Numerical Methods

Krzysztof Tesch
Gdańsk University of Technology

Contents

Contents

Description of fluid/solid at different scales

Finite Difference Method

Finite Volume Method

Finite Element Method

Monte Carlo Method

Lattice Boltzmann Method

Smoothed Particle Hydrodynamics

Turbulence modelling

References

Description of fluid/solid at different scales

Descriptions

Fluid motion may be described by three types of mathematical models according to the observed scales:

- Microscopic description (MD)
- Mesoscopic description
  - kinetic theory
  - LD
  - BD
  - DPD
  - SPH
  - LBM
- Macroscopic description – continuum (FDM, FEM, FVM, LBM)

Microscopic description – MD

Molecular mechanics takes advantage of classical mechanics equations to model molecular systems whereas molecular dynamics simulates movements of atoms in the context of N-body simulation. The motion of molecules is determined by solving the Newtons's equation of motion

$$m\frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} = \mathbf{G}_i + \sum_{j=1\neq i}^{N} \mathbf{f}_{ij} \tag{1}$$

The force exerted on a molecule consists of the external force such as gravity $\mathbf{G}_i$ and the intermolecular force $\mathbf{f}_{ij} = -\nabla V$ usually described by mans of the Lennard–Jones potential

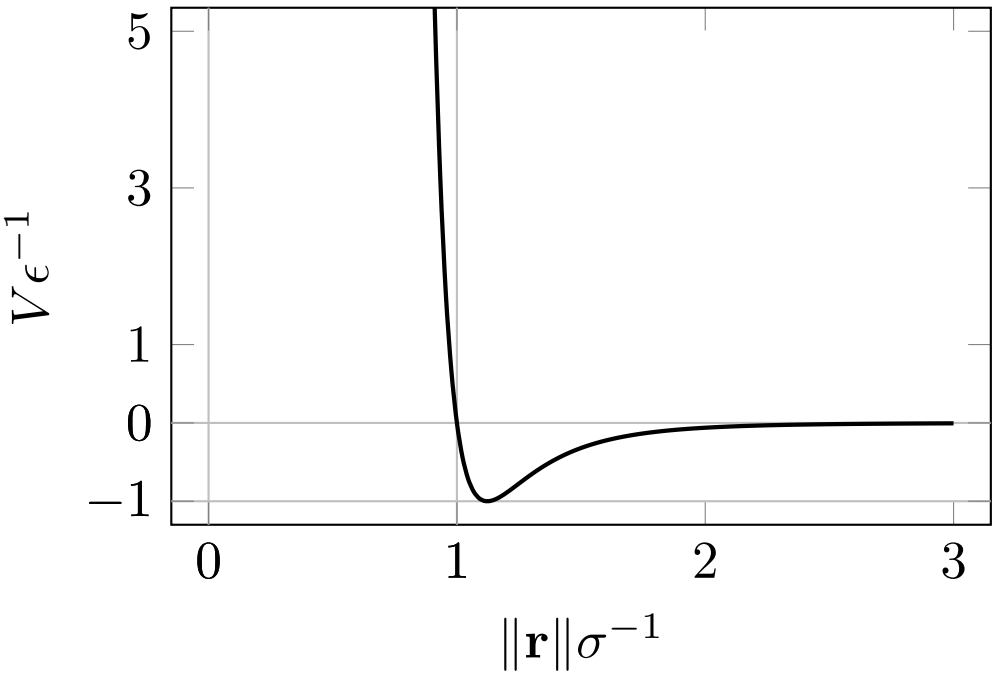
Microscopic description – MD

$$V = 4\epsilon \left(\left(\frac{\sigma}{\|\mathbf{r}\|} \right)^{12} - \left(\frac{\sigma}{\|\mathbf{r}\|} \right)^{6} \right) \tag{2}$$

In the above equations $\|\mathbf{r}\|$ is the distance between particles, ϵ – the depth of the potential well that characterises the interaction strength and σ – the finite distance describing the interaction range.
Further, the ensemble average makes it possible to obtain a macroscopic quantity from the corresponding microscopic variable. The disadvantage of molecular dynamics method is that the total number of molecules even in small volume is too large – proportional to 10^{23}.

Microscopic description – MD

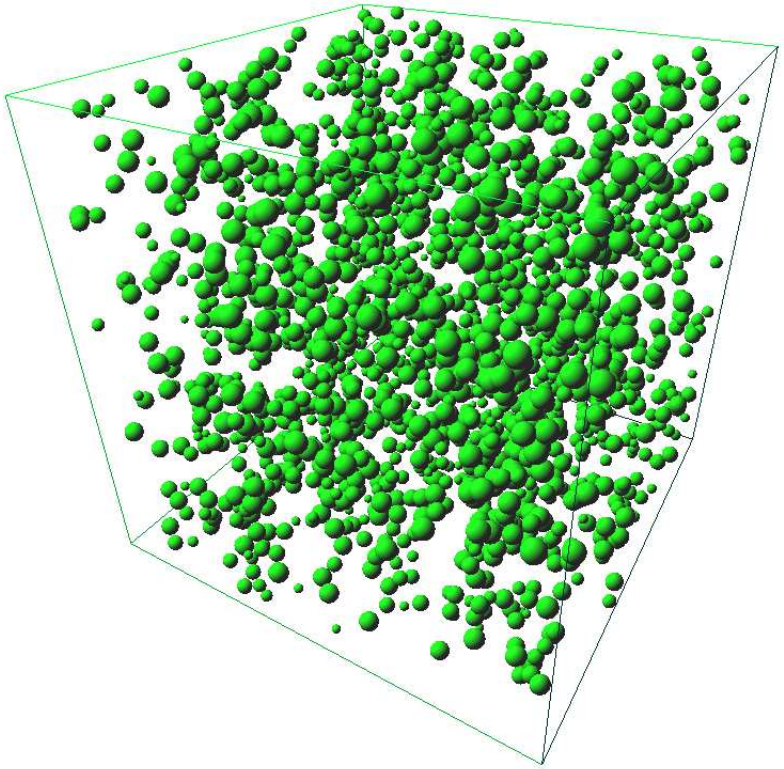
$$V = 4\epsilon \left(\left(\frac{\sigma}{\|\mathbf{r}\|} \right)^{12} - \left(\frac{\sigma}{\|\mathbf{r}\|} \right)^{6} \right) \tag{3}$$

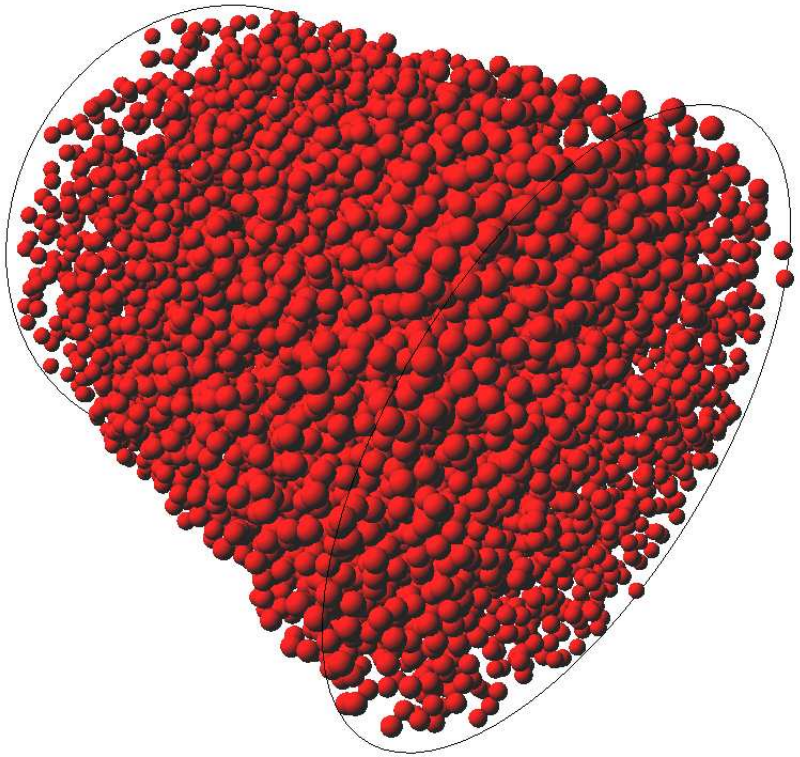


Molecular dynamics pseudocode

$t := 0$;
Calculate initial molecule position $\mathbf{r}$;
while *not the end of calculations* **do**
    $\mathbf{f}_{ij} := -\nabla V$;
    $\mathbf{a} := m^{-1}\mathbf{f}_{ij}$;
    $\mathbf{r} := \mathbf{r} + \mathbf{v}\,\Delta t + \frac{1}{2}\mathbf{a}\,\Delta t^2$;
    $t := t + \Delta t$;

Molecular dynamics - example





Mesoscopic description – LBM

The key concept is the probability distribution function $f^{(N)}$ in the phase space. The phase space is constituted of $3N$ spatial coordinates $\mathbf{q}_1, \ldots, \mathbf{q}_N$ and $3N$ momenta $\mathbf{p}_1, \ldots, \mathbf{p}_N$. The probability distribution function $f^{(N)}$ allows to express the probability to find a particle within the infinitesimal phase space

$$(\mathbf{q}_1, \mathbf{q}_1 + \mathrm{d}\mathbf{q}) \times \ldots \times (\mathbf{q}_N, \mathbf{q}_N + \mathrm{d}\mathbf{q}) \times (\mathbf{p}_1, \mathbf{p}_1 + \mathrm{d}\mathbf{p}) \times \ldots \times (\mathbf{p}_N, \mathbf{p}_N + \mathrm{d}\mathbf{p}) \quad (4)$$

The total number of molecules within the infinitesimal phase space is then

$$f^{(N)}(\mathbf{q}_1, \ldots, \mathbf{q}_N, \mathbf{p}_1, \ldots, \mathbf{p}_N)\, \mathrm{d}q^N\, \mathrm{d}p^N \quad (5)$$

Mesoscopic description – LBM

The time evolution of the probability distribution function $f^{(N)}$ follows the Liouville equation

$$\frac{\mathrm{d}f^{(N)}}{\mathrm{d}t} = \frac{\partial f^{(N)}}{\partial t} + \sum_{i=1}^{N} \left(\frac{\partial f^{(N)}}{\partial \mathbf{p}_i} \cdot \frac{\mathrm{d}\mathbf{p}_i}{\mathrm{d}t} + \frac{\partial f^{(N)}}{\partial \mathbf{q}_i} \cdot \frac{\mathrm{d}\mathbf{q}_i}{\mathrm{d}t} \right) = 0$$

This means that the distribution function is constant along any trajectory in phase space.
The reduced probability distribution function is defined as

$$F_s\left(\mathbf{q}_1, \ldots, \mathbf{q}_s, \mathbf{p}_1, \ldots, \mathbf{p}_s\right) = \int_{\mathbb{R}^{3(N-s)}} \int_{\mathbb{R}^{3(N-s)}} f^{(N)}\left(\mathbf{q}_1, \ldots, \mathbf{q}_N, \mathbf{p}_1, \ldots, \mathbf{p}_N\right) \mathrm{d}q^{N-s}\, \mathrm{d}p^{N-s}$$

Mesoscopic description – LBM

The above function is called the s-particle probability distribution function. A chain of evolution equations for F_s for $1 \leq s \leq N$ is derived and called BBGKY hierarchy. This means that the s^{th} equation for the s-particle distributions contains $s+1$ distribution. That hierarchy may be truncated. Truncating it at the first order results in Boltzmann equation

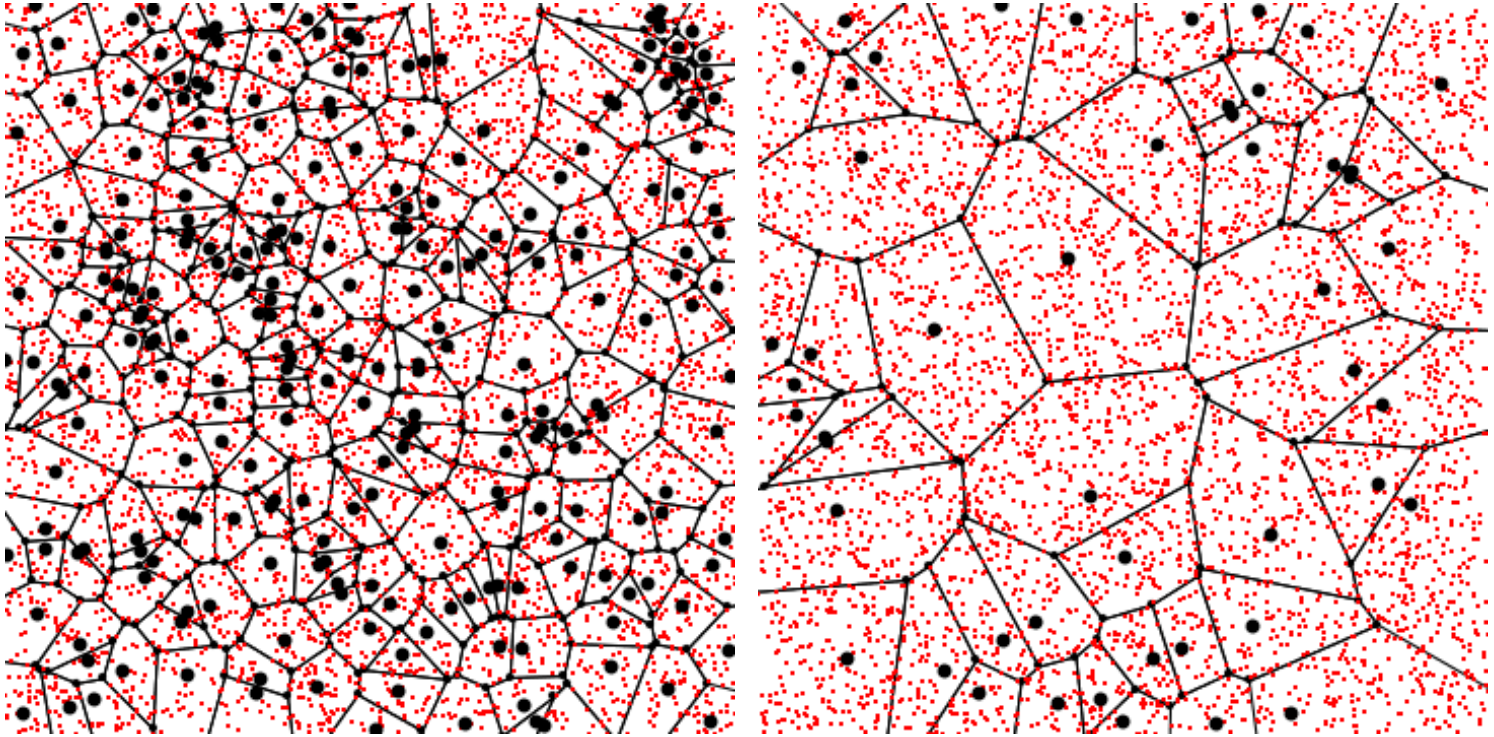
$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \Omega(f) \tag{6}$$

for the probability distribution function

$$f(\mathbf{r}, \mathbf{v}, t) = mNF_1(\mathbf{q}_1, \mathbf{p}_1, t) \tag{7}$$

for binary collisions with uncorrelated velocities before that collision.

Mesoscopic description – DPD



Mesoscopic description – DPD

The DPD (Dissipative Particle Dynamics) method simulate only a reduced number of degrees of freedom (coarse-grained models). The motion of particles is determined by solving the Newtons's equation of motion

$$m\frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} = \mathbf{G}_i + \sum_{j=1\neq i}^{N}\left(\mathbf{f}_{ij}^C + \mathbf{f}_{ij}^D + \mathbf{f}_{ij}^R\right)$$

where the interaction forces are the sum of

- $\mathbf{f}_{ij}^C$ conservative or repulsion forces
- $\mathbf{f}_{ij}^D$ dissipative forces
- $\mathbf{f}_{ij}^R$ random force

Mesoscopic description – DPD

- Dissipative forces

$$\mathbf{f}_{ij}^{D} = -\gamma\omega_D \left(\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}\right) \hat{\mathbf{r}}_{ij} \tag{8}$$

- Random force

$$\mathbf{f}_{ij}^{R} = \sigma\omega_R \hat{\mathbf{r}}_{ij} \frac{\theta_{ij}}{\sqrt{\Delta t}} \tag{9}$$

- Conservative forces

$$\mathbf{f}_{ij}^{C} = \alpha\omega_R \hat{\mathbf{r}}_{ij} \tag{10}$$

$\omega_D = \omega_R^2$ and $\sigma^2 = 2\gamma k_B T$

Mesoscopic description – LD

The Langevin dynamics equation of motion

$$m\frac{\mathrm{d}^2\mathbf{x}_i}{\mathrm{d}t^2} = \mathbf{f}_i^C - \gamma\mathbf{v}_i + \mathbf{f}_i^R \tag{11}$$

where

- Dissipative forces $-\gamma\mathbf{v}_i$
- Random force $\mathbf{f}_i^R$
- Conservative forces

$$\mathbf{f}_i^C = -\nabla V \tag{12}$$

Mesoscopic description – BD

The Brownian dynamics equation of motion

$$\mathbf{0} = \mathbf{f}_i^C - \gamma \mathbf{v}_i + \mathbf{f}_i^R \tag{13}$$

or

$$\gamma \frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t} = \mathbf{f}_i^C + \mathbf{f}_i^R \tag{14}$$

where

- Random force $\mathbf{f}_i^R$
- Conservative forces

$$\mathbf{f}_i^C = -\nabla V \tag{15}$$

Mesoscopic description – SPH

The Smoothed Particle Hydrodynamics equation of motion

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t} = \mathbf{g}_i - \mathbf{f}_{pi} + \mathbf{f}_{\mu i} \tag{16}$$

where

- Body force $\mathbf{g}_i$
- Pressure gradient forces $\mathbf{f}_{pi}$
- Viscous forces $\mathbf{f}_{\mu i}$

Macroscopic description – conservation equations

Conservation of mass

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla\cdot\mathbf{u} = 0 \tag{17}$$

Conservation of linear momentum

$$\rho\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho\mathbf{f} + \nabla\cdot\boldsymbol{\sigma} \tag{18}$$

Decomposition of stress tensor

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta} + \boldsymbol{\tau} \tag{19}$$

Another form of conservation of linear momentum

$$\rho\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho\mathbf{f} - \nabla p + \nabla\cdot\boldsymbol{\tau} \tag{20}$$

Macroscopic description – energy equations

Energy	Equation
Kinetic	$\rho\frac{\mathrm{d}e_k}{\mathrm{d}t} = \rho\mathbf{f}\cdot\mathbf{u} + \nabla\cdot(\boldsymbol{\sigma}\cdot\mathbf{u}) - \nabla\cdot\mathbf{q}$
Total	$\rho\frac{\mathrm{d}e_c}{\mathrm{d}t} = \frac{\partial p}{\partial t} + \nabla\cdot(\boldsymbol{\tau}\cdot\mathbf{u}) - \nabla\cdot\mathbf{q}$
Mechanical	$\rho\frac{\mathrm{d}e_m}{\mathrm{d}t} = \nabla\cdot(\boldsymbol{\sigma}\cdot\mathbf{u}) - \boldsymbol{\sigma}:\mathbf{D}$
Internal	$\rho\frac{\mathrm{d}e}{\mathrm{d}t} = \boldsymbol{\sigma}:\mathbf{D} - \nabla\cdot\mathbf{q}$
Enthalpy	$\rho\frac{\mathrm{d}h}{\mathrm{d}t} = \boldsymbol{\tau}:\mathbf{D} - \nabla\cdot\mathbf{q} + \frac{\mathrm{d}p}{\mathrm{d}t}$

Macroscopic description – general transport equations

$$\frac{\partial(\rho f)}{\partial t} + \nabla \cdot (\rho \mathbf{u} f) = S_f - \nabla \cdot \mathbf{k} \qquad (21)$$

Left hand side represents transient and convection effects. It expresses the rate of change $\rho \frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial(\rho f)}{\partial t} + \nabla \cdot (\rho \mathbf{u} f)$. Right hand side represents sources (positive and negative) and fluxes (transport due to other mechanism than convection).

- mass conservation equation
  $f := 1$, $S_f := 0$, $\mathbf{k} := \mathbf{0}$
- linear momentum conservation equation
  $f \leftarrow \mathbf{u}$, $S_f \leftarrow \rho \mathbf{f}$, $\mathbf{k} \leftarrow -\boldsymbol{\sigma}$
- energy conservation equation
  $f := e_k$, $S_f := \rho \mathbf{f} \cdot \mathbf{u}$, $\mathbf{k} := \mathbf{q} - \boldsymbol{\sigma} \cdot \mathbf{u}$

Macroscopic description – laws of thermodynamics

Second law of thermodynamics

$$\rho \frac{\mathrm{d}s}{\mathrm{d}t} \geq -\nabla \cdot \frac{\mathbf{q}}{T} \tag{22}$$

Entropy balance

$$\rho \frac{\mathrm{d}s}{\mathrm{d}t} = \frac{\phi}{T} - \nabla \cdot \frac{\mathbf{q}}{T} \tag{23}$$

First law of thermodynamics

$$\rho \frac{\mathrm{d}e}{\mathrm{d}t} = \boldsymbol{\tau} : \mathbf{D} - p \nabla \cdot \mathbf{u} - \nabla \cdot \mathbf{q} \tag{24}$$

Macroscopic description – constitutive equations

- Mechanical (rheological) constitutive equations
- Equations of state
- Fluxes

Macroscopic description – mechanical constitutive equations

- Newtonian fluids $\boldsymbol{\tau} = 2\mu\mathbf{D}$
- Non-Newtonian fluids
  - Generalised Newtonian fluids $\boldsymbol{\tau} = 2\mu(\gamma)\mathbf{D}$
  - Differential type fluid $\boldsymbol{\tau} = f(\mathbf{A}_1, \mathbf{A}_2, \ldots)$

$$\mathbf{A}_{i+1} = \frac{\mathrm{d}\mathbf{A}_i}{\mathrm{d}t} + \mathbf{A}_i \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{r}} + \nabla\mathbf{u} \cdot \mathbf{A}_i, \quad i = 1, 2, \ldots$$

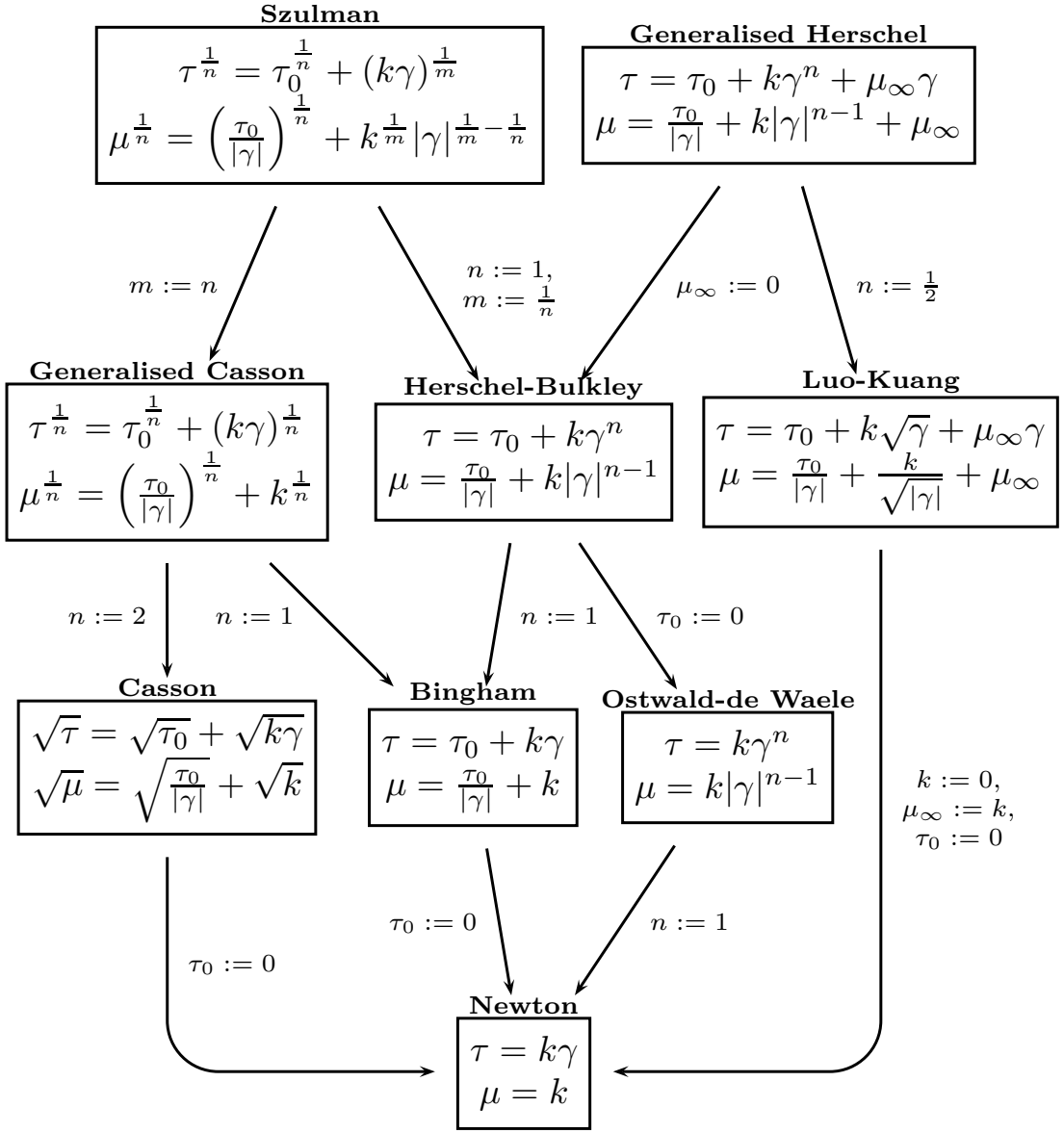
  - Integral type fluids

$$\boldsymbol{\tau} = \int_{-\infty}^{t} f(t-\tau)\left(\boldsymbol{\delta} - \mathbf{C}_t(\tau)\right)\,\mathrm{d}\tau$$

  - Rate type fluids $\dot{\boldsymbol{\tau}} = f\left(\boldsymbol{\tau}, \mathbf{D}, \dot{\mathbf{D}}\right)$

$$\boldsymbol{\tau} + \lambda_1\dot{\boldsymbol{\tau}} = 2\mu\left(\mathbf{D} + \lambda_2\dot{\mathbf{D}}\right)$$

Generalised Newtonian fluids



Macroscopic description – equations of state

- Fundamental equation of state $e = f(s, \rho^{-1})$

$$\frac{\mathrm{d}e}{\mathrm{d}t} = T\frac{\mathrm{d}s}{\mathrm{d}t} + \frac{p}{\rho^2}\frac{\mathrm{d}\rho}{\mathrm{d}t} \tag{25}$$

- Thermal equation of state $p = f(T, \rho^{-1})$

$$p = \rho R T \tag{26}$$

- Caloric equation of state $e = f(T, \rho^{-1})$

$$\mathrm{d}e = c_v\,\mathrm{d}T + \left(T\frac{\partial p}{\partial T} - p\right)\,\mathrm{d}\rho^{-1} \tag{27}$$

Macroscopic description – fluxes

General form $\mathbf{w} = -\mathbf{T} \cdot \nabla\varphi$ due to assumption $\mathbf{w} = f(\nabla\varphi)$. More precisely $\mathbf{w}$ depends only on φ and $\nabla\varphi$.

