6 Ordinary differential equations (ODEs)

6.1 Introduction and definitions

What is an ODE?

- **ODEs** are typically used to mathematically describe the **evolution** of some dynamical variable of interest.

- Examples: Newtonian radiative cooling, radioactive decay

$$\frac{\mathrm{d}q}{\mathrm{d}t}(t) = R\big(q(t), t\big)$$

- Such equations occur in CFD when **integral bulk quantities** are diagnosed.
  - mass of water accumulated in a pumped storage power plant
  - amount of H_2 stored in a gas bottle
  - modulation of heat stored in a thermal facility

What is an ODE? (cont'd)

$$\frac{\mathrm{d}q}{\mathrm{d}t}(t) = R\big(q(t), t\big)$$

- The derivative $\mathrm{d}q/\mathrm{d}t$ of a physical variable q represents a *rate of change* that is equal to a rate function R. This general formulation constitutes a first-order **differential equation**.
- A differential equation is said to be **ordinary**, when it depends on *one parameter only*, here time t.

Numerical solution of an ODE

- We have learned about numerical differentiation and integration in the previous lectures and exercises by applying discretization methods (FDM, quadrature formulas).
- We now strive to apply these methods *formulating an algorithm* that numerically solves an ordinary differential equation. This is called **numerical integration of an ODE**.

General strategy for numerical integration of an ODE I

1. **Formally integrate** the ODE over *one time step* $\Delta t = t^{n+1} - t^n$, where n is the present and $n+1$ the future time.

$$\int_{t^n}^{t^{n+1}} \frac{\mathrm{d}q}{\mathrm{d}t}\,\mathrm{d}t = q(t^{n+1}) - q(t^n) \equiv q^{n+1} - q^n$$

2. **Apply a quadrature rule** to the right-hand side. A simple *explicit Euler method* (lower sum) yields

$$\int_{t^n}^{t^{n+1}} R\big(q(t), t\big)\,\mathrm{d}t \approx R\big(q(t^n), t^n\big) \cdot \Delta t$$

General strategy for numerical integration of an ODE II

3. **Rearrange** by solving for the unknown 'future' value(s).

$$q^{n+1} - q^n = R\big(q(t^n), t^n\big) \cdot \Delta t$$

$$\boxed{\Rightarrow \qquad \underbrace{q^{n+1}}_{\text{new}} = \underbrace{q^n}_{\text{old}} + \underbrace{\Delta t \cdot R\big(q(t^n), t^n\big)}_{\text{update}}}$$

4. **Prescribe** the **initial condition**.

$$q \leftarrow q^0$$

5. **Iterate** by incrementing n until the desired time $t = t_{\text{end}}$ is reached.

$$t \leftarrow t + \Delta t$$
$$n \leftarrow n + 1$$

6 Ordinary differential equations (ODEs)

6.2 ODE systems

What is a system of ODEs?

- In CFD, **systems of ordinary differential equations** occur by *spatial discretization* of the conservation equations for mass, momentum, and energy.

- Every nodal value, like $\rho_{i,j,k,}(t)$, $u_{i,j,k}(t)$, $v_{i,j,k}(t)$, $w_{i,j,k}(t)$, $\ldots$, becomes a **function of time** with an associated *rate equation*.

- ODEs for *neighboring* nodal values located at $i, i \pm 1, \ldots$; $j, j \pm 1, \ldots$; $k, k \pm 1, \ldots$ are **coupled** by the right-hand sides R as result of the discrete *finite-differencing stencils*.

Numerical integration of ODE systems

- We follow the procedure outlined for a *single* ODE, but apply it *simultaneously* to **all** differential equations of the system.
- The equations of the system are hence integrated together 'in parallel'.
- Example: A rank-2 system of coupled ODEs

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t) = y(t)$$

$$\frac{\mathrm{d}y}{\mathrm{d}t}(t) = -k \cdot x(t)$$

Example: Numerical integration of 2 coupled ODEs

1. Integrate over $\Delta t = t^{n+1} - t^n$ and discretize using, for example, an explicit Euler method (lower sum) for the right-hand side

$$x^{n+1} - x^n \approx y^n \cdot \Delta t$$
$$y^{n+1} - y^n \approx -k \cdot x^n \cdot \Delta t$$

2. Rearrange each equation solving for terms with $n+1$

$$x^{n+1} = x^n + \Delta t \cdot y^n$$
$$y^{n+1} = y^n - \Delta t \cdot k \cdot x^n$$

3. We need to prescribe two initial conditions, one for x and one for y

$$x \leftarrow x^0$$
$$y \leftarrow y^0$$

4. Insert all of the above into the previously developed update algorithm

$$t \leftarrow t + \Delta t$$
$$n \leftarrow n + 1$$

6 Ordinary Differential Equations

6.3 Example: Lorenz system with chaotic dynamics

Prelude on instabilities

Instability = unrestricted growth of a perturbation

- *Stability region*:
  - (De-)stabilizing effects are **physically** governed by *viscous* and *inertial* forces in the flow. Their (im-)balance is expressed by the Reynolds (*Re*) number.
  - Also **numerical** algorithms provide (de-)stabilizing effects. In CFD, this is often—*but <u>not</u> exclusively!*—expressed in terms of a Courant–Friedrichs–Levy (CFL) number.
- Instability mechanisms are vast ... more will follow in advanced lectures ond fluid mechanics and CFD.
- A developing instability often provides a possible route to *turbulence*. This can be induced by numerical errors that may trigger physical flow instabilities.

