Dimensionless form of equations

Motivation: sometimes equations are normalized in order to

- facilitate the scale-up of obtained results to real flow conditions
- avoid round-off due to manipulations with large/small numbers
- assess the relative importance of terms in the model equations

Dimensionless variables and numbers

$$t^* = \frac{t}{t_0}, \qquad \mathbf{x}^* = \frac{\mathbf{x}}{L_0}, \qquad \mathbf{v}^* = \frac{\mathbf{v}}{v_0}, \qquad p^* = \frac{p}{\rho v_0^2}, \qquad T^* = \frac{T - T_0}{T_1 - T_0}$$

Reynolds number	$Re = \frac{\rho v_0 L_0}{\mu}$	$\frac{\text{inertia}}{\text{viscosity}}$	Mach number	$M = \frac{\lvert\mathbf{v}\rvert}{c}$
Froude number	$Fr = \frac{v_0}{\sqrt{L_0 g}}$	$\frac{\text{inertia}}{\text{gravity}}$	Strouhal number	$St = \frac{L_0}{v_0 t_0}$
Peclet number	$Pe = \frac{v_0 L_0}{\kappa}$	$\frac{\text{convection}}{\text{diffusion}}$	Prandtl number	$Pr = \frac{\mu}{\rho \kappa}$

Model simplifications

Objective: derive analytical solutions / reduce computational cost

Compressible Navier-Stokes equations

$\rho = const$ → Incompressible Navier-Stokes equations

$\mu = 0$ → Compressible Euler equations

Stokes flow *boundary layer* *inviscid Euler equations* *potential flow*

Derivation of a simplified model

1. determine the type of flow to be simulated
2. separate important and unimportant effects
3. leave irrelevant features out of consideration
4. omit redundant terms/equations from the model
5. prescribe suitable initial/boundary conditions

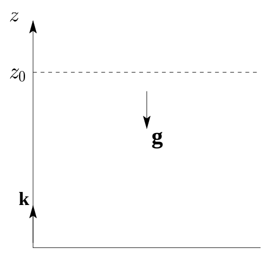
Viscous incompressible flows

Simplification: $\rho = const, \quad \mu = const$

continuity equation $\quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad \longrightarrow \quad \nabla \cdot \mathbf{v} = 0$

inertial term $\quad \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = \rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = \rho \frac{d\mathbf{v}}{dt}$

stress tensor $\quad \nabla \cdot \tau = \mu \nabla \cdot (\nabla \mathbf{v} + \nabla \mathbf{v}^T) = \mu (\nabla \cdot \nabla \mathbf{v} + \nabla \nabla \cdot \mathbf{v}) = \mu \Delta \mathbf{v}$



Let $\quad \rho \mathbf{g} = -\rho g \mathbf{k} = -\nabla(\rho g z) = \nabla p_0$

$p_0 = \rho g (z_0 - z)$ hydrostatic pressure

$\tilde{p} = \frac{p - p_0}{\rho} = \frac{p}{\rho} - g(z_0 - z)$ reduced pressure

$\nu = \mu / \rho$ kinematic viscosity

Incompressible Navier-Stokes equations

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla \tilde{p} + \nu \Delta \mathbf{v} \underbrace{- \beta \mathbf{g}(T - T_0)}_{\text{Boussinesq}} \qquad \text{momentum equations}$$

$$\nabla \cdot \mathbf{v} = 0 \qquad \text{continuity equation}$$

Natural convection problems

Internal energy equation $\rho = \rho(T), \quad \nabla \cdot \mathbf{v} = 0, \quad \kappa = const$

$$\rho \frac{\partial e}{\partial t} + \rho \mathbf{v} \cdot \nabla e = \kappa \Delta T + \rho q + \mu \nabla \mathbf{v} : (\nabla \mathbf{v} + \nabla \mathbf{v}^T), \qquad e = c_v T$$

Temperature equation (convection-diffusion-reaction)

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \tilde{\kappa} \Delta T + \tilde{q}, \qquad \tilde{\kappa} = \frac{\kappa}{\rho c_v}, \quad \tilde{q} = \frac{q}{c_v} + \frac{\nu}{2c_v} |\nabla \mathbf{v} + \nabla \mathbf{v}^T|^2$$

