Second Annual

Stokes Modelling Workshop

for Undergraduate Students

National University of Ireland, Galway

15-18 June 2015

Stokes Applied Mathematics Cluster
School of Mathematics, Statistics and Applied Mathematics
and
NUI Galway SIAM Student Chapter

ORGANISING COMMITTEE:
Shane Burns, Paul Greaney, Niall Madden, Martin Meere

List of Participants

Name	Institution
Mourtadha Badiane	NUI Galway
Alan Brett	NUI Galway
Maria Bridges	Maynooth University
Jack Collins	NUI Galway
Hannah Conroy Broderick	NUI Galway
Brian Dineen	NUI Galway
Shaunagh Downing	University of Limerick
Sinéad Finn	NUI Galway
Michael Flattery	NUI Galway
Charlene Gildea	Maynooth University
Jack Hampson	NUI Galway
Róisín Hill	NUI Galway
Amy Joyce	NUI Galway
Aaron Kilboy	NUI Galway
Jack McCarthy	University of Limerick
Ciaran McDonnell	Maynooth University
Damian O'Connor	University of Limerick
Cian O'Brien	NUI Galway
Séamus Ó Dubhshláine	NUI Galway
Brian Regan	NUI Galway
Jack Roche	NUI Galway
Bram Siebert	NUI Galway
Shishir Suresh	University of Limerick
Szymon Urbas	NUI Galway

Mentors and Speakers

Richard Burke
Shane Burns
Michel Destrade
John Donohue
Niall Madden
Michael Mc Gettrick
Martin Meere
Eoghan Staunton
Michael Tuite
Giuseppe Zurlo

Problem Descriptions

1 Pollution in the Great Lakes

Skills required: Ordinary Differential Equations

The Great Lakes of America provide the main water supply for an estimated 30 million people in the surrounding areas. Unfortunately the same inhabitants dump a large amount of waste and sewage into these lakes. Among the pollutants is the harmful phosphate family, the main killer of marine life in the lakes. Excess of these phosphates also leads to eutrophication, which amongst other things, causes an obnoxious smell.

Figure 1: The Great Lakes

Due to their immense size, it is almost impossible to locate all the causes of pollution. It has been frequently demonstrated that the only feasible solution is to rely on the natural clean up of the lakes. Rivers will normally clean themselves up very quickly once pollution has stopped, but large lakes are less readily decontaminated because of the amount of polluted water already present. To put this into context, the average retention time of water in Lake Michigan is over 30 years, and 189 years for Lake Superior.

Can you come up with a mathematical model of the 'clean-up process' which will aid environmental engineers and policy makers?

Characteristic	Lake Superior	Lake Michigan	Lake Erie	Lake Ontario
Length (km)	560	490	385	309
Breadth (km)	256	188	91	85
Area (km^2)				
Water surface, Canada	28749		12768	10360
Water surface, US	53618	58016	12898	9324
Drainage basin land, Canada	81585		12224	31080
Drainage basin land, US	43253	117845	46620	39370
Drainage basin land and water, Total	207200	175860	87434	90132
Maximum Depth (m)	406	281	60	244
Average Depth (m)	148	84	17	86
Volume of water (km^3)	12221	4871	458	1636
Average annual precipitation (mm)	736	787	863	863
Mean outflow (litre/sec)	2067360	5012640	5550720	6626880
Average retention time of water (year)	189	30.8	2.6	7.8

Table 1: Data on the Great Lakes

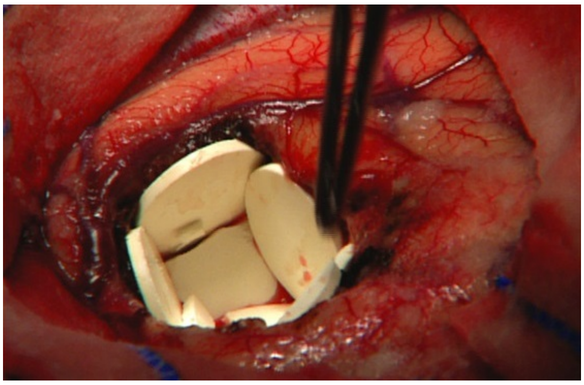
2 Modelling Drug Release from a Polymer

Skills required: Partial Differential Equations, Diffusion Equation

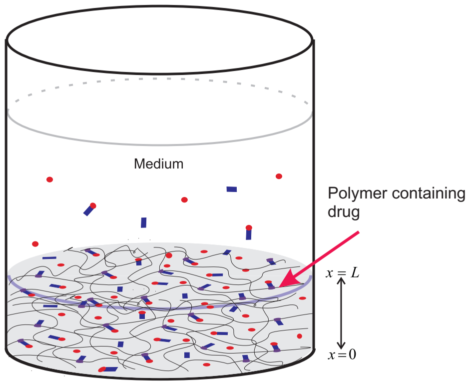
When delivering powerful drugs such as anti-cancer drugs, it is usually better to deliver them *locally* if possible. That is, it usually better to deliver them only to where they are needed rather than delivering them systemically throughout the body. This helps to minimize the undesirable side effects of the drugs.

