Introduction to Computational methods for PDE

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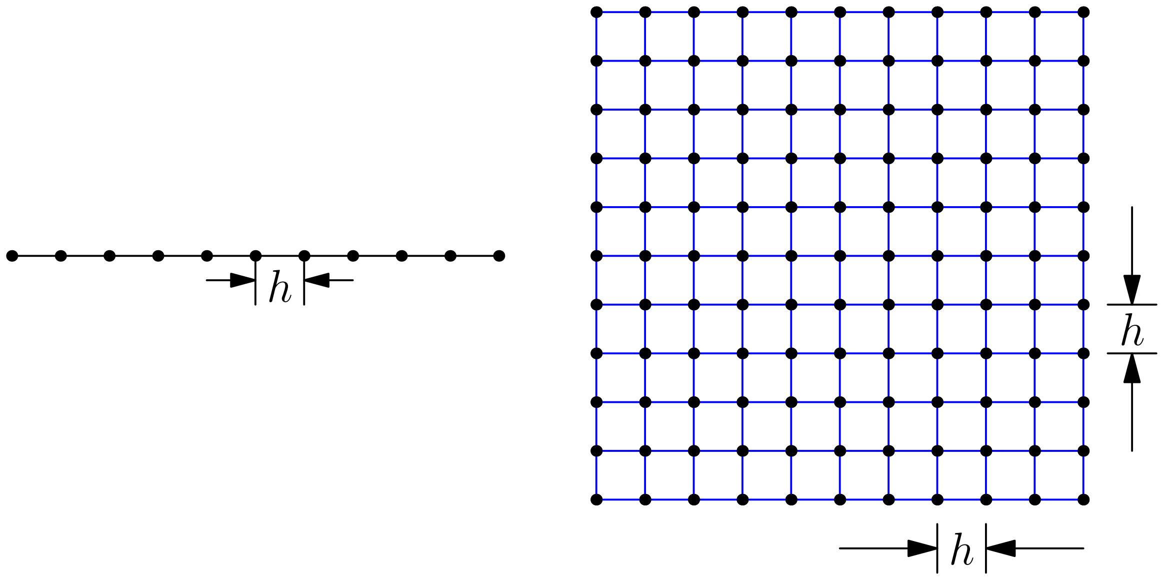
Elements of numerical analysis of PDE

A PDE and its numerical approximation

$$Lu = f \qquad\qquad L_h u_h = f_h$$

u belongs to some infinite dimensional function space, while u_h belongs to some finite dimensional space. Here h denotes the mesh/grid size, or $\frac{1}{h}$ indicates the number of mesh points or the dimension of the finite-dimensional space. It may also be refered to as *number of degrees of freedom*.



Consistency	Stability	Convergence
Accuracy	Efficiency	Scalability

Consistency

Does the numerical scheme approximate the PDE ?

Local truncation error:

$$u = \text{ exact solution} \qquad\qquad L_h u \ne f_h$$

$$\tau_h := L_h u - f_h \ne 0$$

The scheme is ***consistent*** if

$$\tau_h = \mathcal{O}\left(h^p\right) \qquad \text{for some } p > 0$$

since

$$\tau_h \to 0 \quad \text{as} \quad h \to 0$$

Easier to check consistency property. Use of Taylor formula.

Remark: We will use the order symbol $\mathcal{O}\left(\cdot\right)$ frequently. By $\tau_h = \mathcal{O}\left(h^p\right)$ we mean that $\tau_h = Ch^p$ for some C which does not depend on h. Usually we show that

$$\tau_h \le C(u)h^p \qquad C \text{ independent of } h$$

Stability

Is the numerical solution bounded independently of h ?

$$\|u_h\| \le C \|f_h\| \qquad \Longrightarrow \qquad \left\|L_h^{-1}\right\| = \sup_{f_h} \frac{\left\|L_h^{-1} f_h\right\|}{\|f_h\|} \le C$$

C does not depend on h or f_h or u_h.