Linearization: $\rho(T) = \rho(T_0) + \left(\frac{\partial \rho}{\partial T}\right)_{T=T_*} (T - T_0)$ Taylor series

$\rho_0 = \rho(T_0), \qquad \beta \approx -\frac{1}{\rho_0} \left(\frac{\partial \rho}{\partial T}\right)_{T=T_*}$ thermal expansion coefficient

Boussinesq approximation for buoyancy-driven flows

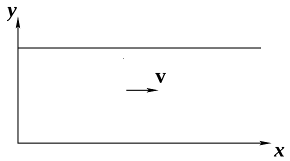
$$\rho(T) = \begin{cases} \rho_0 [1 - \beta (T - T_0)] & \text{in the term } \rho \mathbf{g} \\ \rho_0 & \text{elsewhere} \end{cases}$$

Viscous incompressible flows

Stokes problem   ($Re \to 0$, creeping flows)

$$\frac{d\mathbf{v}}{dt} \approx \frac{\partial \mathbf{v}}{\partial t} \approx 0 \qquad \Rightarrow \qquad \begin{aligned} \frac{\partial \mathbf{v}}{\partial t} &= -\nabla \tilde{p} + \nu \Delta \mathbf{v} && \text{momentum equations} \\ \nabla \cdot \mathbf{v} &= 0 && \text{continuity equation} \end{aligned}$$

Boundary layer approximation   (thin shear layer)



pipe flow

$\mathbf{v} = (u, v)$

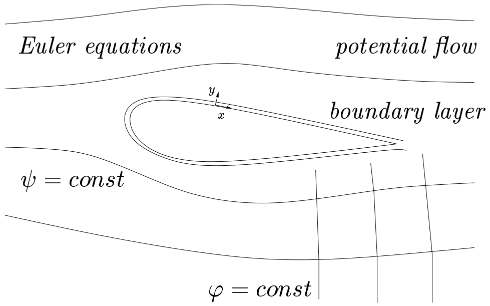
Navier-Stokes equations

$$\begin{aligned} u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} &= -\frac{\partial \tilde{p}}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2} \\ 0 &= -\frac{\partial \tilde{p}}{\partial y} \\ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0 \end{aligned}$$

- $\frac{\partial \mathbf{v}}{\partial t} \approx 0$ and $u \gg v$
- $\nu \frac{\partial^2 u}{\partial x^2}$ can be neglected
- $\frac{\partial \tilde{p}}{\partial y} \approx 0 \quad \Rightarrow \quad \tilde{p} = \tilde{p}(x)$

Inviscid incompressible flows

Incompressible Euler equations



$$\nu = 0 \quad \Rightarrow \quad \begin{aligned} &\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla \tilde{p} \\ &\nabla \cdot \mathbf{v} = 0 \end{aligned}$$

Irrotational / potential flow

$\omega = \nabla \times \mathbf{v} = 0$ (vanishing vorticity)

- $\exists\, \varphi$ such that $\mathbf{v} = -\nabla\varphi$ and $\nabla \cdot \mathbf{v} = -\Delta\varphi = 0$ *Laplace equation*
- in 2D there also exists a *stream function* ψ such that $u = \frac{\partial \psi}{\partial y}, \ v = -\frac{\partial \psi}{\partial x}$

Computation of the pressure

$$\mathbf{v} \cdot \nabla \mathbf{v} = -\mathbf{v} \times \nabla \times \mathbf{v} + \frac{1}{2}\nabla(\mathbf{v} \cdot \mathbf{v}) = \nabla \left(\frac{|\mathbf{v}|^2}{2} \right)$$

$$\frac{\partial \mathbf{v}}{\partial t} = 0 \quad \Rightarrow \quad \tilde{p} = -\frac{|\mathbf{v}|^2}{2} \quad \textit{Bernoulli equation}$$

