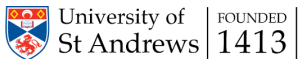


Applications of Mathematics

Theme Head: Irene Kyza

School of Mathematics and Statistics
University of St Andrews



30 September 2026

Overview of the theme

The theme can be divided into two broad categories:

- the formulation and analysis of *mathematical models*
- *methods or tools* needed to analyse and simulate them

Two modules per category; self-contained and independent.

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Two major areas of modelling:

- **continuum mechanics**
- **mathematical biology**

Not comprehensive, but illustrative of a range of approaches.

Two complementary sets of methods:

- **asymptotic and analytic**
- **numerical**

Again not comprehensive, but illustrative. In both cases the aim is to develop *approximate* methods in a systematic, quantitative way.

Continuum Mechanics (semester 1)

- Continuum mechanics describes how deformable media behave:
 - Fluids (liquid/gas)
 - Solids (elastic/plastic)

Continuum hypothesis + Newton II:

- ⇒ $O(10^{24})$ molecules: can't solve $F = ma$ for each
- ⇒ Treat medium as a continuum of parcels, each small on scale of motion, each containing large number of molecules
- ⇒ Then $\mathbf{u}$, p , ρ , etc, considered as functions of $(\mathbf{x}, t)$

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- Huge range of applications (nano-technology to astrophysics)

Continuum Mechanics (semester 1)

Topics:

- **Continuum mechanics:** construction of dynamical models of deformable media
- **Fluid Dynamics:** lubrication theory, aerofoils, hydrodynamic stability
- **Non-Newtonian fluids:** fluid viscosity depends on internal stresses

Mathematical Biology and Physiology (semester 2)

- Mathematical modelling in the life sciences.
- Modelling of just about any aspect of biological systems:
 - Circulation (e.g., blood flow in arteries)
 - Patterns (e.g., rashes)
 - Populations dynamics
 - Cell dynamics (dynamics at cell scale)
 - Diseases/treatments (epidemiology)

Mathematical Biology and Physiology (semester 2)

Topics:

- **Bacterial resistance:** antibiotics
- **Mathematical Physiology:** microscale/macroscale & homogenisation
- **Population Modelling:** epidemiology, evolution, pathogen-host interactions, age-structured models
- **Mathematical Oncology:** cancer modelling

Asymptotic and Analytical Methods (semester 1)

Problems frequently contain a “small parameter” $\epsilon \ll 1$.

- Can change the character of the problem

$$i\epsilon\partial_t u + \epsilon^2\Delta u + Vu = 0.$$

Asymptotic and Analytical Methods (semester 1)

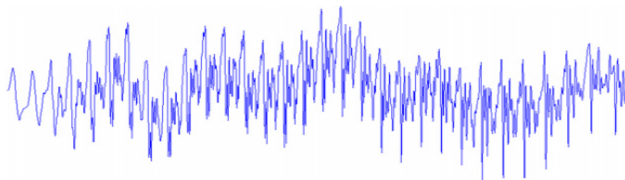
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Some examples:

- In PDEs (e.g. Navier–Stokes, Schrödinger), small terms may give rise to **boundary layers** or **caustics**.



- In forced oscillators, small forcings may lead to **resonance**.

These lectures will provide a toolkit for tackling such problems.

Asymptotic and Analytical Methods (semester 1)

EXAMPLE: Asymptotic expansion of the error function:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \quad (< 1).$$

Seek an expansion to evaluate $\operatorname{erf}(x)$ for large x .

