Introduction to Computational Thinking and Programming for CFD

Module 13251

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1 Introduction

1.1 What is CFD?

What is CFD?

CFD = **C**omputational **F**luid **D**ynamics

What is fluid dynamics?

A synonym is: **fluid *mechanics***

- The science of the laws of *motion* <u>and</u> *equilibriums* of fluids
- A branch of classical mechanics / applied physics

What is a fluid?

Fluid (lat. "‘fluidus"’)

- For example: air, water, oil, ... but is there a definition?
- A modern and technically correct **definition** is given by the German institute for Standardization in **DIN 5492**:

  “Fluid [denotes] the generic term for drippable liquids and gases.”

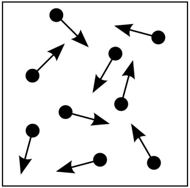
- **States of matter**: liquid and gaseous
- **Response to deformations**: *not* shape elastic

ISS experiment, NASA (www.youtube.com/watch?v=bKk_7NIKY3Y)

What is a fluid?

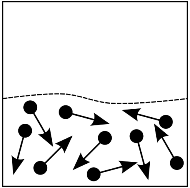
Gas

- always fills a given volume completely
- compressible (= volume elastic)
- weak molecular interaction due to mechanical collisions



Liquid

- forms an interface (may <u>not</u> fill a given volume)
- not or only weakly compressible
- strong molecular interaction through inter-molecular potential



Again: What is CFD?

CFD = **C**omputational **F**luid **D**ynamics

Applications	Single and multi-purpose CFD solver
Methods	Numerical methods · Flow modeling
Foundations	Informatics · Mathematics · Physics

Again: What is CFD?

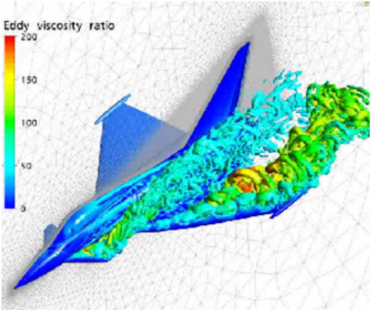
- **Foundations**
  - Physics: governing equations ($\rightarrow$ Gas Dynamics)
  - Mathematics: tensor analysis, discrete mathematics
  - Computer science: languages, algorithms ($\rightarrow$ This course!)
- **Methods** ($\rightarrow$ CFD 1, CFD 2)
  - Discretization of governing equations
  - Numerical algorithms for approximate solutions
  - Influence of numerical errors
- **Applications**
  - CFD software ($\rightarrow$ CFD Project)
  - Modeling strategies ($\rightarrow$ Turbulence Modeling)

1 Introduction

1.2 Overview of CFD applications

Applications in aerospace and automotive engineering

1



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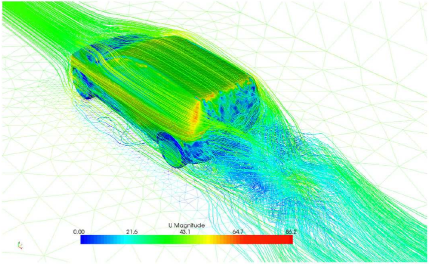

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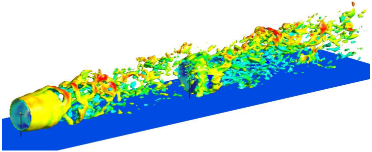
1 – NASA, Langley Research Center, public domain (https://commons.wikimedia.org/w/index.php?curid=494937)
2 – www.computationalfluiddynamics.com.au
3 – www.computerhistory.org

Applications in systems, power, and process engineering


1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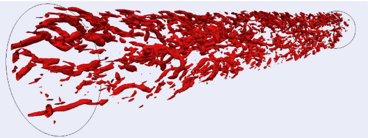
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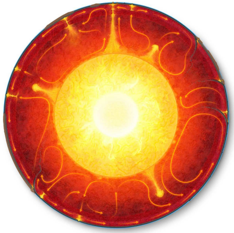
4

1 – NREL (www.nrel.gov)
2 – NeSI (www.nesi.org.nz)
3 – M. Quadrio, Politecnico di Milano (https://home.aero.polimi.it/quadrio)
4 – www.abc.net.au