- Fourier's law

$$\mathbf{q} = -\boldsymbol{\lambda} \cdot \nabla T \tag{28}$$

- Fick's law

$$\mathbf{j}^i = -\rho \mathbf{D}^{ij} \cdot \nabla g^i \tag{29}$$

- Darcy's law

$$\mathbf{u} = -\mu^{-1} \mathbf{K} \cdot \nabla p \tag{30}$$

In the case of isotropy $\mathbf{T} = \alpha\, \boldsymbol{\delta}$ and

$$\mathbf{w} = -\alpha\, \boldsymbol{\delta} \cdot \nabla\varphi = -\alpha \nabla\varphi \tag{31}$$

Macroscopic description – general transport equations

General transport equations

$$\frac{\partial(\rho f)}{\partial t} + \nabla \cdot (\rho \mathbf{u} f) = S_f - \nabla \cdot \mathbf{k} \tag{32}$$

Fluxes

$$\mathbf{k} = -\Gamma \, \boldsymbol{\delta} \cdot \nabla f = -\Gamma \nabla f \tag{33}$$

In the case of isotropy the general transport equations becomes

$$\frac{\partial(\rho f)}{\partial t} + \nabla \cdot (\rho \mathbf{u} f) = S_f + \nabla \cdot (\Gamma \nabla f) \tag{34}$$

Macroscopic description

General form of the Navier–Stokes equation for Newtonian fluids

$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho \mathbf{f} - \nabla p + \nabla \cdot \left(2\mu \mathbf{D}^{\mathrm{D}}\right) \tag{35}$$

- incompressible flow
- creeping flow
- inviscid flow
- Boussinesq approximation
- Oseen approximation
- filtration
- one-dimensional flows
- heat transfer
- surface tension

Macroscopic description

– incompressible fluid ($\rho = \text{const}$)

$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho\mathbf{f} - \nabla p + \nabla \cdot (2\mu\mathbf{D}) \tag{36}$$

$\mu = \text{const}$

$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho\mathbf{f} - \nabla p + \mu\nabla^2\mathbf{u} \tag{37}$$

$\mu = \rho\nu$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f} - \nabla\frac{p}{\rho} + \nu\nabla^2\mathbf{u} \tag{38}$$

$p_k = \frac{p}{\rho} + \mathbf{g} \cdot \mathbf{r}$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = -\nabla p_k + \nu\nabla^2\mathbf{u} \tag{39}$$

Macroscopic description

– creeping flow

$$\rho \frac{\partial \mathbf{u}}{\partial t} = \rho \mathbf{f} - \nabla p + \nabla \cdot (2\mu \mathbf{D}) \tag{40}$$

steady state

$$\nabla p = \nabla \cdot (2\mu \mathbf{D}) \tag{41}$$

2D creeping flow

$$\nabla^4 \psi = 0 \tag{42}$$

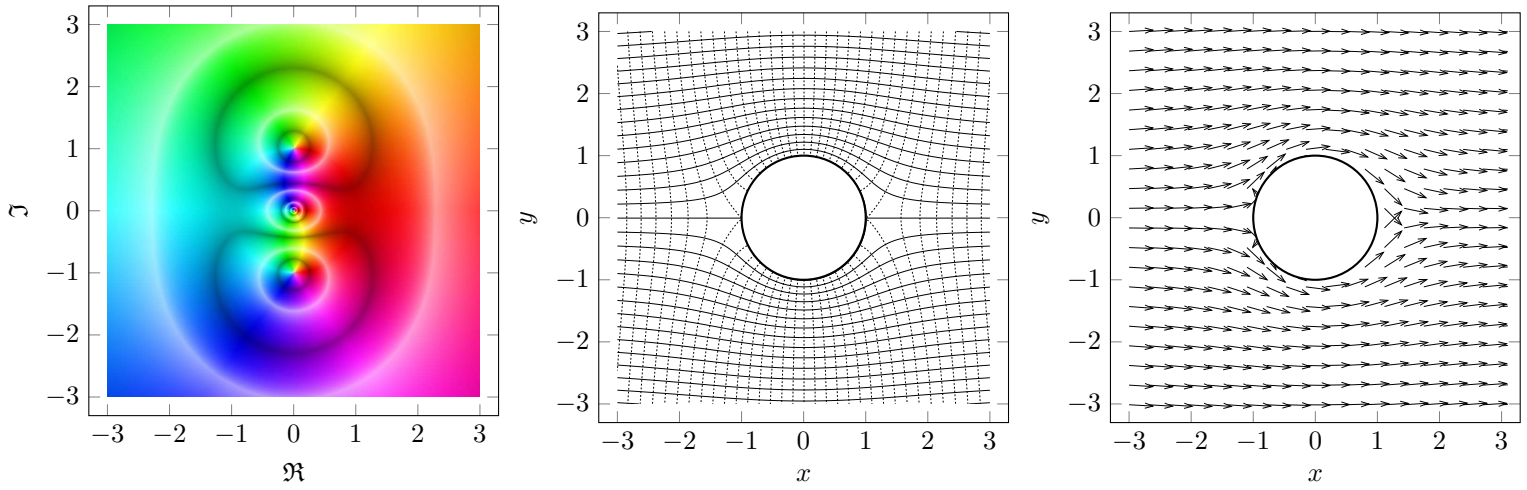
Macroscopic description

– inviscid flow ($\mu = 0$)

$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho \mathbf{f} - \nabla p \tag{43}$$

– potential flows ($\nabla \times \mathbf{u} = \mathbf{0} \iff \mathbf{u} = \nabla \varphi$)

$$\nabla^2 \varphi = \nabla^2 \psi = 0 \tag{44}$$



– Boussinesq approximation

$$\rho\mathbf{f} = \rho\mathbf{g} = \rho_0\mathbf{g} + (\rho - \rho_0)\,\mathbf{g} \tag{45}$$

$$\rho - \rho_0 = -\rho_0\beta(T - T_0) \tag{46}$$

$$\rho_0\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho_0\mathbf{g}\,(1 - \beta(T - T_0)) - \nabla p + \nabla\cdot(2\mu\mathbf{D}) \tag{47}$$

– Oseen approximation (linearisation)

$$\mathbf{u} \cdot \nabla \mathbf{u} \approx \mathbf{u}_\infty \cdot \nabla \mathbf{u} \tag{48}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u}_\infty \cdot \nabla \mathbf{u} = \rho \mathbf{f} - \nabla p + \nabla \cdot \left(2\mu \mathbf{D}^{\mathrm{D}}\right) \tag{49}$$

Macroscopic description

– filtration

$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \rho \mathbf{f} - \nabla p + \mu \nabla^2 \mathbf{u} - R_1 \mathbf{u} \tag{50}$$

– one-dimensional flows

$$\nabla^2 u = a \tag{51}$$

– heat transfer The 'fluid' Fourier equation describes the temperature field in the fluid.

$$c_v \left(\frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho T \mathbf{u}) \right) = \phi_\mu + \nabla \cdot (\lambda \nabla T) \qquad (52)$$

For solids where $\mathbf{u} = \mathbf{0}$ the above equation simplifies to the 'solid' Fourier–Kirchhoff equation

$$c \frac{\partial(\rho T)}{\partial t} = \nabla \cdot (\lambda \nabla T) + S_E \qquad (53)$$

where internal energy sources are given by S_E.

Comments

Generally, the 'fluid' equation should be solved together with 'solid' equation. This is called conjugate heat transfer. Not having to know the heat transfer coefficient is an advantage of this approach. The disadvantage is the necessity of increasing the total number of mesh elements due to the additional solid volume.
It is not always possible because of storage limitations. Then either the temperature or heat flux must be specified at the wall. Alternatives, through boundary conditions, are discussed further such as specified temperature, specified heat flux, specified temperature and heat flux, adiabatic or specified heat transfer coefficient.

– surface tension

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f} - \nabla\frac{p}{\rho} + \nu\nabla^2\mathbf{u} \tag{54}$$

body forces

$$\mathbf{f} = \mathbf{g} + \rho^{-1}\mathbf{f}_\sigma \tag{55}$$

$$\mathbf{f}_\sigma = \sigma\kappa\nabla\alpha \tag{56}$$

$$\kappa = -\nabla\cdot\hat{\boldsymbol{n}} = -\nabla\cdot\frac{\nabla\alpha}{\|\nabla\alpha\|} \tag{57}$$

α transport equation

$$\frac{\partial\alpha}{\partial t} + \nabla\cdot(\alpha\mathbf{u}) = 0 \tag{58}$$

Macroscopic description – dimensionless form of equations

Mass conservation equation

$$\nabla^+ \cdot \mathbf{u}^+ = 0 \tag{59}$$

Linear momentum conservation equation

$$\rho^+ \left(\mathrm{Sh} \frac{\partial \mathbf{u}^+}{\partial t^+} + \mathbf{u}^+ \cdot \nabla^+ \mathbf{u}^+ \right) = = \frac{\rho^+ \mathbf{f}^+}{\mathrm{Fr}} - \mathrm{Eu} \nabla^+ p^+ + \frac{\mu^+}{\mathrm{Re}} \nabla^{2+} \mathbf{u}^+ \tag{60}$$

Fourier–Kirchhoff (internal energy)

$$\rho^+ c_v^+ \left(\mathrm{Sh} \frac{\partial T^+}{\partial t^+} + \mathbf{u}^+ \cdot \nabla^+ T^+ \right) = = \frac{\mathrm{Ec}}{\mathrm{Re}} \phi_\mu^+ + \frac{\lambda^+}{\mathrm{Pr}\,\mathrm{Re}} \nabla^{2+} T^+ \tag{61}$$

Macroscopic description – dimensionless numbers

$$\mathrm{Sh} = \frac{\mathcal{L}}{\mathcal{U}t_0} = \frac{t_{ch}}{t_0} = \frac{\mathcal{L}f}{\mathcal{U}} = \frac{\frac{\mathcal{U}}{t_0}}{\frac{\mathcal{U}^2}{\mathcal{L}}}$$

$$\mathrm{Fr} = \frac{\mathcal{U}^2}{f_0\mathcal{L}} = \frac{\frac{\rho_0\mathcal{U}^2}{\mathcal{L}}}{\rho_0 f_0}$$

$$\mathrm{Re} = \frac{\mathcal{L}\mathcal{U}\rho_0}{\mu_0} = \frac{\mathcal{L}\mathcal{U}}{\nu_0} = \frac{\frac{\rho_0\mathcal{U}^2}{\mathcal{L}}}{\frac{\mu_0\mathcal{U}}{\mathcal{L}^2}}$$

$$\mathrm{Eu} = \frac{p_0}{\rho_0\mathcal{U}^2} = \frac{\frac{p_0}{\mathcal{L}}}{\frac{\rho_0\mathcal{U}^2}{\mathcal{L}}}$$

$$\mathrm{Ec} = \frac{\mathcal{U}^2}{c_{v0}T_0}$$

$$\mathrm{Pr} = \frac{c_{v0}\mu_0}{\lambda_0} = \frac{\nu_0}{\frac{\lambda_0}{c_{v0}\rho_0}}$$

$$\mathrm{Sc} = \frac{\mu_0}{\rho_0 D_0} = \frac{\nu_0}{D_0}$$

$$\mathrm{Da} = \frac{K_0}{\mathcal{L}^2}$$

$$\mathrm{De} = \frac{\lambda_0}{t_0}$$

$$\mathrm{Wi} = \lambda_0\gamma_0$$

Macroscopic description – compatibility conditions

General transport equation

$$\frac{\partial(\rho f)}{\partial t} + \nabla \cdot (\rho \mathbf{u} f) = S_f - \nabla \cdot \mathbf{k} \qquad (62)$$

From Reynolds' transport theorem arises general compatibility condition $\hat{\boldsymbol{n}} \cdot [\rho \mathbf{u} f + \mathbf{k}] = 0$

- Mass conservation: $f := 1$, $S_f := 0$, $\mathbf{k} := \mathbf{0}$. C.C. takes form $\hat{\boldsymbol{n}} \cdot [\rho \mathbf{u}] = 0$ or $\hat{\boldsymbol{n}} \cdot [\mathbf{u}] \equiv [u_n] = 0$
- Linear momentum: $f \leftarrow \mathbf{u}$, $S_f \leftarrow \rho \mathbf{f}$, $\mathbf{k} \leftarrow -\boldsymbol{\sigma}$ and C.C. $\hat{\boldsymbol{n}} \cdot [\rho \mathbf{u}\mathbf{u} - \boldsymbol{\sigma}] = \mathbf{0}$ or $\hat{\boldsymbol{n}} \cdot [\boldsymbol{\sigma}] = [\boldsymbol{\sigma}_n] = \mathbf{0}$
- Energy conservation: $f := e_k$, $S_f := \rho \mathbf{f} \cdot \mathbf{u}$, $\mathbf{k} := \mathbf{q} - \boldsymbol{\sigma} \cdot \mathbf{u}$ and C.C. $\hat{\boldsymbol{n}} \cdot [\rho \mathbf{u} e_k - \boldsymbol{\sigma} \cdot \mathbf{u} + \mathbf{q}] = 0$ or $\hat{\boldsymbol{n}} \cdot [\mathbf{q}]$ or $[\lambda \frac{\partial T}{\partial n}] = 0$

Macroscopic description – boundary conditions

Compatibility conditions are insufficient! Further conditions are needed:

- adhesion $\hat{\boldsymbol{l}} \cdot \mathbf{u} = u_l = 0$
- thermal equilibrium on surfaces $[T] = 0$

Boundary condition related to heat transfer (arise from C.C.)

- Dirichlet: $T = f_1(x, y, z, t)$
- Neumann: $q_n = \hat{\boldsymbol{n}} \cdot \mathbf{q}$ or $q_n = f_2(x, y, z, t)$
- mixed: $\alpha T - \lambda \frac{\partial T}{\partial n} = f_3(P, t)$

Macroscopic description – boundary conditions

Other surfaces than walls

- inlet: $n-1$ conditions where n stands for the number of equations
- outlet: Generally, $\boldsymbol{\sigma}_n = \hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$ plus T distribution. Usually p distribution due to $\boldsymbol{\sigma}_n \approx -p\hat{\boldsymbol{n}}$ plus $\frac{\partial T}{\partial n} = 0$
- symmetry: $\frac{\partial \varphi}{\partial n} = 0$ for all scalar variables φ
- periodicity (translation and rotation): $\varphi(P_1) = \varphi(P_2)$ where P_1 and P_2 are corresponding points on periodic surfaces

Mathematical classification

General partial differential equation

$$F\left(\frac{\partial^k f}{\partial x_1^{n_1}\dots\partial x_n^{n_n}}, \frac{\partial^{k-1} f}{\partial x_1^{m_1}\dots\partial x_n^{m_n}}, \dots, \frac{\partial f}{\partial x_i}, f, \mathbf{x}\right) = 0 \tag{63}$$

- linear
- semi-linear

$$\sum_i a_i(\mathbf{x})\frac{\partial^k f}{\partial x_1^{n_1}\dots\partial x_n^{n_n}} + a_0\left(\frac{\partial^{k-1} f}{\partial x_1^{m_1}\dots\partial x_n^{m_n}}, \dots, \frac{\partial f}{\partial x_i}, f, \mathbf{x}\right) = 0 \tag{64}$$

- quasi-linear
- fully non-linear

Mathematical classification

The Navier–Stokes equations are second order nonlinear partial differential equations. In general, they cannot be easily classified. However they posses properties of semi-linear and linear second order partial differential equations. Sometimes they can be simplified to those and can be divided into:

- hyperbolic
- parabolic
- elliptic

Semi-linear second order PDEs

For two independent variables x, y:

$$A(x,y)\frac{\partial^2 f}{\partial x^2} + B(x,y)\frac{\partial^2 f}{\partial x \partial y} + C(x,y)\frac{\partial^2 f}{\partial y^2} + F\left(x, y, f, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = 0 \quad (65)$$

for all (x,y) over a domain Ω the above equation is:

- hyperbolic if $B^2 - 4AC > 0$
- parabolic if $B^2 - 4AC = 0$
- elliptic if $B^2 - 4AC < 0$

Important elliptic second order PDEs

- Laplace equation

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0 \tag{66}$$

- Poisson equation

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = f(x, y) \tag{67}$$

- Helmholtz equation

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + k^2 f = 0 \tag{68}$$

Important parabolic second order PDEs

- Heat equation

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial^2 f}{\partial x^2} = 0 \tag{69}$$

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial^2 f}{\partial x^2} = g(x,t) \tag{70}$$

- Convection-diffusion equation

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = \nu \frac{\partial^2 f}{\partial x^2} \tag{71}$$

Important hyperbolic second order PDEs

- Wave equation

$$\frac{\partial^2 f}{\partial t^2} - a^2 \frac{\partial^2 f}{\partial x^2} = 0 \tag{72}$$

- Telegraph equations

$$\frac{\partial^2 f}{\partial x^2} - a\frac{\partial^2 f}{\partial t^2} - b\frac{\partial f}{\partial t} - c\, f = 0 \tag{73}$$

- Convection equations

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0 \tag{74}$$

Important mixed type second order PDEs

- Euler-Tricomi equation

$$\frac{\partial^2 f}{\partial x^2} - x\frac{\partial^2 f}{\partial y^2} = 0 \tag{75}$$

It is of hyperbolic type for $x > 0$, parabolic at $x = 0$ and elliptic for $x < 0$.

- Generalised Euler-Tricomi equation

$$\frac{\partial^2 f}{\partial x^2} - g(x)\frac{\partial^2 f}{\partial y^2} = 0 \tag{76}$$

Important mixed type second order PDEs

- Potential gas flow

$$(1 - \mathrm{Ma}_\infty^2)\frac{\partial^2 \varphi'}{\partial x^2} + \frac{\partial^2 \varphi'}{\partial y^2} = 0 \tag{77}$$

It is of hyperbolic type for $\mathrm{Ma}_\infty^2 > 1$, parabolic at $\mathrm{Ma}_\infty^2 = 1$ and elliptic for $\mathrm{Ma}_\infty^2 < 1$
The velocity potential for the x axis dominated flow is

$$\varphi(x, y) = u_\infty x + \varphi'(x, y) \tag{78}$$

Velocity components are then given as

$$u_x(x, y) = \frac{\partial \varphi'}{\partial x} = u_\infty + u_x(x, y) \tag{79}$$

$$u_y(x, y) = \frac{\partial \varphi'}{\partial y} = u_y(x, y) \tag{80}$$

VoF method

VoF – Volume of Fluid

$$\rho = \alpha\rho_l + (1-\alpha)\rho_g \tag{81a}$$
$$\mu = \alpha\mu_l + (1-\alpha)\mu_g \tag{81b}$$

α is a volume fraction

$$\alpha = \begin{cases} 1, & \text{liquid;} \\ 0, & \text{gas;} \\ 0 \leq \alpha \leq 1, & \text{interface} \end{cases} \tag{82}$$

VoF method

Mass conservation

$$\nabla \cdot \mathbf{u} = 0 \tag{83}$$

the Navier–Stokes equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \sigma \kappa \nabla \alpha - \nabla p_{rgh} - \mathbf{g} \cdot \mathbf{h} \nabla \rho + \nabla \cdot (2\mu \mathbf{D}) \tag{84}$$

modified pressure $p_{rgh} = p - \rho \mathbf{g} \cdot \mathbf{h}$
α transport equation

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0 \tag{85}$$

Complex phenomena

- Free surface flows
- Cavitation
- Melting

Mixture mass conservation equation

$$\nabla \cdot \mathbf{u} = 0 \tag{86}$$

Mixture Navier–Stokes equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \underbrace{\sigma \kappa \nabla \alpha}_{=\mathbf{0}, \neq \mathbf{0}} - \nabla p_{rgh} - \mathbf{g} \cdot \mathbf{h} \nabla \rho + \nabla \cdot (2\mu \mathbf{D}) \tag{87}$$

Volume fraction transport equation

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0 \tag{88}$$

Mixture mass conservation equation

$$\nabla \cdot \mathbf{u} = 0 \tag{89}$$

Mixture Navier–Stokes equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \underbrace{\sigma \kappa \nabla \alpha}_{=\mathbf{0}, \neq \mathbf{0}} - \nabla p_{rgh} - \mathbf{g} \cdot \mathbf{h} \nabla \rho + \nabla \cdot (2\mu \mathbf{D}) \tag{90}$$

Volume fraction transport equation

$$\frac{\partial \alpha_l}{\partial t} + \nabla \cdot (\alpha_l \mathbf{u}) = \frac{S_m}{\rho_l} \tag{91}$$

- Merkle $S_m = \ldots$
- Kunz
- Schnerr–Sauer

Melting

Mixture mass conservation equation

$$\nabla \cdot \mathbf{u} = 0 \tag{92}$$

Mixture Navier–Stokes equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \rho_0 \mathbf{g} - \rho_0 \beta (T - T_0)\mathbf{g} - \nabla p + \nabla \cdot (2\mu \mathbf{D}) + \mathbf{S}_u \tag{93}$$

Volume fraction transport equation

$$\frac{\partial \alpha_l}{\partial t} + \nabla \cdot (\alpha_l \mathbf{u}) = \frac{S_m}{\rho_l} \tag{94}$$

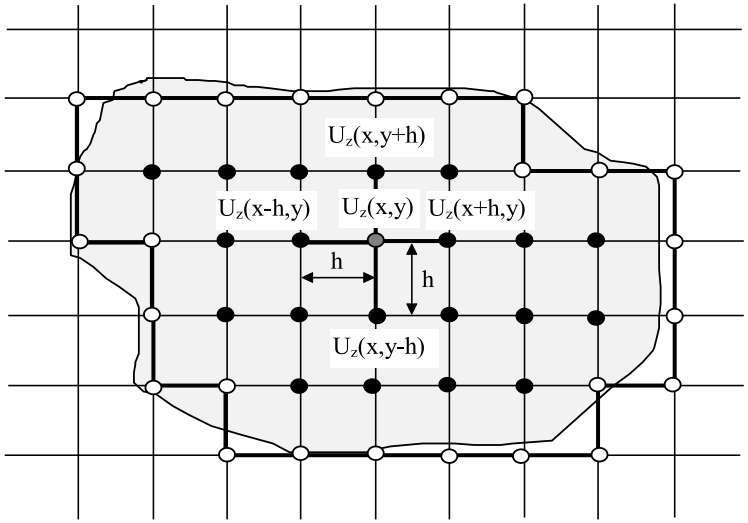
Enthalpy equation

$$\frac{\partial}{\partial t}(\rho c_p T) + \nabla \cdot (\rho c_p T \mathbf{u}) = \nabla \cdot (\lambda \nabla T) + S_h \tag{95}$$

Finite Difference Method

The method

The finite difference method (introduced by Euler in XVIII century) replaces the region by a finite mesh of points at which the dependent variable is approximated.



All partial derivatives at each mesh point are approximated from neighbouring values by means of Taylor's theorem. This means that derivatives at each point are approximated by difference quotients.

Taylor's theorem

Assuming that f has continuous derivatives over certain interval the Taylor expansion is used

$$f(x_0 + \Delta x) = \sum_{n=0}^{m-1} \frac{\mathrm{d}^n f(x_0)}{n!} + \frac{\mathrm{d}^m f(c)}{m!} \qquad (96)$$

where $x = x_0 + \Delta x$, $c = x_0 + \theta \Delta x$ and $\theta \in]0; 1[$. The above equation may also be written as

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + \frac{1}{2} f''(x_0)\Delta x^2 + \frac{1}{6} f'''(x_0)\Delta x^3 + \ldots + \frac{1}{m!} f^{(m)}(c)\Delta x^m \qquad (97)$$

Taylor's theorem

Instead of $f^{(m)}$ at unknown point c it is rewritten in terms of another unknown quantity of order Δx^m

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + f''(x_0)\frac{\Delta x^2}{2} + \ldots + f^{(m-1)}(x_0)\frac{\Delta x^{m-1}}{(m-1)!} + \mathcal{O}(\Delta x^m) \quad (98)$$

Discarding (truncating) $\mathcal{O}(\Delta x^m)$ one gets an approximation to f. The error in this approximation is $\mathcal{O}(\Delta x^m)$. Roughly speaking it says that knowing the value of f and the values of its derivatives at x_0 it is possible to write down the equation for its value at the point $x_0 + \Delta x$.

First order finite difference

Taking under consideration the Taylor expansion up to the first derivative

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + \mathcal{O}(\Delta x^2) \tag{99}$$

then neglecting $\mathcal{O}(\Delta x)$ and rearranging gives the first order finite difference approximation to $f'(x_0)$

$$f'(x_0) \approx \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} \tag{100}$$

This approximation is called a forward approximation. Replacing Δx by $-\Delta x$ in Taylor expansion one gets backward approximation

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x} \tag{101}$$

Second order finite difference

Taking under consideration the Taylor expansion up to the second derivative

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + f''(x_0)\frac{\Delta x^2}{2} + \mathcal{O}(\Delta x^3) \tag{102}$$

then neglecting $\mathcal{O}(\Delta x^2)$. Doing the same for $-\Delta x$ and combining the two above we have

$$f'(x_0) \approx \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x} \tag{103}$$

after neglecting $\mathcal{O}(\Delta x^2)$. This is so called the second order central difference approximation to $f'(x_0)$.

Second order finite difference

Higher order approximation to derivatives is also possible. This can be done by taking more terms in the Taylor expansion. Doing so up to the third we get

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + \frac{1}{2}f''(x_0)\Delta x^2 + \frac{1}{6}f'''(x_0)\Delta x^3 + \mathcal{O}(\Delta x^4) \quad (104)$$

Replacing Δx for $-\Delta x$ and combing the results then dropping $\mathcal{O}(\Delta x^4)$ gives the second order symmetric difference approximation to f''

$$f''(x_0) \approx \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2} \quad (105)$$

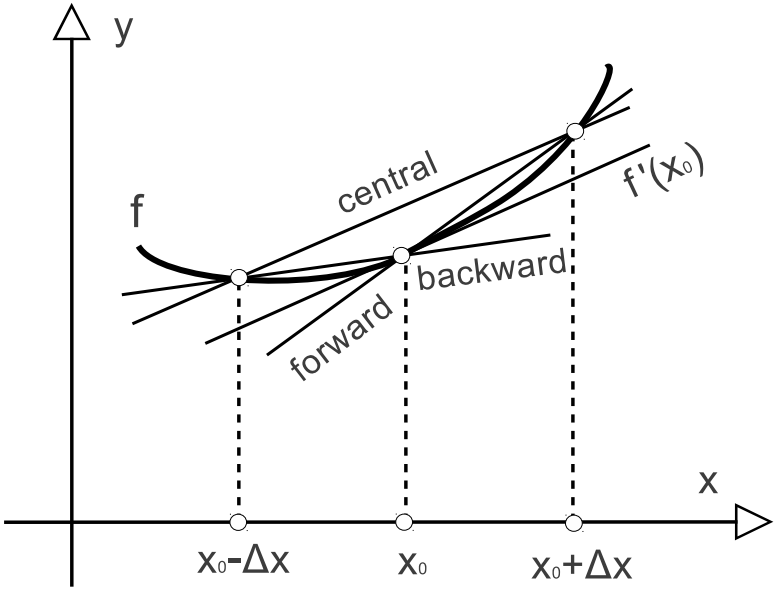
Differences

Selected finite differences approximation to first and second derivatives are given in the following table. These can be used to solve ordinary differential equations by replacing derivatives by their approximations.

	Approximation	Type	Order
$f'(x_0)$	$\frac{f(x_0+\Delta x)-f(x_0)}{\Delta x}$	forward	1^{st}
$f'(x_0)$	$\frac{f(x_0)-f(x_0-\Delta x)}{\Delta x}$	backward	1^{st}
$f'(x_0)$	$\frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x}$	central	2^{nd}
$f''(x_0)$	$\frac{f(x_0+\Delta x)-2f(x_0)+f(x_0-\Delta x)}{\Delta x^2}$	symmetric	2^{nd}

Differences

Equations for f' approximate the slope of the tangent in x_0 by means of chords (backward, forward and central finite difference).



Differences

The typical subscript notation is

$$f(x_0 + m\,h, y_0 + n\,h) \equiv f_{i+m\,j+n} \tag{106}$$

Now it is possible to express selected finite differences approximations to derivatives in somewhat simpler manner

	Approximation	Type	Order
f'_i	$\frac{f_{i+1}-f_i}{h}$	forward	1^{st}
f'_i	$\frac{f_i-f_{i-1}}{h}$	backward	1^{st}
f'_i	$\frac{f_{i+1}-f_{i-1}}{2h}$	central	2^{nd}
f''_i	$\frac{f_{i+1}-2f_i+f_{i-1}}{h^2}$	symmetric	2^{nd}

Convection-diffusion equation

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\cdot(\rho\phi\mathbf{u}) = \nabla\cdot(\Gamma\nabla\phi) \tag{107}$$

- parabolic. Additionally, if $\mathbf{u} = \mathbf{0}$

$$\frac{\partial(\rho\phi)}{\partial t} = \nabla\cdot(\Gamma\nabla\phi) \tag{108}$$

- hyperbolic, if $\Gamma = 0$

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\cdot(\rho\phi\mathbf{u}) = 0 \tag{109}$$

- elliptic, if $\frac{\partial}{\partial t} = 0$ or at the same time $\frac{\partial}{\partial t} = 0$ and $\mathbf{u} = \mathbf{0}$

$$\nabla\cdot(\Gamma\nabla\phi) = 0 \tag{110}$$

Convection equation

If $\Gamma = 0$ and $\rho = 1$ we have

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = 0 \tag{111}$$

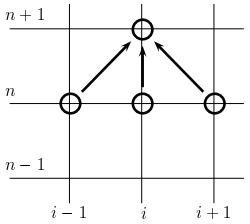
One dimensional version

$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{112}$$

The analytical solution of the above is

$$\phi(x,t) = f(x - u_x t) \tag{113}$$

Convection equation – FTCS scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{114}$$

FTCS discretisation scheme (Forward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = 0 \tag{115}$$

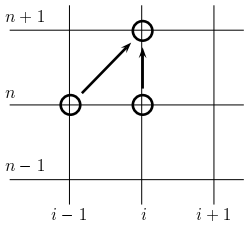
or explicitly

$$\phi_i^{n+1} = \phi_i^n - \tfrac{1}{2}\mathrm{Co}\left(\phi_{i+1}^n - \phi_{i-1}^n\right) \tag{116}$$

where Co is the Courant number

$$\mathrm{Co} = \frac{u_x \Delta t}{\Delta x} \tag{117}$$

Convection equation – FOU scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{118}$$

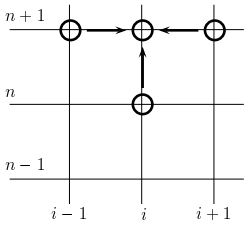
FOU discretisation scheme (First Order Upwind)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} = 0 \tag{119}$$

or explicitly

$$\phi_i^{n+1} = \phi_i^n - \mathrm{Co}\left(\phi_i^n - \phi_{i-1}^n\right) \tag{120}$$

Convection equation – BTCS scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \qquad (121)$$

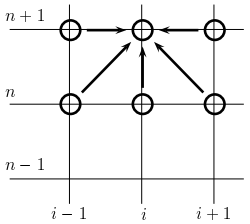
BTCS discretisation scheme (Backward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} = 0 \qquad (122)$$

For comparison, FTCS scheme is

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\Delta x} = 0 \qquad (123)$$

Convection equation – Crank–Nicolson

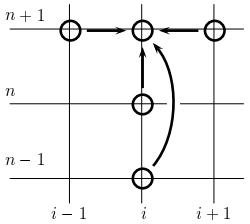


$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \qquad (124)$$

The Crank–Nicolson scheme is a combination of the FTCS and BTCS

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + \frac{1}{2}\left(u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \right) = 0 \qquad (125)$$

Convection equation – backward

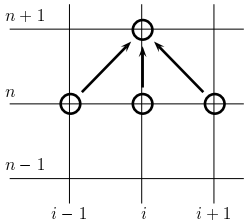


$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \qquad (126)$$

Second-order backward using two previous time-step values ϕ_i^n, ϕ_i^{n-1}

$$\frac{3\phi_i^{n+1} - 4\phi_i^n + \phi_i^{n-1}}{2\Delta t} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} = 0 \qquad (127)$$

Convection equation – Lax–Wendroff



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{128}$$

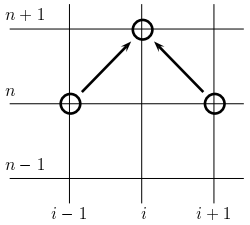
ϕ is expanded up to the third order

$$\frac{\partial \phi_i}{\partial t} \approx \frac{\phi_i^{n+1} - \phi_i}{\Delta t} - \frac{1}{2}\frac{\partial^2 \phi_i}{\partial t^2}\Delta t \tag{129}$$

Also, the centred space approximation is used

$$\phi_i^{n+1} = \phi_i^n - \tfrac{1}{2}\mathrm{Co}\left(\phi_{i+1}^n - \phi_{i-1}^n\right) + \tfrac{1}{2}\mathrm{Co}^2\left(\phi_{i-1}^n - 2\phi_i^n + \phi_{i+1}^n\right) \tag{130}$$

Convection equation – Lax–Friedrichs



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{131}$$

Lax-Friedrichs scheme is a modification of the FTCS scheme

$$\phi_i^{n+1} = \frac{\phi_{i-1}^n + \phi_{i+1}^n}{2} - \frac{1}{2}\mathrm{Co}\left(\phi_{i+1}^n - \phi_{i-1}^n\right) \tag{132}$$

For comparison, FTCS scheme is

$$\phi_i^{n+1} = \phi_i^n - \frac{1}{2}\mathrm{Co}\left(\phi_{i+1}^n - \phi_{i-1}^n\right) \tag{133}$$

Transient diffusion equation

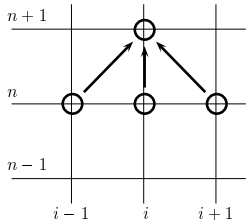
If $\mathbf{u} = \mathbf{0}$ and $\rho = 1$ we have

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (\Gamma \nabla \phi) \tag{134}$$

One dimensional version for $\Gamma = \text{const}$

$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \tag{135}$$

Transient diffusion equation – FTCS



$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \tag{136}$$

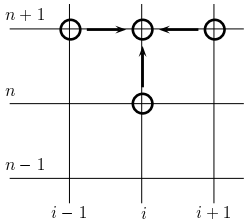
FTCS discretisation scheme (Forward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \Gamma \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \tag{137}$$

or explicitly

$$\phi_i^{n+1} = \phi_i^n + \frac{\Gamma \Delta t}{\Delta x^2} \left(\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n \right) \tag{138}$$

Transient diffusion equation – BTCS

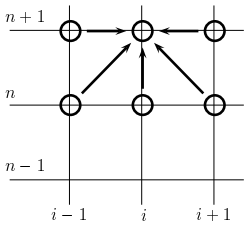


$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \tag{139}$$

BTCS discretisation scheme (Backward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \Gamma \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \tag{140}$$

Transient diffusion equation – Crank–Nicolson

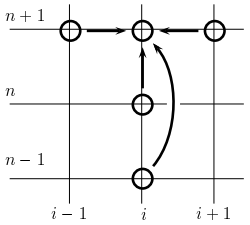


$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \tag{141}$$

The Crank–Nicolson scheme is a combination of the FTCS and BTCS

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{1}{2}\left(\Gamma \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + \Gamma \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \right) \tag{142}$$

Transient diffusion equation – backward



$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \tag{143}$$

Second-order backward using two previous time-step values ϕ_i^n, ϕ_i^{n-1}

$$\frac{3\phi_i^{n+1} - 4\phi_i^n + \phi_i^{n-1}}{2\Delta t} = \Gamma \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \tag{144}$$

Steady diffusion equation

If $\mathbf{u} = \mathbf{0}$, $\rho = 1$ and $\frac{\partial}{\partial t} = 0$ we have

$$\nabla \cdot (\Gamma \nabla \phi) = S_\phi \tag{145}$$

Two types of equations can be distinguished for $\Gamma = \text{const}$

- Poisson equation, $S = \Gamma^{-1} S_\phi$

$$\nabla^2 \phi = S \tag{146}$$

- Laplace equation, $S = 0$

$$\nabla^2 \phi = 0 \tag{147}$$

Poisson equation

Poisson equation is $\nabla^2 \phi_z = a$. Two dimensional versions of this equation is written as

$$\frac{\partial^2 \phi_z}{\partial x^2} + \frac{\partial^2 \phi_z}{\partial y^2} = a \tag{148}$$

The next step would be to replace second order derivatives by symmetric finite difference approximation

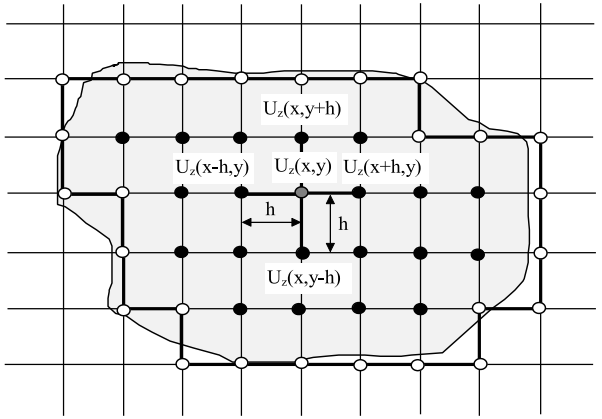
$$\frac{\phi_{i+1j} - 2\phi_{ij} + \phi_{i-1j}}{h^2} + \frac{\phi_{ij+1} - 2\phi_{ij} + \phi_{ij-1}}{h^2} = a \tag{149}$$

It can be rewritten to give ϕ_{ij} as a function of surrounding variables

$$\phi_{ij} = \frac{\phi_{i+1j} + \phi_{i-1j} + \phi_{ij+1} + \phi_{ij-1} - ah^2}{4} \tag{150}$$

Poisson equation - mesh and boundary conditions

The domain is discretised in the x and y directions by means of constant mesh size h (figure on the left). ϕ_z is unknown at black mesh points and known at white points from the boundary condition.