Compressible Euler equations

Simplifications: $\mu = 0, \quad \kappa = 0, \quad \mathbf{g} = 0$

Divergence form

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F} = 0$$

Quasi-linear formulation

$$\frac{\partial U}{\partial t} + \mathbf{A} \cdot \nabla U = 0$$

Conservative variables and fluxes

$$U = (\rho, \rho\mathbf{v}, \rho E)^T$$

$$\mathbf{F} = (F^1, F^2, F^3)$$

$$\mathbf{F} = \begin{bmatrix} \rho\mathbf{v} \\ \rho\mathbf{v} \otimes \mathbf{v} + p\mathcal{I} \\ \rho h \mathbf{v} \end{bmatrix}$$

$$h = E + \tfrac{p}{\rho}$$

$$\gamma = c_p / c_v$$

Jacobian matrices $\quad \mathbf{A} = (A^1, A^2, A^3)$

$$F^d = A^d U, \qquad A^d = \frac{\partial F^d}{\partial U}, \qquad d = 1, 2, 3$$

Equation of state

$$p = (\gamma - 1)\rho \left(E - |\mathbf{v}|^2/2\right)$$

Classification of partial differential equations

PDEs can be classified into hyperbolic, parabolic and elliptic ones

- each class of PDEs models a different kind of physical processes
- the number of initial/boundary conditions depends on the PDE type
- different solution methods are required for PDEs of different type

<u>Hyperbolic equations</u> Information propagates in certain directions at finite speeds; the solution is a superposition of multiple simple waves

<u>Parabolic equations</u> Information travels downstream / forward in time; the solution can be constructed using a marching / time-stepping method

<u>Elliptic equations</u> Information propagates in all directions at infinite speed; describe equilibrium phenomena (unsteady problems are never elliptic)

Classification of partial differential equations

First-order PDEs $a_0 + a_1 \frac{\partial u}{\partial x_1} + \ldots + a_D \frac{\partial u}{\partial x_D} = 0$ are always hyperbolic

Second order PDEs $$-\sum_{i,j=1}^{D} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{k=1}^{D} b_k \frac{\partial u}{\partial x_k} + cu + d = 0$$

coefficient matrix: $A = \{a_{ij}\} \in \mathbb{R}^{D \times D}, \quad a_{ij} = a_{ij}(x_1, \ldots, x_D)$

symmetry: $a_{ij} = a_{ji},$ otherwise set $a_{ij} = a_{ji} := \frac{a_{ij} + a_{ji}}{2}$

PDE type	n^+	n^-	n^0
elliptic	D	0	0
hyperbolic	$D-1$	1	0
parabolic	$D-1$	0	1

n^+ number of positive eigenvalues

n^- number of negative eigenvalues

n^0 number of zero eigenvalues

$n^+ \longleftrightarrow n^-$

Classification of second-order PDEs

2D example

$$-a_{11}\frac{\partial^2 u}{\partial x_1^2} - (a_{12}+a_{21})\frac{\partial^2 u}{\partial x_1 \partial x_2} - a_{22}\frac{\partial^2 u}{\partial x_2^2} + \ldots = 0$$

$$D = 2, \qquad A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \qquad \det A = a_{11}a_{22} - a_{12}^2 = \lambda_1\lambda_2$$

elliptic type	$\det A > 0$	$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$	*Laplace equation*
hyperbolic type	$\det A < 0$	$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$	*wave equation*
parabolic type	$\det A = 0$	$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$	*diffusion equation*
mixed type	$\det A = f(y)$	$-y\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$	*Tricomi equation*

Classification of first-order PDE systems

Quasi-linear form $$A_1 \frac{\partial U}{\partial x_1} + \ldots + A_D \frac{\partial U}{\partial x_D} = B$$ $U \in \mathbb{R}^m, \quad m > 1$

Plane wave solution $U = \hat{U} e^{is(\mathbf{x},t)}, \quad \hat{U} = const, \quad s(\mathbf{x},t) = \mathbf{n} \cdot \mathbf{x}$

where $\mathbf{n} = \nabla s$ is the normal to the characteristic surface $s(\mathbf{x},t) = const$

$$B = 0 \quad \rightarrow \quad \left[\sum_{d=1}^{D} n_d A_d\right] \hat{U} = 0, \qquad \det\left[\sum_{d=1}^{D} n_d A_d\right] = 0 \quad \longrightarrow \quad \mathbf{n}^{(k)}$$

Hyperbolic systems There are D real-valued normals $\mathbf{n}^{(k)}, \quad k = 1, \ldots, D$ and the solutions $\hat{U}^{(k)}$ of the associated systems are linearly independent