CFD for heat transfer and energy storage applications

Environmental and geophysical flows


1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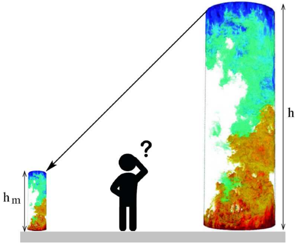
Technical flows



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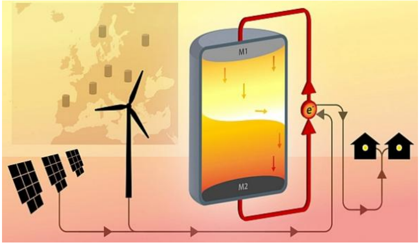

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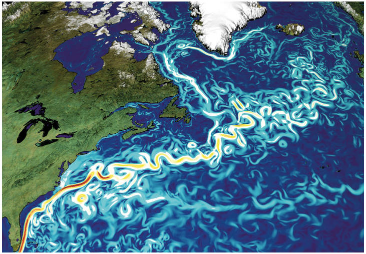
1 – Pyroconvection cloud, Noriyuki Todo, NOAA
3 – Scaling in thermal convection, R. J. A. M. Stevens et al., DLES 2019
2 – Mantle convection, Cambridge Volcano Seismology, UK
4 – Liquid metal battery, Nick Flaherty (eenewseurope.com)

Applications in climate system research (atmos/ocean)

1



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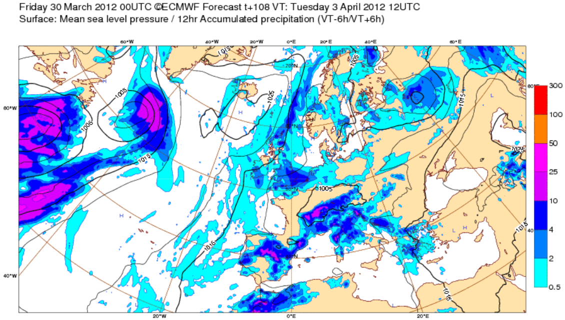

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1 – Hurricane “Sandy” (`www.amerika21.de`) 2 – GEOMAR (`www.geomar.de`) 3 – ECMWF (`www.ecmwf.int`)

1 Introduction

1.3 Summary of the governing equations

Physical background

- **CFD** is based on *fluid mechanics*. Hence, it should obey the same *physical principles*:
  1. **Conservation of mass.**
  2. **Conservation of momentum.**
  3. **Conservation of energy.**
- *Fluid mechanics* is a classical theory that describes the motion of continuous media (gases and liquids) by a few field variables.
- The *governing equations* are the **Navier–Stokes equations**[1]. All of the above examples can be described by these equations.

[1] See below and additional material in Moodle.

Physical principles of CFD

- **Conservation of mass** takes into account that mass can be rearranged by but *not* vanish (neglecting nuclear decay).

  change of mass = sum of in- and outfluxes across the surface of a fluid element

- **Conservation of momentum** follows from *Newton's axioms of classical mechanics*, in particular the 2nd axiom.

  change of momentum = sum of forces acting on a fluid element

- **Conservation of energy** requires an account for thermodynamic properties in addition to macroscopic motions. This is achieved by the *first law of thermodynamics*.

  change of energy = sum of mechanical work performed on and heat supplied to a fluid element

Governing equations in general differential form

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0 \qquad \text{mass}$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} \circ \boldsymbol{u}) = -\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \boldsymbol{\tau} + \rho \boldsymbol{f} \qquad \text{momentum}$$

$$\begin{aligned} \frac{\partial (\rho \hat{e})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \hat{e} \boldsymbol{u}) &= -\boldsymbol{\nabla} \cdot (p \boldsymbol{u}) + \boldsymbol{\nabla} \cdot (\boldsymbol{u} \cdot \boldsymbol{\tau}) + \boldsymbol{u} \cdot \rho \boldsymbol{f} \\ &\quad - \boldsymbol{\nabla} \cdot \boldsymbol{q}_T + \rho \dot{Q} \qquad \text{energy} \end{aligned}$$

$$\text{with} \quad \hat{e} = \frac{u^2}{2} + e(T) \qquad \text{total energy} \quad + \quad \text{EoS}^*$$

- The set of conservation equations constitutes a hyperbolic system of partial differential equations.
- The conservation equations alone are <u>not closed</u>.
- Additional conditions are obtained from *equations of state* (EoS*) (like the ideal gas caloric, $e = C_V T$, and thermal, $p = \rho R_s T$, EoS) that define the thermodynamic properties of the fluid.