For instance the Dirichlet boundary condition specifies the values of ϕ_z directly. In this case $\phi_z = 0$ meaning no slip wall. If the boundary values are known then discrete Poisson equation gives a system of linear equations for ϕ_{ij}.

Poisson equation - solution methods

The accuracy of results depends on the size of the mesh represented here by h. Mesh size should be decreased until there is no significant influence on numerical results. The set of linear equations can be solved either directly by means of an appropriate method (Gauss elimination for instance) or indirectly by means of iterative solution methods or the relaxation method (point-Jacobi iteration)

$$\phi_{ij}^{n+1} = \frac{\phi_{i+1j}^{n} + \phi_{i-1j}^{n} + \phi_{ij+1}^{n} + \phi_{ij-1}^{n} - ah^2}{4} \tag{151}$$

or point-Gauss–Seidel (faster than point-Jacobi)

$$\phi_{ij}^{n+1} = \frac{\phi_{i+1j}^{n} + \phi_{i-1j}^{n+1} + \phi_{ij+1}^{n} + \phi_{ij-1}^{n+1} - ah^2}{4} \tag{152}$$

Poisson equation - solution methods

Another indirect method is so called Successive Over-Relaxation method

$$\phi_{ij}^{n+1} = (1-w)\phi_{ij}^{n} + w\frac{\phi_{i+1j}^{n} + \phi_{i-1j}^{n+1} + \phi_{ij+1}^{n} + \phi_{ij-1}^{n+1} - ah^2}{4} \quad (153)$$

where w is a relaxation parameter. For $w \in]1,2[$ we have over-relaxation and for $w = 1$ this method corresponds to the point-Gauss–Seidel method. One can also consider under-relaxation method for $w \in]0,1[$.
The best choice of w value needs numerical experiments. It also depends on specific problems.

Poisson FDM pseudocode

Data: Read input variables and BCs

$w := 1$; $n := 1$;

repeat

  $R := 0$;

  for $i := 1$ **to** i_{max} **do**

    for $j := 1$ **to** j_{max} **do**

      if not $\text{boundary}(\phi_{ij}^n)$ **then**

        $\phi_{ij}^{n+1} := \frac{\phi_{i+1j}^n + \phi_{i-1j}^{n+1} + \phi_{ij+1}^n + \phi_{ij-1}^{n+1} - ah^2}{4}$;

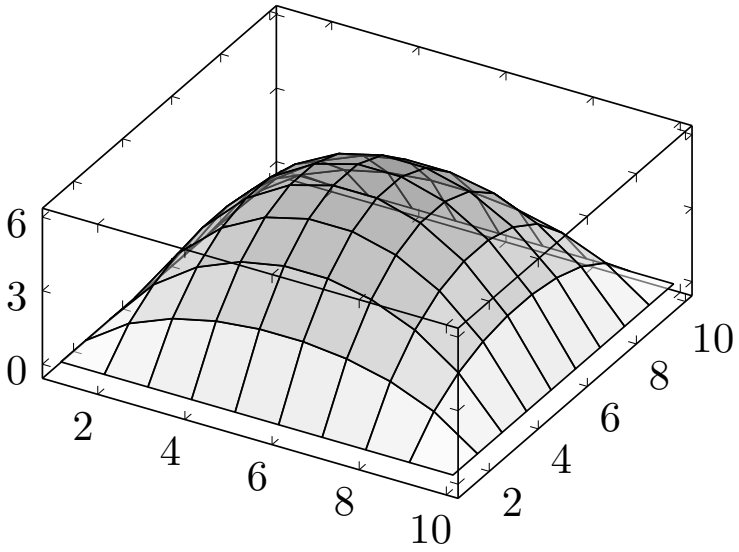
        $R := \max\left(|\phi_{ij}^{n+1} - \phi_{ij}^n|, R\right)$;

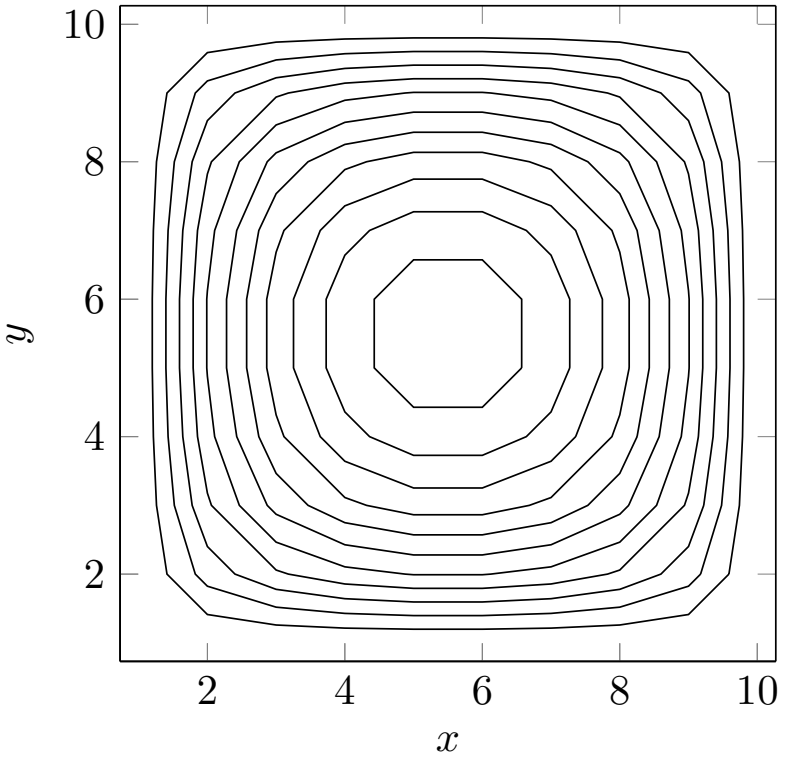
        $\phi_{ij}^{n+1} := (1-w)\phi_{ij}^n + w\,\phi_{ij}^{n+1}$;

  $n := n + 1$;

until $n \leq n_{max}$ **and** $R > R_{min}$;

Results - Poisson equation





Laplace equation

Laplace equation is $\nabla^2\varphi = 0$. Two dimensional versions of this equation is written as

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} = 0 \tag{154}$$

Replacing second order derivatives by symmetric finite difference approximation

$$\frac{\varphi_{i+1j} - 2\varphi_{ij} + \varphi_{i-1j}}{h^2} + \frac{\varphi_{ij+1} - 2\varphi_{ij} + \varphi_{ij-1}}{h^2} = 0 \tag{155}$$

It can be rewritten to give φ_{ij} as a function of surrounding variables

$$\varphi_{ij} = \frac{\varphi_{i+1j} + \varphi_{i-1j} + \varphi_{ij+1} + \varphi_{ij-1}}{4} \tag{156}$$

Laplace eq. – Neumann boundary condition

Neumann boundary condition specifies values of the derivative $\frac{\partial}{\partial n}$ of a solution φ on boundary $\partial\Omega$ to fulfil

$$\frac{\partial \varphi}{\partial n} = N(x, y) \tag{157}$$

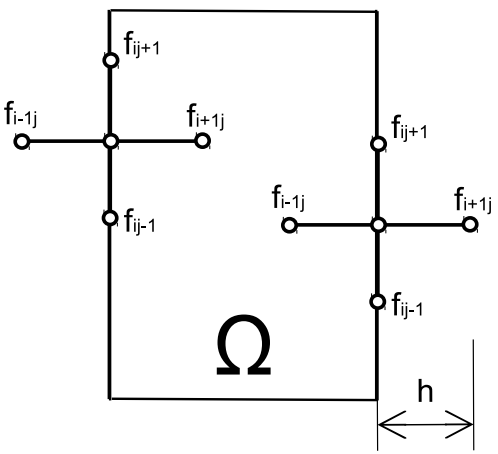
where the normal derivatives is defined as

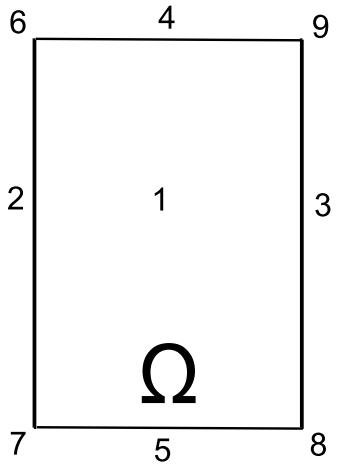
$$\frac{\partial \varphi}{\partial n} = \hat{\boldsymbol{n}} \cdot \nabla \varphi = n_x \frac{\partial \varphi}{\partial x} + n_y \frac{\partial \varphi}{\partial y} \tag{158}$$

and $(x, y) \in \partial\Omega$. If $\mathbf{u} = \nabla\varphi$ we get

$$\frac{\partial \varphi}{\partial n} = \hat{\boldsymbol{n}} \cdot \mathbf{u} = n_x u_x + n_y u_y \tag{159}$$

Laplace eq. – Neumann boundary condition





We have two equation for a point located on boundary '2'

$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1j} - 2f_{ij} + f_{i-1j}}{h^2}$$
$$\frac{\partial f}{\partial x} = \frac{f_{i+1j} - f_{i-1j}}{2h} = N_{ij}$$

Point f_{i-1j} is located outside the Ω area. Eliminating it we get

$$\frac{\partial^2 f}{\partial x^2} = \frac{2f_{i+1j} - 2N_{ij}h - 2f_{ij}}{h^2}$$

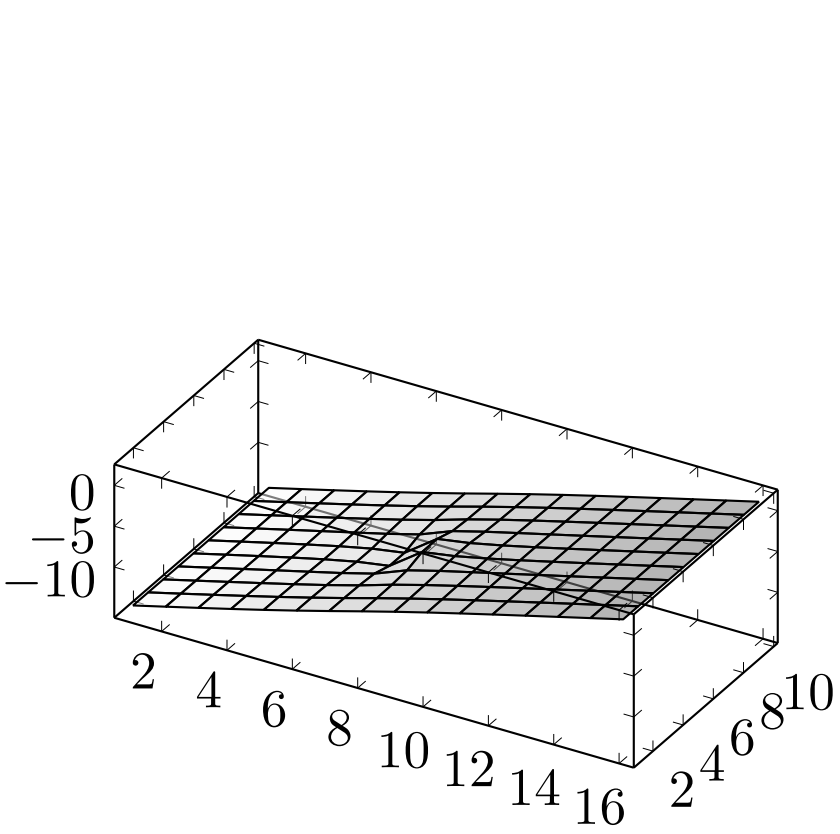
and

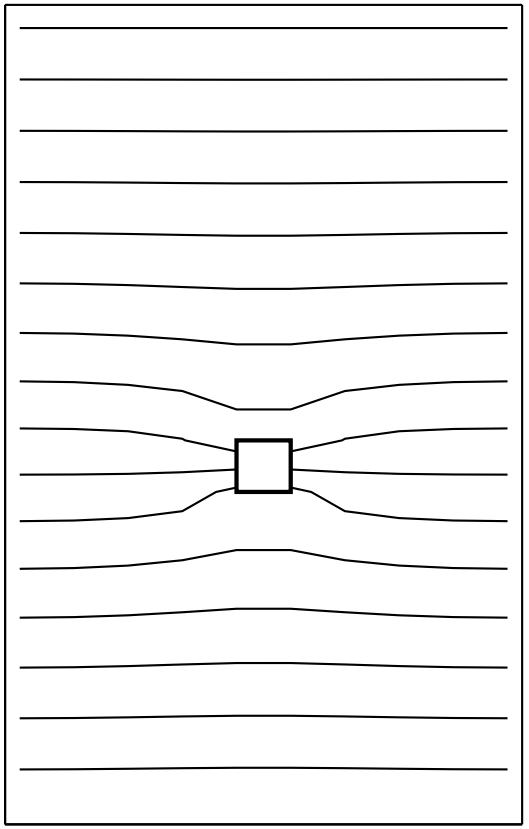
$$f_{ij} = \frac{2f_{i+1j} + f_{ij+1} + f_{ij-1} - 2N_{ij}h}{4}$$

Laplace FDM pseudocode

Data: Read input variables and BCs
$w := 1$; $n := 1$;
repeat
  $R := 0$;
  for $i := 1$ **to** i_{max} **do**
    for $j := 1$ **to** j_{max} **do**
      if $\text{boundary}(\varphi_{ij}^n) \neq 0$ **then**
        switch φ_{ij}^n **do**
          case 1*:* **do** $\varphi_{ij}^{n+1} := \frac{\varphi_{i+1j}^n + \varphi_{i-1j}^{n+1} + \varphi_{ij+1}^n + \varphi_{ij-1}^{n+1}}{4}$;
          ;
          case 2*:* **do** $\varphi_{ij}^{n+1} := \frac{2\varphi_{i+1j}^n + \varphi_{ij+1}^n + \varphi_{ij-1}^{n+1} - 2h\mathrm{N}_{ij}}{4}$;
          ;
          ⋮
      $R := \max\left(|\varphi_{ij}^{n+1} - \varphi_{ij}^n|, R\right)$;
      $\varphi_{ij}^{n+1} := (1-w)\varphi_{ij}^n + w\,\varphi_{ij}^{n+1}$;
  $n := n + 1$;
until $n \leq n_{max}$ **and** $R > R_{min}$;

Results - Laplace equation





Biharmonic equation

The biharmonic equation is $\nabla^4\psi \equiv \nabla^2 \cdot \nabla^2\psi = 0$. Two dimensional versions of this equation is written as

$$\frac{\partial^4\psi}{\partial x^4} + 2\frac{\partial^4\psi}{\partial x^2\partial y^2} + \frac{\partial^4\psi}{\partial y^4} = 0 \qquad (161)$$

It is a fourth-order elliptic partial differential equation that describes creeping flows in terms of a stream function ψ where the velocity components are $u_x = \frac{\partial\psi}{\partial y}$ and $u_y = -\frac{\partial\psi}{\partial x}$.
The Dirichlet boundary condition specifies both: a stream function ψ and its normal derivative $\frac{\partial\psi}{\partial n}$. Two conditions are needed due to the fourth order of the biharmonic equation.

Biharmonic equation - approximation to derivatives

The finite difference approximations to $\frac{\partial^4\psi}{\partial x^4}$, $\frac{\partial^4\psi}{\partial y^4}$ are

$$\frac{\partial^4\psi}{\partial x^4} = \frac{\psi_{i+2j} + \psi_{i-2j} - 4\psi_{i+1j} - 4\psi_{i-1j} + 6\psi_{ij}}{h^4} \quad (162a)$$

$$\frac{\partial^4\psi}{\partial y^4} = \frac{\psi_{ij+2} + \psi_{ij-2} - 4\psi_{ij+1} - 4\psi_{ij-1} + 6\psi_{ij}}{h^4} \quad (162b)$$

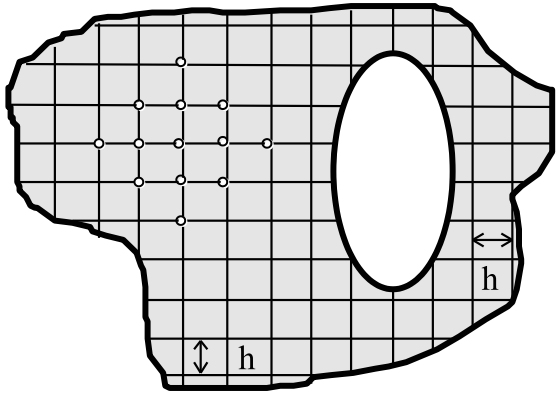
The fourth order mixed derivative is approximated as

$$\frac{\partial^4\psi}{\partial x^2\partial y^2} = \frac{\psi_{i+1j+1} + \psi_{i-1j-1} + \psi_{i-1j+1} + \psi_{i+1j-1}}{h^4} + \frac{4\psi_{ij} - 2\psi_{i+1j} - 2\psi_{i-1j} - 2\psi_{ij+1} - 2\psi_{ij-1}}{h^4} \quad (163)$$

Biharmonic equation - discrete equation

From the discrete biharmonic equations ψ_{ij} can be expressed as a function of surrounding variables

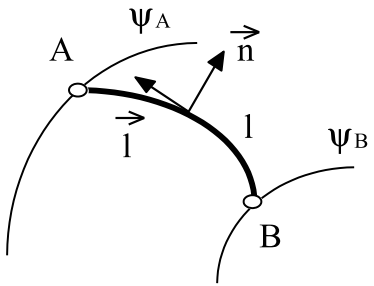
$$\psi_{ij} = \frac{-\psi_{i+2j} - \psi_{i-2j} - \psi_{ij+2} - \psi_{ij-2} + 4\psi_{ij}}{20} + 8\frac{\psi_{i-1j} + \psi_{ij+1} + \psi_{ij-1} + \psi_{i+1j}}{20} - 2\frac{\psi_{i+1j+1} + \psi_{i-1j-1} + \psi_{i-1j+1} + \psi_{i+1j-1}}{20} \quad (164)$$



Biharmonic equation - boundary conditions

From the below figure two purely geometric relationships arise $\frac{\partial \psi}{\partial n} = \hat{\boldsymbol{n}} \cdot \nabla \psi = -u_l$, $\frac{\partial \psi}{\partial l} = \hat{\boldsymbol{l}} \cdot \nabla \psi = u_n$. For an impermeable boundary one gets $u_n = 0 \Rightarrow \frac{\partial \psi}{\partial l} = 0$. The general relationship between volumetric flow rate and the stream functions is

$$\dot{V} = \int_L \mathbf{u} \cdot \hat{\boldsymbol{n}} \, \mathrm{d}L = \int_L \frac{\partial \psi}{\partial l} \, \mathrm{d}L = \int_L \mathrm{d}\psi = \psi_A - \psi_B \quad (165)$$



Biharmonic FDM pseudocode

Data: Read input variables and BCs

$w := 1$; $n := 1$;

repeat

  $R := 0$;

  for $i := 1$ **to** i_{max} **do**

    for $j := 1$ **to** j_{max} **do**

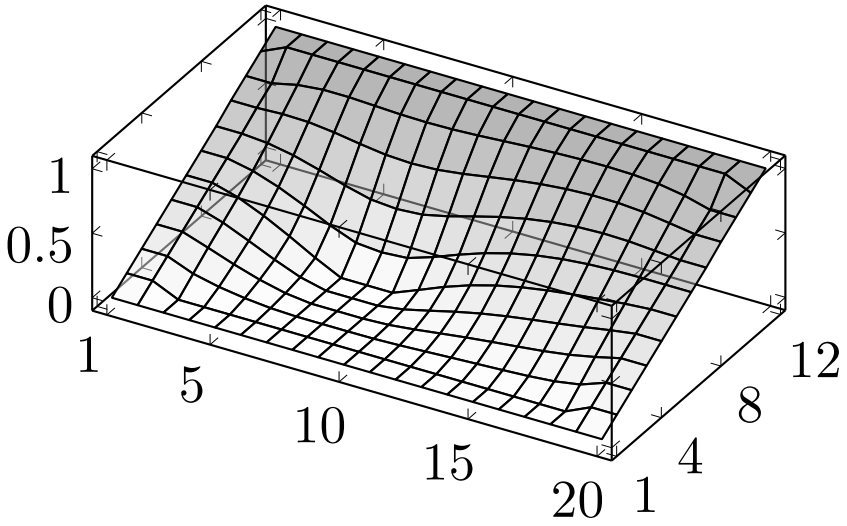
      if not $\mathrm{boundary}(\psi_{ij}^n)$ **then**

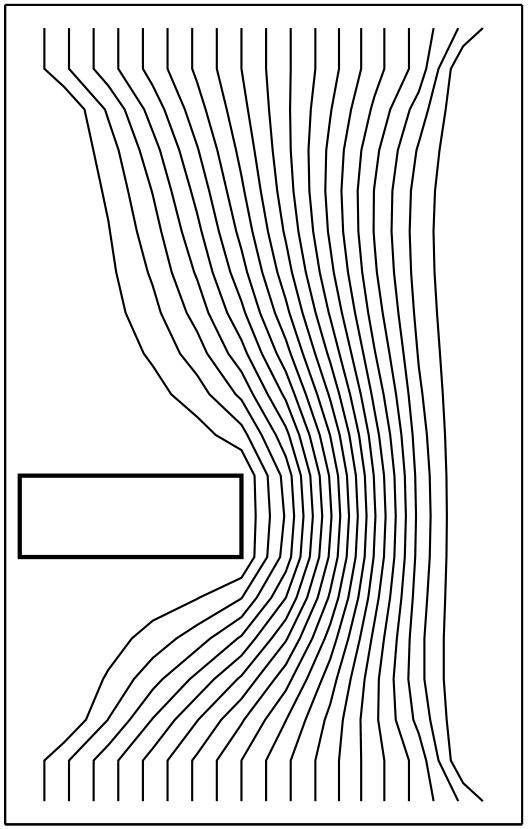
$$\psi_{ij}^{n+1} := \frac{-\psi_{i+2j}^n - \psi_{i-2j}^n - \psi_{ij+2}^n - \psi_{ij-2}^n + 4\psi_{ij}^n}{20} +$$
$$8\frac{\psi_{i-1j}^n + \psi_{ij+1}^n + \psi_{ij-1}^n + \psi_{i+1j}^n}{20} -$$
$$2\frac{\psi_{i+1j+1}^n + \psi_{i-1j-1}^n + \psi_{i-1j+1}^n + \psi_{i+1j-1}^n}{20};$$
$$R := \max\left(|\psi_{ij}^{n+1} - \psi_{ij}^n|, R\right);$$
$$\psi_{ij}^{n+1} := (1-w)\psi_{ij}^n + w\,\psi_{ij}^{n+1};$$

  $n := n + 1$;

until $n \leq n_{max}$ **and** $R > R_{min}$;

Results - biharmonic equation





Convection-diffusion equation

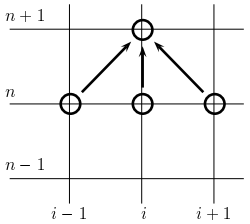
If $\Gamma = \nu = \text{const}$ and $\rho = 1$ we have

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = \nu \nabla^2 \phi \tag{166}$$

One dimensional version

$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \tag{167}$$

Convection-diffusion equation – FTCS



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \tag{168}$$

Forward time centred space discretisation scheme

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = \nu \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \tag{169}$$

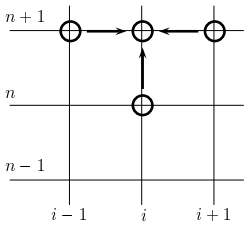
or explicitly

$$\phi_i^{n+1} = \phi_i^n - \frac{\mathrm{Co}}{2}\left(\phi_{i+1}^n - \phi_{i-1}^n\right) + \frac{1}{\mathrm{Re}}\left(\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n\right) \tag{170}$$

where

$$\mathrm{Re} = \frac{\Delta x^2}{\nu\, \Delta t} \tag{171}$$

Convection-diffusion equation – BTCS



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \tag{172}$$

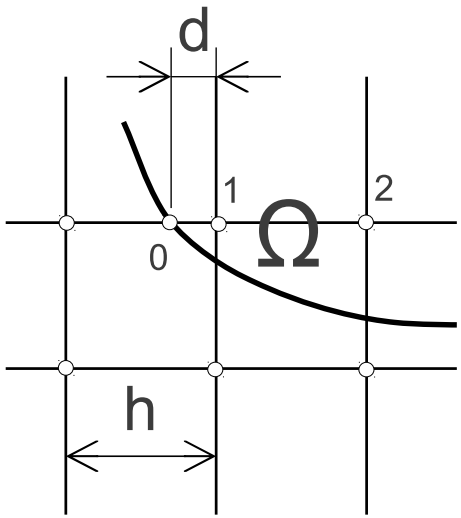
Backward time centred space discretisation scheme

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} = \nu \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \tag{173}$$

or

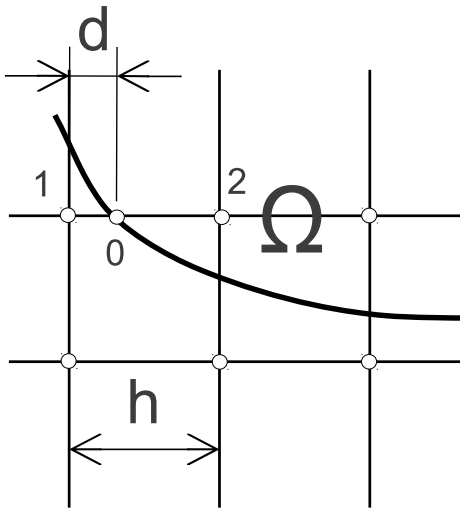
$$\phi_i^{n+1} - \phi_i^n + \frac{\mathrm{Co}}{2}\left(\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}\right) = \frac{1}{\mathrm{Re}}\left(\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}\right) \tag{174}$$