- Stability is required to ensure that numerical computations do not blow up during an iterative process; round-off errors should not magnify.
- It is desirable that numerical scheme inherits the stability properties of the exact solution: boundedness, positivity, monotonicity, etc.
- Stability is required to show convergence

$$u_h \to u \qquad \text{as} \qquad h \to 0$$

Convergence

Does the numerical solution approach the exact solution

$$u_h \to u \quad \text{as} \quad h \to 0$$

Define the ***discretization error*** or ***global error***

$$e_h := u - u_h$$

Then

$$L_h e_h = L_h u - L_h u_h = L_h u - f_h = \tau_h \qquad \text{i.e.} \qquad \boxed{L_h e_h = \tau_h}$$

so that for a stable scheme

$$\|e_h\| \le C \|\tau_h\|$$

If the scheme is consistent, then

$$\|e_h\| \le C \|\tau_h\| = Ch^p \to 0 \quad \text{as} \quad h \to 0$$

Lax equivalence theorem

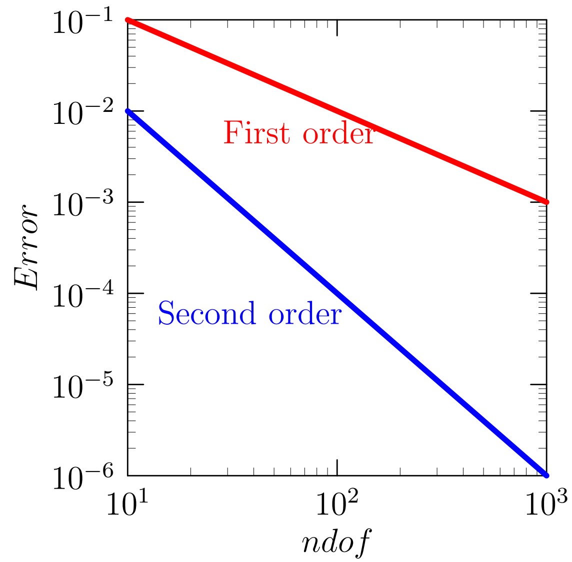
For a linear scheme approximating a linear PDE

consistency + stability $\Longrightarrow$ convergence

Accuracy

Truncation error for a consistent scheme

$$\tau_h = \mathcal{O}(h^p), \quad p > 0$$



Discretization error of a consistent and stable scheme

$$\|e_h\| \le C \|\tau_h\| = \mathcal{O}(h^p)$$

p measures the rate of convergence wrt h.

- We would like to have p as large as possible, since this leads to a smaller error, as $h < 1$.
- $p = 1$: first order accurate. They have very high errors and require very large grids (small h) to reduce error to acceptable levels.
- Most schemes used in practice have $p = 2$: second order accurate.

$$h \to h/2 \qquad e_{h/2} = \frac{1}{4} e_h$$

- Schemes with $p > 2$ are refered to as high-order accurate or high resolution schemes. But not robust for practical problems.

Building confidence

How can you trust a numerical solution ?

- Construct schemes which have as many qualitative properties of the PDE model as possible: stability, invariance, conserved quantities, positivity, monotonicity, etc.
- Do as much theoretical analysis as possible: stability, error estimates
- For problems that really matter, it is usually not possible to make a complete theoretical analysis;
  - do lots of numerical experiments.
  - compare with analytical results
  - compare with experimental results
  - compare with results from other numerical simulations
- Studying linear models and linear schemes is a first step, and a necessary condition.
- Linearize non-linear models and schemes; study their properties
- Many numerical schemes constructed for linear problems and/or scalar problems; they are also applied to non-linear and systems of PDEs without full theoretical justification (Hyperbolic conservation laws).

Verification and Validation

1. Verification
   - Are you solving the PDE correctly ? Consistency analysis
   - Purely a mathematical step (you can prove theorems) without relation to the real world.
   - Compare numerical solution with analytical solutions
   - Method of manufactured solutions: R is some differential operator

     $$R(u) = 0 \quad \Longrightarrow \quad R(u^*) = f(u^*) \qquad \text{Solve} \quad R(u) = f(u^*)$$

     u is unknown; u^* is some assumed function, $f(u^*)$ is a known source term.
   - Perform numerical study of convergence: Plot error $\|e_h\|$ wrt h and find convergence rate. Compare with theoretical analysis. See figure (1)

     $$\frac{\|e_h\|}{\|e_{h/2}\|} = 2^p \quad \Longrightarrow \quad p = \frac{\log\left(\frac{\|e_h\|}{\|e_{h/2}\|}\right)}{\log(2)}$$

2. Validation
   - Are you solving the correct (PDE) model ?
   - This is a modeling/physics issue.
   - All PDE models are approximations to reality.
   - How well does the PDE model + numerical solution represent reality ?
   - Compare numerical solution with (lots of) experiments.