Remarks on the equations of motion

The governing equations are *conservation equations* that describe the evolution of the *conserved quantities*.

The following **conserved quantities**, **equations**, and **physical principles** can be identified ...

mass	**continuity eq.**	**mass conservation**
momentum	**momentum eq.**	**Newton's second axiom**
energy	**energy eq.**	**first law of thermodynamics**

Different **formulations** are possible ...

differential	for a point (local)	only for continuous solutions
integral	for a finite volume	also for <u>dis</u>continuous solutions
Eulerian	global reference frame	prognostic
Lagrangian	local (FE) reference frame	mostly diagnostic

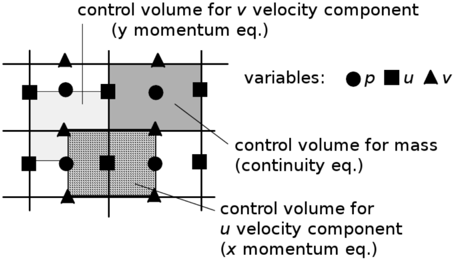
1 Introduction

1.4 Overview of essential CFD methods

Overview of discretization strategies

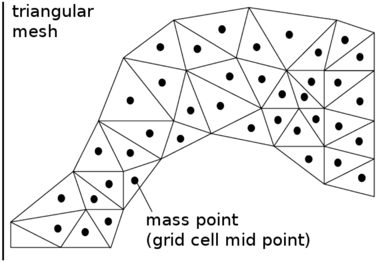
FDM

structured grid



FVM

unstructured grid



After: C. Beffa, *2-D Shallow Water Equations*, Numerical Hydraulics Script, FLUVIAL (`www.fluvial.ch`)

Discretization strategies for structured grids

Finite Difference Method (FDM)

- Start from: *differential form* of the governing equations
- Approximation of the *derivative* by a *difference stencil*

$$\frac{\partial u}{\partial y} \approx \frac{u(x, y + \Delta y, z, t) - u(x, y, z, t)}{\Delta y}$$

- Efficient and of high accuracy, but only for simple geometries and continuous (differentiable) solutions
- In-house research codes

Discretization strategies for unstructured grids

Finite Volume Method (FVM)

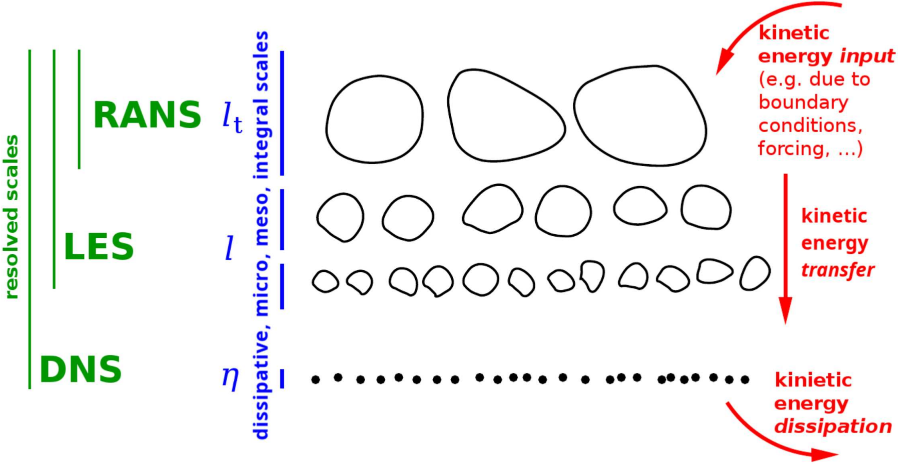
- Start from: *integral form* of the governing equations
- Approximation of the *integral* by a *quadrature rule*

$$\int_{\Delta V} \rho(x, y, z, t)\,\mathrm{d}V \approx \rho(x_0, y_0, z_0, t)\,\Delta x\,\Delta y\,\Delta z$$