Complex geometry



Point 1 is located inside the Ω area

$$f_1 = \frac{h\, f_0 + d\, f_2}{h + d} \qquad (175)$$



Point 1 is located outside the Ω area

$$f_1 = \frac{h\, f_0 - d\, f_2}{h - d} \qquad (176)$$

Stability analysis

The decomposition of ϕ_j^n into a Fourier series is

$$\phi_j^n = \sum_{m=-N}^{N} A_m^n e^{ik_m j \Delta x} \tag{177}$$

where the wave number k_m is

$$k_m = \frac{m\pi}{N\,\Delta x} = \frac{\theta}{\Delta x} \tag{178}$$

A single mode determines the time evolution of ϕ_j^n

$$\phi_j^n = A_m^n e^{ij\theta} \tag{179}$$

A numerical scheme is stable if and only if

$$\left| \frac{A_m^{n+1}}{A_m^n} \right| = |G| \leq 1 \tag{180}$$

Stability analysis – FTCS

- convection equation

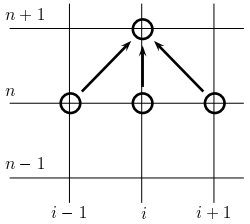
$$|G| = \sqrt{1 + \mathrm{Co}^2 \sin^2 \theta} \geq 1 \tag{181}$$

- diffusion equation

$$2\,\mathrm{Re}^{-1} \leq 1 \tag{182}$$

- convection-diffusion equation

$$\mathrm{Co}^2 \leq 2\,\mathrm{Re}^{-1} \leq 1 \tag{183}$$



Stability analysis – BTCS

- convection equation

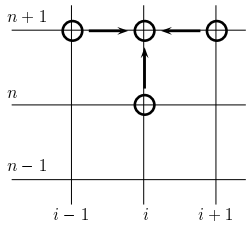
$$|G|^2 = \frac{1}{1 + \mathrm{Co}^2 \sin^2 \theta} \leq 1 \qquad (184)$$

- diffusion equation

$$|G| \leq 1 \qquad (185)$$

- convection-diffusion equation

$$|G|^2 = \frac{1}{\left(1 + 4\,\mathrm{Re}^{-1} \sin^2 \frac{\theta}{2}\right)^2 + \mathrm{Co}^2 \sin^2 \theta} \leq 1 \qquad (186)$$



Stability analysis – Crank–Nicolson

- convection equation

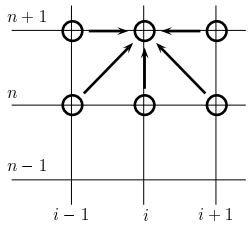
$$|G| = 1 \tag{187}$$

- diffusion equation

$$|G| \leq 1 \tag{188}$$

- convection-diffusion equation

$$|G| \leq 1 \tag{189}$$



Modified equation

- Using a specific discretisation scheme one obtains a discrete counterpart of the original PDE;
- Taylor's expansion is applied around ϕ_i^{n+1} and substituted into the specific scheme;
- Resulting equation is rearranged in order to recover the original PDE;
- The remaining terms are the truncation errors associated with the specific discretisation scheme;
- The modified equation is actually solved rather than the original PDE;
- Numerical diffusion and dispersion can be analysed now;

Model equations

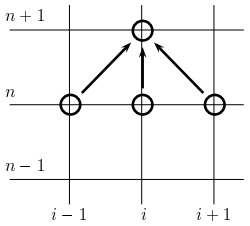
Convection-diffusion equation

$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = \underbrace{\nu \frac{\partial^2 \phi}{\partial x^2}}_{\text{diffusion}} \tag{190}$$

Korteweg-de Vries equation

$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = \underbrace{-\varepsilon \frac{\partial^3 \phi}{\partial x^3}}_{\text{dispresion}} \tag{191}$$

Convection equation – FTCS scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{192}$$

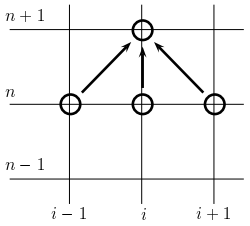
FTCS discretisation scheme (Forward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = 0 \tag{193}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = -\tfrac{1}{2} u_x \Delta x \, \mathrm{Co} \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} - \tfrac{1}{6} u_x \Delta x^2 \left(2\,\mathrm{Co}^2 + 1\right) \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \ldots \tag{194}$$

Convection equation – FTCS scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{195}$$

FTCS discretisation scheme (Forward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = 0 \tag{196}$$

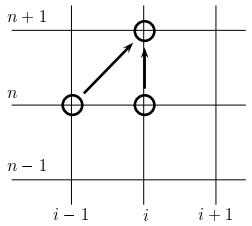
The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = \nu_N \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} - \varepsilon_N \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \dots \tag{197}$$

or

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = \nu_N \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} \tag{198}$$

Convection equation – FOU scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{199}$$

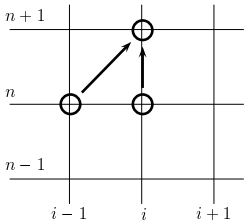
FOU discretisation scheme (First Order Upwind)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} = 0 \tag{200}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = \tfrac{1}{2} u_x \Delta x \left(1 - \mathrm{Co}\right) \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} + \tfrac{1}{6} u_x \Delta x^2 \left(3\,\mathrm{Co} - 2\,\mathrm{Co}^2 - 1\right) \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \ldots \tag{201}$$

Convection equation – FOU scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{202}$$

FOU discretisation scheme (First Order Upwind)

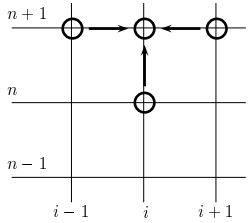
$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} = 0 \tag{203}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = \nu_N \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} - \varepsilon_N \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \dots \tag{204}$$

What if $\mathrm{Co} = 1$?

Convection equation – BTCS scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{205}$$

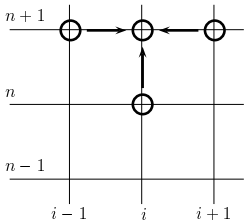
BTCS discretisation scheme (Backward Time Centred Space)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} = 0 \tag{206}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = \tfrac{1}{2} u_x \Delta x \, \mathrm{Co} \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} + \tfrac{1}{6} u_x \Delta x^2 \left(\mathrm{Co}^2 - 1\right) \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \ldots \tag{207}$$

Convection equation – BTCS scheme



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{208}$$

BTCS discretisation scheme (Backward Time Centred Space)

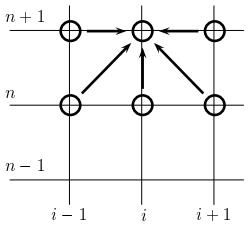
$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} = 0 \tag{209}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = \nu_N \frac{\partial^2 \phi_i^{n+1}}{\partial x^2} - \varepsilon_N \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \dots \tag{210}$$

What if $\mathrm{Co} = 1$?

Convection equation – Crank–Nicolson



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{211}$$

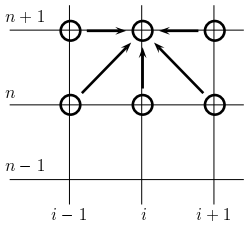
The Crank-Nicolson scheme is a combination of the FTCS and BTCS

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + \frac{1}{2}\left(u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \right) = 0 \tag{212}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = -\tfrac{1}{6} u_x \Delta x^2 \left(\tfrac{1}{2}\,\mathrm{Co}^2 + 1 \right) \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \ldots \tag{213}$$

Convection equation – Crank–Nicolson



$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = 0 \tag{214}$$

The Crank–Nicolson scheme is a combination of the FTCS and BTCS

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + \frac{1}{2}\left(u_x \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u_x \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \right) = 0 \tag{215}$$

The modified equation

$$\frac{\partial \phi_i^{n+1}}{\partial t} + u_x \frac{\partial \phi_i^{n+1}}{\partial x} = -\varepsilon_N \frac{\partial^3 \phi_i^{n+1}}{\partial x^3} + \ldots \tag{216}$$

Navier-Stokes equations

Typical numerical approaches for the incompressible Navier–Stokes equations:

- Ω_z-ψ (vorticity-stream function) formulation method
- Artificial compressibility method
- Pressure/velocity correction (operator splitting methods)
  - Projection methods
  - Explicit and implicit operator splitting methods
  - Fractional step method
  - PISO, SIMPLE, PIMPLE (PIso + siMPLE)

Bad idea

The incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{217}$$

Explicit forward difference in time

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \mathbf{u}^n \cdot \nabla \mathbf{u}^n = -\frac{1}{\rho} \nabla p^n + \nu \nabla^2 \mathbf{u}^n \tag{218}$$

Problems:

$\nabla \cdot \mathbf{u}^{n+1} \neq 0,$
$p^{n+1} = ?$

Better idea

The incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{219a}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{219b}$$

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \mathbf{u}^n \cdot \nabla \mathbf{u}^n = -\frac{1}{\rho} \nabla p^{n+1} + \nu \nabla^2 \mathbf{u}^n \tag{220a}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0 \tag{220b}$$

Problems:

$\nabla^2 p^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot (\mathbf{u}^n - \Delta t\, \mathbf{u}^n \cdot \nabla \mathbf{u}^n + \Delta t\, \nu \nabla^2 \mathbf{u}^n)$
BCs?

Semi implicit – non-linear

The incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{221a}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{221b}$$

Semi implicit approach

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \underbrace{\mathbf{u}^n \cdot \nabla \mathbf{u}^n}_{\text{non-linear}} = -\frac{1}{\rho} \nabla p^{n+1} + \nu \nabla^2 \mathbf{u}^{n+1} \tag{222a}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0 \tag{222b}$$

Semi implicit – linearised

The incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{223a}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{223b}$$

Semi implicit approach

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \underbrace{\mathbf{u}^n \cdot \nabla \mathbf{u}^{n+1}}_{\text{linearised}} = -\frac{1}{\rho} \nabla p^{n+1} + \nu \nabla^2 \mathbf{u}^{n+1} \tag{224a}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0 \tag{224b}$$

Fully implicit – non-linear

The incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{225a}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{225b}$$

Fully implicit approach

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \mathbf{u}^{n+1} \cdot \nabla \mathbf{u}^{n+1} = -\frac{1}{\rho} \nabla p^{n+1} + \nu \nabla^2 \mathbf{u}^{n+1} \tag{226a}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0 \tag{226b}$$

Artificial compressibility method

The incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{227a}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{227b}$$

Explicit forward difference in time

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \mathbf{u}^n \cdot \nabla \mathbf{u}^n = -\frac{1}{\rho_0} \nabla p^n + \nu \nabla^2 \mathbf{u}^n \tag{228a}$$

$$\beta \frac{p^{n+1} - p^n}{\Delta t} + \nabla \cdot \mathbf{u}^n = 0 \tag{228b}$$

Projection method

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\mathbf{u}^n \cdot \nabla \mathbf{u}^n + \nu \nabla^2 \mathbf{u}^n \tag{229}$$

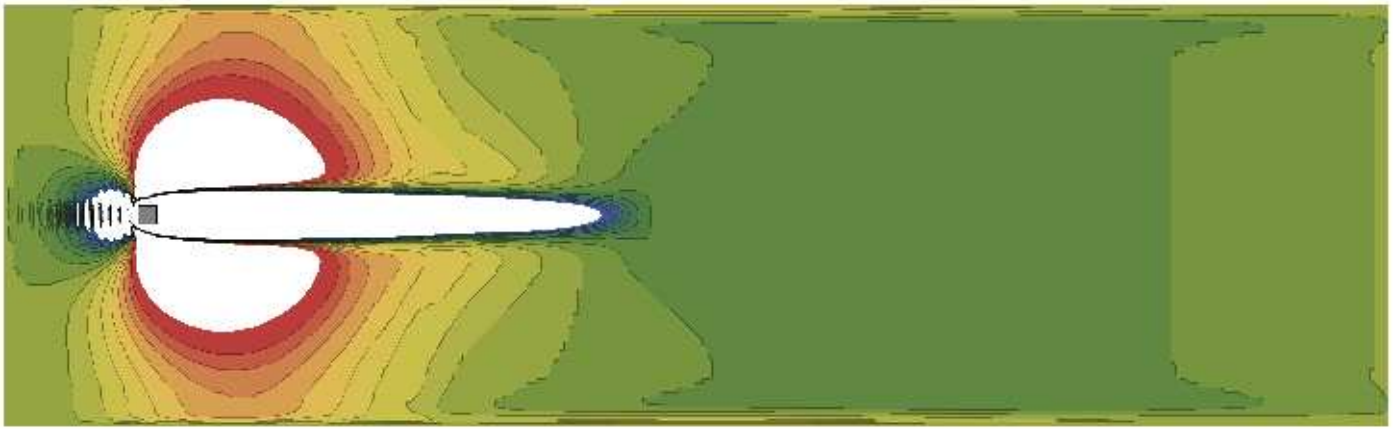
$\nabla \cdot \mathbf{u}^* \neq 0$, BC

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\frac{1}{\rho} \nabla p^{n+1} \tag{230}$$

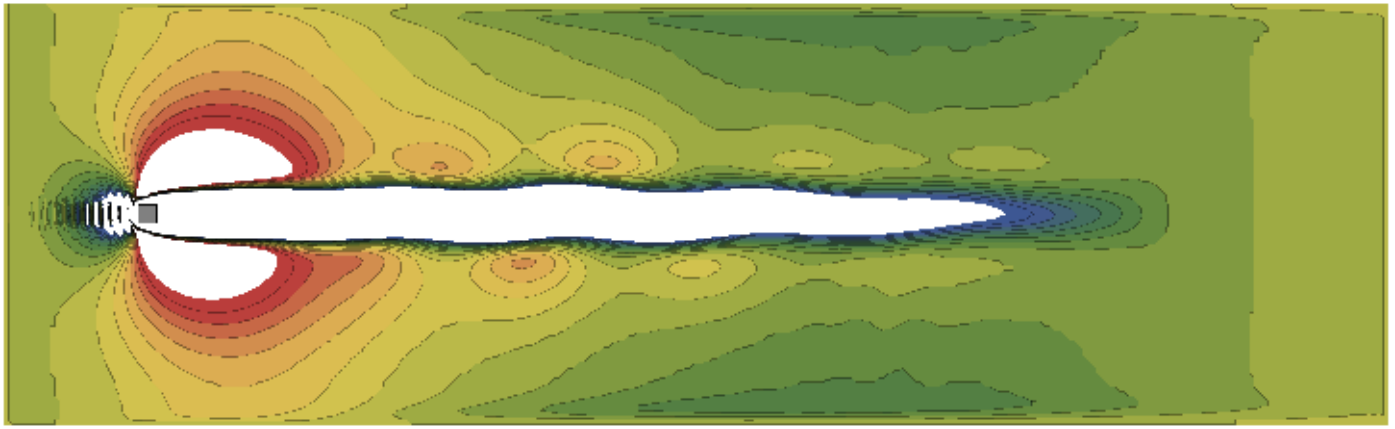
$\nabla \cdot \mathbf{u}^{n+1} = 0$, $\neg$BC

$$\nabla^2 p^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot \mathbf{u}^* \tag{231}$$

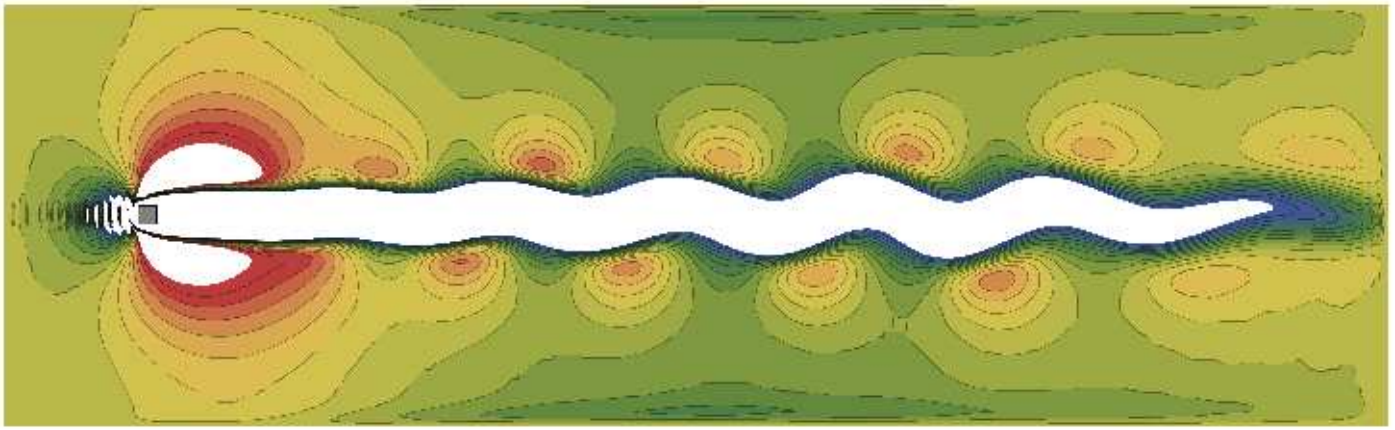
Square cylinder



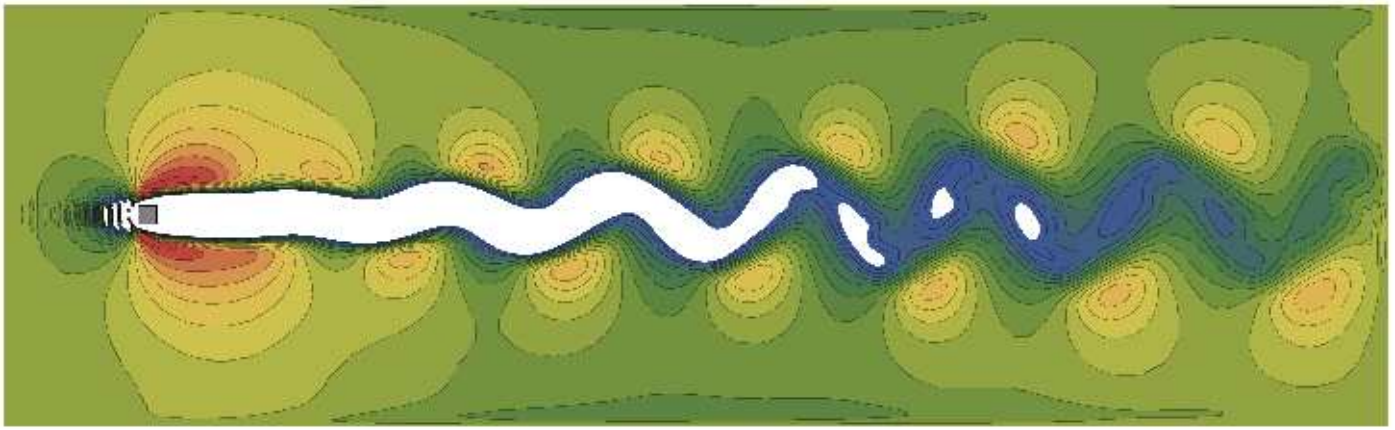
Square cylinder



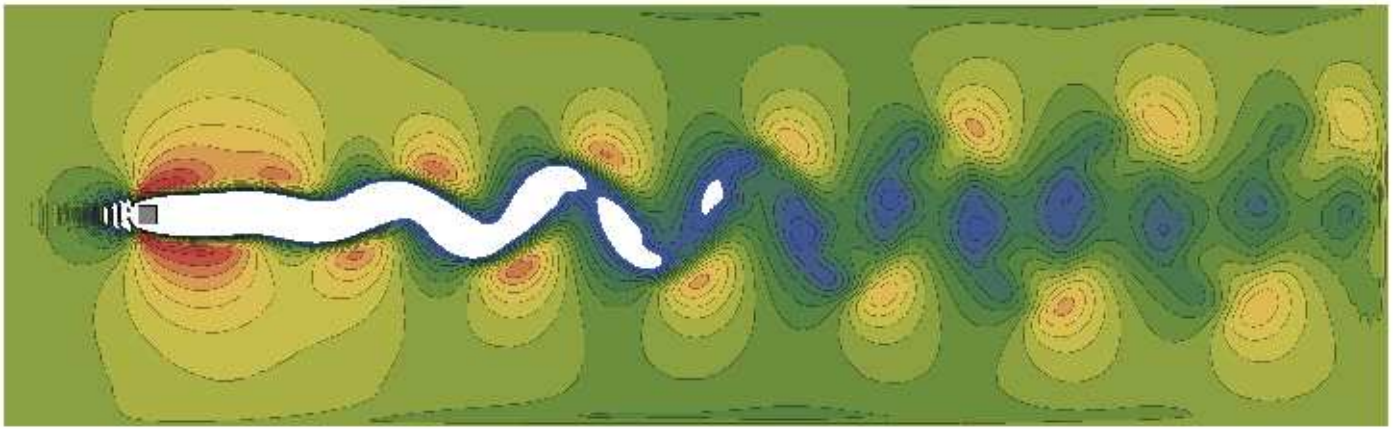
Square cylinder



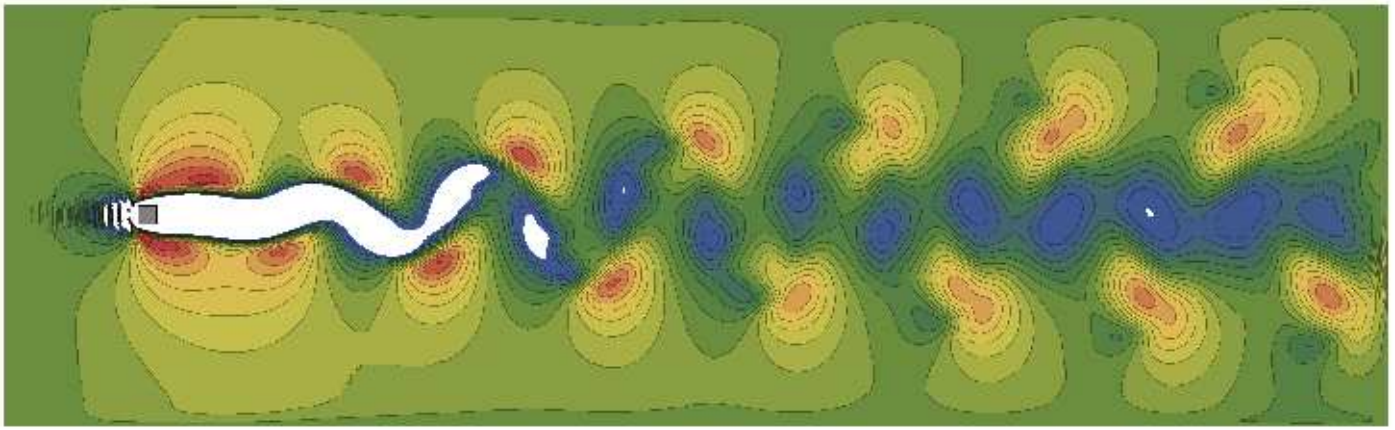
Square cylinder



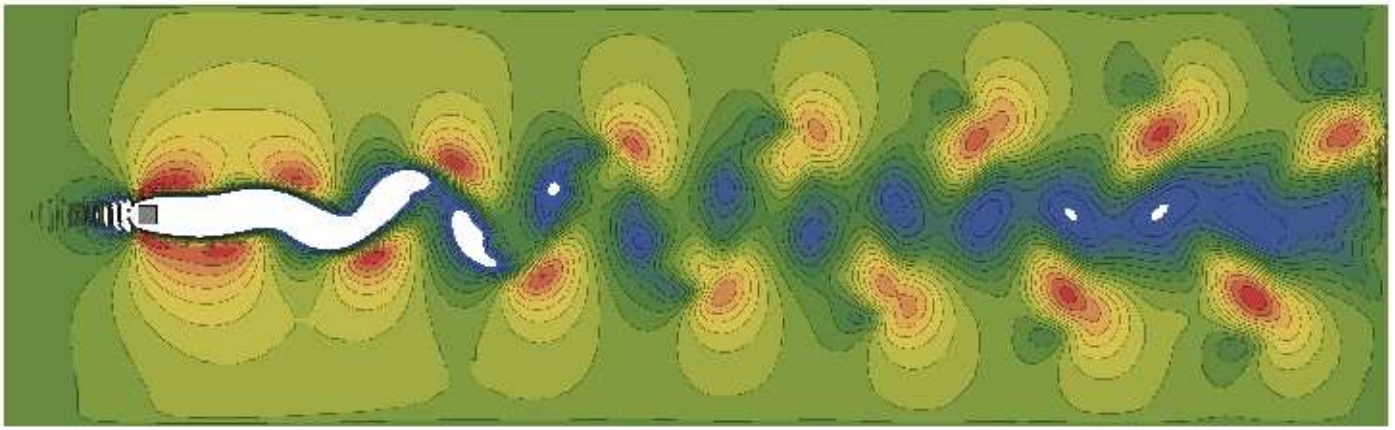
Square cylinder



Square cylinder



Square cylinder



Decomposition method

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\mathbf{u}^n \cdot \nabla \mathbf{u}^n - \frac{1}{\rho}\nabla p^n + \nu \nabla^2 \mathbf{u}^n \qquad (232)$$

$$\nabla \cdot \mathbf{u}^* \neq 0$$

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\mathbf{u}^n \cdot \nabla \mathbf{u}^n - \frac{1}{\rho}\nabla p^{n+1} + \nu \nabla^2 \mathbf{u}^n \qquad (233)$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0$$

$$\mathbf{u}^c = \mathbf{u}^{n+1} - \mathbf{u}^* = -\frac{1}{\rho}\Delta t \, \nabla \left(p^{n+1} - p^n \right) \qquad (234)$$

$$\nabla \cdot \mathbf{u}^c = -\nabla \cdot \mathbf{u}^* = -\frac{1}{\rho}\Delta t \, \nabla^2 \left(p^{n+1} - p^n \right) \qquad (235)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* + \mathbf{u}^c$$

Vorticity-stream function formulation

The incompressible 2D Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{236a}$$

$$\Omega_z = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \tag{236b}$$

2D Helmholtz equation ($u_x = \frac{\partial \psi}{\partial y}$, $u_y = -\frac{\partial \psi}{\partial x}$)

$$\frac{\partial \Omega_z}{\partial t} + \mathbf{u} \cdot \nabla \Omega_z = \nu \nabla^2 \Omega_z \tag{237a}$$

$$\nabla^2 \psi = -\Omega_z \tag{237b}$$

$$\frac{\Omega_z^{n+1} - \Omega_z^n}{\Delta t} + \mathbf{u}^n \cdot \nabla \Omega_z^n = \nu \nabla^2 \Omega_z^n \tag{238a}$$

$$\nabla^2 \psi^{n+1} = -\Omega_z^{n+1} \tag{238b}$$

Finite Volume Method

Transport eqution

Since all the transport equation have common terms, the general transport equation for a quantity ϕ has the form of

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\cdot(\rho\phi\mathbf{u}) = \nabla\cdot(\Gamma\nabla\phi) + S_\phi \qquad (239)$$

Four transport effects can be summarised at least, namely

- unsteadiness $\frac{\partial}{\partial t}(\rho\phi)$,
- convection $\nabla\cdot(\rho\phi\mathbf{u})$,
- diffusion $\nabla\cdot(\Gamma\nabla\phi)$.
- overall source term S_ϕ. In the above Γ is the diffusivity for ϕ.

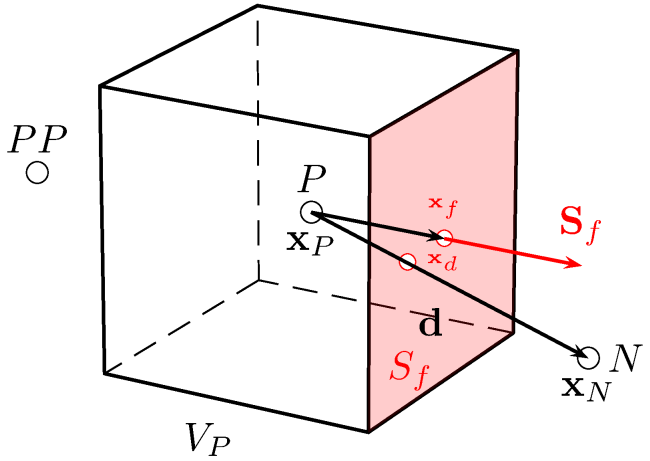
Integral form

The integral form of the transport equation over a control volume V_P is now expressed as

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_P}\rho\phi\,\mathrm{d}V+\iiint\limits_{V_P}\nabla\cdot(\rho\phi\mathbf{u})\,\mathrm{d}V=\iiint\limits_{V_P}\nabla\cdot(\Gamma\nabla\phi)\,\mathrm{d}V+\iiint\limits_{V_P}S_\phi\,\mathrm{d}V \quad (240)$$

where a finite volume V_P and its measure is $|V_P|$.

Integral form



- the finite volume centroid P located at $\mathbf{x}_P$,
- the vector $\mathbf{d}$ connects the centroid P with its neighbour centroid N,
- the surface S_f is oriented by means of a surface normal vector $\mathbf{S}_f$ pointing outward and the face S_f centroid is located at $\mathbf{x}_f$.

Spatial terms

The order of discretisation is usually equal or higher in comparison with the order of the discretised equation. Exceptions to this rule are sometimes permitted.
In order to keep the second order accuracy of spatial dicretisation the following variation of ϕ around P is assumed

$$\phi(\mathbf{x}) = \phi_P + (\mathbf{x} - \mathbf{x}_P) \cdot (\nabla\phi)_P \qquad (241)$$

This can be proved by means of Taylor series expansion. Also, the unknown variable ϕ_P, located at the centroid $\mathbf{x}_P$ of a control volume V_P, is calculated as $\phi_P = \phi(\mathbf{x}_P)$.

Volume integrals

In order to transform volume integrals into surface integrals the Gauss's (divergence) theorem is applied

$$\iiint_{V_P} \nabla \cdot \mathbf{w} \, \mathrm{d}V = \oiint_{\partial V_P} \mathbf{w} \cdot \, \mathrm{d}\mathbf{S} \tag{242}$$

where $\mathrm{d}\mathbf{S}$ stands for the differential of the surface area vector pointing outward. Now the general transport equation can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t} \iiint_{V_P} \rho\phi \, \mathrm{d}V + \oiint_{\partial V_P} \rho\phi\mathbf{u} \cdot \, \mathrm{d}\mathbf{S} = \oiint_{\partial V_P} \Gamma\nabla\phi \cdot \, \mathrm{d}\mathbf{S} + \iiint_{V_P} S_\phi \, \mathrm{d}V \tag{243}$$

Volume integrals

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_P}\rho\phi\,\mathrm{d}V+\oiint\limits_{\partial V_P}\rho\phi\mathbf{u}\cdot\,\mathrm{d}\mathbf{S}=\oiint\limits_{\partial V_P}\Gamma\nabla\phi\cdot\,\mathrm{d}\mathbf{S}+\iiint\limits_{V_P}S_\phi\,\mathrm{d}V \quad (244)$$

The following definition of an average value ϕ_P of the function ϕ located at the centroid of V_P is assumed

$$\phi_P=\frac{1}{|V_P|}\iiint\limits_{V_P}\phi\,\mathrm{d}V \quad (245)$$

The volume integral is expressed by means of the averaged value $\bar{\phi}$ of unknown function ϕ and the control volume measure $|V_P|$. Next, the averaged value is replaced by the value at V_P centroid ϕ_P.