Numerical study of convergence rate

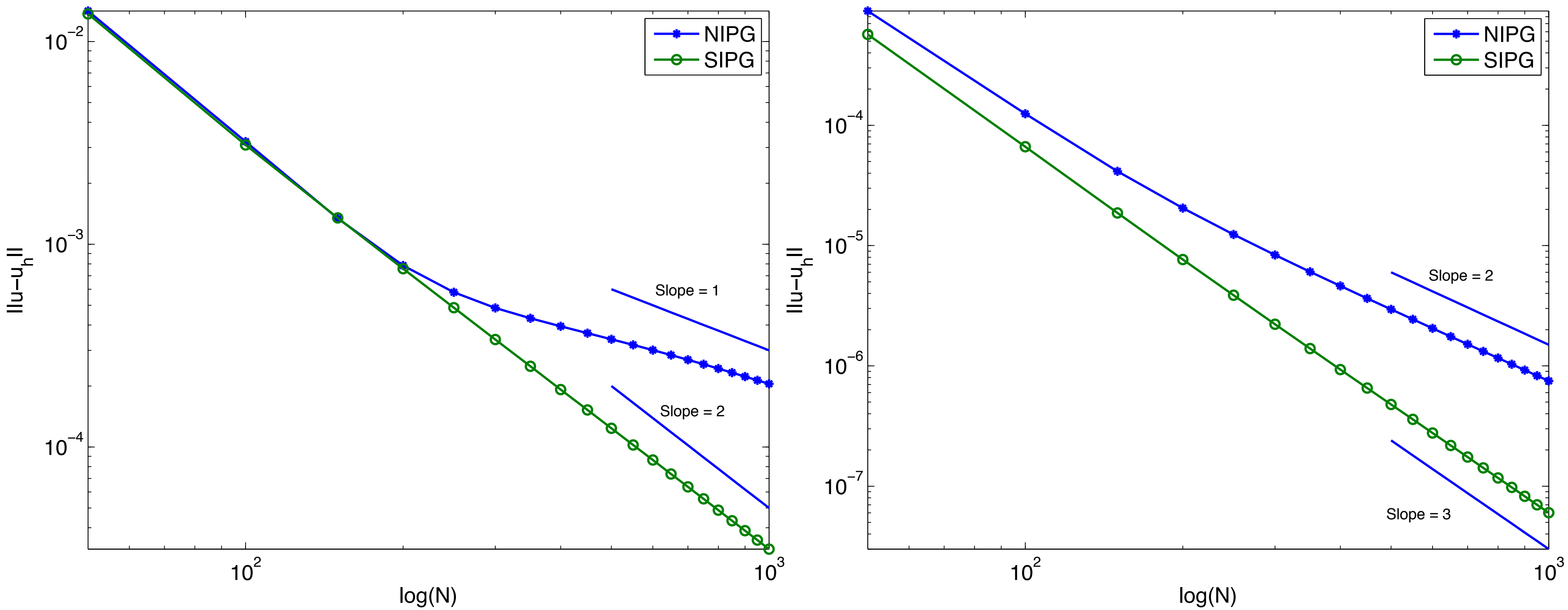


Figure : Convergence of a DG scheme for convection-diffusion equation

QoI, error estimate, grid convergence

- Usually one is interested in some integral quantities: force, heat flux, mass flow rate, etc.

$$F = \int_\Gamma p(x,y,z) n \mathrm{d}s, \quad p = \text{pressure}, \quad n = \text{unit normal to } \Gamma$$

  Full solution $p(x,y,z)$ is rarely of interest (to engineers).

- For practical problems, it is enough to compute F to within some error tolerance $|F - F_h| < \text{TOL}$.
- An ideal numerical scheme gives *good a posteriori* error estimates

$$a_h(u_h) \le |F - F_h| \le A_h(u_h)$$

  FEM provides good theoretical framework for error estimation.