- Supports complex geometries and discontinuous solutions (like shocks), but order of accuracy is often limited
- Multi-purpose CFD codes (e.g. OpenFOAM, ANSYS Fluent)

Simulation methods for turbulent flows

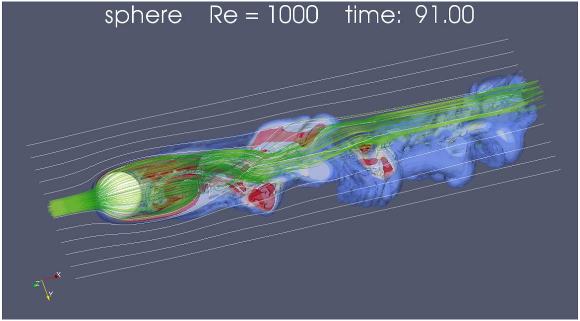
– see also: Turbulence Modeling –



After: J. Fröhlich, TU Dresden

LES in industry: Turbulent wake

OpenFOAM LES with Smagorinsky SGS model, $Re = \frac{U_\infty D}{\nu} = 1000$



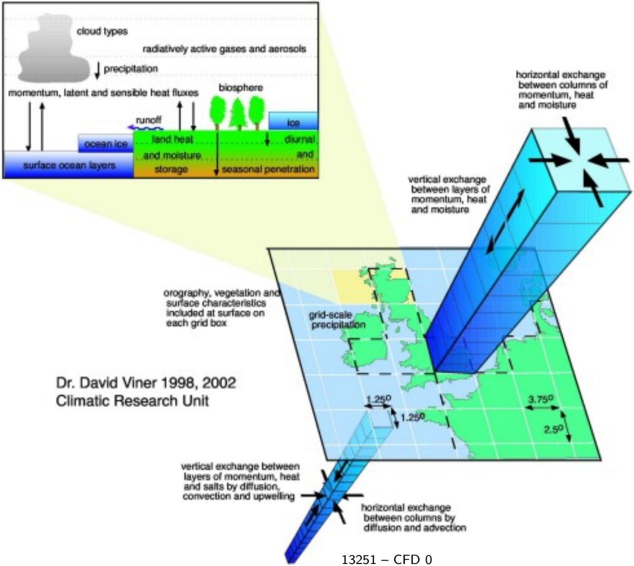
streamlines (green/white): velocity $|\boldsymbol{u}|$ **isosurfaces (blue/red):** enstrophy $|\boldsymbol{\nabla} \times \boldsymbol{u}|^2$

Reference: H. Oertel, *Strömungsmechanik*, Vieweg + Teubner, 2011

(Unsteady) RANS in climate research: Global predictions

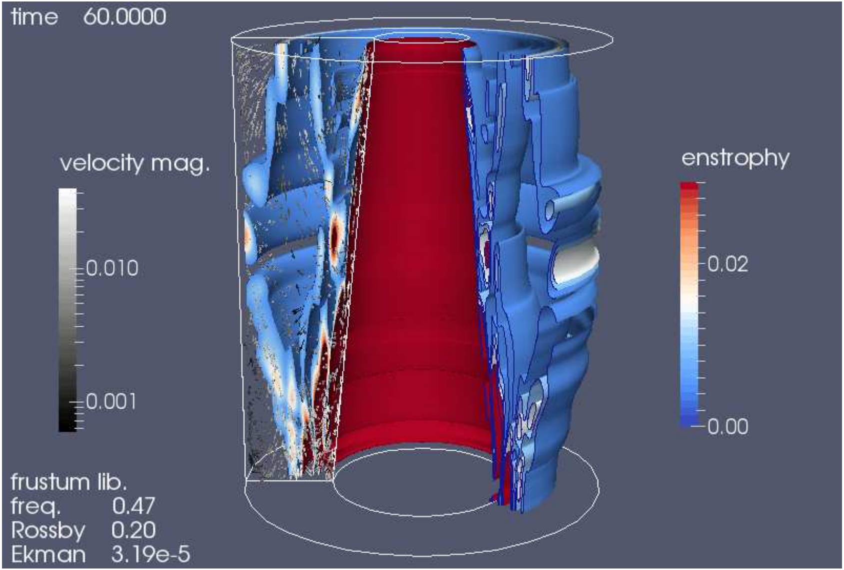
- ≈ 250–600 km horizontal and ≈ 10–1000 m vertical resolution
- ≈ 30 min time step