Volume integrals

If the source term S_ϕ, i.e. the fourth integral in the general transport equation, depends on the unknown function ϕ it should be linearised first

$$S_\phi(\phi) = S_C + S_P\phi \tag{246}$$

Subsequently, it can be integrated similarly and the discretised source terms is now

$$\iiint_{V_P} S_\phi \,\mathrm{d}V = S_C|V_P| + S_P|V_P|\phi_P \tag{247}$$

If, however, the source term S_ϕ does not depend on ϕ the discretised form is simpler since $S_P = 0$.

Volume integrals

For the sake of simplicity let us assume further incompressibility $\rho = \mathrm{const}$. This assumptions is also valid for gases provided that $\mathrm{Ma} < 0.3$. Furthermore, if the control volume V_P is constant in time, i.e. is not deforming, then it is now possible to express the general transport equation as

$$\rho \frac{\mathrm{d}\phi_P}{\mathrm{d}t}|V_P| + \rho \oiint_{\partial V_P} \phi \mathbf{u} \cdot \mathrm{d}\mathbf{S} = \oiint_{\partial V_P} \Gamma \nabla \phi \cdot \mathrm{d}\mathbf{S} + S_C|V_P| + S_P|V_P|\phi_P \quad (248)$$

Convection terms

Convection terms involving $\nabla \cdot (\rho\phi\mathbf{u})$ are already transformed by means of the Gauss's theorem and expressed as surface integrals. The surface integral over the individual surface S_f is now expressed by means of the vector $\mathbf{w}_f$ value located the face S_f centroid and the surface area vector $\mathbf{S}_f$ pointing outward, namely

$$\iint_{S_f} \mathbf{w} \cdot \mathrm{d}\mathbf{S} = \mathbf{w}_f \cdot \mathbf{S}_f \tag{249}$$

This also means that the vector $\mathbf{w}$ distribution over the surface S_f is now expressed by means of a single value $\mathbf{w}_f$.

Convection terms

Since the boundary ∂V_P of a control volume V_P consists of f planar surfaces S_f, i.e. $\bigcup_f S_f = \partial V_P$, the convection terms is now given by the following approximation being second order accurate

$$\oiint_{\partial V_P} \phi \mathbf{u} \cdot \, \mathrm{d}\mathbf{S} = \sum_f \phi_f \mathbf{u}_f \cdot \mathbf{S}_f \tag{250}$$

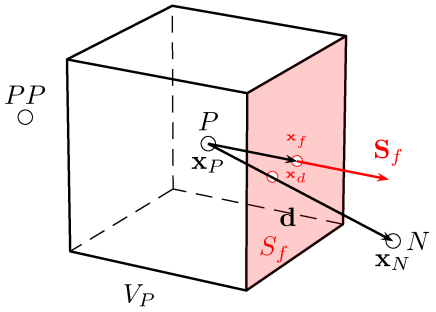
The term $\phi_f \mathbf{u}_f \cdot \mathbf{S}_f$ is also referred to as a face flux. The general transport equations is now given by

$$\rho \frac{\mathrm{d}\phi_P}{\mathrm{d}t} |V_P| + \rho \sum_f \phi_f \mathbf{u}_f \cdot \mathbf{S}_f = \oiint_{\partial V_P} \Gamma \nabla \phi \cdot \, \mathrm{d}\mathbf{S} + S_C |V_P| + S_P |V_P| \phi_P \tag{251}$$

Convection terms

What is important, is the fact that the discretised convection term needs to be interpolated further by means of cell centred values because the values ϕ_f are located at the face centroids. Several methods are in common use. These include, among others:

- linear interpolation or central differencing (CD),
- upwind differencing (UD),
- blending differencing,
- second order upwind differencing (SOU) or linear upwind differencing (LUD).



Convection terms – linear interpolation

A linear distribution of ϕ between two points P and N is assumed. This leads to the following face value ϕ_f

$$\phi_f = f_x \phi_P + (1 - f_x)\phi_N \tag{252}$$

where the weighting factor f_x is a ratio of respective distances

$$f_x = \frac{\|\mathbf{x}_d - \mathbf{x}_N\|}{\|\mathbf{d}\|} \tag{253}$$

This method is known to be second order accurate. Nonetheless, it may lead to non-physical oscillations for some convection dominated flows or in the presence of strong gradients.

Convection terms – upwind differencing

This interpolation depends on the flow direction $\mathbf{u}_f \cdot \mathbf{S}_f$. The face value ϕ_f is interpolated by means of the upstream node P or N, depending of the flow direction, namely

$$\phi_f = \begin{cases} \phi_P; & \mathbf{u}_f \cdot \mathbf{S}_f \geq 0, \\ \phi_N; & \mathbf{u}_f \cdot \mathbf{S}_f < 0 \end{cases} \tag{254}$$

Boundedness of the solution is guaranteed, however, it comes at a price of having to sacrifice accuracy. This is because the numerical diffusion term is implicitly introduced. Additionally, upwind differencing is only first order accurate.

Convection terms – blending differencing

This type of interpolation tries to maintain reasonable accuracy and boundedness of the solution at the same time. Typically, it combines upwind differencing and central differencing in the following manner

$$\phi_f = \gamma \phi_{fCD} + (1 - \gamma)\phi_{fUD} \tag{255}$$

Other methods also exist. In the above equation γ is the so called flux limiter also referred to as a blending coefficient. The idea of flux limiter makes it possible, among others, to limit towards first order upwind in regions of rapidly changing gradients.

Convection terms – SOU or LUD

Second order upwind differencing (SOU) or linear upwind differencing (LUD). More information is required than the nearest neighbours of the control volume. This leads to higher order accuracy. The face value ϕ_f depends on the flow direction and is interpolated by means of two the upstream nodes P, PP or N, NN

$$\phi_f = \begin{cases} \phi_P + \frac{1}{2}\left(\phi_P - \phi_{PP}\right); & \mathbf{u}_f \cdot \mathbf{S}_f > 0, \\ \phi_N + \frac{1}{2}\left(\phi_N - \phi_{NN}\right); & \mathbf{u}_f \cdot \mathbf{S}_f < 0 \end{cases} \tag{256}$$

LUD interpolation is second order accurate and unbounded.

Convection terms – limiters

Flux limiter formulation ($\mathbf{u}_f \cdot \mathbf{S}_f > 0$)

$$\phi_f = \phi_P + \frac{1}{2}\psi(r)\left(\phi_P - \phi_{PP}\right) \tag{257}$$

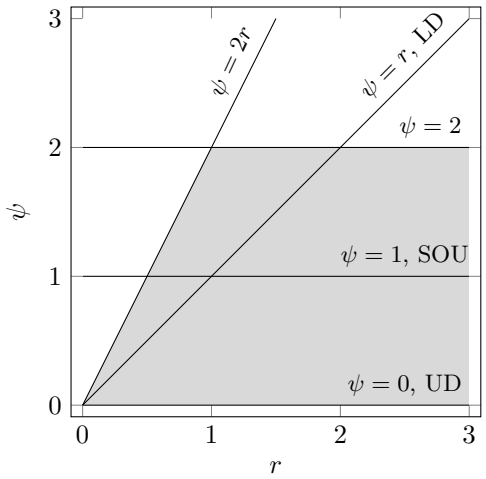
where ψ is a limiter function. The limiter ψ is a function of gradients ratio r (1D version)

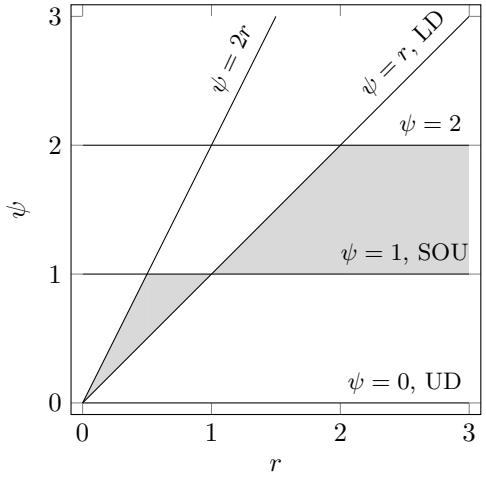
$$r = \frac{\phi_N - \phi_P}{\phi_P - \phi_{PP}} \tag{258}$$

General 3D version

$$r = 2\frac{\mathbf{d} \cdot (\nabla\phi)_P}{\mathbf{d} \cdot (\nabla\phi)_f} - 1 \tag{259}$$

Convection terms – TVD
Total Variation Diminishing





A limiter is symmetric if

$$\psi\left(\frac{1}{r}\right) = \frac{\psi(r)}{r} \qquad (260)$$

TVD conditions:

- $0 \leq \psi(r) \leq 2r$,
- $0 \leq \psi(r) \leq 2$

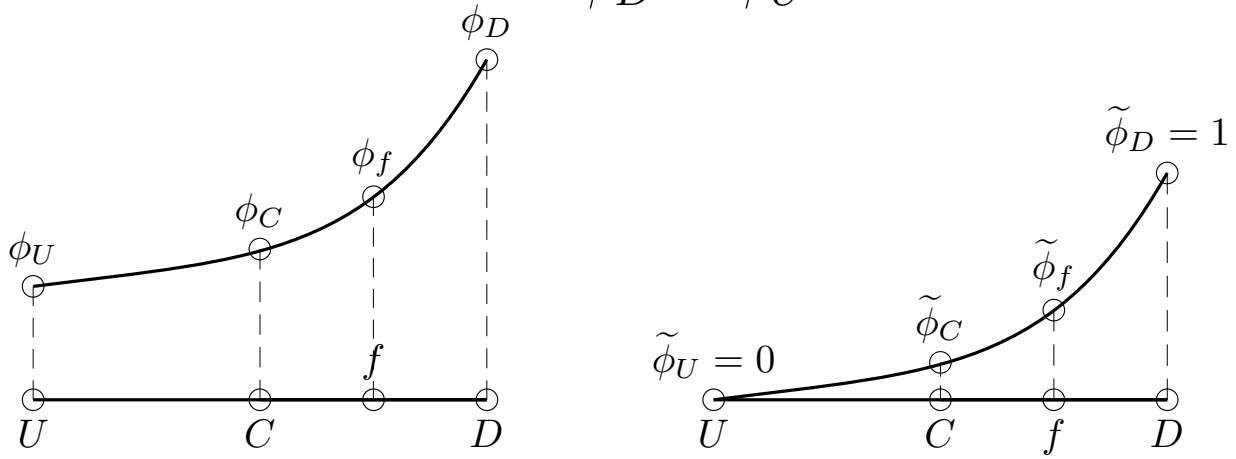
Second order TVD conditions:

- $0 \leq \psi(r) \leq 2r, \;\; r \in [0;1]$,
- $1 \leq \psi(r) \leq r, \;\; r \in [1;2]$,
- $0 \leq \psi(r) \leq 2, \;\; r > 2$,
- $\psi(1) = 1$

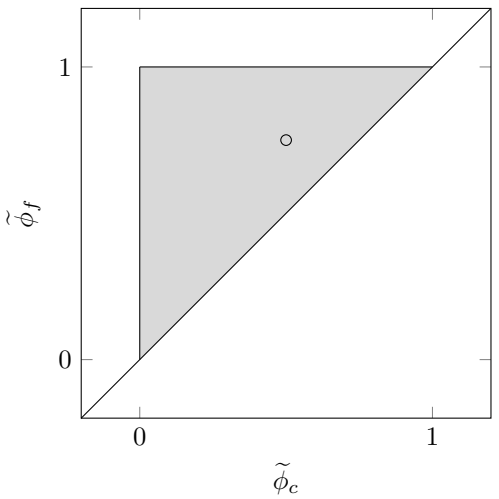
Convection terms – NVF
Normalised Variables Formulation

$$\widetilde{\phi}_C = \frac{\phi_C - \phi_U}{\phi_D - \phi_U} \tag{261}$$

$$\widetilde{\phi}_f = \frac{\phi_f - \phi_U}{\phi_D - \phi_U} \tag{262}$$



Convection terms – NVD
Normalised Variables Diagram



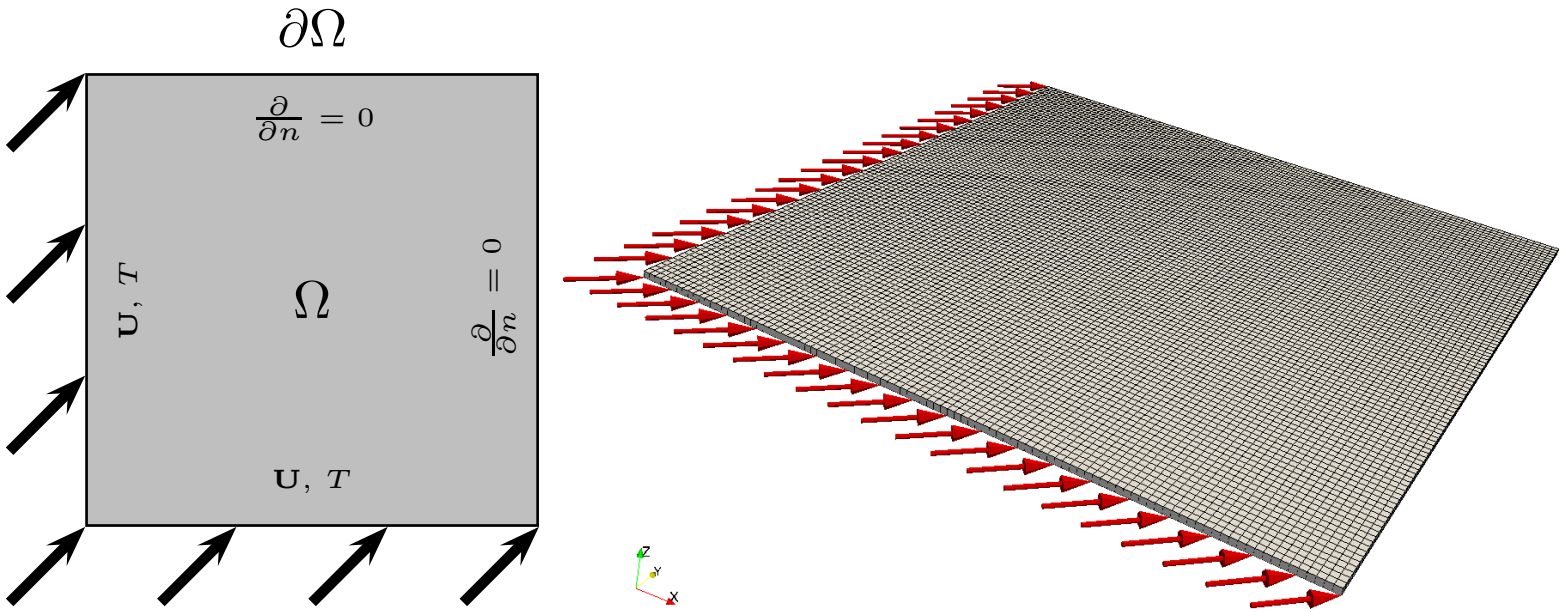
NVD conditions:

- $\widetilde{\phi}_f$ is continuous,
- $\widetilde{\phi}_C \leq \widetilde{\phi}_f(\widetilde{\phi}_C) \leq 1$, $\widetilde{\phi}_C \in [0;1]$,
- $\widetilde{\phi}_f(\widetilde{\phi}_C) = \widetilde{\phi}_C$, $\widetilde{\phi}_C \notin [0;1]$

Second (or above) order NVD conditions:

- all above,
- $\widetilde{\phi}_f(0.5) = 0.75$

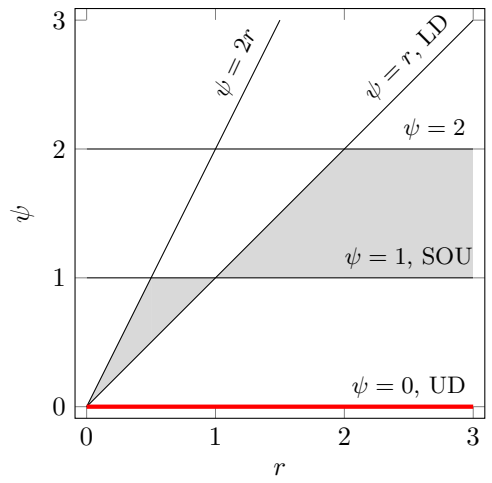
Convection terms – example



$$\frac{\partial (\rho\phi)}{\partial t} + \nabla \cdot (\rho\phi\mathbf{u}) = \nabla \cdot (\Gamma \nabla\phi) + S_\phi \qquad (263)$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi\mathbf{u}) = 0 \qquad (264)$$

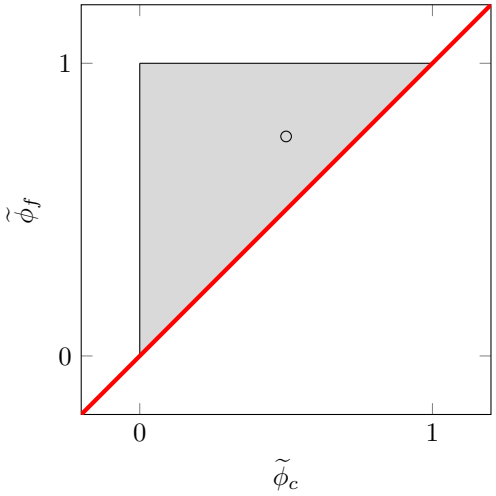
Convection terms – UD



Upwind Differencing (First Order Upwind)

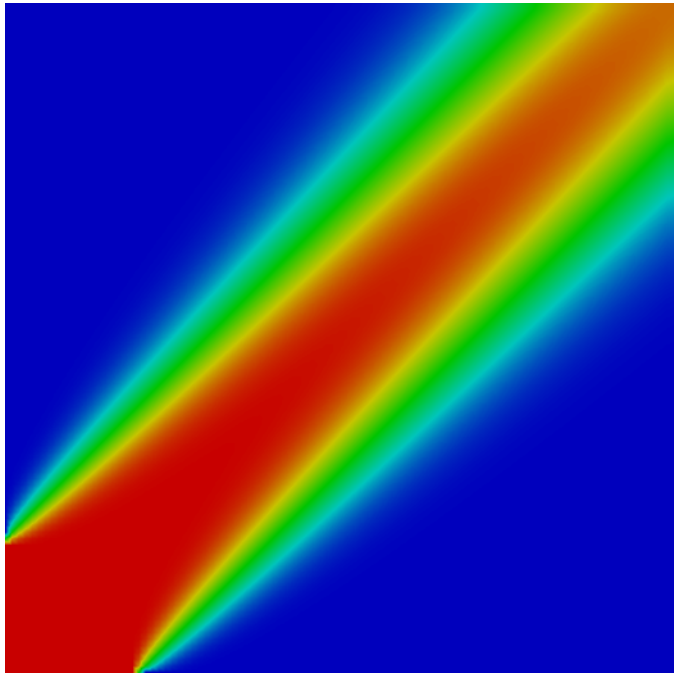
$$\psi(r) = 0$$

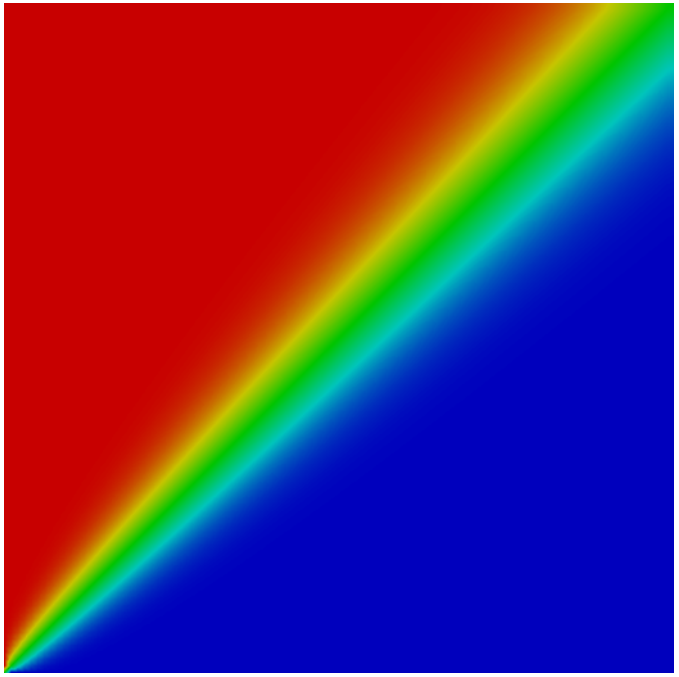
- TVD, NVD,
- 1^{st} order

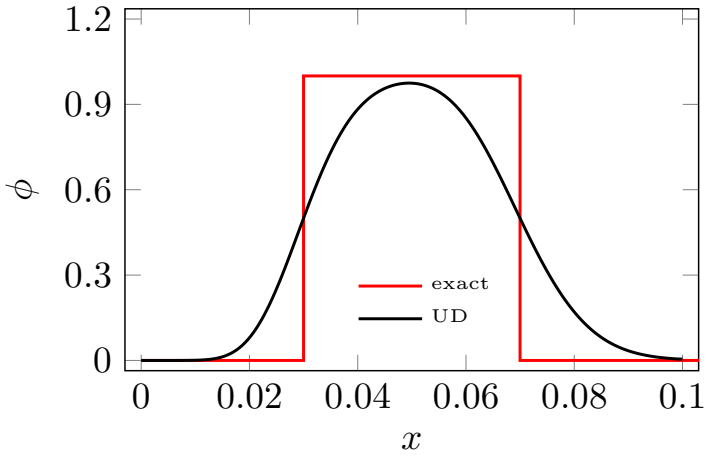


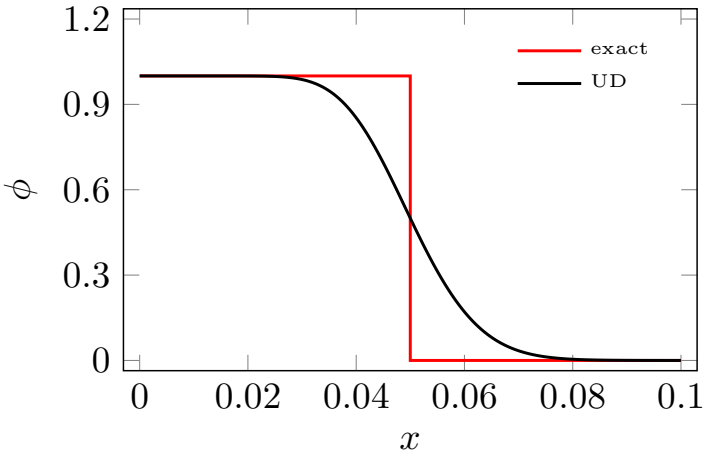
$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \widetilde{\phi}_C$$

Convection terms – UD

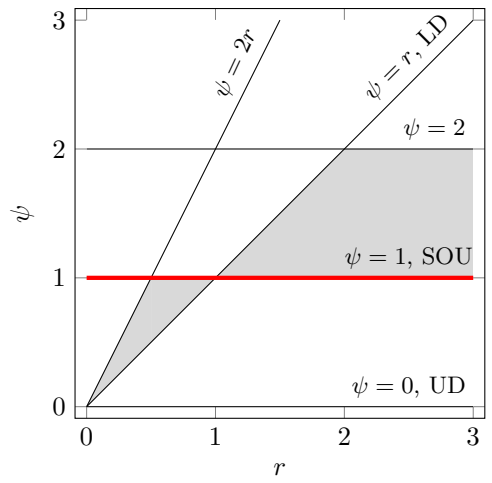








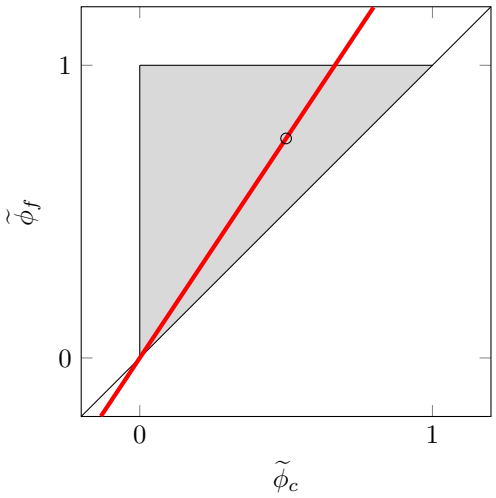
Convection terms – SOU



Second Order Upwind (Linear Upwind Differencing)

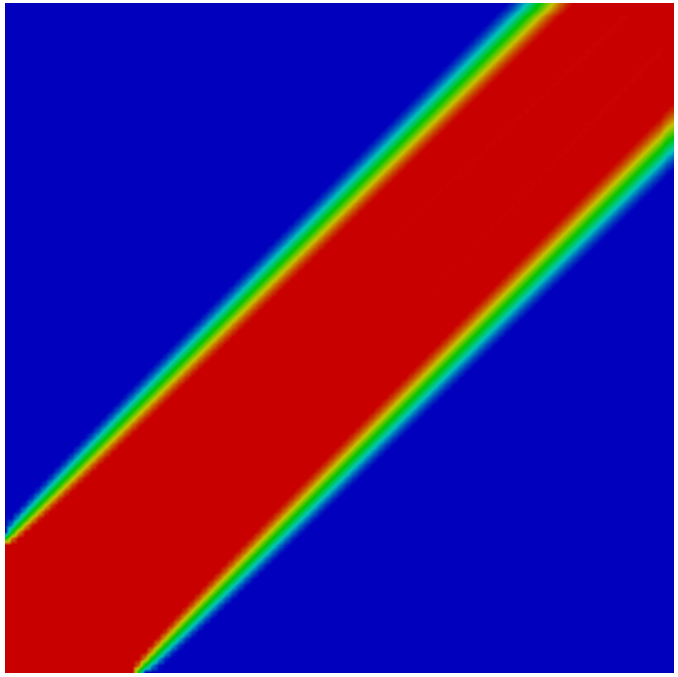
$$\psi(r) = 1$$

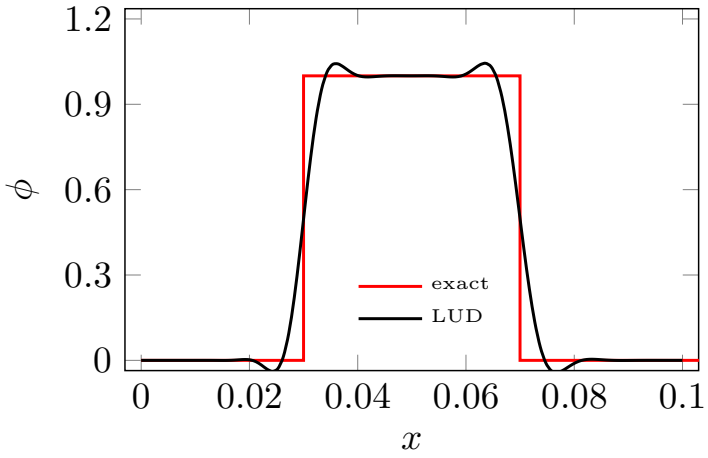
- Not TVD, not NVD,
- 2^{nd} order

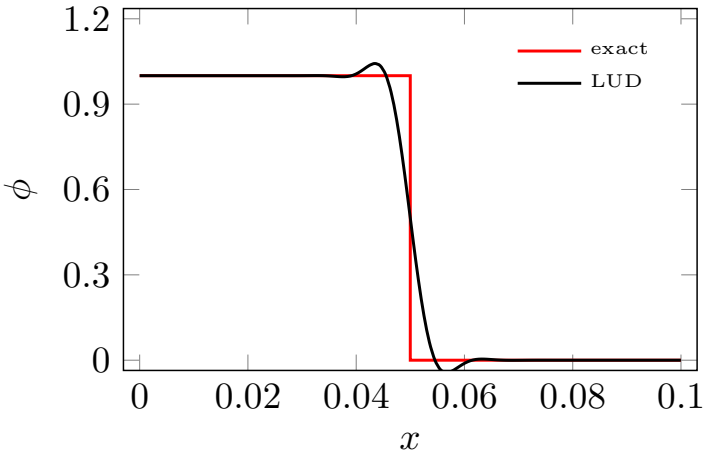


$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \tfrac{3}{2}\widetilde{\phi}_C$$

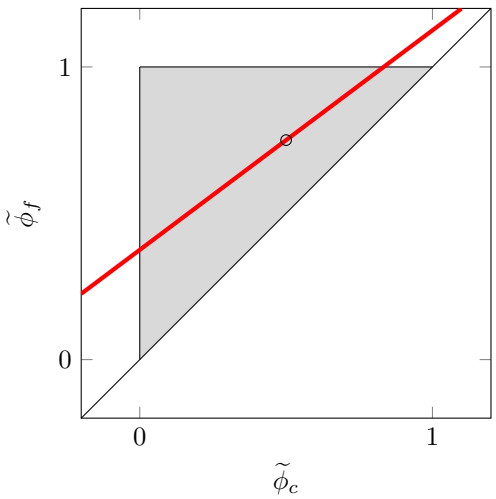
Convection terms – SOU







Convection terms – QUICK



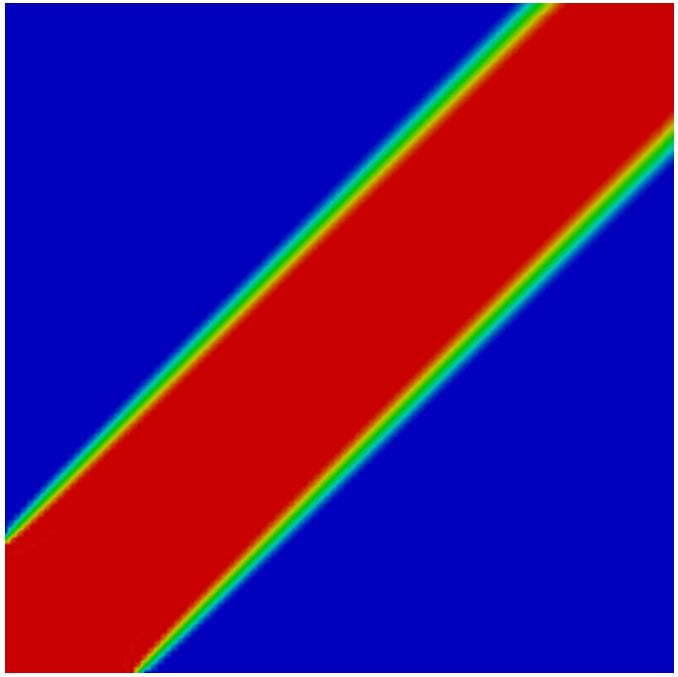
Quadratic Upwind Interpolation for Convective Kinematics (Quadratic Upwind Differencing)
For a uniform mesh