- ***Grid convergence study***: Plot F_h as a function of h; find h below which there is no significant change in F_h

Some references

- Uncertainty and Error in CFD Simulations
  http://www.grc.nasa.gov/WWW/wind/valid/tutorial/errors.html
- Examining Spatial (Grid) Convergence
  http://www.grc.nasa.gov/WWW/wind/valid/tutorial/spatconv.html

Some PDE models

from fluid dynamics

Description of flow

- Gas treated as a continuum
- At every point of space occupied by gas, define density

$$\rho(x, y, z, t) = \lim_{\text{volume} \to 0} \frac{\text{mass}}{\text{volume}}$$

- Cartesian components of Velocity vector

$$u(x, y, z, t)$$
$$v(x, y, z, t)$$
$$w(x, y, z, t)$$

- Pressure

$$p(x, y, z, t) = \lim_{\text{area} \to 0} \frac{\text{Force}}{\text{area}}$$

Description of flow

- Temperature: $T(x, y, z, t)$
- Thermodynamics: relates ρ, p, T through an ***equation of state***, e.g.,

$$p = f(\rho, T)$$

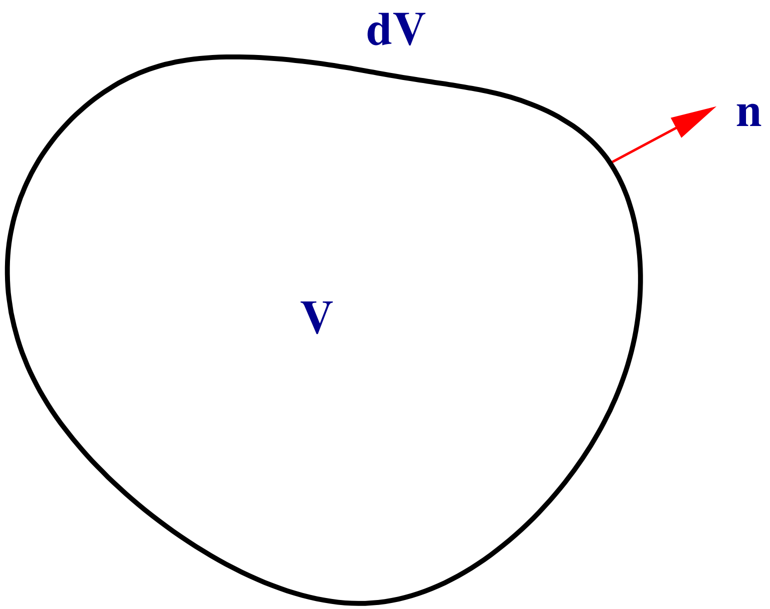
- Five quantities: ρ, u, v, w, p completely specify the state of the fluid
- Require five equations to describe the evolution of the state