https://www.ipcc-data.org/guidelines/pages/gcm_guide.html

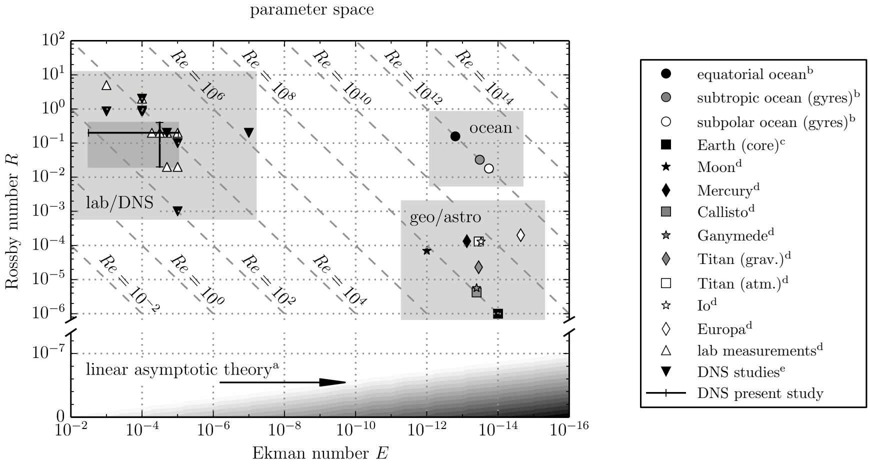


DNS in research: Inertial wave excitation

3-D structure of an inertial wave attractor – M. Klein, PhD thesis, 2016



Costs? Accessible parameter space (inertial waves)



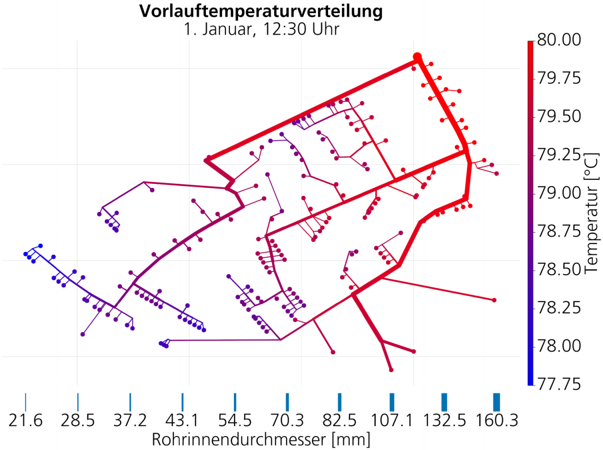
M. Klein, PhD thesis, 2016

1 Introduction

1.5 Reduced-order modeling, dynamical systems, and link to this course

Multi-energy systems – district heating network

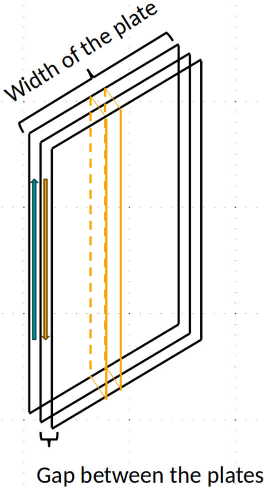
- **Heat exchangers** connect consumers to **district heating network**
- Grid operation demands control ⇝ ***fast dynamic models***



Courtesy of M. Rose & W. Hagemann (Fraunhofer IEG) – DySONiC
`https://www.ieg.fraunhofer.de/de/projekte-veroeffentlichungen/referenzprojekte/dysonic-betriebssimulation-optimierung-fernwaermenetze.html`

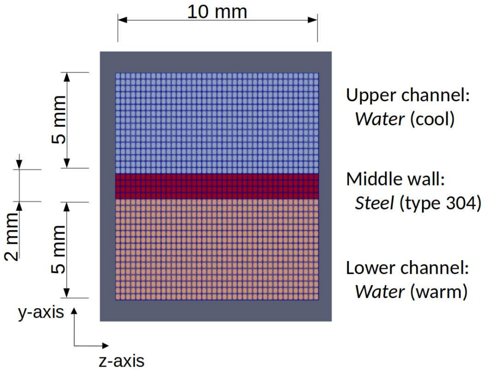
Counter-flow plate heat exchanger

Source: RomanM82, CC BY-SA 4.0
https://commons.wikimedia.org/w/index.php?curid=68483905