Parabolic systems There are less than D real-valued solutions $\mathbf{n}^{(k)}$ and $\hat{U}^{(k)}$

Elliptic systems No real-valued normals $\mathbf{n}^{(k)} \Rightarrow$ no wave-like solutions

Second-order PDE as a first-order system

Quasi-linear PDE of 2nd order $\quad a\frac{\partial^2\varphi}{\partial x^2} + 2b\frac{\partial^2\varphi}{\partial x\partial y} + c\frac{\partial^2\varphi}{\partial y^2} = 0$

Equivalent first-order system for $\quad u = \frac{\partial\varphi}{\partial x}, \quad v = \frac{\partial\varphi}{\partial y}$

$$\begin{cases} a\frac{\partial u}{\partial x} + 2b\frac{\partial u}{\partial y} + c\frac{\partial v}{\partial y} = 0 \\ -\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = 0 \end{cases} \qquad \underbrace{\begin{bmatrix} a & 0 \\ 0 & 1 \end{bmatrix}}_{A_1} \frac{\partial}{\partial x} \underbrace{\begin{bmatrix} u \\ v \end{bmatrix}}_{U} + \underbrace{\begin{bmatrix} 2b & c \\ -1 & 0 \end{bmatrix}}_{A_2} \frac{\partial}{\partial y} \underbrace{\begin{bmatrix} u \\ v \end{bmatrix}}_{U} = 0$$

Matrix form $\quad A_1\frac{\partial U}{\partial x} + A_2\frac{\partial U}{\partial y} = 0, \quad U = \hat{U}e^{i\mathbf{n}\cdot\mathbf{x}} = \hat{U}e^{i(n_x x + n_y y)} \quad$ plane wave

The resulting problem $\quad [n_x A_1 + n_y A_2]\hat{U} = 0 \quad$ admits nontrivial solutions if

$$\det[n_x A_1 + n_y A_2] = \det\begin{bmatrix} an_x + 2bn_y & cn_y \\ -n_y & n_x \end{bmatrix} = 0 \quad \Rightarrow \quad an_x^2 + 2bn_x n_y + cn_y^2 = 0$$

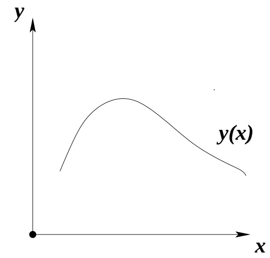
$$a\left(\frac{n_x}{n_y}\right)^2 + 2b\left(\frac{n_x}{n_y}\right) + c = 0 \qquad \Rightarrow \qquad \frac{n_x}{n_y} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Second-order PDE as a first-order system

Characteristic lines

$$ds = \frac{\partial s}{\partial x}dx + \frac{\partial s}{\partial y}dy = n_x dx + n_y dy = 0 \qquad \text{tangent}$$

$$\frac{dy}{dx} = -\frac{n_x}{n_y} = -\frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad \text{curve}$$



The PDE type depends on $D = b^2 - 4ac$

$D > 0$	two real characteristics	hyperbolic equation
$D = 0$	just one root $\frac{dy}{dx} = \frac{b}{2a}$	parabolic equation
$D < 0$	no real characteristics	elliptic equation

Transformation to an ‘unsteady’ system

$$\frac{\partial U}{\partial x} + \tilde{A}\frac{\partial U}{\partial y} = 0, \qquad \tilde{A} = A_1^{-1}A_2 = \begin{bmatrix} \frac{1}{a} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 2b & c \\ -1 & 0 \end{bmatrix} = \begin{bmatrix} \frac{2b}{a} & \frac{c}{a} \\ -1 & 0 \end{bmatrix}$$

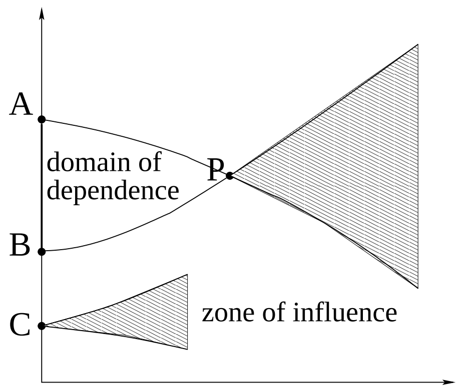
$$\det[\tilde{A} - \lambda I] = \lambda^2 - \left(\frac{2b}{a}\right)\lambda + \frac{c}{a} = 0 \quad \Rightarrow \quad \lambda_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Geometric interpretation for a second-order PDE