Textbook example: Kelvin–Helmholtz shear instability

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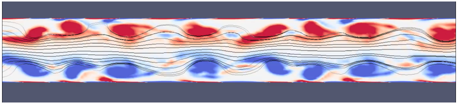
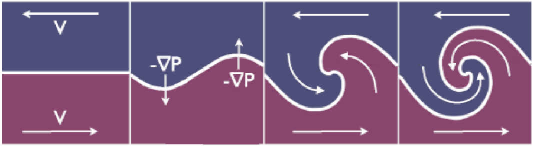
(https://commons.wikimedia.org/w/index.php?curid=575598)

2-D LES with OpenFOAM ($Re = 1335$) exhibiting pile-up of numerical errors followed by physical instability.

Video: `anim_kh-chan_OFles2d.mp4`





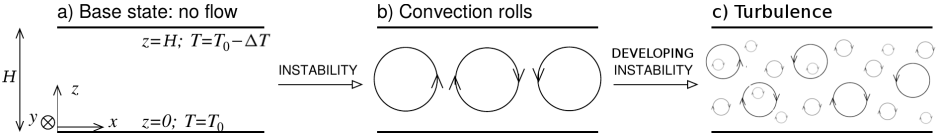
from: J. R. Johnson *et al.*, Kelvin Helmholtz instability in planetary magnetospheres, *Space Sci. Rev.*, 184:1–31, 2014.

- Laboratory experiment of the Kelvin–Helmholtz instability:
  https://www.youtube.com/watch?v=UbAfvcaYr0O
  (M. Hallworth & G. Worster, University of Cambridge, UK)

Bénard instability (unstable buoyancy stratification)

- The flow due to the instability is called *Rayleigh–Bénard convection*.
- Rayleigh and Prandtl number: $Ra = \dfrac{g\,\alpha\,\Delta T\,H^3}{\nu\,\Gamma}$ $\qquad Pr = \dfrac{\nu}{\Gamma}$

from: O. Shishkina, MPI-DS, Göttingen, Germany, 2018



adapted from: A. Juel, University of Manchester, UK, 2012

Lorenz' view on chaotic Rayleigh–Bénard convection

- **Reference:** E. N. Lorenz (1963), "Deterministic nonperiodic flow", *J. Atmos. Sci.*, **20**:130
- Lorenz aimed to study bulk flow properties of Rayleigh–Bénard convection, in particular, the emergence of nonperiodic flow as route to chaos and turbulence.
- The basis is the **Navier–Stokes equations** for a Newtonian fluid assuming small flow velocities and the **Boussinesq limit** of weak density and temperature fluctuations.
- Lorenz simplified (spatially integrated) the governing equations obtaining one equation for the "temperature", one for the "buoyancy", and another for the "kinetic energy".
- Control parameters are proportional to the Prandtl number, the Rayleigh number, and the height of the fluid layer.

The Lorenz system

- The **Lorenz system** is given by the following 3 coupled ordinary rate equations:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = s \cdot (y - x)$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = (r - z) \cdot x - y$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = x \cdot y - b \cdot z$$

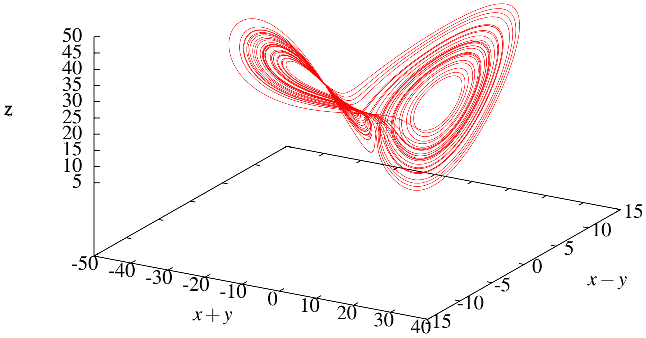
- **Dimensionless dynamical variables:** $x(t)$, $y(t)$, $z(t)$
- **Dimensionless control parameters:** s, r, b

6 Ordinary Differential Equations

6.4 Numerical solution of the Lorenz system

Numerical solution of the Lorenz system

Details? See Exercise 06!



Lorenz attractor for the parameters $b = 8/3$, $r = 28$, $s = 10$ using initial conditions $x^0 = -8$, $y^0 = -1$, $z^0 = 33$.

Keywords

- ODE
- Systems of ODEs
- Explicit numerical integration of ODEs
- Lorenz system