Courtesy by C. Tang (BTU)

Domain regions and mesh



Courtesy by C. Tang (BTU)

- **Length $L = 200\,\mathrm{mm}$**
- **Hydraulic diameter $D_h = 6.7\,\mathrm{mm}$**
- Typical values $D_h \simeq 4\ldots10\,\mathrm{mm}$

  Kakac & Liu (2012) *Heat Exchangers: Selection, Rating, and Thermal Design*, CRC Press

- Flow velocity $U = 0.1\,\mathrm{m/s}$
- **Reynolds number $Re = 670$ (subcritical)**
- **Resolution**
  $36 \times 36 \times 800 \approx 1\mathrm{M}$ cells

CFD-based approach: OpenFOAM *chtMultiRegionFoam*

- **Conjugate heat transfer (CHT)** $\rightsquigarrow$ fluid-solid coupling
- Pressure loss

Solid: Fourier eq.

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho c_p} \boldsymbol{\nabla} \cdot \boldsymbol{q}_{\mathrm{cond}}$$

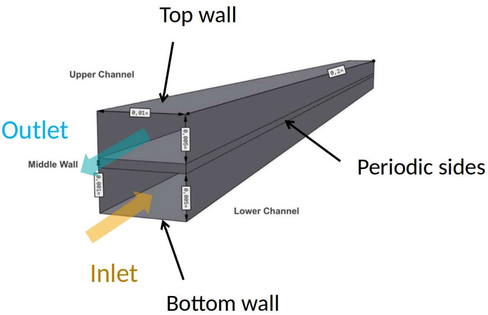
Fluid: Filtered Navier–Stokes eqs. for incompressible flow
$\rightsquigarrow$ large-eddy simulation (LES)

$$\begin{aligned}
\boldsymbol{\nabla} \cdot \boldsymbol{u} &= 0 \\
\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} &= -\frac{1}{\rho}\boldsymbol{\nabla} p - \frac{1}{\rho}\boldsymbol{\nabla} \cdot (\boldsymbol{\tau}_{\mathrm{visc}} + \boldsymbol{\tau}_{\mathrm{SGS}}) \\
\frac{\partial T}{\partial t} + (\boldsymbol{u} \cdot \boldsymbol{\nabla}) T &= -\frac{1}{\rho c_p}\boldsymbol{\nabla} \cdot (\boldsymbol{q}_{\mathrm{cond}} + \boldsymbol{q}_{\mathrm{SGS}})
\end{aligned}$$

... using *pressure-based* solver and SGS turbulence modeling

Darwish & Moukalled (2000) *Numer. Heat Transf. B: Fundamentals* **37**:103–139

Initial and boundary conditions



Courtesy by C. Tang (BTU)

Boundary conditions

- *Solid front & back:* adiabatic
- *Top & bottom:* adiabatic no-slip wall
- *Inlet:* tabulated **time-dependent inflow**
- *Outlet:* zero gradient

Initial conditions

- Uniform velocity and temperature

Model order reduction

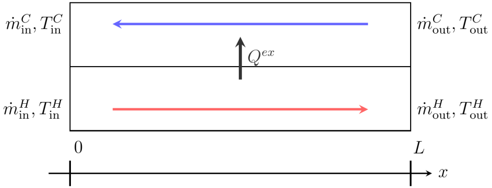
- CFD model has ≈ 1,000,000 degrees of freedom $\rightsquigarrow$ *too expensive!*
- **Collapsing the spatial dependence:** lumped modeling

$\rightsquigarrow$ control-volume-based approach

$$\frac{\mathrm{d}T^C_{\mathrm{out}}}{\mathrm{d}t} + \frac{\dot{m}^C}{\rho^C V^C}\left(T^C_{\mathrm{out}} - T^C_{\mathrm{in}}\right) = \frac{Q^{\mathrm{ex}}}{\rho^C c^C_p A^C_\perp}$$

$$\frac{\mathrm{d}T^H_{\mathrm{out}}}{\mathrm{d}t} + \frac{\dot{m}^H}{\rho^H V^H}\left(T^H_{\mathrm{out}} - T^H_{\mathrm{in}}\right) = -\frac{Q^{\mathrm{ex}}}{\rho^H c^H_p A^H_\perp}$$