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○ **First attempt:** Taylor expand e^{-t^2} and integrate term-by-term:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \left[x - \frac{x^3}{3} + \frac{1}{5} \frac{x^5}{2!} - \dots + \frac{(-1)^n}{2n+1} \frac{x^{2n+1}}{n!} + \dots \right]$$

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- **Convergent:** gets arbitrarily close to $\operatorname{erf}(x)$ for any x
- $x = 4$: needs > 40 terms for a reasonable approximation
- $x = 4$: first 16 terms sum to 10^5

Asymptotic and Analytical Methods (semester 1)

○ **Alternative approach:** Write

$$\operatorname{erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$$

and integrate by parts n times:

$$\begin{aligned} \int_x^\infty e^{-t^2} dt &= \int_x^\infty \frac{te^{-t^2}}{t} dt \\ &= e^{-x^2} \left[\frac{1}{2x} - \frac{1}{4x^3} + \frac{3}{8x^5} + \dots + \frac{(-1)^{n-1} 1.3.5 \dots (2n-3)}{2^n x^{2n-1}} \right] + R_n \end{aligned}$$

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- $x = 4$: first 2 terms give $\operatorname{erf}(4)$ to within 10^{-7}

Asymptotic and Analytical Methods (semester 1)

Topics:

- **Multiple scales:** modulation and resonance
- **Matched Asymptotics:** boundary layers
- **WKB Theory:** rapidly oscillating solutions, ray theory
- **Approximation of Integrals:** Watson's lemma, steepest descent
- **Intermediate Asymptotics:** self-similarity of solutions
- **Resummation:** techniques for series

Numerical Methods (semester 2)

- **Ways to solve mathematical models numerically.**
- Often there is a *compromise* between ease of implementation and efficiency.
- Or between speed (computational cost) and accuracy.

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Topics:

- **Ordinary DEs:** Explicit, implicit and multistep methods
- **Stochastic DEs:** Brownian Motion, Stochastic Integrals, Stochastic DEs and simulations
- **Partial DEs:** Finite Difference and Finite Element methods
- **Linear Algebra:** Numerical Solution of Linear Systems and Eigenvalue problems.

Numerical Methods (semester 2)

○ Numerical methods for PDEs

Many models in applied mathematics are based on PDEs.

- Many pieces of software claim to be able to solve PDEs.
- Pretty pictures are not always accurate!!!
- It is good to know what are some standard things that can go wrong.

Numerical Methods (semester 2)

○ Numerical methods for PDEs

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These lectures will look at some of the basic questions:

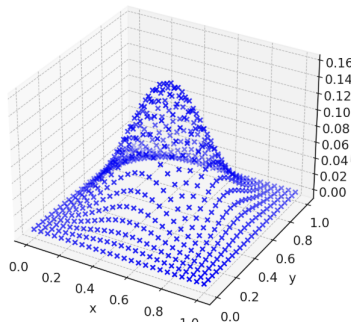
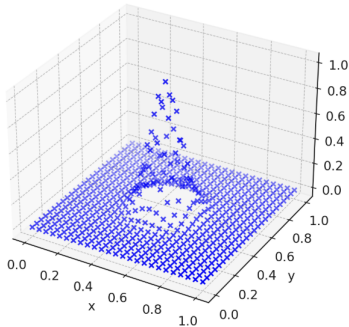
- How can we **discretise** PDEs to give systems of algebraic equations?
- How can we solve the resulting systems **efficiently**?
- How do we prove these methods have desirable properties, like
 - **Consistency** (representing the desired PDE)
 - **Stability** (not being hypersensitive to data)
 - **Convergence** (error decreasing as resolution increases)

Numerical Methods (semester 2): Finite Differences

○ **EXAMPLE:** FTCS method for the **heat equation**: $\partial_t u = \Delta u$ (homogeneous Dirichlet BCs):

$$\frac{U_{i,j}^{n+1} - U_{i,j}^n}{\Delta t} = \frac{U_{i+1,j}^n - 2U_{i,j}^n + U_{i-1,j}^n}{(\Delta x)^2} + \frac{U_{i,j+1}^n - 2U_{i,j}^n + U_{i,j-1}^n}{(\Delta y)^2}.$$

- If $\Delta x = \Delta y$, choose $\Delta t < \frac{(\Delta x)^2}{2}$ to ensure *stability* and hence *convergence*.



