Scalar Transport Equation

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Background

Scalar Transport Equation

- Scalar transport equation in the standard form will be our model for discretisation. Conservation laws, governing the continuum mechanics adhere to the standard form: good example
- Standard form is not the only one available: modelled equations may be more complex or some source/sink terms can be recognised as transport. This leads to other forms, but the basics are still the same
- Moving away from physics, almost identical equations can be found in other areas: for example financial modelling
- The common factor for all equations under consideration is the same set of operators: temporal derivative, gradient, divergence, Laplacian, curl, as well as various source and sink terms

Nomenclature

- **Scalar, vector, tensor** represent a property in a point. In the equations under consideration, we will need tensors only up to second order
  - Scalars in lowercase: a
  - Vectors in bold: $\mathbf{a} = a_i$
  - Tensors in bold capitals: $\mathbf{A} = A_{ij}$
- All vectors will be written in the global Cartesian coordinate system and in 3-D space
- **Inner and outer product** of vectors and tensors. Vector notation will be used – feel free to shadow in the Einstein notation in the notes and I will help
  - Scalar product: $a\mathbf{b} = a\, b_i$
  - Inner vector product, producing a scalar: $\mathbf{a}\bullet\mathbf{b} = a_i\, b_i$
  - Outer vector product, producing a second rank tensor: $\mathbf{ab} = a_i\, b_i$
  - Inner product of a vector and a tensor (mind the index)
    - product from the left: $\mathbf{a}\bullet\mathbf{C} = a_i\, C_{ij}$
    - product from the right: $\mathbf{C}\bullet\mathbf{a} = a_j\, C_{ij}$

Nomenclature

- **Field algebra**
  - Continuum mechanics deals with field variables: according to the continuity assumption, a variable (*e.g.* pressure) is defined in each point in space for each moment in time
  - I will use ϕ as a name for the generic variable
  - From the field definition $\phi = \phi(\mathbf{x}, t)$, which means that we can define the spatial and temporal derivative
- **Divergence and gradient**
  - For convenience, we need to define the gradient operator $\nabla\bullet$ operator to extract the spatial component of the derivative as a vector. Formally this would be $\frac{\partial \phi}{\partial \mathbf{x}}$

$$\nabla = \frac{\partial}{\partial \mathbf{x}} = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}$$

Thus, for a scalar field ϕ, $\nabla\phi$ is a vector field

$$\nabla \phi = \frac{\partial \phi}{\partial \mathbf{x}}$$

Nomenclature

- If we imagine ϕ defined in a 2-D space as a 2-D surface, for each point the gradient vector points in the direction of the steepest ascent, *i.e.* up the slope
- For vector and tensor fields, we define the inner and outer product with the gradient operator. Please pay attention to the definition of the gradient: multiplication from the left!
- Gradient operator for a vector field $\mathbf{u}$ creates a second rank tensor field

$$\nabla \mathbf{u} = \frac{\partial}{\partial x_i} u_j = \frac{\partial u_j}{\partial x_i}$$

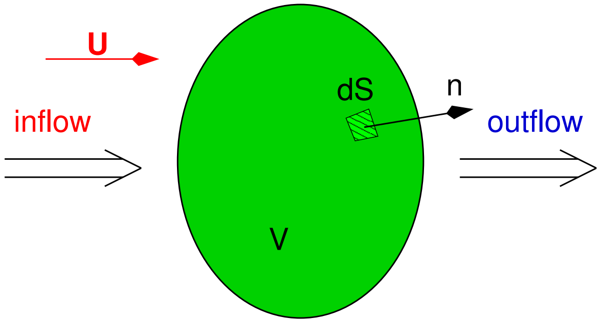
- Divergence operator for a vector field $\mathbf{u}$ creates a scalar field

$$\nabla \bullet \mathbf{u} = \frac{\partial u_i}{\partial x_i}$$

Reynolds Transport Theorem

Handling Convective Transport

- Reynolds transport theorem is a first step to assembling the standard transport equation
- Examine a region of space: a Control Volume (CV)