Divergence theorem

- In Cartesian coordinates, $\vec{q} = (u, v, w)$

$$\nabla \cdot \vec{q} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

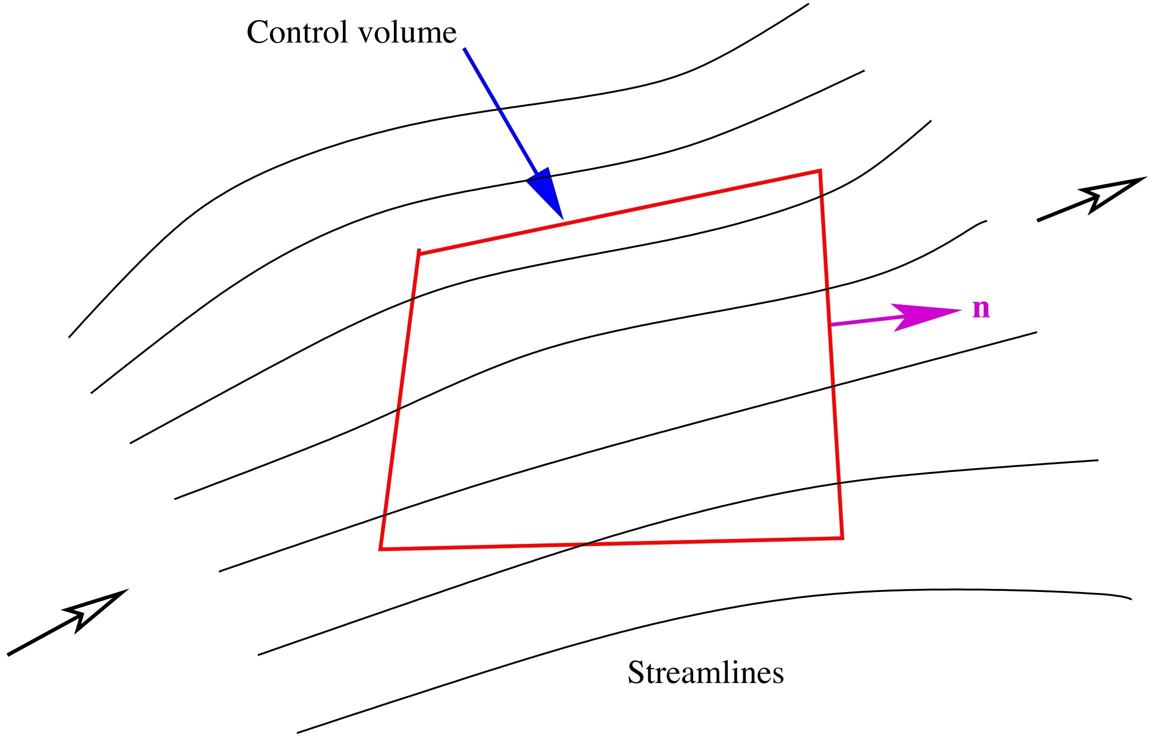
- Divergence theorem



$$\boxed{\int_V \nabla \cdot \vec{q} \mathrm{d}V = \oint_{\partial V} \vec{q} \cdot \hat{n} \mathrm{d}S}$$

Conservation laws

- Basic laws of physics are conservation laws:
  mass, momentum, energy, charge



Rate of change of ϕ in V = -(net out flux across ∂V)

$$\frac{\partial}{\partial t}\int_V \phi \mathrm{d}V = -\oint_{\partial V} \vec{F}\cdot\hat{n}\mathrm{d}S$$

Conservation laws

- If $\vec{F}$ is differentiable, use divergence theorem

$$\frac{\partial}{\partial t}\int_V \phi \mathrm{d}V = -\int_V \nabla \cdot \vec{F} \mathrm{d}V$$

or

$$\int_V \left[\frac{\partial \phi}{\partial t} + \nabla \cdot \vec{F}\right] \mathrm{d}V = 0, \quad \text{for every control volume } V$$

$$\boxed{\frac{\partial \phi}{\partial t} + \nabla \cdot \vec{F} = 0}$$

- In Cartesian coordinates, $\vec{F} = (f, g, h)$

$$\boxed{\frac{\partial \phi}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z} = 0}$$

Mass conservation equation

- $\phi = \rho$, $\vec{F} = \rho\vec{q}$

$$\vec{F} \cdot \hat{n}\mathrm{d}S = \text{amount of mass flowing across } \mathrm{d}S \text{ per unit time}$$

$$\frac{\partial}{\partial t}\int_V \rho \mathrm{d}V + \oint_{\partial V} \rho\vec{q} \cdot \hat{n}\mathrm{d}S = 0$$

- Using divergence theorem

$$\frac{\partial}{\partial t}\int_V \rho \mathrm{d}V + \int_V \nabla \cdot (\rho\vec{q})\mathrm{d}V = 0$$

or

$$\int_V \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\vec{q})\right] \mathrm{d}V = 0$$

Mass conservation equation

- Differential form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{q}) = 0$$

- In Cartesian coordinates, $\vec{q} = (u, v, w)$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0$$

- Non-conservative form

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} + w\frac{\partial \rho}{\partial z} + \rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) = 0$$

or in vector notation

$$\frac{\partial \rho}{\partial t} + \vec{q} \cdot \nabla \rho + \rho \nabla \cdot \vec{q} = 0$$

Momentum conservation

- Newton's law of motion

Rate of change of momentum	=	Total body force	+	Total surface force

Body forces like gravity
Surface forces: pressure and viscous shearing

- x, y, z momentum equations

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(p + \rho u^2) + \frac{\partial}{\partial y}(\rho u v) + \frac{\partial}{\partial z}(\rho u w) = \frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{xy} + \frac{\partial}{\partial z}\tau_{xz} + \rho f_x$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v u) + \frac{\partial}{\partial y}(p + \rho v^2) + \frac{\partial}{\partial z}(\rho v w) = \frac{\partial}{\partial x}\tau_{yx} + \frac{\partial}{\partial y}\tau_{yy} + \frac{\partial}{\partial z}\tau_{yz} + \rho f_y$$

$$\frac{\partial}{\partial t}(\rho w) + \frac{\partial}{\partial x}(\rho w u) + \frac{\partial}{\partial y}(\rho w v) + \frac{\partial}{\partial z}(p + \rho w^2) = \frac{\partial}{\partial x}\tau_{zx} + \frac{\partial}{\partial y}\tau_{zy} + \frac{\partial}{\partial z}\tau_{zz} + \rho f_z$$