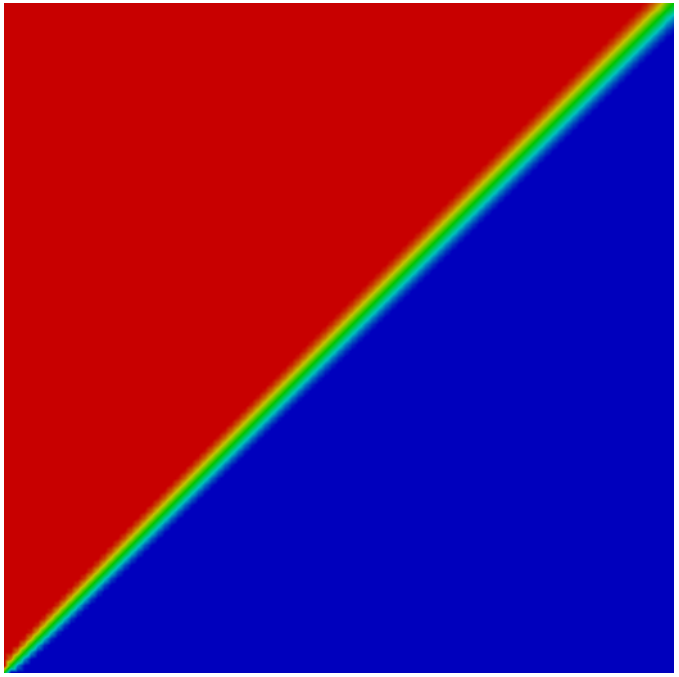
$$\phi_f = \frac{3}{8}\phi_D + \frac{3}{4}\phi_C - \frac{1}{8}\phi_U$$

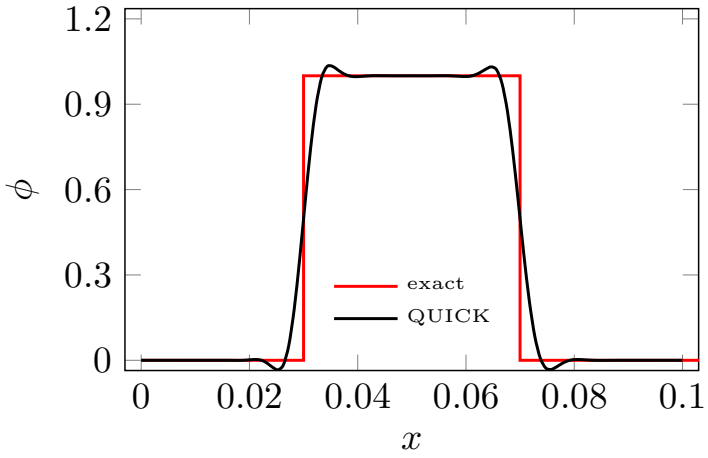
- not NVD,
- 3^{rd} order

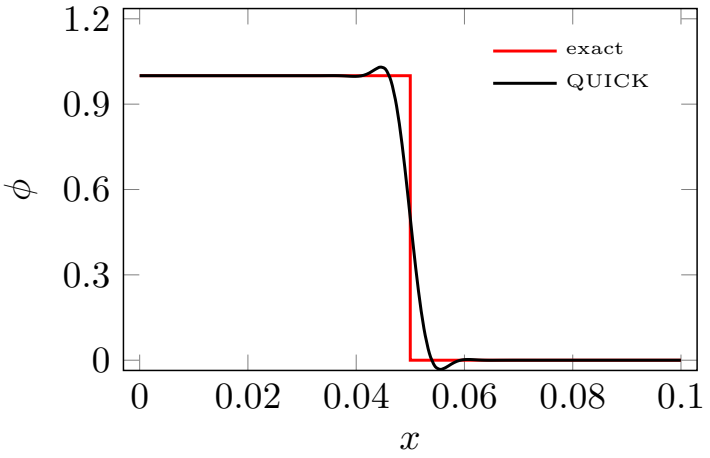
$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \frac{3}{8}\left(1 + 2\widetilde{\phi}_C\right)$$

Convection terms – QUICK

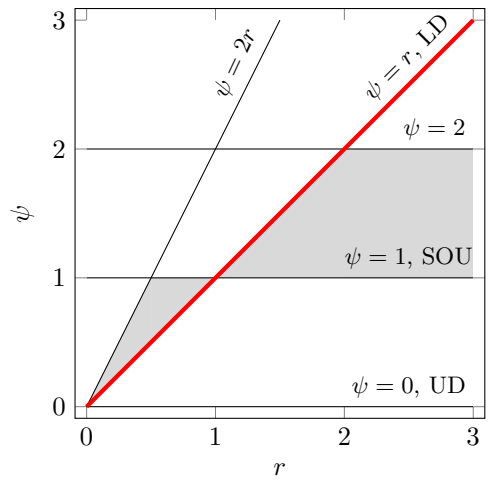








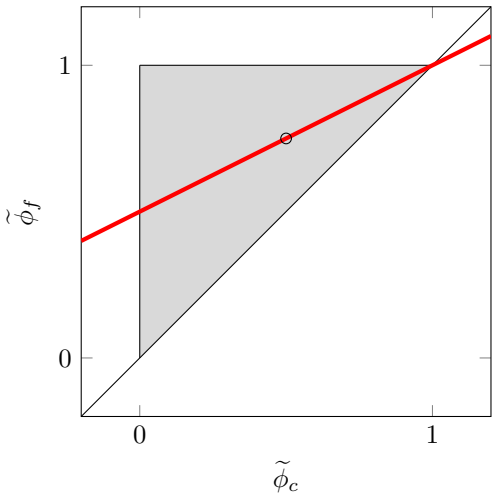
Convection terms – LD



Linear Differencing (Central Differencing)

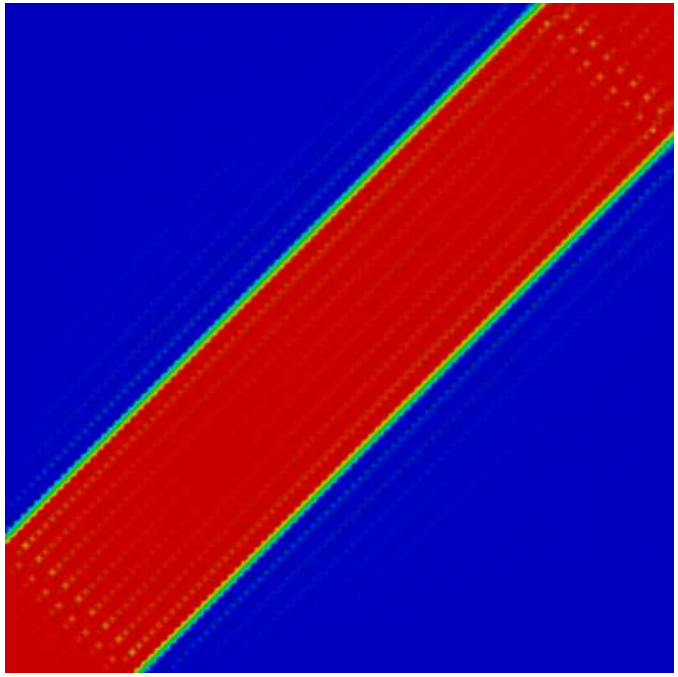
$$\psi(r) = r$$

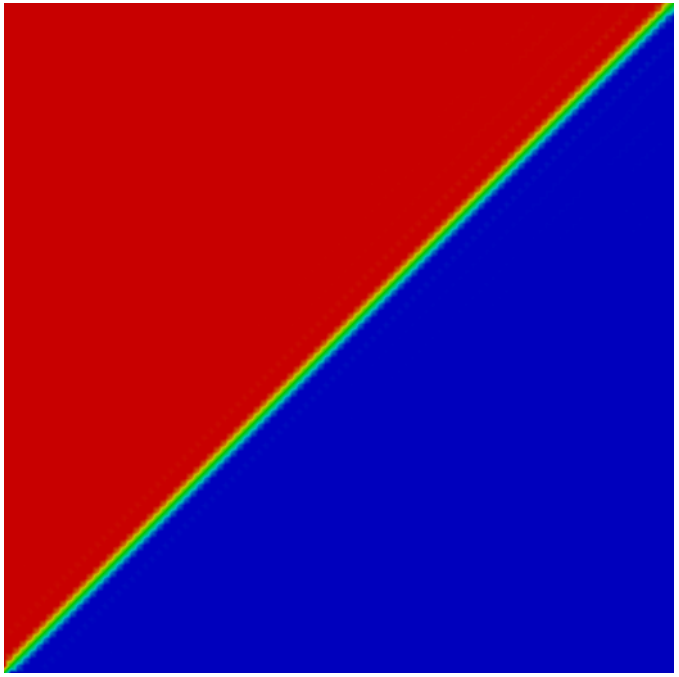
- Not TVD, not NVD,
- 2^{nd} order

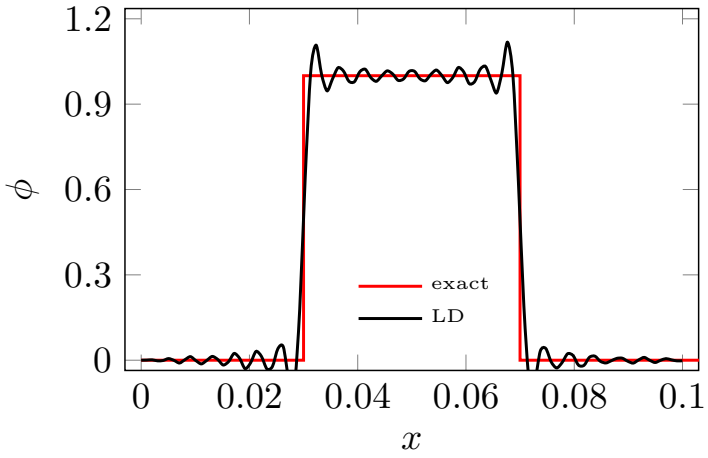


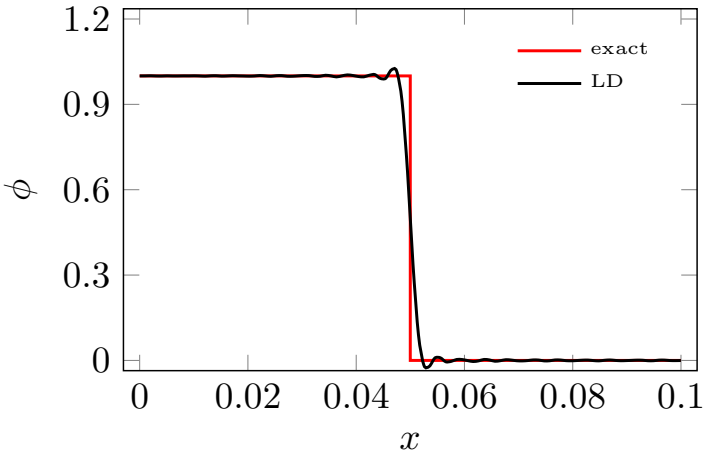
$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \frac{1}{2}\left(1 + \widetilde{\phi}_C\right)$$

Convection terms – LD

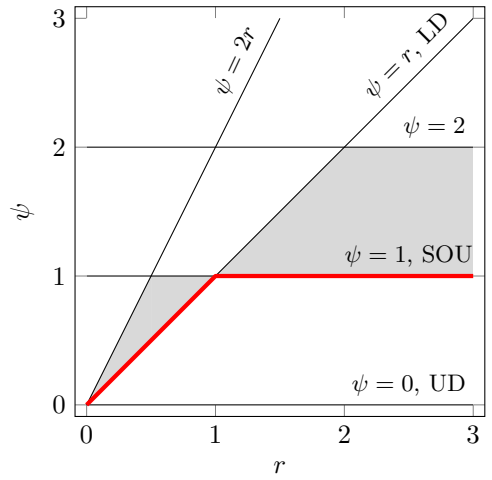






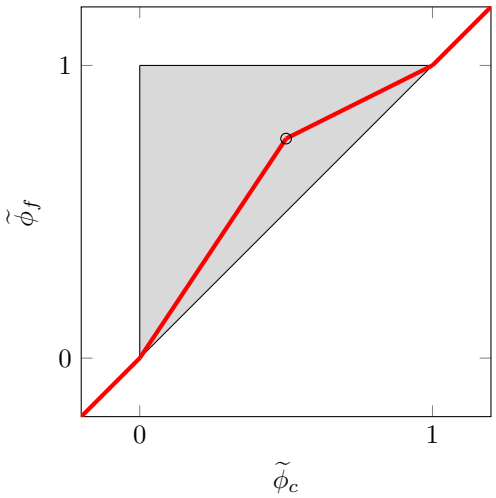


Convection terms – minmod



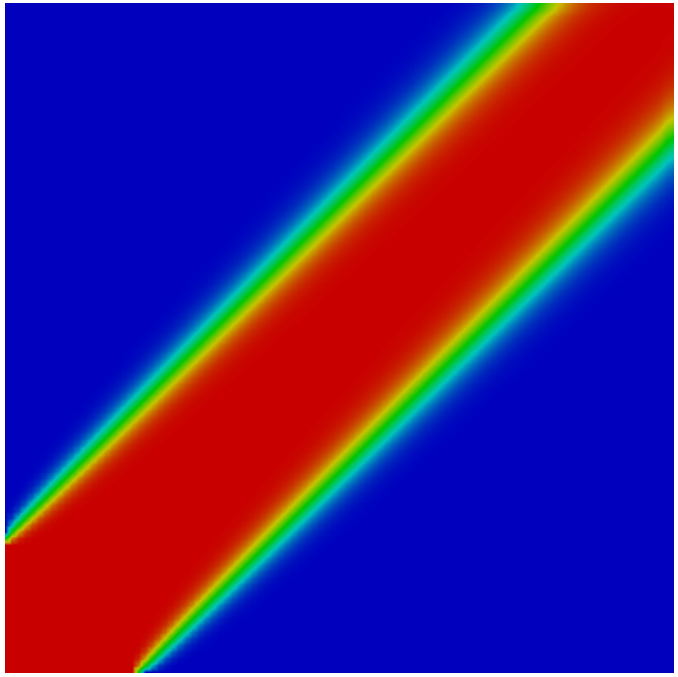
$$\psi(r) = \max(0, \min(1, r))$$

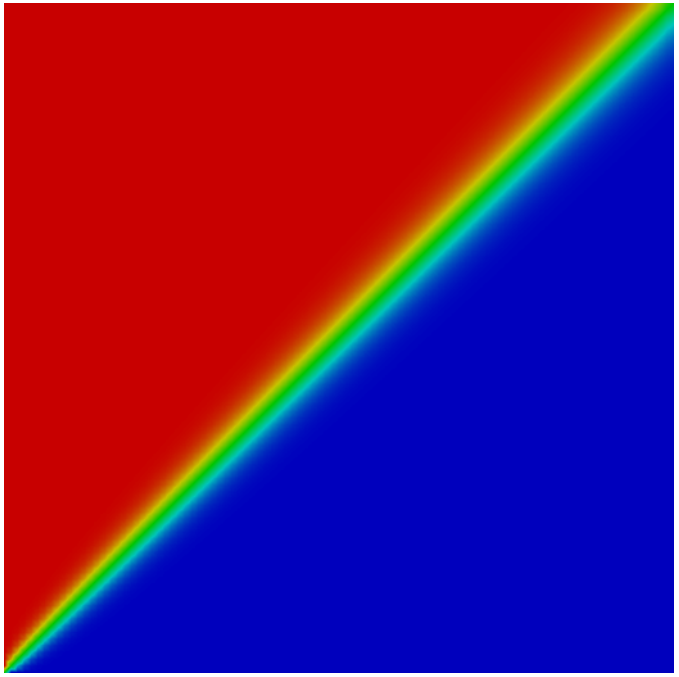
- TVD, NVD,
- 2^{nd} order,
- piecewise linear

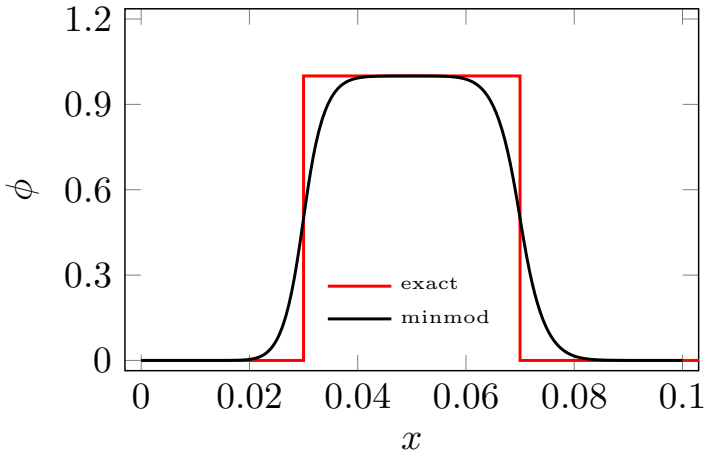


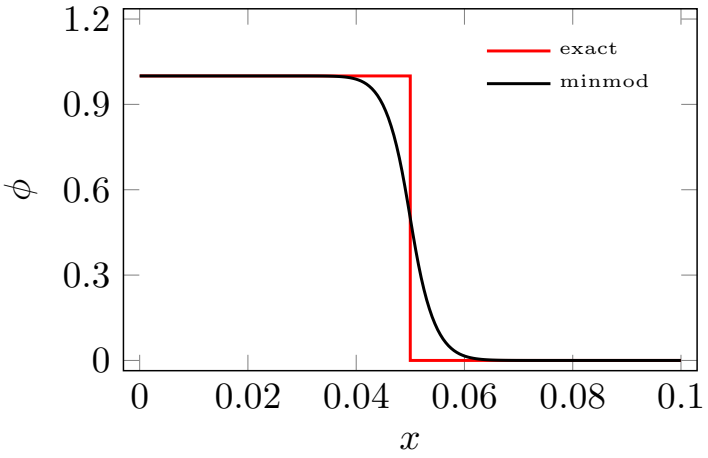
$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \begin{cases} \frac{3}{2}\widetilde{\phi}_C; & 0 \leq \widetilde{\phi}_C < \frac{1}{2}, \\ \frac{1}{2}\left(1 + \widetilde{\phi}_C\right); & \frac{1}{2} \leq \widetilde{\phi}_C \leq 1, \\ \widetilde{\phi}_C; & \text{otherwise} \end{cases}$$

Convection terms – minmod

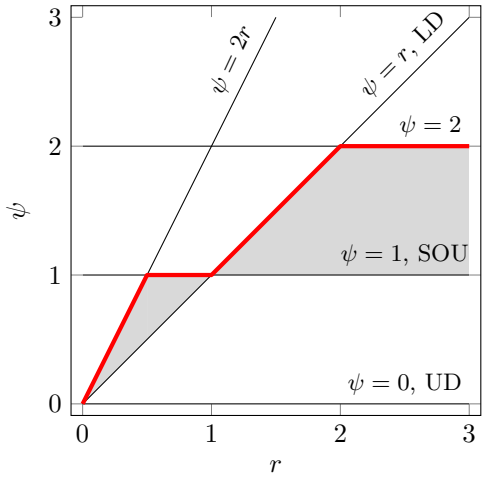








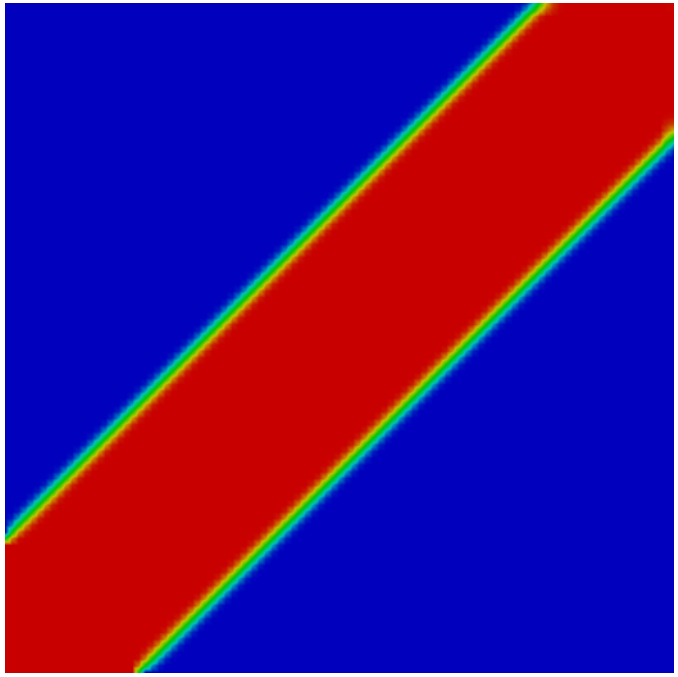
Convection terms – superbee

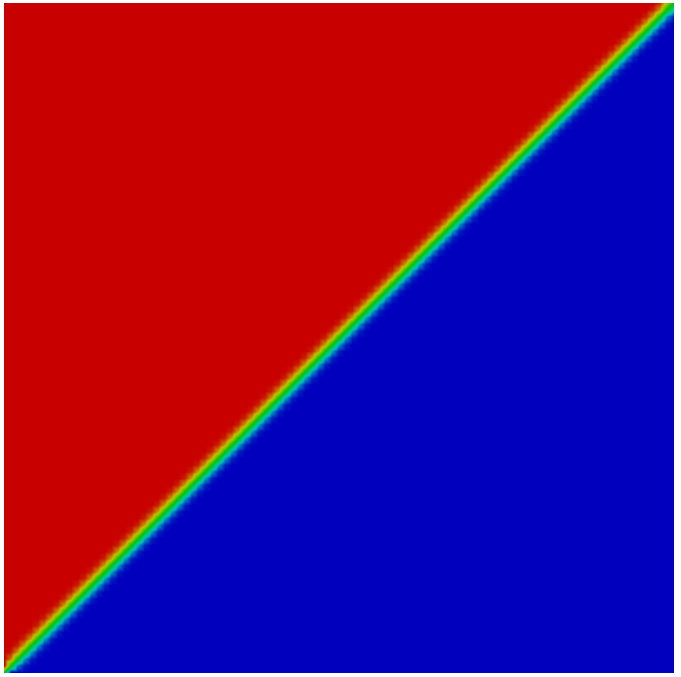


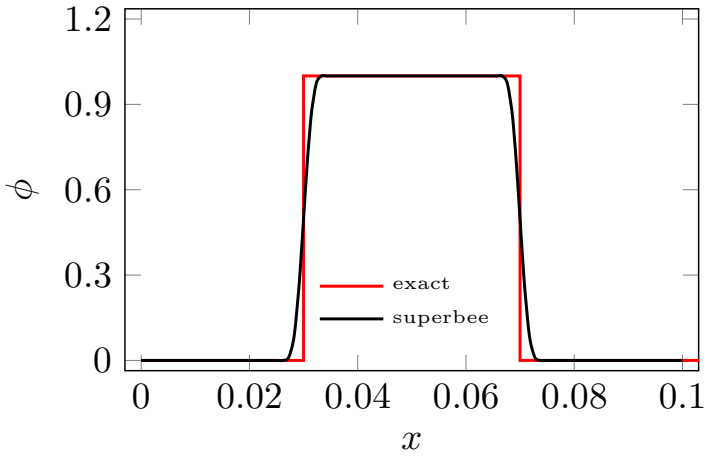
$$\psi(r) = \max(0, \min(2r, 1), \min(r, 2))$$

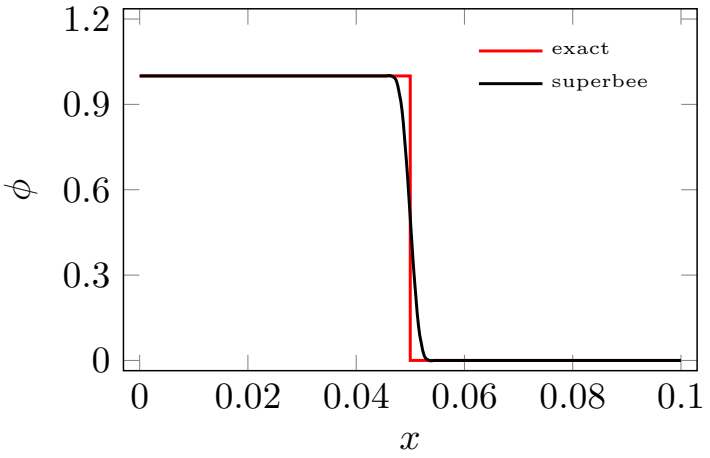
- TVD,
- 2^{nd} order,
- symmetric.
- piecewise linear

Convection terms – superbee

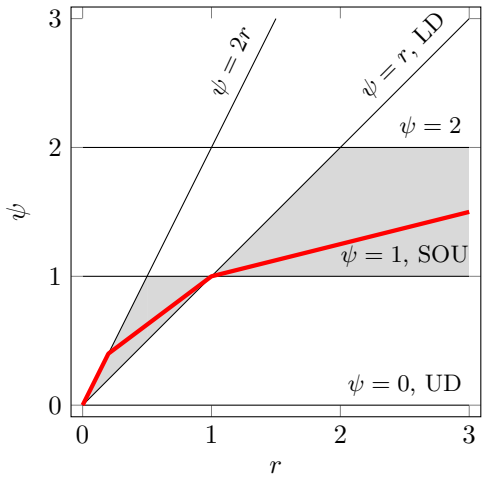








Convection terms – UMIST

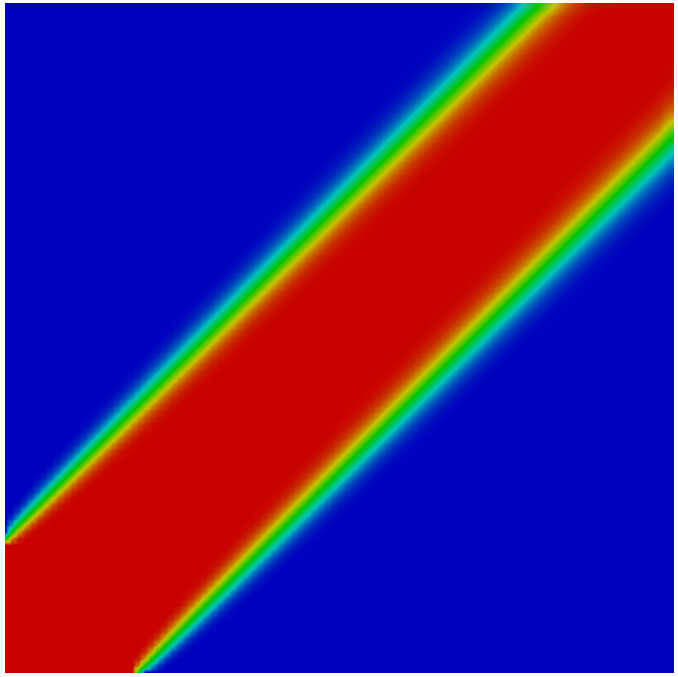


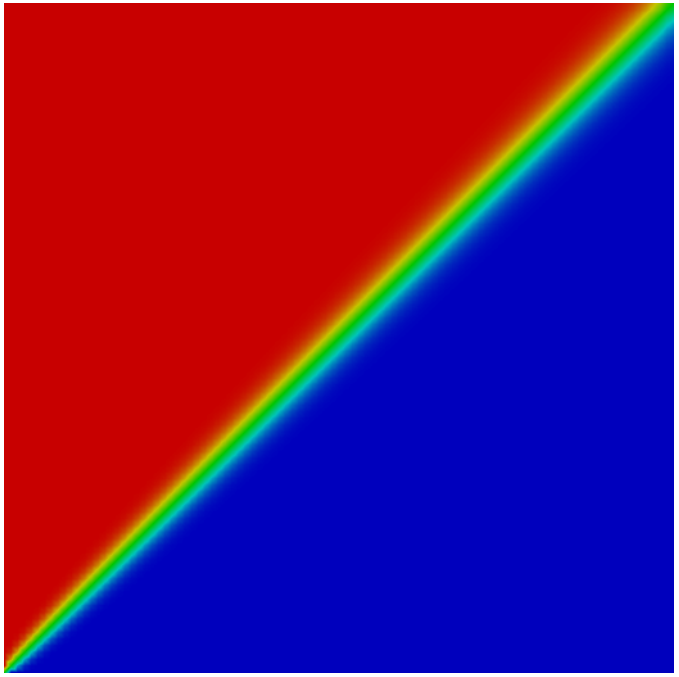
Upstream Monotonic Interpolation Scalar Transport

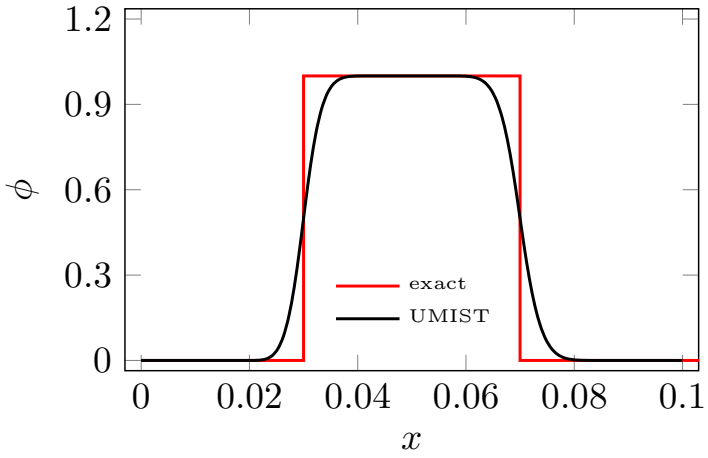
$$\psi(r) = \max(0, \min(2r, \tfrac{1}{4}+\tfrac{3}{4}r, \tfrac{3}{4}+\tfrac{1}{4}r, 2))$$

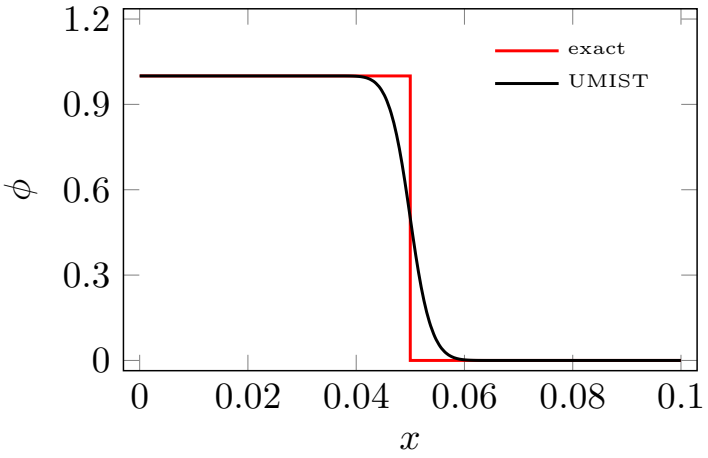
- TVD,
- 2^{nd} order,
- $\lim_{r\to\infty} \psi(r) = 2$,
- piecewise linear