The rate of change of a general property ϕ in the system is equal to the rate of change of ϕ in the control volume plus the rate of net outflow of ϕ through the surface of the control volume.

$$\frac{d}{dt}\int_{V_m} \phi \, dV = \int_{V_m} \frac{\partial \phi}{\partial t} \, dV + \oint_{S_m} \phi(\mathbf{n} \bullet \mathbf{u}) dS$$

$$\frac{d}{dt}\int_{V} \phi \, dV = \int_{V} \left[\frac{\partial \phi}{\partial t} + \nabla \bullet (\phi \mathbf{u}) \right] \, dV$$

Reynolds Transport Theorem

Handling Convective Transport

- Transformation from the surface integral into the volume integral used above is called the Gauss' Theorem

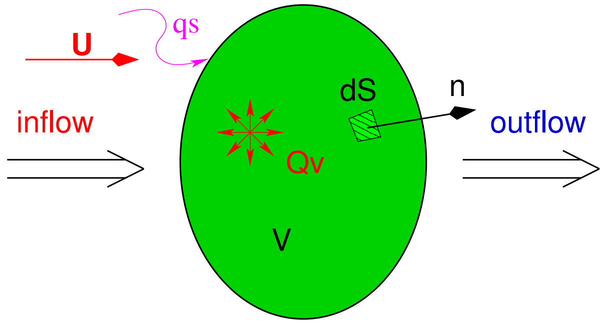
$$\int_{V_P} \nabla \bullet \mathbf{a} \, dV = \oint_{\partial V_P} d\mathbf{s} \bullet \mathbf{a} = \oint_{\partial V_P} d\mathbf{n} \bullet \mathbf{a} \, dS$$

- $\mathbf{u}$ in the equation above represents the **convective velocity**: flux going in is negative ($\mathbf{u} \bullet \mathbf{n} < 0$). The convective velocity in general terms can be considered as a coordinate transformation.
- $\mathbf{u}$ is also a function of space and time: our coordinate transformation is not trivial. Examples: "solid body motion", solid rotation, cases where $\mathbf{u}$ is not divergence-free

Sources and Sinks

Volume and Surface Terms

- Apart from convection (above), we can have local sources and sinks of ϕ.
- Volume source: distributed through the volume, *e.g.* gravity
- Surface source: act on external surface S, *e.g.* heating. Typically modelled using gradient-based models



$$\frac{d}{dt}\int_V \phi \, dV = \int_V q_v \, dV - \oint_S (\mathbf{n} \bullet \mathbf{q}_s) dS$$

$$\frac{\partial \phi}{\partial t} + \nabla \bullet (\phi \mathbf{u}) = q_v - \nabla \bullet \mathbf{q}_s$$

Diffusive Transport

Modelling Diffusive Transport

- Gradient-based transport is a model for surface source/sink terms
- Consider a case where ϕ is a concentration of a scalar variable and a closed domain. Diffusion transport says that ϕ will be transported from regions of high concentration to regions of low concentration until the concentration is uniform everywhere.
- Taking into account that $\nabla\phi$ point up the concentration slope, and the transport will be in the opposite direction, we can define the following diffusion model

$$\mathbf{q}_s = -\gamma \, \nabla\phi$$

where γ is the diffusivity

Generic Transport Equation

Generic Transport

- Assembling the above yields the transport equation in the standard form

$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{temporal derivative}} + \underbrace{\nabla \bullet (\phi \mathbf{u})}_{\text{convection term}} - \underbrace{\nabla \bullet (\gamma \nabla \phi)}_{\text{diffusion term}} = \underbrace{q_v}_{\text{source term}}$$

- Temporal derivative represents inertia of the system
- Convection term represents the convective transport by the prescribed velocity field (coordinate transformation). The term has got **hyperbolic** nature: information comes from the vicinity, defined by the direction of the convection velocity
- Diffusion term represents gradient transport. This is an **elliptic** term: every point in the domain feels the influence of every other point instantaneously
- Sources and sinks account for non-transport effects: local volume production and destruction of ϕ

Conservation Equations

Conservation Equations in Continuum Mechanics

- Conservation of mass: continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u}) = 0$$

