

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

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

Reynolds number $Re = \frac{\rho v_0 L_0}{\mu} \quad \frac{\text{inertia}}{\text{viscosity}}$

Mach number $M = \frac{|\mathbf{v}|}{c}$

Froude number $Fr = \frac{v_0}{\sqrt{L_0 g}} \quad \frac{\text{inertia}}{\text{gravity}}$

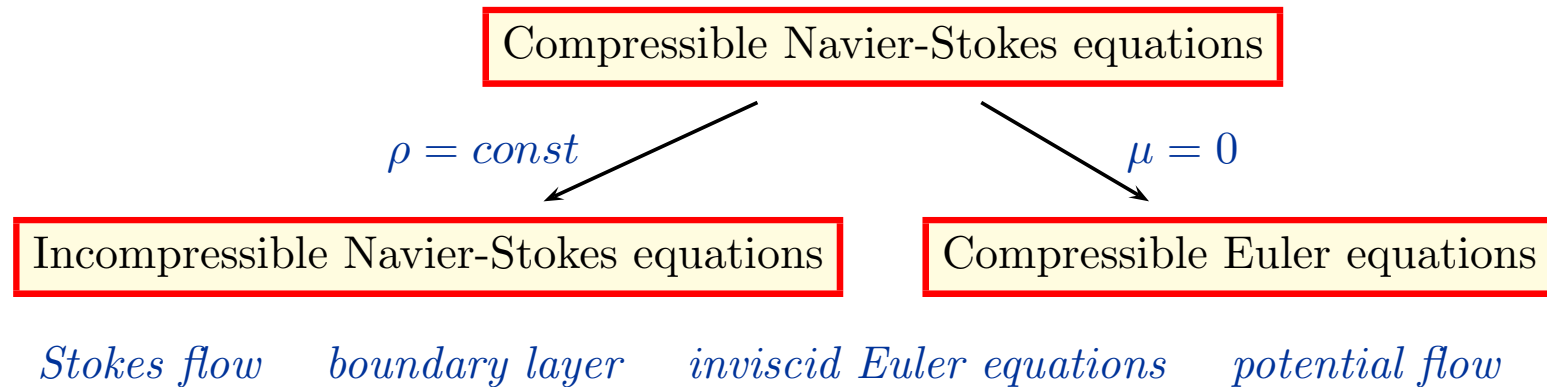
Strouhal number $St = \frac{L_0}{v_0 t_0}$

Peclet number $Pe = \frac{v_0 L_0}{\kappa} \quad \frac{\text{convection}}{\text{diffusion}}$

Prandtl number $Pr = \frac{\mu}{\rho \kappa}$

Model simplifications

Objective: derive analytical solutions / reduce computational cost



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

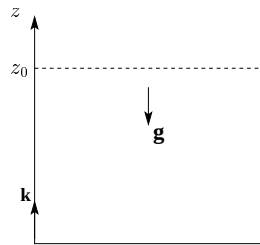
Viscous incompressible flows

Simplification: $\rho = \text{const}$, $\mu = \text{const}$

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

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

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



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

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

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

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

Natural convection problems

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

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

Temperature equation (convection-diffusion-reaction)

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

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

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

Boussinesq approximation for buoyancy-driven flows

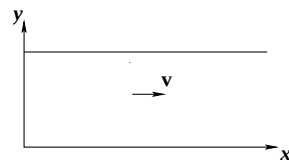
$$\rho(T) = \begin{cases} \rho_0 [1 - \beta(T - T_0)] & \text{in the term } \rho \mathbf{g} \\ \rho_0 & \text{elsewhere} \end{cases}$$

Viscous incompressible flows

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

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

Boundary layer approximation (thin shear layer)



pipe flow

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

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

Navier-Stokes equations

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial \tilde{p}}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2}$$

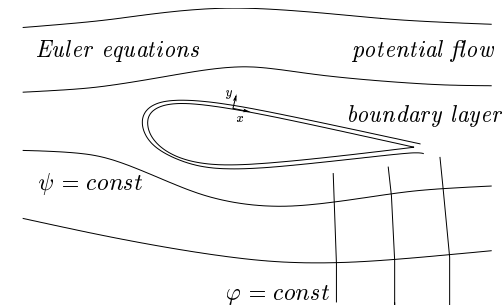
$$0 = -\frac{\partial \tilde{p}}{\partial y}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

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

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

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

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

$$\begin{aligned} U &= (\rho, \rho \mathbf{v}, \rho E)^T \\ \mathbf{F} &= (F^1, F^2, F^3) \end{aligned} \quad \mathbf{F} = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + p \mathcal{I} \\ \rho h \mathbf{v} \end{bmatrix} \quad \begin{aligned} h &= E + \frac{p}{\rho} \\ \gamma &= c_p / c_v \end{aligned}$$