Convection terms – UMIST

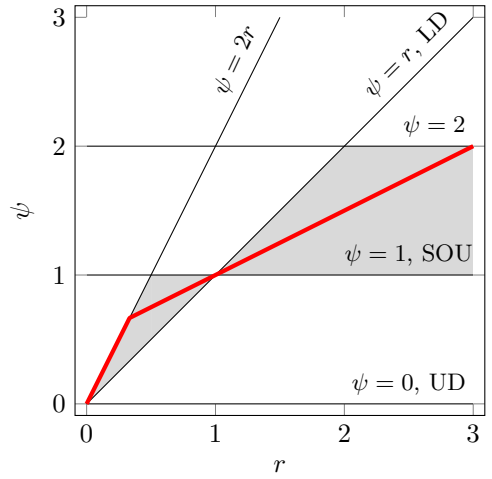


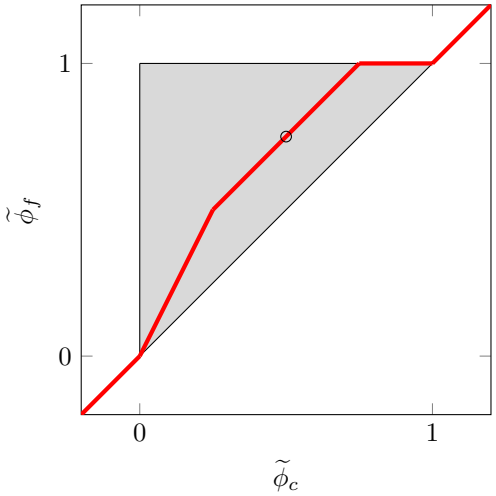






Convection terms – MUSCL





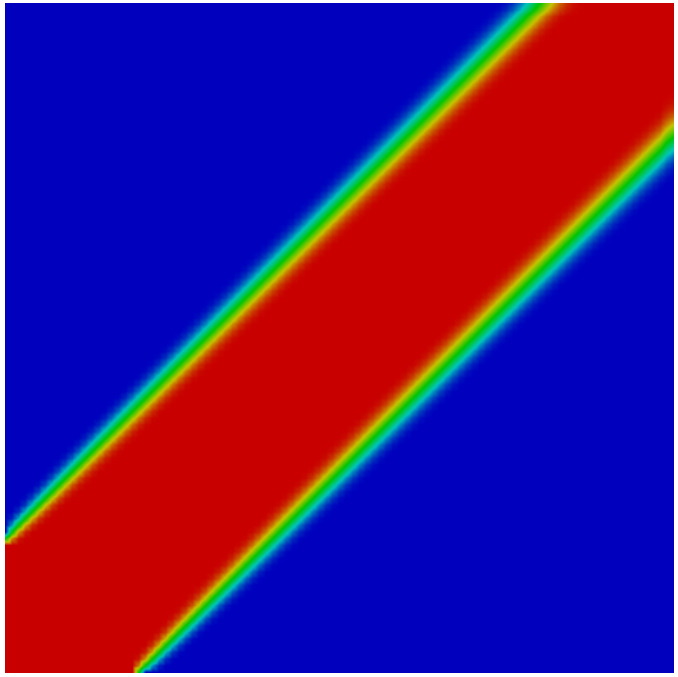
Monotonic Upwind Scheme for Conservation Laws

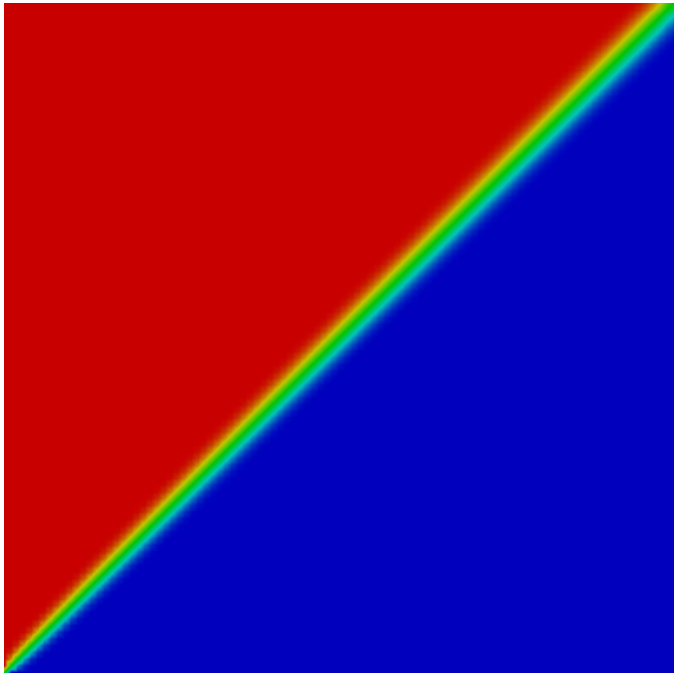
$$\psi(r) = \max(0, \min(2r, \tfrac{1}{2}+\tfrac{1}{2}r, 2))$$

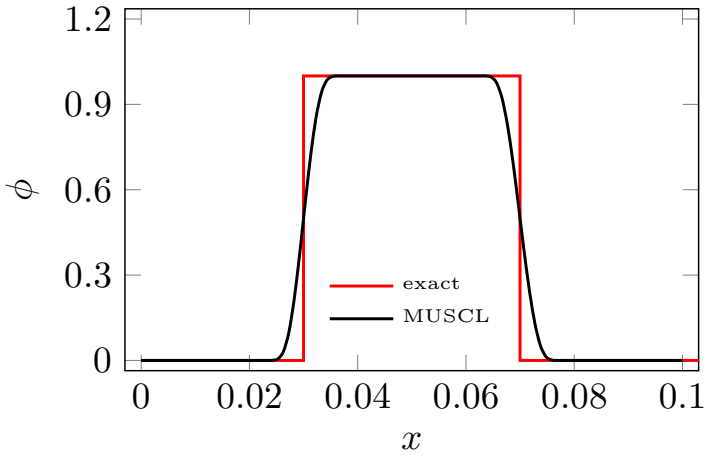
- TVD, NVD,
- 2^{nd} order,
- $\lim_{r\to\infty} \psi(r) = 2$,
- piecewise linear

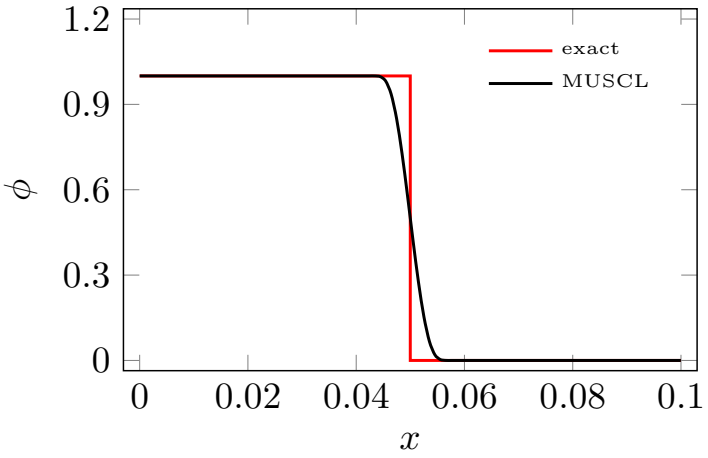
$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \begin{cases} 2\widetilde{\phi}_C; & 0 \le \widetilde{\phi}_C < \frac{1}{4}, \\ \frac{1}{4} + \widetilde{\phi}_C; & \frac{1}{4} \le \widetilde{\phi}_C < \frac{3}{4}, \\ 1; & \frac{3}{4} \le \widetilde{\phi}_C \le 1, \\ \widetilde{\phi}_C; & \text{otherwise} \end{cases}$$

Convection terms – MUSCL

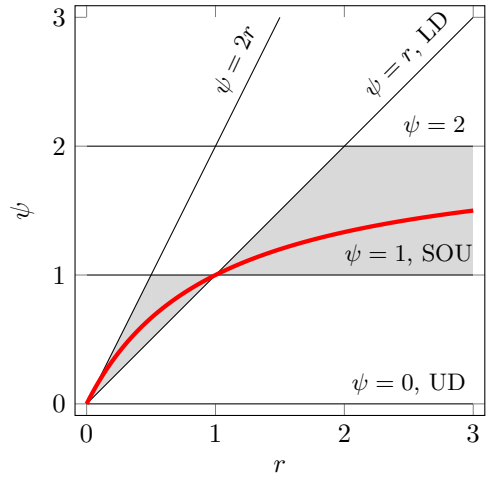






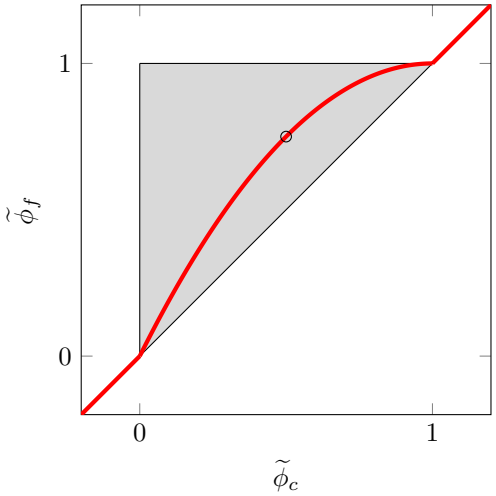


Convection terms – van Leer



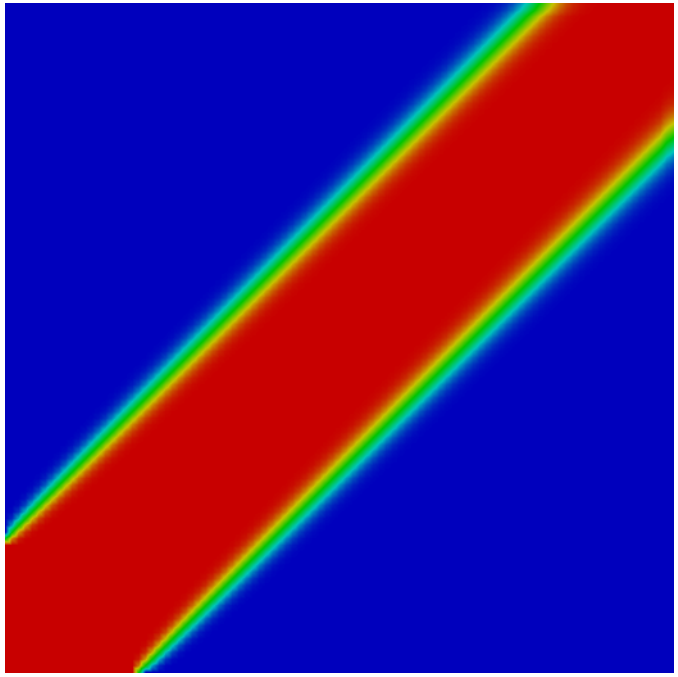
$$\psi(r) = \frac{r + |r|}{1 + |r|}$$

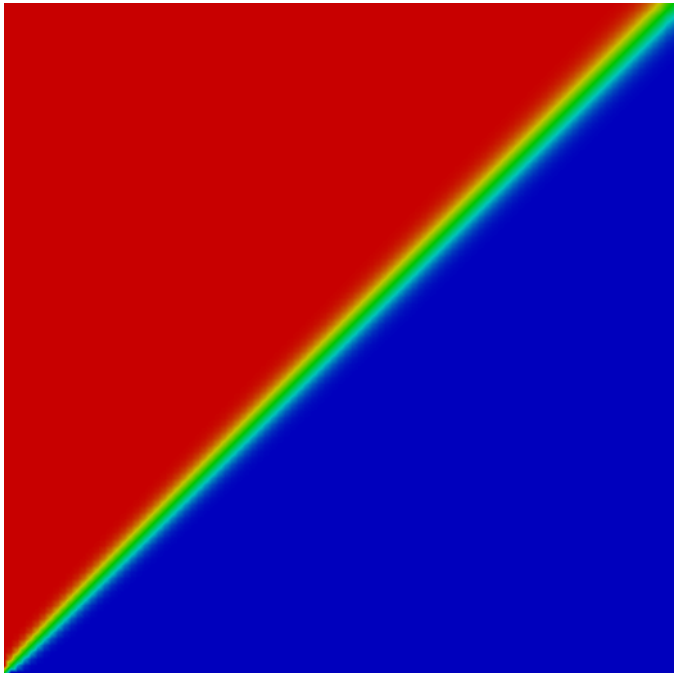
- TVD, NVD,
- 2^{nd} order,
- symmetric,
- $\lim_{r\to\infty} \psi(r) = 2$

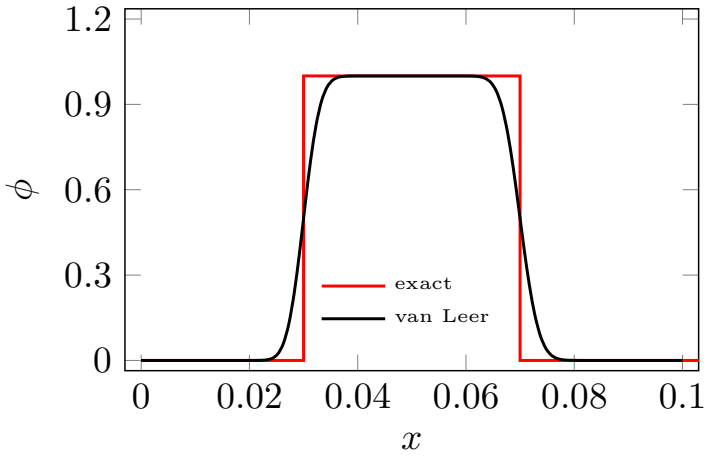


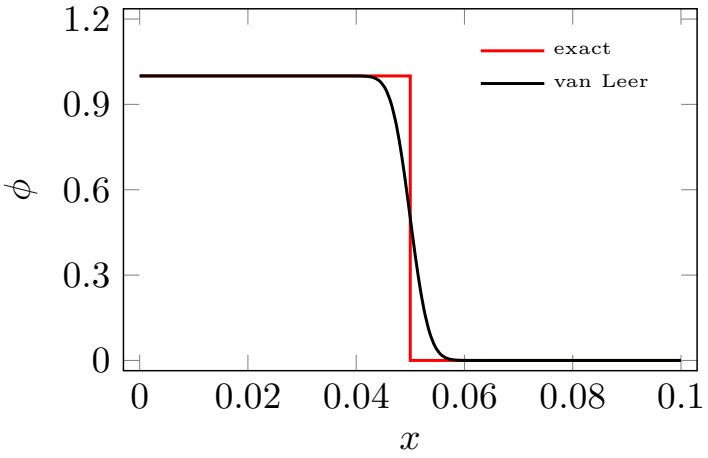
$$\widetilde{\phi}_f(\widetilde{\phi}_C) = \begin{cases} \widetilde{\phi}_C \left(2 - \widetilde{\phi}_C\right); & 0 \leq \widetilde{\phi}_C \leq 1, \\ \widetilde{\phi}_C; & \text{otherwise} \end{cases}$$

Convection terms – van Leer









Diffusion terms

Diffusion terms involving $\nabla \cdot (\Gamma \nabla \phi)$ are treated in the same way as convection terms

$$\oiint_{\partial V_P} \Gamma \nabla \phi \cdot \, \mathrm{d}\mathbf{S} = \sum_f \Gamma_f \left(\nabla \phi\right)_f \cdot \mathbf{S}_f \qquad (265)$$

Most importantly, the discretised diffusion term needs to be interpolated further by means of cell centred values. The spatially discretised general transport equations is now given by

$$\rho \frac{\mathrm{d}\phi_P}{\mathrm{d}t} |V_P| + \rho \sum_f \phi_f \mathbf{u}_f \cdot \mathbf{S}_f = \sum_f \Gamma_f \left(\nabla \phi\right)_f \cdot \mathbf{S}_f + S_C |V_P| + S_P |V_P| \phi_P \qquad (266)$$

Diffusion terms

If the considered mesh is orthogonal the dot product of the face centred gradient $(\nabla\phi)_f$ and surface normal vector $\mathbf{S}_f$, being in fact the surface normal gradient, is calculated according to the following equation

$$(\nabla\phi)_f \cdot \mathbf{S}_f = \frac{\phi_N - \phi_P}{\|\mathbf{d}\|}\|\mathbf{S}_f\| \tag{267}$$

which takes under considerations two two centroids P and N values around the surface S_f. This approach is the central difference approximation of the first order derivative and is know to be second order accurate.

Diffusion terms

For generic non-orthogonal meshes a correction is introduced. The two contributing parts are considered based upon the following decomposition $\mathbf{S}_f = \mathbf{S}_\perp + \mathbf{k}$. Here, $\mathbf{S}_\perp$ is parallel with $\mathbf{d}$. Finally, the corrected equation is

$$(\nabla\phi)_f \cdot \mathbf{S}_f = \frac{\phi_N - \phi_P}{\|\mathbf{d}\|}\|\mathbf{S}_\perp\| + (\nabla\phi)_f \cdot \mathbf{k} \qquad (268)$$

The right hand side of the above formula represents the orthogonal and non-orthogonal contributions. The latter requires the face centred gradient interpolation. This is usually achieved by the linear interpolation of cell centred gradients $(\nabla\phi)_P$ and $(\nabla\phi)_N$, i.e.

$$(\nabla\phi)_f = f_x\,(\nabla\phi)_P + (1 - f_x)\,(\nabla\phi)_N \qquad (269)$$

Diffusion terms

$$(\nabla\phi)_f = f_x\,(\nabla\phi)_P + (1 - f_x)\,(\nabla\phi)_N \qquad (270)$$

Two most commonly met methods of cell centred gradients evaluations are Gaussian integration and least squares method:

- Gaussian integration,
- least squares method.

Diffusion terms – Gaussian integration

Gaussian integration. Cell centred gradients are evaluated by means of the Gauss's theorem for $\mathbf{w} = \phi\mathbf{c}$ where $\mathbf{c}$ stands for a constant vector

$$\iiint_{V_P} \nabla\phi \, \mathrm{d}V = \oiint_{\partial V_P} \phi \, \mathrm{d}\mathbf{S} \tag{271}$$

These terms are converted by means of Gaussian integration. Secondly, the average value of $\nabla\phi$ is replaced by the cell centred value $(\nabla\phi)_P$

$$(\nabla\phi)_P = \frac{1}{|V_P|} \iiint_{V_P} \nabla\phi \, \mathrm{d}V = \frac{1}{|V_P|} \oiint_{\partial V_P} \phi \, \mathrm{d}\mathbf{S} = \frac{1}{|V_P|} \sum_f \phi_f \mathbf{S}_f \tag{272}$$

Diffusion terms – least squares method

Equation

$$\phi_N = \phi_P + (\mathbf{x}_N - \mathbf{x}_P) \cdot (\nabla\phi)_P \tag{273}$$

allows for extrapolation of the values ϕ_P by means of their gradients $(\nabla\phi)_P$ to the neighbouring points ϕ_N. Introducing the following vector connecting point P with its neighbours N, namely $\mathbf{d}_N = \mathbf{x}_N - \mathbf{x}_P$, it is now possible to provide N equations

$$\mathbf{d}_N \cdot (\nabla\phi)_P = \phi_N - \phi_P \tag{274}$$

where N stands for the total number of neighbours of P and is always larger or equal four. This is because the simplest polyhedral volume consists of four faces.

Diffusion terms – least squares method

Since N is larger than the three components of the gradient $(\nabla\phi)_P$ to be computed, it is necessary to minimise the sum of the square of weighted errors for all N neighbours. In order to find the gradient $(\nabla\phi)_P$ a linear system of equations is formulated

$$\mathbf{A} \cdot (\nabla\phi)_P = \mathbf{y} \tag{275}$$

where known $N \times 3$ matrix is $\mathbf{A} = (\mathbf{d}_N, \ldots)^{\mathrm{T}}$, the unknown 3×1 gradient is $(\nabla\phi)_P$ and finally the known $N \times 1$ vector is $\mathbf{y} = (\phi_N - \phi_P, \ldots)^{\mathrm{T}}$.

Diffusion terms – least squares method

The sum of squared residuals or the the norm to be minimised is defined by

$$\left\| \mathbf{A} \cdot (\nabla\phi)_P - \mathbf{y} \right\|^2 = \sum_N \left(\mathbf{d}_N \cdot (\nabla\phi)_P - (\phi_N - \phi_P) \right)^2 \quad (276)$$

Finally, the unknown gradient $(\nabla\phi)_P$ is the solution of the following linear equations system

$$\left(\mathbf{A}^{\mathrm{T}} \cdot \mathbf{A} \right) \cdot (\nabla\phi)_P = \mathbf{A}^{\mathrm{T}} \cdot \mathbf{y} \quad (277)$$

Temporal discretisation

Time dependent (transient) problems require temporal discretisation of the general transport equation. Integration it with respect to time from t to $t + \Delta t$ results in

$$\rho|V_P| \int_t^{t+\Delta t} \frac{\mathrm{d}\phi_P}{\mathrm{d}t}\,\mathrm{d}t = \int_t^{t+\Delta t} \left(-\rho \sum_f \phi_f \mathbf{u}_f \cdot \mathbf{S}_f \right) \mathrm{d}t + \int_t^{t+\Delta t} \sum_f \Gamma_f \left(\nabla\phi\right)_f \cdot \mathbf{S}_f \,\mathrm{d}t + \int_t^{t+\Delta t} \left(S_C|V_P| + S_P|V_P|\phi_P\right) \mathrm{d}t \tag{278}$$

The right hand side of the above represents the time integral of all the spatial values.

Temporal discretisation

The following abbreviations are assumed:

- the new value $\phi_P^{n+1} = \phi_P(t + \Delta t)$, i.e. value the solver is calculating for,
- old value $\phi_P^n = \phi_P(t)$, i.e. known from the previous time step,
- old old value $\phi_P^{n-1} = \phi_P(t - \Delta t)$ known from the time step prior to the previous.

Temporal discretisation

The left hand side of the dicretised equation can be evaluated directly and the right hand side integrand is denoted as $f(\phi_f, \phi_P)$

$$\rho \left(\phi_P^{n+1} - \phi_P^n\right) |V_P| = \int_t^{t+\Delta t} f(\phi_f(t), \phi_P(t)) \, \mathrm{d}t \qquad (279)$$

This time, however, the right hand side cannot be integrated directly. This means that it has to be approximated by $F(\phi_f, \phi_P)\Delta t$. Above equation now reads

$$\rho \frac{\phi_P^{n+1} - \phi_P^n}{\Delta t} |V_P| = F(\phi_f, \phi_P) \qquad (280)$$

Temporal discretisation

Several treatments of the spatial derivatives in a transient problem are possible. The most popular are:

- explicit Euler,
- implicit Euler,
- Crank–Nicolson (linear interpolation),
- backward differencing.

Euler methods as well as Crank–Nicolson method require only values of the unknown function at two different times ϕ_P^{n+1} and ϕ_P^n and are referred to as two-level methods. Backward differencing is the so called three-level method because it require the values of the unknown function ϕ_P at three different times, namely ϕ_P^{n+1}, ϕ_P^n and ϕ_P^{n-1}.

Temporal discretisation – explicit Euler

The right hand side of previous equation is approximated explicitly by means of old values ϕ^n which is denoted as $F(\phi_f^n, \phi_P^n)$. The discrete version of the general transport equation is

$$\rho \frac{\phi_P^{n+1} - \phi_P^n}{\Delta t} |V_P| + \rho \sum_f \phi_f^n \mathbf{u}_f \cdot \mathbf{S}_f = \sum_f \Gamma_f \left(\nabla \phi\right)_f^n \cdot \mathbf{S}_f + S_C |V_P| + S_P |V_P| \phi_P^n \quad (281)$$

The method is first order accurate in time. However, it is also unstable if $\mathrm{Co} > 1$. Despite this, explicit Euler discretisation is very easy to implement and does not require substantial computer resources.

Temporal discretisation – implicit Euler

This time the right hand side of previous equation is approximated implicitly by means of current values ϕ^{n+1} which is denoted as $F(\phi_f^{n+1}, \phi_P^{n+1})$. The discrete version of the general transport equation is

$$\rho \frac{\phi_P^{n+1} - \phi_P^n}{\Delta t} |V_P| + \rho \sum_f \phi_f^{n+1} \mathbf{u}_f \cdot \mathbf{S}_f =$$

$$\sum_f \Gamma_f \left(\nabla \phi\right)_f^{n+1} \cdot \mathbf{S}_f + S_C |V_P| + S_P |V_P| \phi_P^{n+1} \quad (282)$$

The method is first order accurate in time and is unconditionally stable in contrast to explicit method. Implicit Euler discretisation is more complicated to implement in comparison with its explicit formulation and requires iterative approach.

Temporal discretisation – Crank–Nicolson

Formally, the method utilises the trapezoid rule. This is equivalent to an arithmetical average of current and old values

$$\rho \frac{\phi_P^{n+1} - \phi_P^n}{\Delta t} |V_P| = \frac{F\left(\phi_f^n, \phi_P^n\right) + F\left(\phi_f^{n+1}, \phi_P^{n+1}\right)}{2} \quad (283)$$

The method is known to be second order accurate in time and unconditionally stable.

Temporal discretisation – backward differencing

The integrand $\frac{\mathrm{d}\phi_P}{\mathrm{d}t}$ of the left hand side of the previous equation is discretised first rather than being evaluated directly

$$\frac{\mathrm{d}\phi_P}{\mathrm{d}t} = \frac{3\phi_P^{n+1} - 4\phi_P^n + \phi_P^{n-1}}{2\Delta t} \tag{284}$$

Now the left hand side of the previous equation can be integrated. The implicit discrete version of the general transport equation is

$$\rho\frac{3\phi_P^{n+1} - 4\phi_P^n + \phi_P^{n-1}}{2\Delta t}|V_P| + \rho\sum_f \phi_f^{n+1}\mathbf{u}_f \cdot \mathbf{S}_f =$$

$$\sum_f \Gamma_f \left(\nabla\phi\right)_f^{n+1} \cdot \mathbf{S}_f + S_C|V_P| + S_P|V_P|\phi_P^{n+1} \tag{285}$$

The method is known to be second order accurate in time.

The method in 2D

Let us consider differential form of the general transport equation

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\phi\mathbf{u}) = \nabla \cdot (\Gamma \nabla\phi) + S_\phi \qquad (286)$$

To obtain the integral form of this equation one needs Gauss's (divergence) theorem. Two dimensional version has the following form

$$\iint_{\Omega_i} \nabla \cdot \mathbf{w}\, \mathrm{d}\Omega = \oint_{\partial\Omega_i^+} \mathbf{w} \cdot \mathrm{d}\mathbf{L} \qquad (287)$$

where $\mathrm{d}\Omega \equiv \mathrm{d}x\,\mathrm{d}y$ and $\mathrm{d}\mathbf{L} \equiv \hat{\boldsymbol{n}}\,\mathrm{d}L \equiv \hat{\boldsymbol{\imath}}\,\mathrm{d}y - \hat{\boldsymbol{\jmath}}\,\mathrm{d}x$

Integral form in 2D

Integrating over the two dimensional domain (finite 'volume') Ω_i and utilising Gauss's theorem results in

$$\frac{\mathrm{d}}{\mathrm{d}t}\iint_{\Omega_i}\rho\phi\,\mathrm{d}\Omega+\oint_{\partial\Omega_i^+}\rho\phi\mathbf{u}\cdot\,\mathrm{d}\mathbf{L}=\oint_{\partial\Omega_i^+}\Gamma\nabla\phi\cdot\,\mathrm{d}\mathbf{L}+\iint_{\Omega_i}S_\phi\,\mathrm{d}\Omega \quad (288)$$

First and last integral in the above equation suggest the following definition of an average $\bar{\phi}_i$ value of f over Ω_i

$$\bar{\phi}_i=\frac{1}{|\Omega_i|}\iint_{\Omega_i}\phi\,\mathrm{d}\Omega \quad (289)$$

The average value ϕ_i is typically located at the centre of the volume Ω_i.

Spatial discretisation in 2D

The next step would be the spatial discretisation over the volume Ω_i boundary $\partial\Omega_i$. The line integral represents the total flux out of volume Ω_i and is replaced by a sum

$$\oint_{\partial\Omega_i^+} \mathbf{w} \cdot \mathrm{d}\mathbf{L} \approx \sum_k \mathbf{w}_k \cdot \Delta\mathbf{L}_k \tag{290}$$

Boundary $\partial\Omega_i$ consists of lines indexed by subscript k. There are at least three lines (triangle). The vector $\mathbf{w}$ is either $\phi\mathbf{u}$ or $\Gamma\nabla\phi$. Because that vector $\mathbf{w}$ is typically not constant along each line it has to be approximated by a single value $\mathbf{w}_k$ at the centre of each line.

Time discretisation

The last step would be time discretisation. Among many possibilities the simplest is the first order forward finite difference approximation

$$\frac{\mathrm{d}\bar{\phi}_i}{\mathrm{d}t} \approx \frac{\bar{\phi}_i^{n+1} - \bar{\phi}_i^n}{\Delta t} \tag{291}$$

Time step of this approximation is denoted here as Δt. Finally, one gets the following discretised version of transport equation (i.e. Finite Volume Scheme)

$$\rho \frac{\bar{\phi}_i^{n+1} - \bar{\phi}_i^n}{\Delta t} |\Omega_i| + \rho \sum_k (\phi \mathbf{u})_k \cdot \Delta \mathbf{L}_k = \sum_k (\Gamma \nabla \phi)_k \cdot \Delta \mathbf{L}_k + \bar{S}_{\phi i} |\Omega_i| \tag{292}$$

$|\Omega_i|$ stands for the area of control volume Ω_i

2D FVM diffusion problem

Two dimensional and steady state diffusion equation of a f quantity arises, as previously, from the general transport equation (convection-diffusion equation)

$$\nabla \cdot (\Gamma \nabla \phi) + S_\phi = 0 \tag{293}$$

If the diffusion coefficient is constant $\Gamma = 1$ and the source term $S_\phi = a$ then the above equation simplifies to

$$\nabla \cdot \nabla \phi + a = 0 \tag{294}$$

or $\nabla^2 \phi = -a$ which is Poisson equation.