- Conservation of linear momentum

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \bullet (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{g} + \nabla \bullet \boldsymbol{\sigma}$$

- Energy conservation equation

$$\frac{\partial (\rho e)}{\partial t} + \nabla \bullet (\rho e \mathbf{u}) = \rho \mathbf{g} \bullet \mathbf{u} + \nabla \bullet (\boldsymbol{\sigma} \bullet \mathbf{u}) - \nabla \bullet \mathbf{q} + \rho Q$$

Boundary Conditions

Role of Boundary Conditions

- The role of boundary conditions is to isolate the system from the rest of the Universe. Without them, we would have to model everything
- Position of boundaries and specified condition requires engineering judgement. Badly placed boundaries will compromise the solution or cause "numerical problems". Example: locating an outlet boundary across a recirculation zone.
- Incorporating the knowledge of boundary conditions from experimental studies or other sources into a simulation is not trivial: it is not sufficient to pick up some arbitrary data and force in on a simulation. Choices need to be based on physical understanding of the system

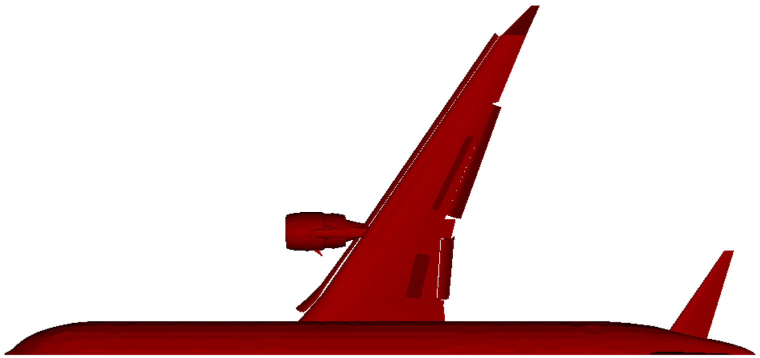
Numerical Boundary Conditions

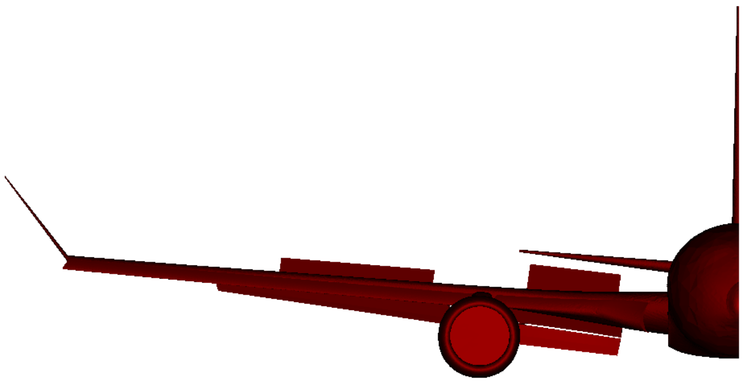
- Dirichlet condition: fixed boundary value of ϕ
- Neumann: zero gradient or no flux condition: $\mathbf{n}\bullet\mathbf{q}_s = 0$
- Fixed gradient or fixed flux condition: $\mathbf{n}\bullet\mathbf{q}_s = q_b$. Generalisation of the Neumann condition
- Mixed condition: Linear combination of the value and gradient condition