Energy conservation

- Energy

$$E = \text{internal} + \text{kinetic} + \text{etc.}$$

Rate of change of energy	=	Flux of energy due to flow	+	Work done by surface and body forces	+	Transfer of heat by conduction

- Energy equation

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}[(E+p)u] + \frac{\partial}{\partial y}[(E+p)v] + \frac{\partial}{\partial z}[(E+p)w] = \text{etc.}$$

Navier-Stokes equations

$$
\begin{aligned}
\text{Mass:} \quad & \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{q}) && = 0 \\
\text{Momentum:} \quad & \frac{\partial}{\partial t}(\rho \vec{q}) + \nabla \cdot (\rho \vec{q}\vec{q}) + \nabla p && = \nabla \cdot \tau \\
\text{Energy:} \quad & \frac{\partial E}{\partial t} + \nabla \cdot (E + p)\vec{q} && = \nabla \cdot (\vec{q} \cdot \tau) + \nabla \cdot \vec{Q}
\end{aligned}
$$

Constitutive laws

- Newton's law

$$\tau = \mu(\nabla\vec{q} + (\nabla\vec{q})^\top) - \frac{2}{3}\mu(\nabla\cdot\vec{q})$$

$$\mu = \text{coefficient of dynamic viscosity}$$

- Fourier law of heat conduction

$$\vec{Q} = -k\nabla T$$

$$k = \text{coefficient of thermal conduction}$$

- μ, k are ***material properties***. They can be computed experimentally or from kinetic theory.

Convection and diffusion

$$\begin{aligned}
\text{Mass:} \quad & \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{q}) && = 0 \\
\text{Momentum:} \quad & \frac{\partial}{\partial t}(\rho \vec{q}) + \nabla \cdot (\rho \vec{q}\vec{q}) + \nabla p && = \nabla \cdot \tau \\
\text{Energy:} \quad & \frac{\partial E}{\partial t} + \nabla \cdot (E + p)\vec{q} && = \nabla \cdot (\vec{q} \cdot \tau) + \nabla \cdot \vec{Q}
\end{aligned}$$

Convection and diffusion

- Continuity equation in non-conservative form

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} + w\frac{\partial \rho}{\partial z} + \rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) = 0$$

$\Longrightarrow$ Linear convection equation

$$\boxed{\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} = 0}$$

- x momentum equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \ldots \quad = \quad \mu\frac{\partial^2 u}{\partial x^2} + \ldots$$

$\Longrightarrow$ Non-linear convection and diffusion phenomena

$$\boxed{\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0} \quad \text{and} \quad \boxed{\frac{\partial u}{\partial t} = \mu\frac{\partial^2 u}{\partial x^2}} \quad \text{and} \quad \boxed{\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \mu\frac{\partial^2 u}{\partial x^2}}$$

Differential and integral form

- Differential form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \vec{F} = 0$$

This is the basis of Finite Difference Methods

$$\frac{\partial}{\partial t}(\text{conserved quantity}) + \text{divergence}(\text{flux}) = 0$$