Domain of dependence: $\mathbf{x} \in \bar{\Omega}$ which may influence the solution at point P

Zone of influence: $\mathbf{x} \in \bar{\Omega}$ which are influenced by the solution at point P

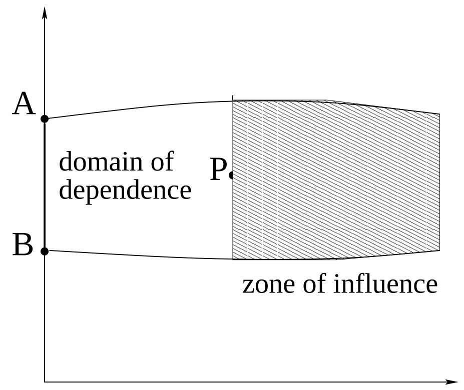
Hyperbolic PDE



steady supersonic flows

unsteady inviscid flows

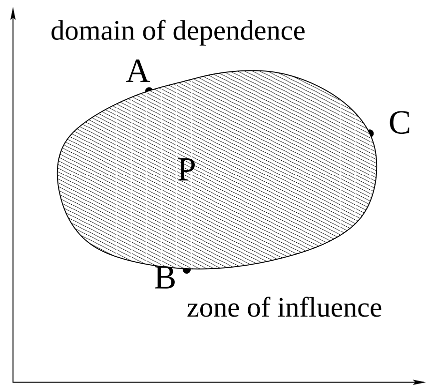
Parabolic PDE



steady boundary layer flows

unsteady heat conduction

Elliptic PDE



steady subsonic/inviscid

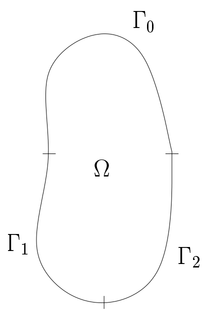
incompressible flows

Space discretization techniques

Objective: to approximate the PDE by a set of algebraic equations

$$\begin{cases} \mathcal{L}u = f & \text{in } \Omega & \text{stationary (elliptic) PDE} \\ u = g_0 & \text{on } \Gamma_0 & \text{Dirichlet boundary condition} \\ \mathbf{n} \cdot \nabla u = g_1 & \text{on } \Gamma_1 & \text{Neumann boundary condition} \\ \mathbf{n} \cdot \nabla u + \alpha u = g_2 & \text{on } \Gamma_2 & \text{Robin boundary condition} \end{cases}$$

Boundary value problem BVP = PDE + boundary conditions

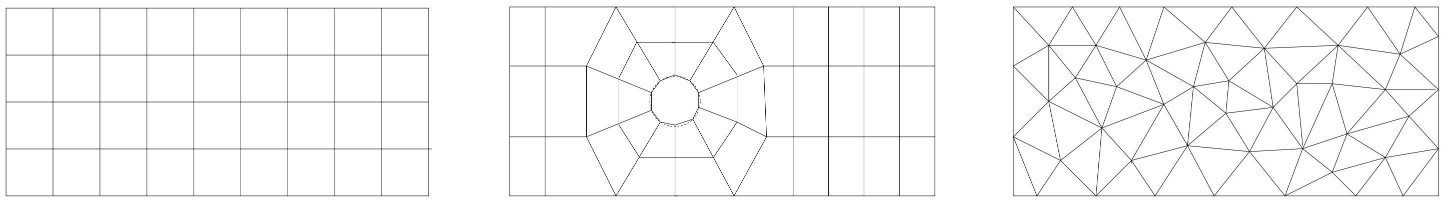


Getting started: 1D and 2D toy problems

1. $-\Delta u = f$ Poisson equation
2. $\nabla \cdot (u\mathbf{v}) = \nabla \cdot (d\nabla u)$ convection-diffusion