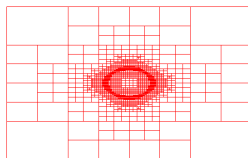
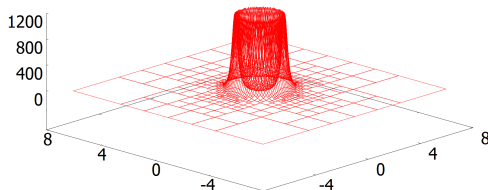
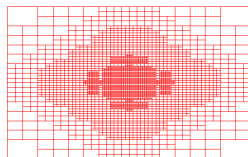
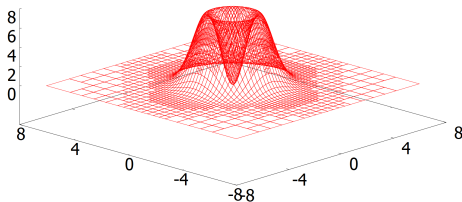
Gaussian bump (IC; left) and FTCS approximation (after 50 steps; right)

Numerical Methods (semester 2):

Finite Elements: **More Advance Techniques!**

Semilinear parabolic equations: **Regional blowup**

- $\partial_t u - \Delta u = u^2$ in $\Omega \times (0, T]$, $\Omega = (-8, 8) \times (-8, 8)$
- $u_0(x, y) = 10(x^2 + y^2)e^{-0.5(x^2 + y^2)} \rightsquigarrow$ **Blowup set: circle centred on $(0, 0)$**

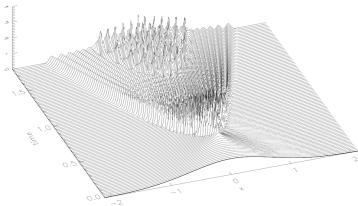


Numerical Methods (semester 2):

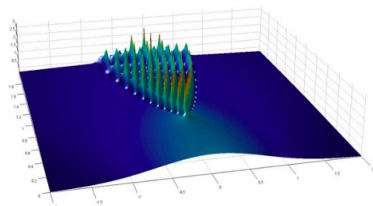
Finite Elements: **More Advance Techniques!**

- Complicated geometries
- Sharply localised features

• *Semiclassical behaviour of NLS*



Cai, McLaughlin & McLaughlin, 2002



Bertola & Tovbis, 2013

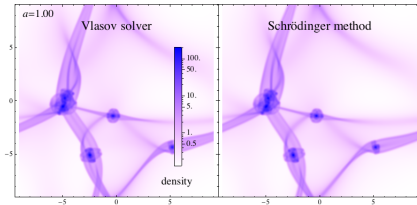
NLS dispersive breaking

Numerical Methods (semester 2):

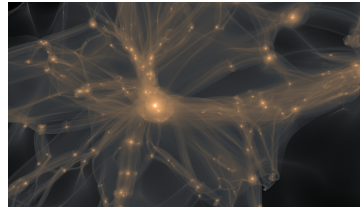
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• Cosmology: *Galaxy formation*



Kopp, Vattis & Scordis, 2017



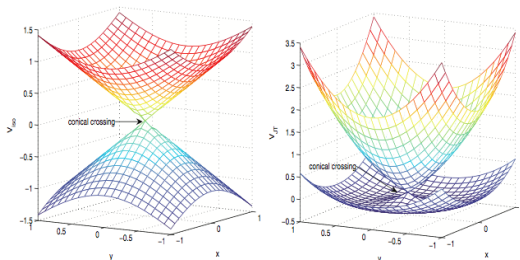
From the page of Dr. R. Kaehler

2d & 3d simulations for galaxy formation

Numerical Methods (semester 2): Advance Techniques!

