TMA4195 - Mathematical Modelling

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Trondheim,
November 21, 2018

Mathematical Modelling

...can be roughly described as the art of

- translating practical problems from applied areas into mathematical formulations, and
- using these formulations together with theoretical and numerical methods in order to get further insight into the problem and answer concrete practical questions.

Typical procedure:

1. Identification of the problem and the relevant quantities.
2. Formulation of the relation between these quantities.
3. Simplification and model reduction.
4. Theoretical analysis and/or numerical approximation.
5. Comparison of the results with real data.
6. Revision and refinement of the model.

Outline

Basic laws of physics

- Newton's laws of motion:
  - Change of momentum = sum of all forces.
  - Momentum = mass $\times$ velocity.
- Laws of electrodynamics.
- Laws of thermodynamics.
- Experimentally derived approximate relations.
- ...

Population dynamics

- Modelling of changes in populations/sub-populations (diseases,...).
- Logistic equation (maximal carrying capacity K):

$$\dot{P} = \alpha(1 - P/K)P.$$

- Predator–prey systems:

$$\begin{aligned} \dot{P} &= \alpha P - \beta PQ, \\ \dot{Q} &= \gamma PQ - \delta Q. \end{aligned}$$

- ...additional terms depending on interactions between different populations and environmental effects.

Chemical reactions

- Processes of the form

$$S_1 + S_2 + \ldots + S_n \quad \underset{\beta}{\overset{\alpha}{\rightleftharpoons}} \quad P_1 + P_2 + \ldots + P_m.$$

- For substances with low concentration in a well mixed solution, effective reaction rate are proportional to the product of concentrations of the input.
- Reaction rates may be (often are) temperature dependent.

Conservation laws

- Describe large scale behaviour in time and space of a large number of particles/independent actors.
- Quantities of interests can be well described on a large scale by their densities.
- In any given region, the change of the quantities of interest can only be due to:
  - ... production within that region,
  - ... flux through the boundary of that region.

Integral and differential forms

- Total change + flux = production.
- φ ... density of interest.
- j ... flux density.
- Q production rate.
- Integral form:

$$\frac{d}{dt}\int_R \varphi \, dV + \int_{\partial R} j \cdot n \, d\sigma = Q(R).$$

- Assume production rate of the form $Q(R) = \int_R q$.
- Apply divergence theorem to the boundary integral.
- Obtain

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot j = q.$$

Eulerian and Lagrangian forms

Euler formulation:

- Fix a control volume and formulate the conservation law within this region.

Lagrange formulation:

- Select a collection of particles and follow these particles as they move; formulate the conservation law for the *moving* particles.

Switch between formulations: *Reynold's transport theorem*:

$$\frac{d}{dt}\int_{R(t)} \varphi \, dV = \int_{R(t)} \frac{\partial}{\partial t}\varphi \, dV + \int_{\partial R(t)} \varphi \, v \cdot n \, d\sigma$$

with $v \ldots$ velocity of particles.

Conservation of mass

- Change of mass + flux through boundary = production.
- ρ ... density.
- ρv ... flux density.
- Integral form:

$$\frac{d}{dt}\int_R \rho\, dV + \int_{\partial R} \rho v \cdot n\, d\sigma = \int_R q.$$

- Differential form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = q.$$

- Incompressible materials, $\rho = \text{const}$:

$$\rho\,(\nabla \cdot v) = q.$$

Conservation of momentum

- Lagrangian formulation:

$$\frac{d}{dt}\int_{R(t)} \rho v \, dV = F(R(t), t).$$

- F ... total force acting on region $R(t)$.
- Eulerian formulation:

$$\frac{d}{dt}\int_{R} \rho v \, dV + \int_{\partial R} (\rho v)(v \cdot n) \, d\sigma = F(R, t).$$

Stresses

- Total forces can be decomposed as

$$F(R) = F_B(R) + F_S(R) = \int_R f_B \, dV + \int_{\partial R} T \cdot n \, d\sigma.$$

- f_B ... body forces (gravity, electro-magnetic forces, fictitious forces,...).
- T ... stress tensor.
- In fluid dynamics typically: $T = -p \, \mathrm{Id} + T_V$ with pressure p and viscous stresses T_V.
- Differential formulation:

$$\frac{d}{dt}(\rho v_i) + \nabla \cdot \big((\rho v_i) v\big) = f_B + \nabla \cdot t_i.$$

Outline

Dimensional consistency

- We always deal with physical quantities consisting of values and units.
- All relations have to hold independent of the choice of units.
- Buckingham's Π-theorem:

  Every relation between physical quantities is equivalent to a relation between dimensionless quantities.