Computational meshes

Degrees of freedom for the approximate solution are defined on a computational mesh which represents a subdivision of the domain into cells/elements



structured *block-structured* *unstructured*

Structured (regular) meshes

- families of gridlines do not cross and only intersect with other families once
- topologically equivalent to Cartesian grid so that each gridpoint (or CV) is uniquely defined by two indices in 2D or three indices in 3D, e.g., (i, j, k)
- can be of type H (nonperiodic), O (periodic) or C (periodic with cusp)
- limited to simple domains, local mesh refinement affects other regions

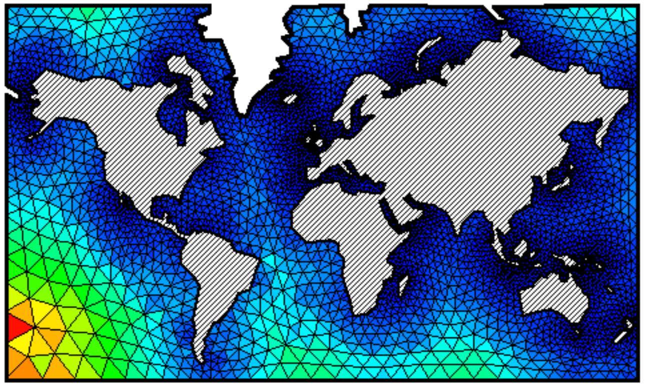
Computational meshes

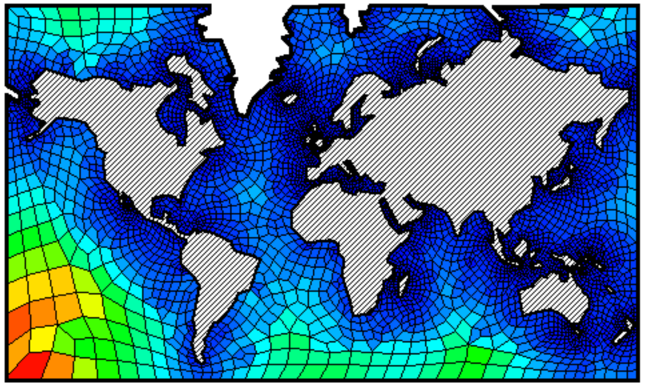
Block-structured meshes

- multilevel subdivision of the domain with structured grids within blocks
- can be non-matching, special treatment is necessary at block interfaces
- provide greater flexibility, local refinement can be performed blockwise

Unstructured meshes

- suitable for arbitrary domains and amenable to adaptive mesh refinement
- consist of triangles or quadrilaterals in 2D, tetrahedra or hexahedra in 3D
- complex data structures, irregular sparsity pattern, difficult to implement

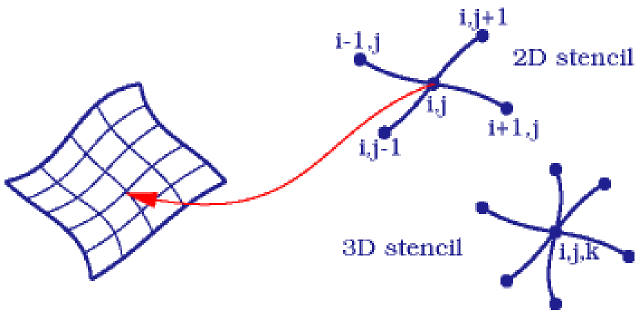




Discretization techniques

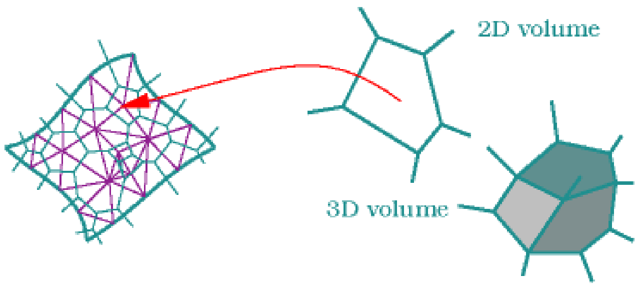
Finite differences / differential form

- approximation of nodal derivatives
- simple and effective, easy to derive
- limited to (block-)structured meshes



Finite volumes / integral form

- approximation of integrals
- conservative by construction
- suitable for arbitrary meshes



Finite elements / weak form

- weighted residual formulation
- remarkably flexible and general
- suitable for arbitrary meshes