● Two-level Schrödinger system with conical crossings

- Potential matrix $V(\mathbf{x})$ has eigenvalues $\lambda_{1,2}(\mathbf{x}) = a(\mathbf{x}) \pm \sqrt{v_1^2(\mathbf{x}) + v_2^2(\mathbf{x})}$
- Two energy levels are said to **cross** at a point $\mathbf{x}_* \in \mathbb{T}^2$ if $\lambda_1(\mathbf{x}_*) = \lambda_2(\mathbf{x}_*)$
- Such a crossing is called **conical** if $\nabla_{\mathbf{x}} v_1(\mathbf{x}_*)$ and $\nabla_{\mathbf{x}} v_2(\mathbf{x}_*)$ are **linearly independent**.



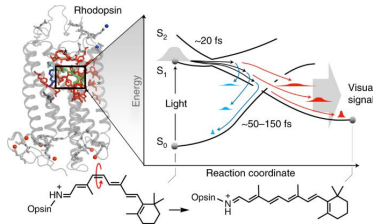
The conical crossings for two different potentials; $\lambda_1(\mathbf{x}), \lambda_2(\mathbf{x})$ are plotted (Jin, Qi & Zhang, 2011)

○ Close to conical crossings: Numerical behaviour as in a **non-smooth problem** (Schrödinger equation with low regularity data)

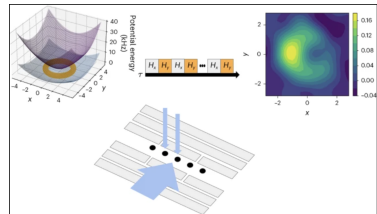
Numerical Methods (semester 2): Advance Techniques!

○ APPLICATIONS: Several chemical reactions, including:

- Vision (Retinal photoisomerisation)
- Photochemistry and light-harvesting
- DNA photostability
- Quantum Simulation and Quantum Computing



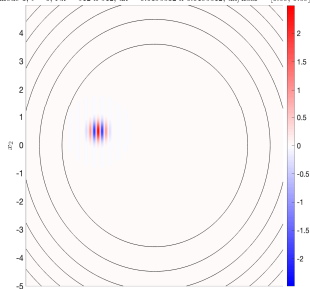
Polli et al., 2010, Nature



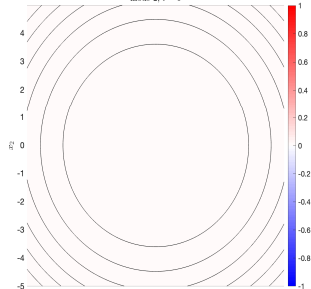
Whitlow et al., 2023, Nature Chemistry

✱ Conical crossings: Exactly where the *interesting chemistry happens*

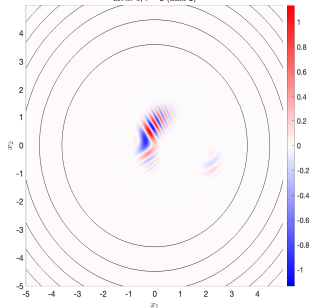
mode 1, $t = 0$, $N_x = 512 \times 512$, $dx = 0.0195312 \times 0.0195312$, $dx/hbar = [0.39, 0.39]$



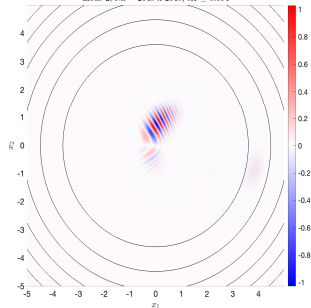
mode 2, $t = 0$



mode 1, $t = 2$ (final 2)



mode 2, $N_x = 2048 \times 2048$, $err \leq 0.004$



Prior knowledge, delivery and assessment

Assumed knowledge of standard, core undergraduate material:

- Calculus, ODEs, PDEs
- Linear Algebra
- Complex Variables

More details on the module pages.

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Assessment: two assignments per module

- Mix of analytic and computational work
- Normally at least two weeks to complete each