Boundary Conditions

More Numerical Boundary Conditions

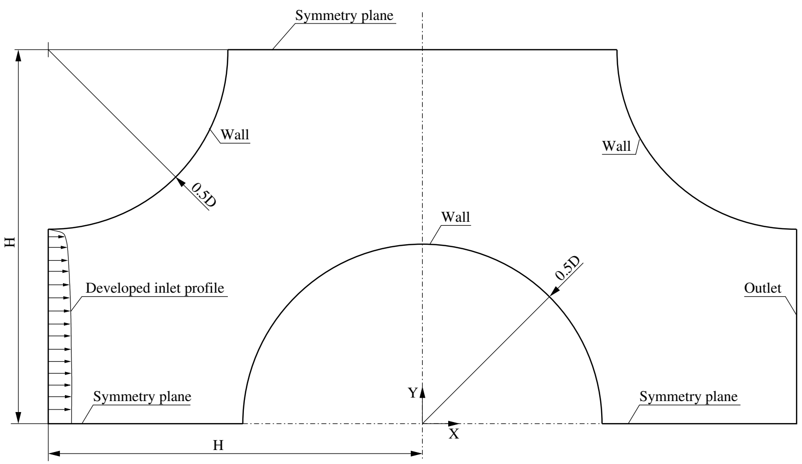
- The idea is to limit or decrease the size of the computational domain (saving on the cell count) by using the properties of the solution and boundary conditions
- **Symmetry plane.** In cases where the geometry and boundary conditions are symmetric and the flow is steady (or the equation is linear in the symmetrical direction), only a section of the problem may be modelled. The simplification will not work if the expected flow pattern is not symmetric as well: manoeuvring aircraft, cross-wind etc.

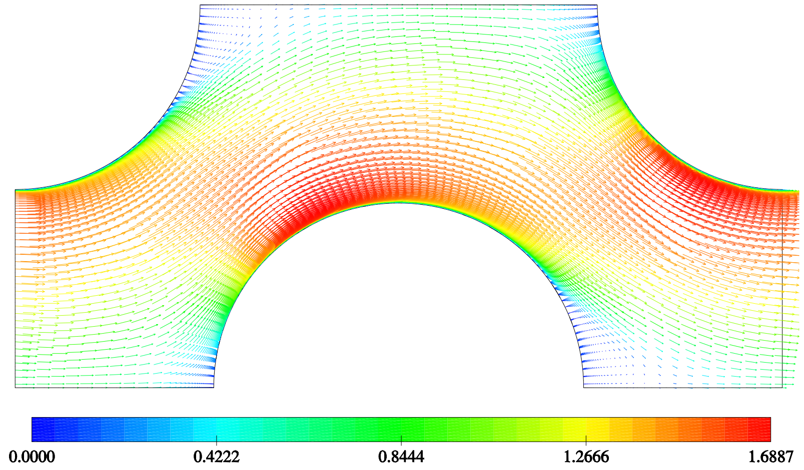




More Numerical Boundary Conditions

- **Cyclic and periodic conditions.** In cases of repeating geometry (*e.g.* tube bundle heat exchangers) or fully developed conditions, the size of domain can be reduced by modelling only a representative segment of the geometry. In order to account for periodicity, a "self-coupled" condition can be set up on the boundary. In special cases, a jump condition can be specified for variables that do not exhibit cyclic behaviour. Example: pressure in fully developed channel flow





- Implicit implementation of the condition (depending on the current value) improves the numerical properties of the condition
- A more general (re-mapping) form of the condition can also be specified, but not in the implicit form