Useful for problems with smooth solutions

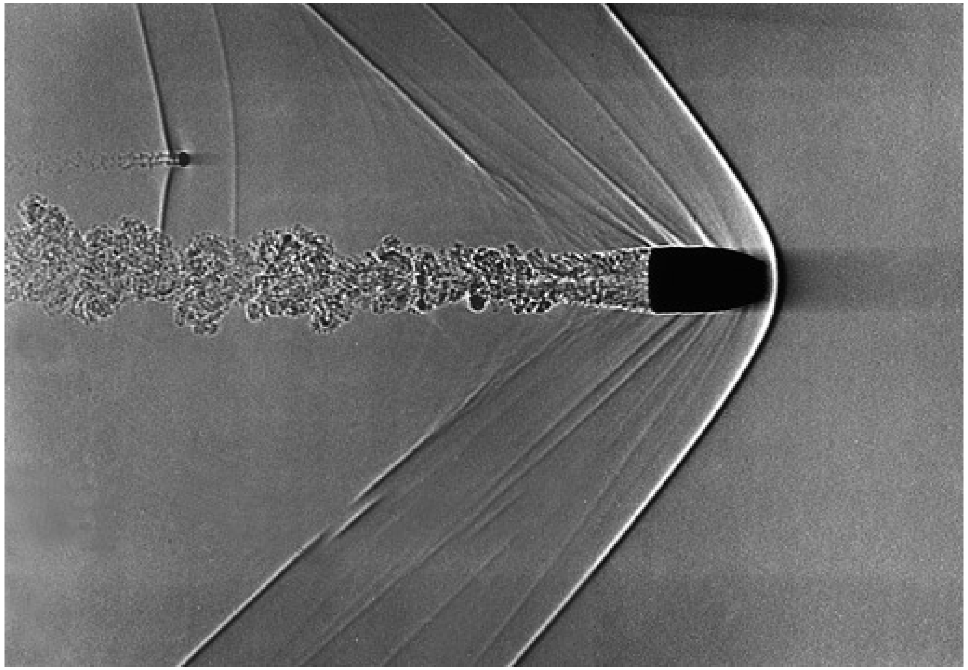
- Integral form

$$\frac{\partial}{\partial t} \int_V \phi \mathrm{d}V = - \oint_{\partial V} \vec{F} \cdot \hat{n} \mathrm{d}S$$

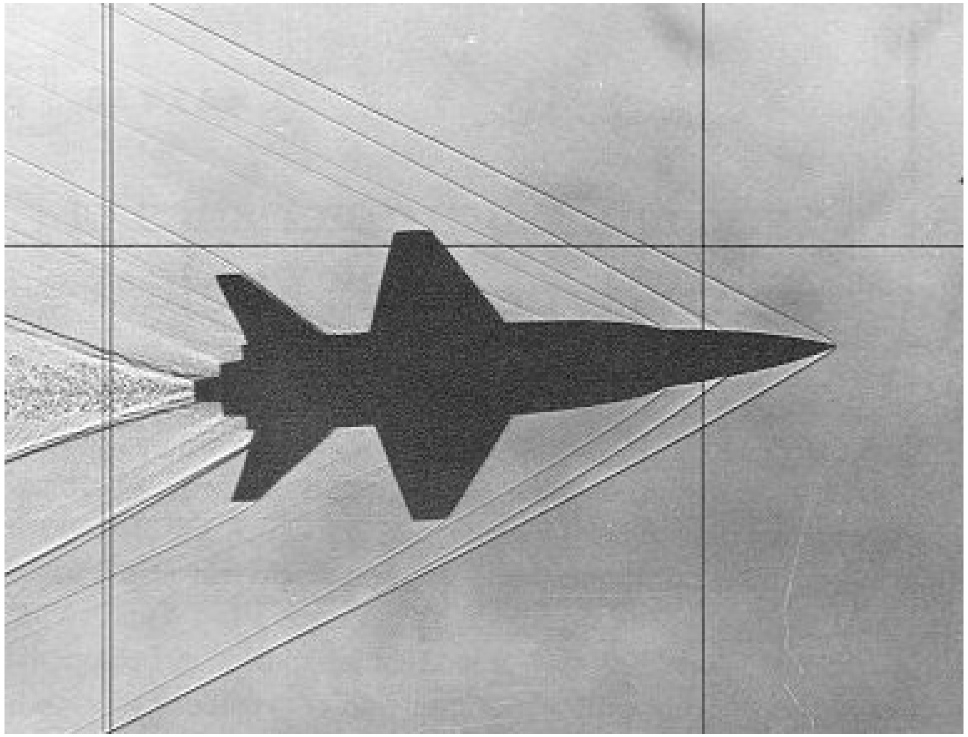
This is the basis of Finite Volume Methods. Can be applied for problems with discontinuous solutions, like hyperbolic equations.

Finite Element Method also belongs to this class since it uses notion of weak solutions, which are defined in terms of integrals.

Flow with shocks



Flow with shocks



X-15 model at mach = 3.5