Gliadel wafers are an example of a local drug delivery system. These wafers are made from a polymeric material and contain a potent anti-cancer drug. They are used to treat brain cancers; see Figure (a). After the surgeon removes the brain tumour, he lines the perimeter of the tumour cavity with the wafers. In the weeks and months following surgery, the drug releases from the wafers into the surrounding tissue killing residual cancer cells and helping to prevent the regrowth of the tumour.

A pharmaceutical company is developing a polymeric drug delivery system much like the gliadel system described above. In their system, a polymeric wafer contains a drug that can diffuse into surrounding tissue to have a therapeutic effect. To evaluate the rate at which the drug releases from the polymer, the pharmaceutical company conducts a series of release experiments. In a release experiment, the drug-infused polymer is placed at the base of a flat-bottomed glass container, as shown in Figure (b). Water is poured over the polymer, and this water is continuously stirred using a stirrer bar. The drug then releases into the water from the polymer via diffusion, and the release rate is evaluated by periodically measuring the amount of drug in the water.



(a) Gliadel wafers being placed on the perimeter of a brain tumour cavity. Drug molecules diffuse through the wafers into the surrounding tissue killing residual cancer cells.



(b) A release experiment. The polymer containing the drug is placed at the base of a container, and the drug subsequently releases into an overlaying release medium.

Your task is to mathematically model the drug release experiment described above. In particular, you are asked to address the following questions:

1. How much drug has released into the release medium by time t? How does this quantity depend on the thickness of the polymer, the initial concentration of drug in the polymer, and the diffusive properties of the drug molecules? What parameter regime will lead to drug release over a period of a few months?
2. Explore how the drug release rate depends on the geometry of the polymer. For part 1 above, you may assume that the polymer is simply a one-dimensional planar system. However, explore also the cases of a spherical polymer, a cubical polymer, and a cylindrical polymer.

3 Aircraft Wing Vibrations During Landing

Skills required: Partial Differential Equations, 1D Beam Equation

During the landing stage of an airplane, the impact of the main gears with the landing strip determines an impulsive concentrated load that induces a complex pattern of vibrations of the whole structure.

A very delicate engineering problem is to study the consequences of the impulsive load on the mechanical resistance of the various parts of the aircraft. Focus your attention on the wings, which can be modelled as slender elastic beams, and try to describe their elastic vibrations under the received impulsive force. In doing so, you can neglect the role of friction forces and of the air lift.

Your tasks are:

1. to create a sound mathematical model for the wings bending vibrations under the impulsive load that is received by the main gear;
2. to produce an animation showing the bending vibrations of the wings;
3. to determine the maximum impulsive force that the wings are able to sustain without breaking; in this perspective, which is the most critical instant after the impact?

4 Connectivity of Flight Networks

Skills required: Linear Algebra, Graph Theory, Numerical Analysis, Programming

There are various algorithms for determining if a graph (network) is connected, and applications of these algorithms are found in many areas of applied mathematics. In this project you will work on algorithms for comparing graphs and determining which is more connected. We shall focus on commercial flight networks and the ways an airline can optimise its connectivity by strategic deployment of its fleet.