Boundary Conditions

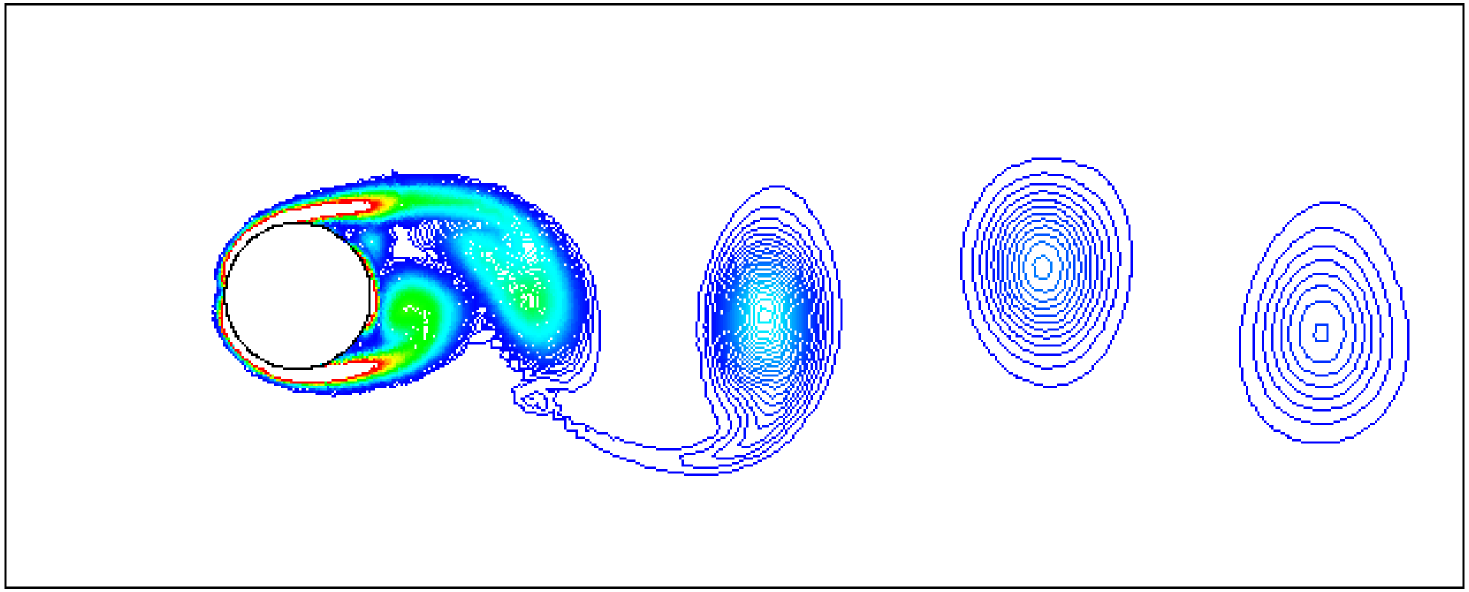
Physical Boundary Conditions

- Currently, we are dealing with a passive transport of a scalar variable: physical meaning of the boundary condition is trivial
- In case of coupled equation sets or a clear physical meaning, it is useful to associate physically meaningful names to the sets of boundary conditions for individual equations. Examples
  - Subsonic velocity inlet: fixed value velocity, zero gradient pressure, fixed temperature
  - Supersonic outlet: all variables zero gradient
  - Heated wall: fixed value velocity, zero gradient pressure, fixed gradient temperature (fixed heat flux)

Initial Condition

Specifying Initial Conditions

- Boundary conditions are only a part of problem specification. **Initial conditions** specify the variation of each solution variable in space. In some cases, this may be irrelevant:
  - Steady-state simulation result should not depend on the initial condition
  - In oscillatory transient cases (*e.g.* vortex shedding), the initial condition is irrelevant



- . . . but in other simulations it is essential: relaxation problems

Enforcing Physical Bounds

Physical Bounds in Solution Variables

- When transport equations are assembled, they represent real physical properties. A set of equations under consideration relies on the fact that physical variables obey certain bounds: if the bounds are violated, the system exhibits unrealistic behaviour
- Examples of variables with physical bounds
  - Negative density value: $-3\,\mathrm{kg/m^3}$
  - Negative absolute temperature
  - Negative kinetic energy (to turbulent kinetic energy
  - Concentration value below zero or above one: Two phase flow, using a scalar concentration ϕ to indicate the presence of fluid A

$$\phi = 1.05, \rho_1 = 1\,\mathrm{kg/m^3}, \rho_2 = 1000\,\mathrm{kg/m^3}$$

$$\begin{aligned}\rho &= \phi\,\rho_1 + (1-\phi)\,\rho_2 \\ &= 1.05 * 1 + (1 - 1.05) * 1000 \\ &= 1.05 - 0.05 * 1000 = 1.05 - 50 = -48.95\,\mathrm{kg/m^3}\end{aligned}$$

Enforcing Physical Bounds

Physical Bounds in Solution Variables

- Our task is not only to recognise this in the original equations but to enforce it during the solution process
- For vector and tensor variables, the physical bounds are not as straightforward and may be more difficult to enforce
- **Diffusion coefficient and stability.** An example of how the iterative process breaks down is a case of negative diffusion introducing positive feed-back in the system. The diffusion model:

  $$\mathbf{q}_s = -\gamma \, \nabla \phi,$$

  assumes positive value of γ. For cases where γ is genuinely negative (*e.g.* financial modelling equations), there is still a way to solve them: marching in time backwards!
- **Bounding source and sink terms.** For a scalar variable with bounds, *e.g.* $0 \geq \phi \geq 1$, a sanity check can be performed on the volumetric source term: as ϕ approaches its bounds, q_v must tend to zero