$\rightsquigarrow$ 2 ODEs + CHT model for Q^{ex}



Courtesy by C. Tang (BTU)

Control-oriented model

- **Parameterize** the effects of geometry, fluid prop., flow state, ...
- **Generalized ODE:** (suppressing superscripts C, H)

$$\frac{\mathrm{d}\,T_{\mathrm{avg}}}{\mathrm{d}t} = \frac{\dot{m}}{\boldsymbol{a}}\,(T_{\mathrm{in}} - T_{\mathrm{out}}) - \boldsymbol{b}\,(T_{\mathrm{avg}} - T'_{\mathrm{avg}})$$

$\rightsquigarrow$ 2 degrees of freedom

Model 1: Classical approach

$$T_{\mathrm{out}} = 2\,T_{\mathrm{avg}} - T_{\mathrm{in}}$$

Model 2: Upstream approx.

$$T_{\mathrm{out}} = T_{\mathrm{avg}}$$

Model 3: Power balance

$$T_{\mathrm{out}} = \frac{T_{\mathrm{avg}} - T_{\mathrm{in}}}{\xi} + T_{\mathrm{in}}$$

Mozley (1956) *Industr. Eng. Chem.* **48**(6):1035–1041

Michel & Kugi (2013) *Int. J. Heat Mass Transf.* **61**:323–331

System identification

Goal

- Relate inflow ($\dot{m}$) to outlet temperature (T_{out})

  $\rightsquigarrow$ bridge gap between CFD & ODE models

Grey box approach

- Parameters ***a*** and ***b*** have physical meaning; depend on ...
  - Channel volume
  - Surface area
  - Fluid density
  - Fluid heat capacity
  - ***Heat transfer coefficient*** $\rightsquigarrow$ *flow state* $\rightsquigarrow$
    $Nu = C_h \, Re^{p} \, Pr^{1/3} \, f(\mu, \cdots)$

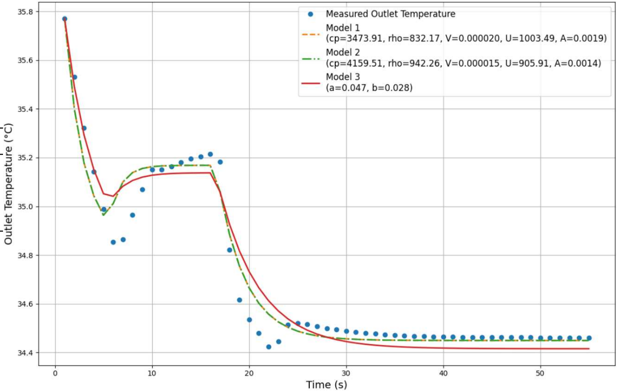
Dynamic simulation:
Validation reproducing CFD-based **outlet temperature**

Case 2 (≈ **0.92 Wh**)

Time [s]	Velocity [m/s]
0–5	0.10
5–16	0.25
16–55	0.15

$T_{\text{in}}^{H} = \underline{35.7^\circ C}$

start at 1st CFD output



C. Tang (2025), Master Thesis, BTU Cottbus-Senftenberg

The Lorenz system as toy problem ⇝ **lecture/exercise 6**

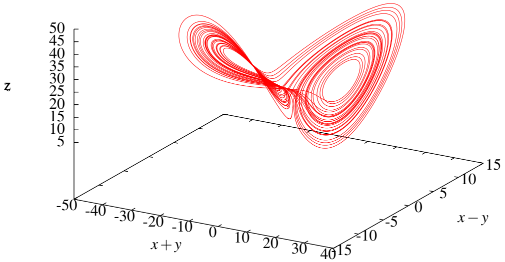
- The Lorenz system is a <u>**reduced-order dynamical model**</u>:

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

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

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

- Variables: x, y, z
- Parameters: s, r, b



Lorenz attractor

Keywords

- What is CFD?
- Navier–Stokes equations
- Discretization (FDM, FVM)
- Simulation (DNS) and modeling (LES, RANS)
- Reduced-order modeling (ROM)