- Can always reduce the number of relevant parameters.
- Choice of dimensionless parameters is not unique; some choices are "better" than others.

Scaling

- Given a set of relations between physical quantities, find a reasonable choice of units/scales:
  - Obtain dimensionless relations.
  - Reduce the number of parameters.
  - Scales should be chosen in such a way that the interesting quantities are well scaled.
- Scaling usually based on balancing considerations.
- Time is often scaled such that maximal velocities are of order one.
- Scaling is specific to the physical situation; the same equations can entail completely different scalings.
- Sometimes, different scalings are necessary to describe a single phenomenon.

Outline

Basic idea

- After rescaling, we have obtained a relation

$$\Phi(y; \varepsilon, \mu, \nu, \dots) = 0$$

  with dimensionless parameters ε, μ, ν, ...
- In the situation we are interested in, we have $\varepsilon \ll \mu \sim \nu \sim \cdots$.
- Approximate the relation by

$$\Phi_0(y_0; \mu, \nu, \dots) := \Phi(y_0; 0, \mu, \nu, \dots) = 0.$$

- Obtain approximation y_0 for sufficiently small parameters ε.

Higher order perturbations

Obtain better approximations by including higher order terms:
Try to write solution as

$$y = y_0 + \varepsilon y_1 + \varepsilon^2 y_2 + \dots$$

and relation as

$$\Phi_0(y_0; \dots) + \varepsilon \Phi_1(y_0, y_1; \dots) + \varepsilon^2 \Phi_2(y_0, y_1, y_2; \dots) + \dots = 0.$$

Solve

$$\begin{aligned} \Phi_0(y_0; \dots) &= 0 \qquad \text{for } y_0, \\ \Phi_1(y_0, y_1; \dots) &= 0 \qquad \text{for } y_1, \\ \Phi_2(y_0, y_1, y_2; \dots) &= 0 \qquad \text{for } y_2, \\ &\vdots \end{aligned}$$

Conflicting scales

- Perturbation approach cannot be used immediately if we have different scales at different parts of the solution.
- Typical situation: small parameter ε in front of highest order derivative $y^{(k)}$:
  - Approximation $\varepsilon y^{(k)} \sim 0$ makes only sense if $y^{(k)} \ll 1/\varepsilon$.
  - Setting $\varepsilon = 0$ leads to overdetermined equation because of conflicting initial or boundary conditions.
- Reasonable scalings include different small parameters in different parts of the solutions.
- Obtain different approximations that have to be fitted together.

Outer and inner solutions

- Have identified a boundary (or interior) layer where the approximation $\varepsilon = 0$ leads to inconsistencies.
- Use regular perturbations to obtain an outer solution outside of the boundary layer.
- Rescale the equation, and use regular perturbations for the rescaled equation to obtain an inner solution within the boundary layer.
- Adjust free constants by matching the solutions in an intermediate region.

Outline

Stationary states

- Long term behaviour of many systems is given by their (asymptotically) stable stationary states.
- For an explicit first order system of ODEs

  $$\dot{y} = F(y),$$

  the stationary states/equilibrium points are the solutions of $F(y) = 0$.
- For a parabolic/hyperbolic PDE

  $$\frac{\partial y}{\partial t} = F(x, y, \nabla y, \nabla^2 y, \ldots),$$

  the stationary states are the time independent solutions $y = y(x)$ of $F(x, y, \ldots) = 0$.

Linearisation

- Assume that y_e is a stationary state of the system

$$\dot{y} = F(y).$$

The linearisation of the system around y_e is the linear system

$$\dot{z} = JF(y_e)z,$$

where JF is the Jacobian of F.

- For PDEs we obtain a linearisation by Taylor expansion w.r.t. δ of

$$\frac{\partial}{\partial t}(y_e + \delta z) = F(x, y_e + \delta z, \nabla y_e + \delta \nabla z, \ldots)$$

and collecting all terms of order δ.

Linear stability for ODEs

- An equilibrium point y_e is (asymptotically) stable, if all solutions of the system that start close to y_e remain bounded (converge to y_e).[1]
- For linear systems, stability is completely determined by (geometric and algebraic) eigenvalues of the system.
- Non-linear case: Denote by λ_i the eigenvalues of $JF(y_e)$.
  - If $\Re\lambda_i < 0$ for all i, then y_e is asymptotically stable.
  - If $\Re\lambda_i > 0$ for any i, then y_e is unstable.

[1] This is not a precise definition!

