
- KAUST (Saudi Arabia)
- Microsoft Research Cambridge
- The Francis Crick Institute (under construction)
- Fios Genomics
- Financial Network Analysis
- DZB (co-operative bank network)

Academic

- Universität Potsdam, TU Berlin, Jülich, UPMC Paris, Montpellier 2, UC Irvine, Wuhan University, ...

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First semester modules

15 credits each, semester = term

- Dynamical modelling of non-equilibrium systems
- Simulation methods for non-equilibrium systems
- Statistical learning and data-driven analysis
- Rare events and large deviations in non-equilibrium systems*
- Modelling quantum systems*

*Students choose one for examination, but need to audit other – for cohort coherence and flexibility

- Mathematical foundation course (as needed)
- **Timetable** includes flexible slots for additional seminars or tutorials

Second semester modules

15 credits each

- Advanced topics in non-equilibrium systems
- Topics covered (students choose 3 for examination):
 - Aging processes
 - Fluctuation theorems
 - Green's functions
 - Non-equilibrium networks
 - Advanced simulation methods
 - Non-stationary time series
- One optional module – chosen in consultation with senior CDT tutor

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Transferable skills training

- Co-ordinated by KCL **Graduate School**
- National framework: Researcher Development Programme
- Targeted via annual **Training Needs Analysis**

Topics include:

- Time management; Being an effective researcher
- Presentation skills; Good science writing
- Databases and e-resources
- Getting the most out of conferences
- Additional science background including LTCC (**London Taught Course Centre**) courses
- Language courses (English Language Centre), ...

We are excited about building CANES

- Thank you to everyone for their support so far
- Good start so far (recruitment of first cohort, workshops and events in the pipeline)
- Much more to do – we look forward to working with all of you