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

Equation of state

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

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

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

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

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

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

Classification of partial differential equations

First-order PDEs $a_0 + a_1 \frac{\partial u}{\partial x_1} + \dots + a_D \frac{\partial u}{\partial x_D} = 0$ 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: $A = \{a_{ij}\} \in \mathbb{R}^{D \times D}$, $a_{ij} = a_{ij}(x_1, \dots, x_D)$

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

PDE type	n^+	n^-	n^0
<i>elliptic</i>	D	0	0
<i>hyperbolic</i>	$D - 1$	1	0
<i>parabolic</i>	$D - 1$	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

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

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

elliptic type	det $A > 0$	$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$	<i>Laplace equation</i>
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hyperbolic type	det $A < 0$	$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$	<i>wave equation</i>
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parabolic type	det $A = 0$	$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$	<i>diffusion equation</i>
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mixed type	det $A = f(y)$	$-y \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$	<i>Tricomi equation</i>
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Classification of first-order PDE systems

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

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

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

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

Hyperbolic systems There are D real-valued normals $\mathbf{n}^{(k)}, \quad k = 1, \dots, D$
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 $a \frac{\partial^2 \varphi}{\partial x^2} + 2b \frac{\partial^2 \varphi}{\partial x \partial y} + c \frac{\partial^2 \varphi}{\partial y^2} = 0$

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

$$\left\{ \begin{array}{l} a \frac{\partial u}{\partial x} + 2b \frac{\partial u}{\partial y} + c \frac{\partial v}{\partial y} = 0 \\ -\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = 0 \end{array} \right. \quad \underbrace{\begin{bmatrix} a & 0 \\ 0 & 1 \end{bmatrix}}_{A_1} \underbrace{\frac{\partial}{\partial x} \begin{bmatrix} u \\ v \end{bmatrix}}_U + \underbrace{\begin{bmatrix} 2b & c \\ -1 & 0 \end{bmatrix}}_{A_2} \underbrace{\frac{\partial}{\partial y} \begin{bmatrix} u \\ v \end{bmatrix}}_U = 0$$

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

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

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

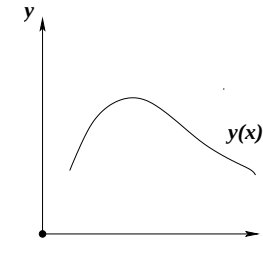
$$a \left(\frac{n_x}{n_y} \right)^2 + 2b \left(\frac{n_x}{n_y} \right) + c = 0 \quad \Rightarrow \quad \frac{n_x}{n_y} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Second-order PDE as a first-order system

Characteristic lines

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

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



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

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

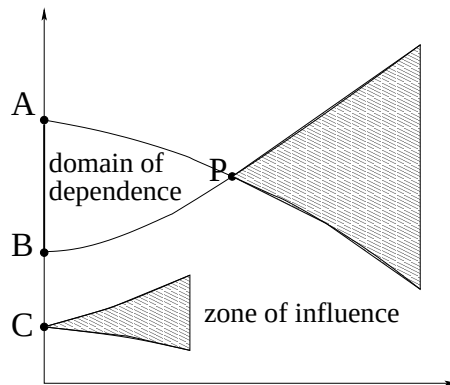
$$\det[\tilde{A} - \lambda I] = \lambda^2 - \left(\frac{2b}{a}\right) \lambda + \frac{c}{a} = 0 \quad \Rightarrow \quad \lambda_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Geometric interpretation for a second-order PDE

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

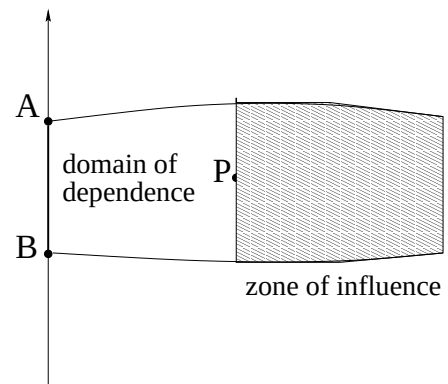
Zone of influence: $\mathbf{x} \in \bar{\Omega}$ which are influenced by the solution at point P

Hyperbolic PDE



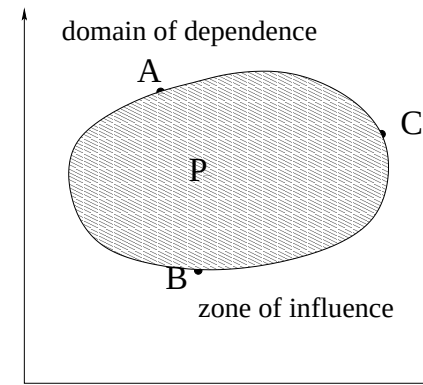
steady supersonic flows
unsteady inviscid flows