Bifurcations

- Consider parameter dependent system

$$\dot{y} = F(y; \mu)$$

  with equilibrium points y_μ.
- Bifurcation diagram: plot of the solutions of $F(y; \mu) = 0$ as μ varies.
- Bifurcation points: parameters/points (μ, y_μ) where a change of μ changes the character of the equilibrium points:
  - Regular turning points: stable and unstable equilibrium merge and then vanish.
  - Transcritical bifurcations: stable and unstable equilibrium merge and then change roles.
  - Pitchfork bifurcations: stable (unstable) equilibrium point becomes unstable (stable), new set of stable (unstable) equilibrium points emerges.
  - ...

Method of characteristics

- Consider hyperbolic PDE of the form

$$\frac{\partial h}{\partial t} + a(t,x,h)\frac{\partial h}{\partial x} = b(t,x,h).$$

- Equation for characteristics given by

$$\begin{aligned} \dot{x} &= a(t,x,z), & x(0) &= x_0, \\ \dot{z} &= b(t,x,z), & z(0) &= h_0(x_0). \end{aligned}$$

- Solution of the equation given by

$$h(x(t),t) = z(t)$$

if possible.

Shocks

Shocks form when characteristics collide at some point $(\bar{x}, \bar{t})$.

Basic model:

- Up to the time $\bar{t}$, the density ρ is continuous.
- After the time $\bar{t}$, the density has a discontinuity (*shock*) along a curve $(s(t), t)$ starting at $(\bar{x}, \bar{t})$.
- Immediately to the left of the shock, the density and flux density are

  $$\rho^-(t) := \rho(s(t)^-, t) \qquad j^-(t) := j(t, x, \rho(s(t)^-, t));$$

  immediately to the right, they are

  $$\rho^+(t) := \rho(s(t)^+, t) \qquad j^+(t) := j(t, x, \rho(s(t)^+, t)).$$

- The shock develops at speed

  $$\dot{s}(t) = \frac{j^+(t) - j^-(t)}{\rho^+(t) - \rho^-(t)} =: \frac{[j](t)}{[\rho](t)}.$$

Rarefaction waves

Rarefaction waves are formed, when a region of the (x, t) half-plane is not covered by characteristics.

Basic situation for equation of the form

$$\rho_t + j(\rho)_x = q(\rho):$$

- We have a discontinuity at a point x_0 in the initial data.
- Characteristics starting near x_0 leave in opposite directions, creating a "dead sector" in between.
- Model the solution in the dead sector as

$$\rho(x,t) = \varphi\Big(\frac{x - x_0}{t}\Big)$$

such that the PDE holds.

Boundary conditions

- Solution of hyperbolic PDE requires:
  - Initial conditions at $t = 0$.
  - Boundary conditions.
- Need to differentiate between inflow and outflow boundaries:
  - At outflow boundaries, characteristics move away of the domain of the PDE; boundary values cannot have any effect.
  - At inflow boundaries, characteristics move into the domain of the PDE; boundary values are necessary.
  - Shocks at inflow boundaries are possible.
- Boundary conditions often given as flux conditions.
  - Fluxes have to be translated first into ordinary boundary values.
  - Additional modelling assumptions can be necessary.

Outline

Numerics of PDEs

- Mathematical models tend to lead to (possibly non-linear) PDEs.
- Need *accurate* and *fast* numerical solvers for PDEs.

Possible courses:

- (Finite differences (TMA4212, spring).)
- Finite elements (TMA4220, autumn):
  - Numerical solution of PDEs on irregular domains.
  - Specifically elliptic and parabolic equations.
  - Most common solution methods in engineering applications.
- Numerical linear algebra (TMA4205, autumn):
  - Efficient numerical solution of large systems obtained from the discretisation of PDEs.
  - Numerical treatment of (large) eigenvalue problems.

Optimal control

Given a PDE (or ODE) modelling a specific situation of interest.

- Can control certain parameters of the problem (e.g. right hand side, boundary values).
- Want to reach a specific solution (as close as possible).

Possible course:

- Optimisation II (TMA4183, spring):
  - Existence of optimal controls.
  - Analysis of optimality conditions.
  - Fundamental numerical solution methods.

Modelling weeks

- Organised annually by ECMI (European Consortium of Mathematics in industry, `www.ecmiindmath.org`).
- One week collaboration with international students on a project based on real world problems.
- Presentations of all the different projects at the end of the week.
- Afterwards summary in form of a project report.
- Winter modelling week in Darmstadt, Feb 24–Mar 03 2019.
  - `http://www.graduate-school-ce.de/ecmi2019`
- Regular modelling week in Grenoble, July 2019 (exact date TBA).