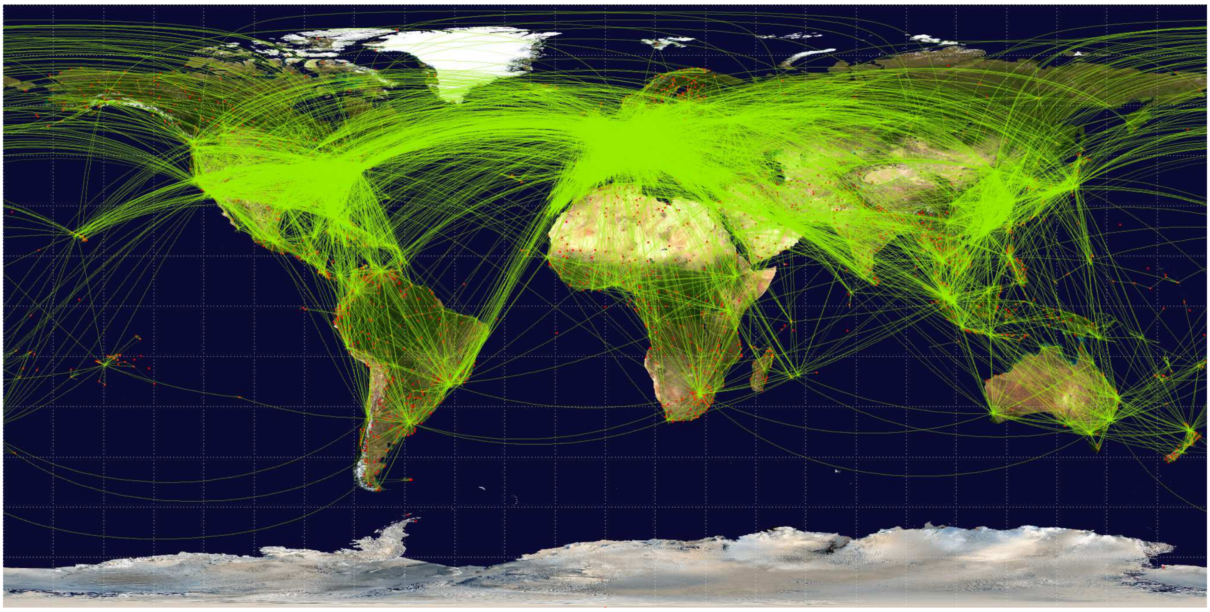


Figure 3: Airline flight map showing the 59000 busiest routes worldwide.

The aim of the project is to build an adjacency based mathematical model of the air route network, develop an algorithm to quantify the connectivity of this network, and use this connectivity measure to compare the existing network with more optimal artificial networks.

To make the problem more tractable, we will restrict our analysis to European flights for a single commercial airline (Ryanair) and you will engage in the following tasks:

1. Data gathering: construct several networks based on real data that you can use to test your algorithms.
2. Modelling: devise a mathematical description of the connectivity of your network, that allows you to consider two similar networks.
3. Implementation: produce running code (in Matlab, for example), that simulates your algorithm(s).
4. Description and presentation.

5 Counting Structural Isomers

Skills required: Graph Theory, Computing, and a little Group Theory

Alkanes are a simple class of chemical compounds given by the chemical formula C_nH_{2n+2} for $n = 1, 2, \ldots$. The first few cases are familiar examples: methane CH_4, ethane C_2H_6, and propane C_3H_8, shown below:

$$\begin{array}{ccccc} & & H & & \\ & & | & & \\ H & - & C & - & H, \\ & & | & & \\ & & H & & \end{array} \qquad \begin{array}{ccccccc} & & H & & H & & \\ & & | & & | & & \\ H & - & C & - & C & - & H, \\ & & | & & | & & \\ & & H & & H & & \end{array}$$

$$\begin{array}{ccccccccc} & & H & & H & & H & & \\ & & | & & | & & | & & \\ H & - & C & - & C & - & C & - & H. \\ & & | & & | & & | & & \\ & & H & & H & & H & & \end{array}$$

For general C_nH_{2n+2} there exist several different isomers, i.e. arrangements of the carbon chains into inequivalent configurations. This first occurs for $n = 4$.

If we remove or replace **one** hydrogen atom, then a number of molecules $C_nH_{2n+1}X$ of interest to chemists, known as monosubstituted alkanes, result. Thus replacing one hydrogen atom by an OH group results in an alcohol whereas replacing it by a metal results in a organo-metallic compound.

$$\begin{array}{ccccc} & & H & & \\ & & | & & \\ X & - & C & - & H, \\ & & | & & \\ & & H & & \end{array} \qquad \begin{array}{ccccccc} & & H & & H & & \\ & & | & & | & & \\ X & - & C & - & C & - & H \\ & & | & & | & & \\ & & H & & H & & \end{array}$$

Your tasks are as follows:

1. Formulate the isomers C_nH_{2n+2} in terms of tree diagrams with vertices of degree 4 (i.e. 4 branches from each vertex), and hence by hand determine the number of isomers for $n = 4, 5$.

2. Formulate the isomers $C_nH_{2n+1}X$ for a monosubstituted alkane in terms of tree diagrams with one root with vertices of degree 4 (i.e. 4 branches from each vertex), and hence by hand determine the number of such isomers for $n = 4, 5$.

3. Explore methods for determining the number of such graphs. (Try Googling Polya's Theory of Counting!)