Examples

Examples of Convective-Diffusive Transport

- Convection-dominated problems
- Diffusion problems
- Negative diffusion coefficient
- Convection-diffusion and Peclet number
- Source and sink terms: preserving the boundedness

Vector and Tensor Transport

Generic Transport Equation for Vector and Tensor Properties

- A transport equation for a vector and tensor quantity very similar to the scalar form: ϕ becomes $\mathbf{d}$. However, having $\mathbf{d}$ as a transported variable allows the introduction of come interesting new terms
  - Variable convected by itself: $\nabla\bullet(\mathbf{d}\,\mathbf{d})$
  - Laplace transpose: $\nabla\bullet\left[\gamma(\nabla\mathbf{d})^T\right]$
  - Divergence (trace): $\lambda\mathbf{I}\nabla\bullet\mathbf{d}$
- The tricky terms will introduce non-linearity or inter-component coupling and produce interesting solutions
- For now, we can consider the question of coupling: are the components of the transported vector coupled or decoupled?

Introducing Non-Linearity

Non-Linear Transport

- The non-linearity in convection, $\nabla \bullet (\mathbf{u}\,\mathbf{u})$ is the most interesting term in the Navier-Stokes equations. Complete wealth of interaction in incompressible flows stems from this term. This includes all turbulent interaction: in nature, this is an inertial effect
- In compressible flows, additional effects, related to inter-equation coupling appear: shocks, contact discontinuities.
- Another form of non-linearity introduces the diffusion coefficient γ as a direct or indirect function of the solution: much less interesting

Introducing Non-Linearity

Non-Linear Source and Sink Terms

- As mentioned before, for bounded scalar variables, source and sink terms need to tend to zero as ϕ approaches its bounds. Therefore, cases where q_v is a function of ϕ are a rule rather than exception
- $q_v = q_v(\phi)$ usually leads to the decomposition of the term into a source and sink. This strictly only makes sense when ϕ is bounded below by zero and has no upper bound, but it is instructive. The linearisation is only first-order, *i.e.* q_u and q_p can still depend on ϕ.

$$q_v = q_u - q_p \phi$$

  where both $q_u \geq 0$ and $q_p \geq 0$. This kind of linearisation also follows from numerical considerations and will be re-visited later

Coupled Equations Sets

Inter-Equation Coupling

- Inter-equation coupling introduces additional complexity: a set of physical phenomena which depend on each other.
- Complexity, strength of coupling and non-linearity varies wildly, to the level of inability to handle certain models numerically. The most difficult ones involve separation of scales, where the fastest interaction (*e.g.* chemical reaction) occurs at time-scales several order of magnitude faster than the slowest (*e.g.* turbulent fluid flow)

Example

Two Coupled Scalar Equations

- $k - \epsilon$ model of turbulence:
  - k: turbulence kinetic energy
  - ϵ: dissipation turbulence kinetic energy
  - $\mathbf{u}$: velocity. Consider it fixed for the moment
  - C_μ, C_1, C_2: model coefficients.
  - k-equation:

$$\frac{\partial k}{\partial t} + \nabla\bullet(\mathbf{u}\,k) - \nabla\bullet(\mu_t \nabla k) = G - \epsilon$$

where

$$\mu_t = C_\mu \frac{k^2}{\epsilon}$$

and

$$G = \mu_t [\nabla\mathbf{u} + (\nabla\mathbf{u})^T] : \nabla\mathbf{u}$$

  - ϵ-equation:

$$\frac{\partial \epsilon}{\partial t} + \nabla\bullet(\mathbf{u}\,\epsilon) - \nabla\bullet(\mu_t \nabla \epsilon) = C_1\, G \frac{\epsilon}{k} - C_2 \frac{\epsilon^2}{k}$$