Parabolic PDE



steady boundary layer flows
unsteady heat conduction

Elliptic PDE



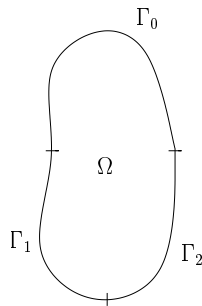
steady subsonic/inviscid
incompressible flows

Space discretization techniques

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

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

Boundary value problem BVP = PDE + boundary conditions

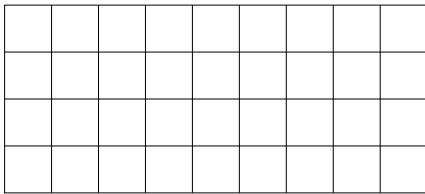


Getting started: 1D and 2D toy problems

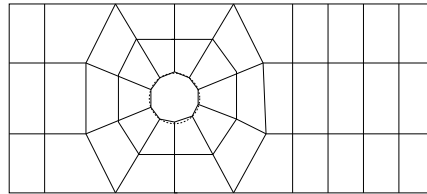
1. $-\Delta u = f$ Poisson equation
2. $\nabla \cdot (u\mathbf{v}) = \nabla \cdot (d\nabla u)$ convection-diffusion

Computational meshes

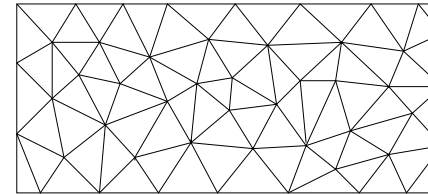
Degrees of freedom for the approximate solution are defined on a computational mesh which represents a subdivision of the domain into cells/elements



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

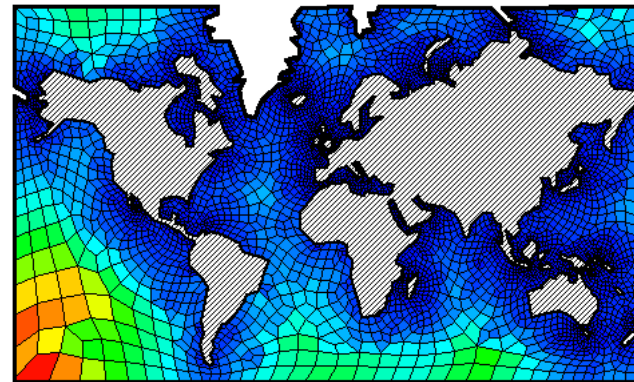
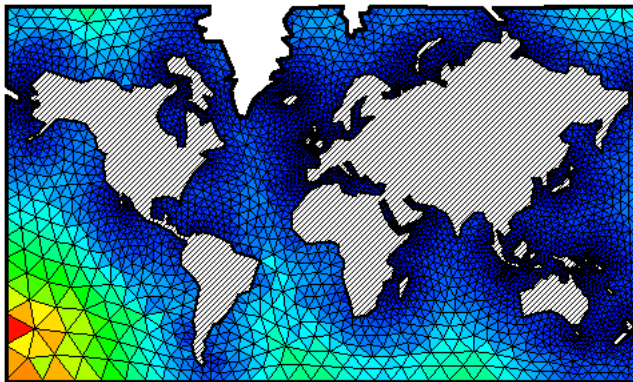
Computational meshes

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

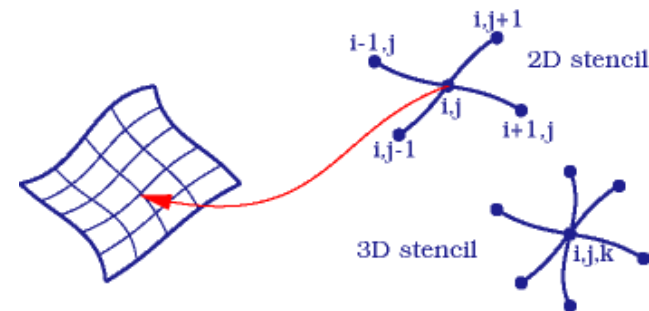
- suitable for arbitrary domains and amenable to adaptive mesh refinement
- consist of triangles or quadrilaterals in 2D, tetrahedra or hexahedra in 3D
- complex data structures, irregular sparsity pattern, difficult to implement



Discretization techniques

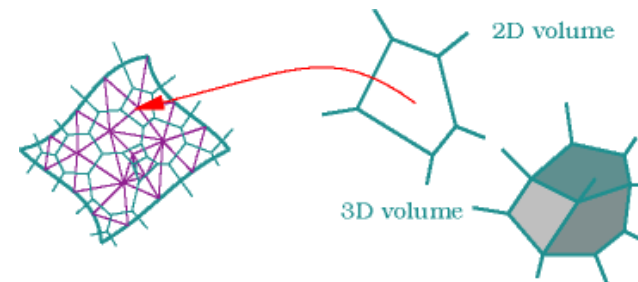
Finite differences / differential form

- 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

