Centre Organisation

SCI-SYM

Director :
H.J.Ruskin

Assoc. Dir:
R.J. Walshe

Assoc. Dir.
M.Crane

P.A. Leader
T.Downes

P.A. Leader
C. Brennan

P.A. Leader
M. O'Connell

Co-PI
A.Barat

P.A. Leader
Y.Delaure

Co-PI
J. Murphy

Co-PI
D.Perrin

Graduate Researchers

Thematic Areas:

1. *Bioinformatics & Microscopic Biosystems ,*

2. *Social, Economic & Environmental Systems,*

3. *Complexity & Computation in Physics*

Centre Objectives

- Improve/enhance **DCU's** ***theoretical & computational*** modelling expertise for ***complex problems***

- Provide ***computational link for existing centres***, (benefiting from personnel expertise already).

- Build up ***HPC research cluster*** facility of *intermediate* international capability

- Target diverse ***funding opportunities*** and new strategic collaborations

Theme 1: Bioinformatics & Microscopic Biosystems

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Epigenome

Heritable Epigenetic Changes

Genome

Microarray Data Analysis

Molecular Evolution

Comparative Functional Genomics & Evolution

Immune System

Multiple Infection Network

Drug Delivery

Drug Dissolution Modelling

Bacterial

Bacteria-Antibiotic Interaction

<u>Theme 1:</u> (cont'd)

- <u>Principal Area 1:</u> Epigenetics (*Prof. H. Ruskin et al*)
  - *PathEpigen* (db/mining for G-Eg pathways for cancer phenotypes)
  - `P=G+Env+EpiG` (agent-based models, probabilistic bayesian networks)

- <u>Principal Area 2:</u> Microarrays (*Prof. H. Ruskin et al*)
  - Storage, Retrieval & Visualisation of MA data (dbs)
  - Preprocessing Techinques for MA data (stat. methods)
  - Network Models for MA data (ann's/grn's)
  - MA Data Clustering Techniques (biclustering, graph theory)

- <u>Principal Area 3:</u> Molecular Evolution (*M. O'Connell BT*)
  - Origin & evolution of inherited disease (dbs, datamining)
  - Ancestral protein resurrection (Likelihood, Bayesian methods)
  - Evolution & timing of developmental genes (comparative genomics)
  - Effect of mating systems on protein evolution (stat. methods)

Theme 1: (cont'd)

- Principal Area 4: Bacteria-AB Interaction *(R. Walshe et al)*
  - "Bottom-up" Modelling of Cell-Culture (hpc, agent-based models)
  - Diffusion Models for AB Spread (DE Models)

- Principal Area 5: Drug Delivery Systems *(M. Crane et al)*

  - Mathematical Modelling of Dissolution Environments (DE models)
  - Probabilistic Dissolution Models (direct & inv MC models, hpc)
  - Therapeutic Implant Integration Model (hpc, Bayesian & DE models)

- Principal Area 6: Immune Modelling *(Prof. H. Ruskin et al)*
  - Shape-Space Models of Immune Memory (hpc, agent-based models)
  - Individual response to Viral Infection (agent-based models)
  - Response to Combined Therapy, Treatment Delay (DE models)

Theme 2: Social, Economic & Environmental Systems

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Environment

Wave Structure
Interaction

Natural

Harmful

Algal

Bloom

Human

Disease Spread

In Populations

Socioeconomic

Multiple-scaling in
Financial Markets

Social

Network Models of
Social Interaction

<u>Theme 2:</u> (cont'd)

- <u>Principal Area 7:</u> Environmental (*Y. Delaure, MME, R. Walshe*)
  - Heat/fluid flow solvers: convective heat transfer in bubble flow interacting with natural convection flow from heated plates.
  - Multifluid flows: waves & rising bubbles (Krylov Subspace models).
  - Algal Blooms (agent-based models)

- <u>Principal Area 8:</u> Social (*Prof. H. Ruskin, D. Perrin*)
  - Disease Spread (game theoretic & DE models)
  - Simulation of Social Networks (avatars, complex network models)
  - Traffic & Driver Behaviour Modelling (agent-based models)

- <u>Principal Area 9:</u> Economic (*M. Crane, Prof H. Ruskin*)
  - Trader Motivation/Behaviour (agent-based models)
  - Hedge fund data (wavelet & spectral models)
  - Multiple-Asset Class Crashes (random matrix & portfolio theory)

Theme 3: Complexity & Computation in Physics

Radio Frequency Propagation

Astrophysics

Radio Frequency Propagation

Pulsed Stellar Jet

<u>Theme 3:</u> (cont'd)

- <u>Principal Area 10:</u> Radio Frequency *(Dr. C. Brennan, EE)*

    - EM wave scattering (ROMs)

    - UWB signal propagation in indoor environments (ray tracing)

    - EM wave scattering problems (krylov subspace models)

    - EM wave scattering from complex dielectric bodies (IE models)

- <u>Principal Area 11:</u> Astrophysics *(Dr. T. Downes, Maths)*

    - Stellar jet launching - beyond magnetic flux freezing (MHD)

    - Turbulence in molecular clouds

    - Multifluid instabilities: organised into turbulent motion in clouds

Graduate Education Basis

- ## M.Sc. in Bioinformatics (MBIO)
  - First in Ireland
  - First Twin Stream intake in Europe
  - Over 100 graduands so far (25% into 4th Level)
- ## M.Sc. in Computational Science & Complex Systems (MCSCS)
  - First Twin Stream intake in Europe
  - Intake Sept 2009
- ## Interns etc
  - "Seed-bed"/High Risk Research projects
  - With PG Researchers
  - Supervised by Faculty/PD Researchers etc
  - Often produce conference/journal publications

Current Funding Sources

SCI-SYM

- Internal
  - Faculty of Engineering and Computing
  - Faculty of Science and Health
  - DCU RAP /Career Start

- National
  - Enterprise Ireland
  - Science Foundation Ireland
  - Irish Research Council for Science Engineering and Technology
  - Higher Education Authority (PRTLI)

- International
  - ESF, European Complexity Network/IRCSET

- Questions?
- More info at:
  - **www.computing.dcu.ie/Research/SCISYM**
- Contact Details
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