2D FVM diffusion problem

The discrete version of the diffusion equation (simplified version of general transport equation) is

$$\sum_k (\Gamma \nabla \phi)_k \cdot \Delta \mathbf{L}_k + \bar{S}_{\phi ij} |\Omega_{ij}| = 0 \tag{295}$$

For a structural and Cartesian mesh (next slide) the normal $\Delta \mathbf{L}_k$ vectors are

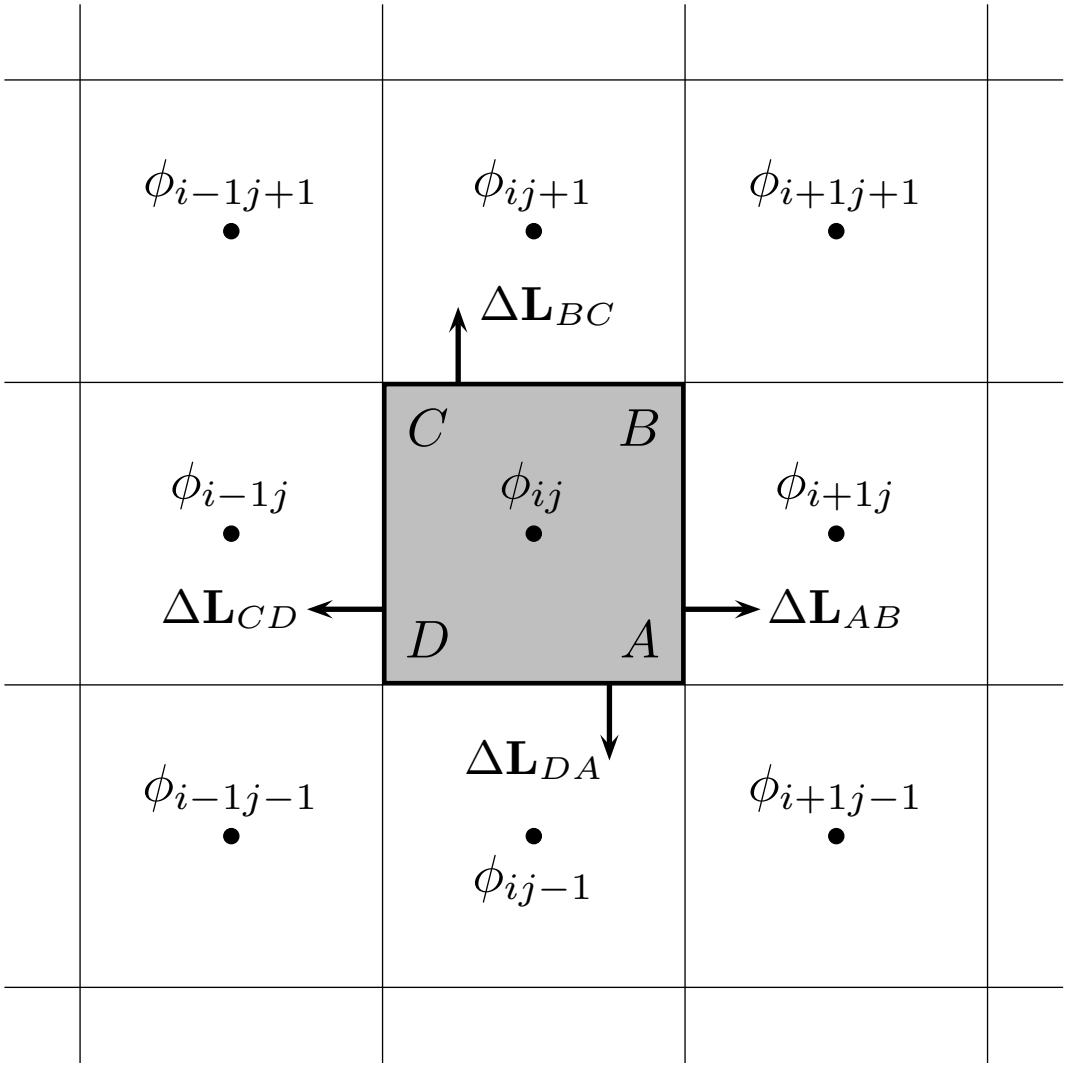
$$\Delta \mathbf{L}_{AB} = |\overline{AB}| \hat{\boldsymbol{\imath}} = \Delta y_i \, \hat{\boldsymbol{\imath}} \tag{296a}$$

$$\Delta \mathbf{L}_{BC} = |\overline{BC}| \hat{\boldsymbol{\jmath}} = \Delta x_i \, \hat{\boldsymbol{\jmath}} \tag{296b}$$

$$\Delta \mathbf{L}_{CD} = |\overline{CD}| \, (-\hat{\boldsymbol{\imath}}) = -\Delta y_i \, \hat{\boldsymbol{\imath}} \tag{296c}$$

$$\Delta \mathbf{L}_{DA} = |\overline{DA}| \, (-\hat{\boldsymbol{\jmath}}) = -\Delta x_i \, \hat{\boldsymbol{\jmath}} \tag{296d}$$

2D FVM diffusion problem



2D FVM diffusion problem

The discrete version of two dimensional diffusion equation is now

$$\Gamma\frac{\partial\phi_{i+\frac{1}{2}j}}{\partial x}\Delta y_i+\Gamma\frac{\partial\phi_{ij+\frac{1}{2}}}{\partial y}\Delta x_i-\Gamma\frac{\partial\phi_{i-\frac{1}{2}j}}{\partial x}\Delta y_i- \Gamma\frac{\partial\phi_{ij-\frac{1}{2}}}{\partial y}\Delta x_i+\bar{S}_{\phi ij}|\Omega_{ij}|=0 \quad (297)$$

where the area of volume Ω_{ij} is $|\Omega_{ij}|=\Delta x_i\Delta y_i$ and the diffusion coefficient is constant $\Gamma=1$. If so, then

$$\frac{\partial\phi_{i+\frac{1}{2}j}}{\partial x}\Delta y_i+\frac{\partial\phi_{ij+\frac{1}{2}}}{\partial y}\Delta x_i-\frac{\partial\phi_{i-\frac{1}{2}j}}{\partial x}\Delta y_i - \frac{\partial\phi_{ij-\frac{1}{2}}}{\partial y}\Delta x_i+\bar{S}_{\phi ij}\Delta x_i\Delta y_i=0 \quad (298)$$

2D FVM diffusion problem

The average value of S_ϕ at the centre of finite volume is approximated by means of known values of S_ϕ at the boundary of finite volume

$$\bar{S}_{\phi ij} = \frac{1}{4}\left(S_{\phi i-\frac{1}{2}j-\frac{1}{2}} + S_{\phi i+\frac{1}{2}j-\frac{1}{2}} S_{\phi i-\frac{1}{2}j+\frac{1}{2}} + S_{\phi i+\frac{1}{2}j+\frac{1}{2}}\right) \tag{299}$$

Derivatives at the boundary of finite volume are approximated by means of the second order scheme as

$$\frac{\partial \phi_{i+\frac{1}{2}j}}{\partial x} \approx \frac{\phi_{i+1j} - \phi_{ij}}{x_{i+1j} - x_{ij}} = \frac{\phi_{i+1j} - \phi_{ij}}{\Delta x_{i+1}} \tag{300a}$$

$$\frac{\partial \phi_{ij+\frac{1}{2}}}{\partial y} \approx \frac{\phi_{ij+1} - \phi_{ij}}{y_{ij+1} - y_{ij}} = \frac{\phi_{ij+1} - \phi_{ij}}{\Delta y_{j+1}} \tag{300b}$$

2D FVM diffusion problem

$$\frac{\partial \phi_{i-\frac{1}{2}j}}{\partial x} \approx \frac{\phi_{ij} - \phi_{i-1j}}{x_{ij} - x_{i-1j}} = \frac{\phi_{ij} - \phi_{i-1j}}{\Delta x_{i-1}} \tag{301a}$$

$$\frac{\partial \phi_{ij-\frac{1}{2}}}{\partial y} \approx \frac{\phi_{ij} - \phi_{ij-1}}{y_{ij} - y_{ij-1}} = \frac{\phi_{ij} - \phi_{ij-1}}{\Delta y_{j-1}} \tag{301b}$$

The specific form of a finite volume scheme is now

$$\bar{S}_{\phi ij}\Delta x_i \Delta y_i + \frac{\phi_{i-1j}\Delta y_i}{\Delta x_{i-1}} + \frac{\phi_{i+1j}\Delta y_i}{\Delta x_{i+1}} + \frac{\phi_{ij-1}\Delta x_i}{\Delta y_{j-1}} + \frac{\phi_{ij+1}\Delta x_i}{\Delta y_{j+1}} - \phi_{ij}\left(\frac{\Delta y_i}{\Delta x_{i-1}} + \frac{\Delta y_i}{\Delta x_{i+1}} + \frac{\Delta x_i}{\Delta y_{j-1}} + \frac{\Delta x_i}{\Delta y_{j+1}}\right) = 0 \tag{302}$$

2D FVM diffusion problem

It can also be rewritten to give ϕ_{ij} as a function of surrounding variables

$$\phi_{ij} = \frac{\frac{\phi_{i-1j}\Delta y_i}{\Delta x_{i-1}} + \frac{\phi_{i+1j}\Delta y_i}{\Delta x_{i+1}} + \frac{\phi_{ij-1}\Delta x_i}{\Delta y_{j-1}} + \frac{\phi_{ij+1}\Delta x_i}{\Delta y_{j+1}} + \bar{S}_{\phi ij}\Delta x_i \Delta y_i}{\frac{\Delta y_i}{\Delta x_{i-1}} + \frac{\Delta y_i}{\Delta x_{i+1}} + \frac{\Delta x_i}{\Delta y_{j-1}} + \frac{\Delta x_i}{\Delta y_{j+1}}} \quad (303)$$

For $\Delta x_i = \Delta y_i = \Delta x_{i-1} = \Delta x_{i+1} = \Delta y_{i-1} = \Delta y_{i+1} = h$ (i.e. uniform mesh) the finite volume scheme reduced to a finite difference scheme for Poisson equation

$$\phi_{ij} = \frac{\phi_{i-1j} + \phi_{i+1j} + \phi_{ij-1} + \phi_{ij+1} + \bar{S}_{\phi ij}h^2}{4} \quad (304)$$

2D FVM pseudocode

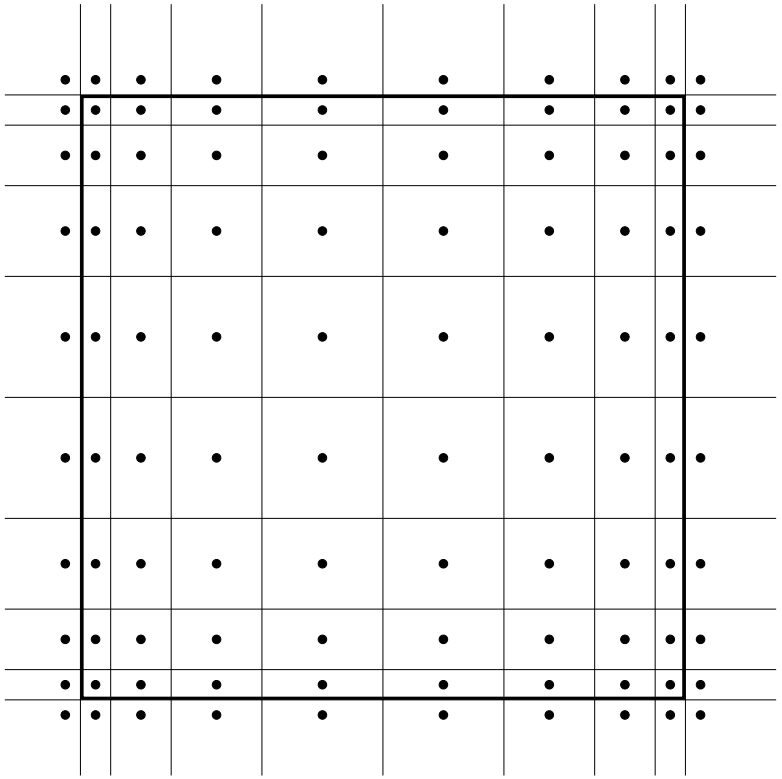
Data: Read volumes data and BCs
Create nodes and ghost nodes;
$n := 1$;
repeat
  $R := 0$;
  for $i := 2$ **to** $i_{max} - 1$ **do**
    for $j := 2$ **to** $j_{max} - 1$ **do**

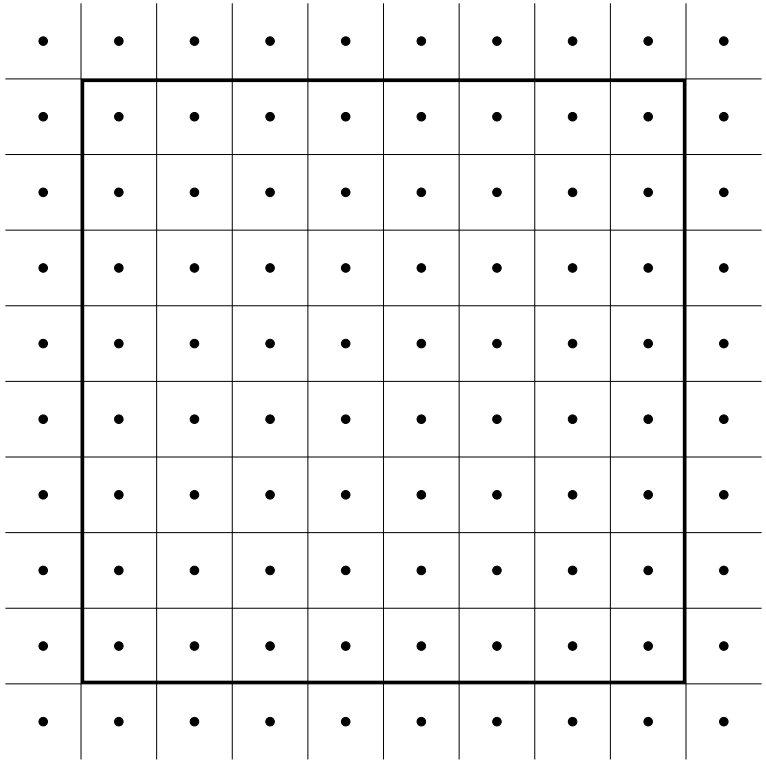
$$\phi_{ij}^{n+1} := \frac{\frac{\phi_{i-1j}^{n}\Delta y_i}{\Delta x_{i-1}} + \frac{\phi_{i+1j}^{n}\Delta y_i}{\Delta x_{i+1}} + \frac{\phi_{ij-1}^{n}\Delta x_i}{\Delta y_{j-1}} + \frac{\phi_{ij+1}^{n}\Delta x_i}{\Delta y_{j+1}} + \bar{S}_{\phi ij}\Delta x_i \Delta y_i}{\frac{\Delta y_i}{\Delta x_{i-1}} + \frac{\Delta y_i}{\Delta x_{i+1}} + \frac{\Delta x_i}{\Delta y_{i-1}} + \frac{\Delta x_i}{\Delta y_{i+1}}};$$

      $R := \max\left(|\phi_{ij}^{n+1} - \phi_{ij}^{n}|, R\right)$;

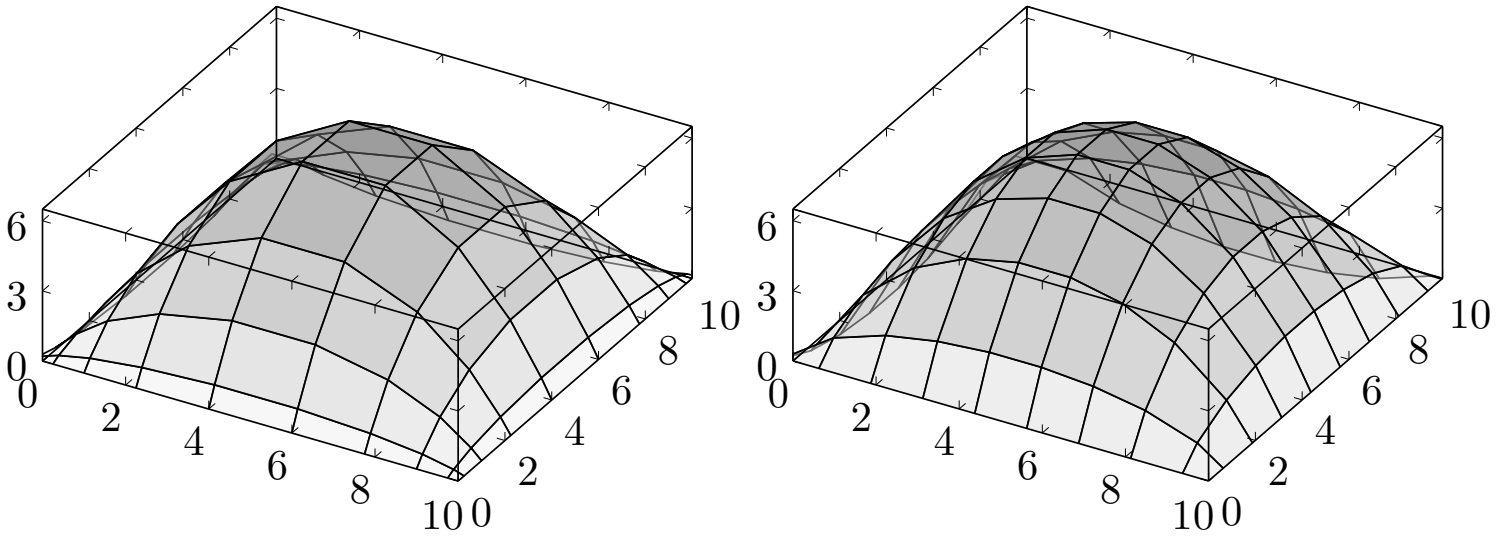
  Update ghost nodes;
  $n := n + 1$;
until $n \leq n_{max}$ **and** $R > R_{min}$;

Nonuniform and uniform volumes and nodes

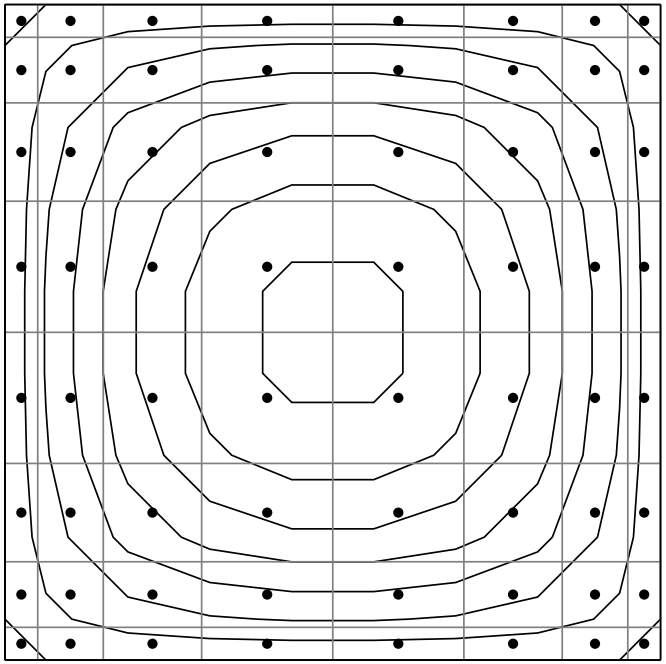


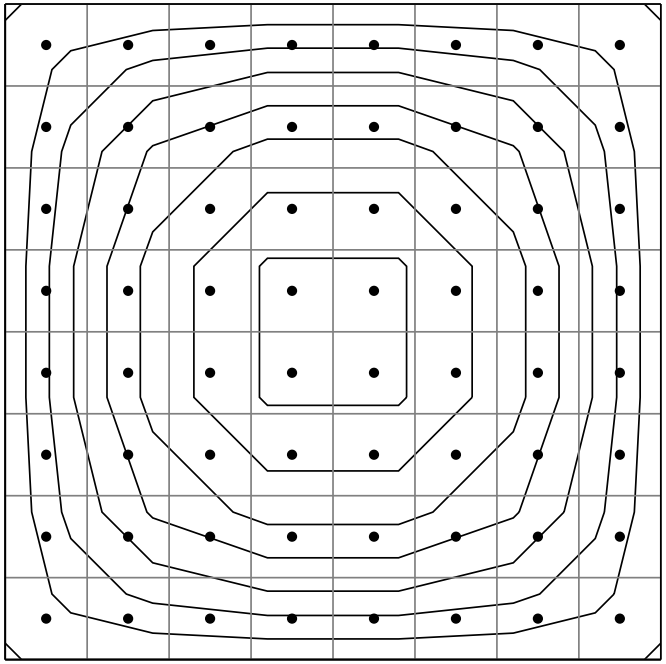


Results for nonuniform and uniform mesh

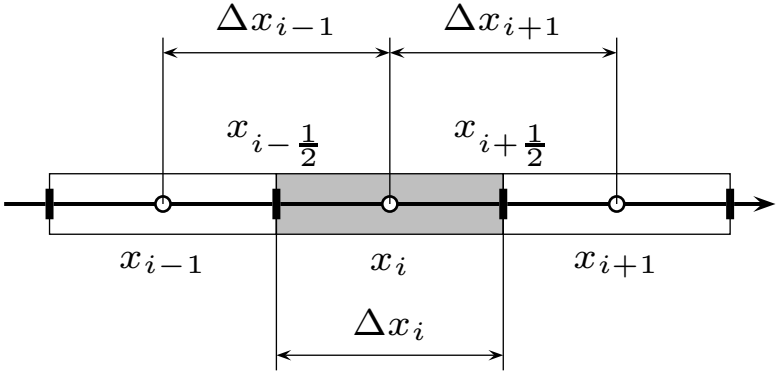


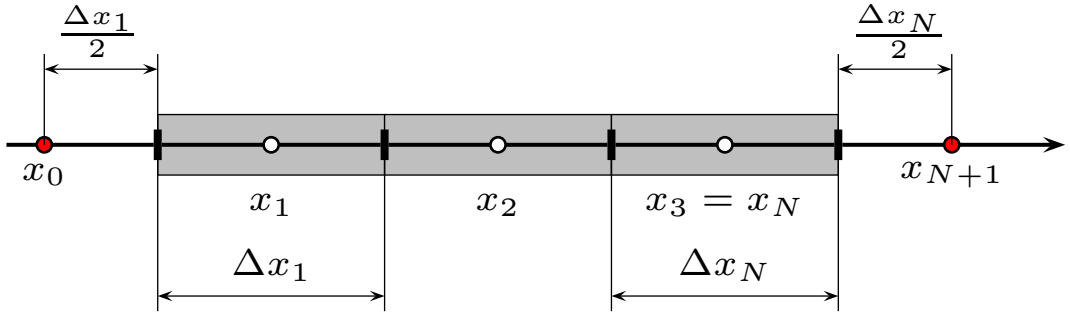
Results for nonuniform and uniform mesh





1D FVM diffusion problem





1D FVM diffusion problem

One dimensional and steady state diffusion equation of a f quantity arises from the general transport equation (convection-diffusion equation)

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi \tag{305}$$

If the diffusion coefficient Γ is constant then the above equation simplifies to

$$\nabla \cdot (\Gamma \nabla \phi) + S_\phi = 0 \tag{306}$$

or more precisely

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right) + S_\phi = 0 \tag{307}$$

1D FVM diffusion problem

The integral form of one dimensional diffusion equation takes the following form

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\mathrm{d}}{\mathrm{d}x}\left(\Gamma\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)\,\mathrm{d}x + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} S_\phi\,\mathrm{d}x = 0 \qquad (308)$$

There is no need to take advantage of Gauss's theorem. This is because the first term can be integrated directly

$$\left(\Gamma\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_{i+\frac{1}{2}} - \left(\Gamma\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_{i-\frac{1}{2}} + \bar{S}_{\phi i}\,\Delta x_i = 0 \qquad (309)$$

where $\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$

1D FVM diffusion problem - Dirichlet BC

The average value of S_f at the centre of finite volume can be approximated by means of trapezoidal rule by means of known values of S_f at the boundary of finite volume

$$\bar{S}_{fi} = \frac{S_{fi-\frac{1}{2}} + S_{fi+\frac{1}{2}}}{2} \tag{310}$$

Let us consider ODE

$$y''(x) + 20x = 0 \tag{311}$$

subjected to the Dirichlet boundary conditions $y(0) = y(1) = 0$. The specific solution is

$$y(x) = -\frac{10}{3}(x^3 - x) \tag{312}$$

1D FVM diffusion problem

In other word, the diffusion coefficient $\Gamma = 1$ and source term $S_f = 20x$. If so, then discrete version of one dimensional diffusion equation is now

$$\frac{\mathrm{d}\phi_{i+\frac{1}{2}}}{\mathrm{d}x} - \frac{\mathrm{d}\phi_{i-\frac{1}{2}}}{\mathrm{d}x} + \bar{S}_{\phi i}\,\Delta x_i = 0 \tag{313}$$

Derivatives or diffusive fluxes at the boundary of finite volume are approximated by means of the second order scheme as

$$\frac{\mathrm{d}\phi_{i+\frac{1}{2}}}{\mathrm{d}x} \approx \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \tag{314a}$$

$$\frac{\mathrm{d}\phi_{i-\frac{1}{2}}}{\mathrm{d}x} \approx \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} \tag{314b}$$

1D FVM diffusion problem

The specific form of a finite volume scheme is now

$$\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} + \bar{S}_{\phi i}\, \Delta x_i = 0 \tag{315}$$

It can also be rewritten to give ϕ_i as a function of surrounding variables

$$\phi_i = \frac{\Delta x_{i+1}\phi_{i-1} + \Delta x_{i-1}\phi_{i+1} + \bar{S}_{\phi i}\Delta x_{i-1}\Delta x_{i+1}\Delta x_i}{\Delta x_{i-1} + \Delta x_{i+1}} \tag{316}$$

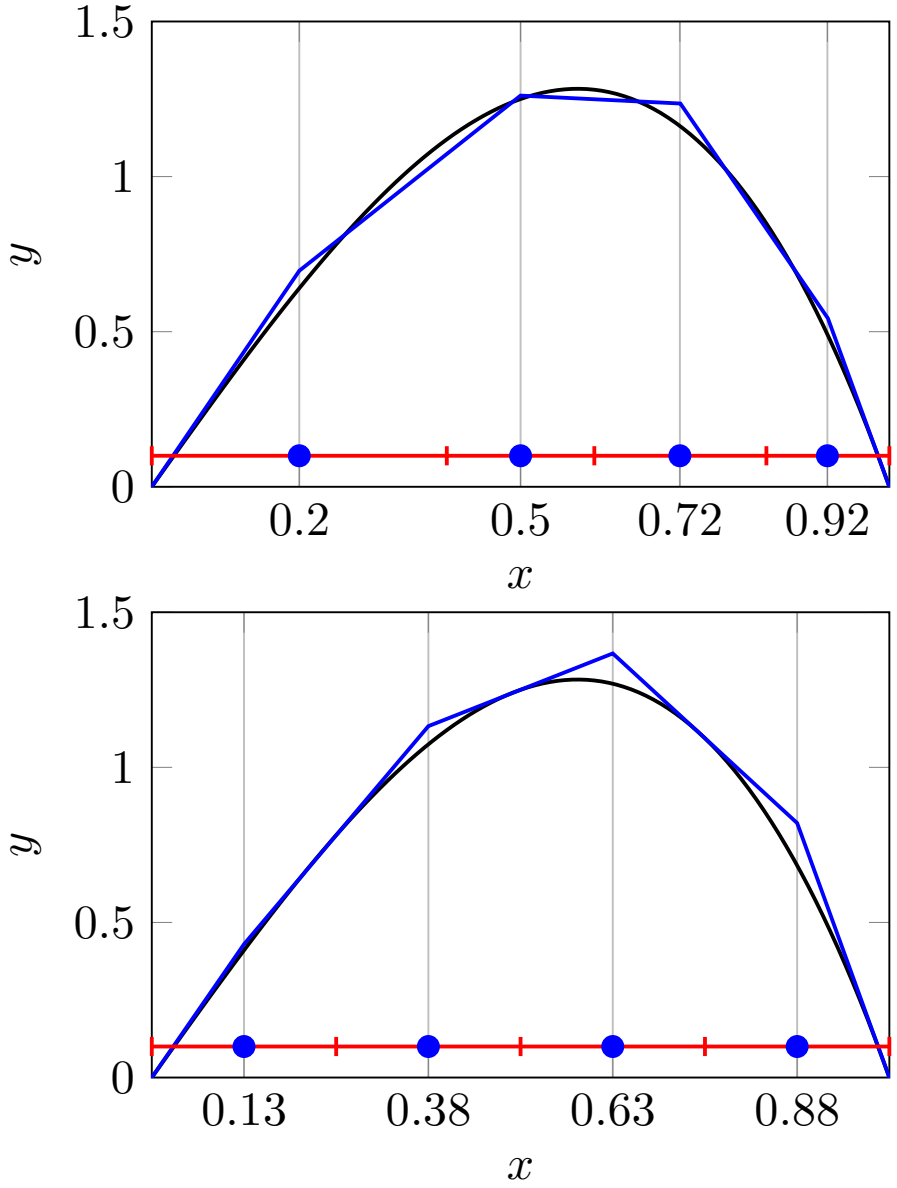
where $\Delta x_{i-1} = x_i - x_{i-1}$ and $\Delta x_{i+1} = x_{i+1} - x_i$.
For $\Delta x_{i-1} = \Delta x_{i+1} = \Delta x_i = h$ (i.e. uniform mesh) the finite volume scheme is reduced to a finite difference scheme

$$\phi_i = \frac{\phi_{i-1} + \phi_{i+1} + \bar{S}_{\phi i} h^2}{2} \tag{317}$$

1D FVM pseudocode

Data: Read volumes data and BCs
Create nodes and ghost nodes;
$n := 1$;
repeat
  $R := 0$;
  for $i := 2$ **to** $i_{max} - 1$ **do**
    $\phi_i^{n+1} := \frac{\Delta x_{i+1}\phi_{i-1}^n + \Delta x_{i-1}\phi_{i+1}^n + \bar{S}_{\phi i}\Delta x_{i-1}\Delta x_{i+1}\Delta x_i}{\Delta x_{i-1} + \Delta x_{i+1}}$;
    $R := \max\left(|\phi_i^{n+1} - \phi_i^n|, R\right)$;
  Update ghost nodes;
  $n := n + 1$;
until $n \leq n_{max}$ **and** $R > R_{min}$;

Results for nonuniform and uniform grids



1D FVM diffusion problem - Neumann BC

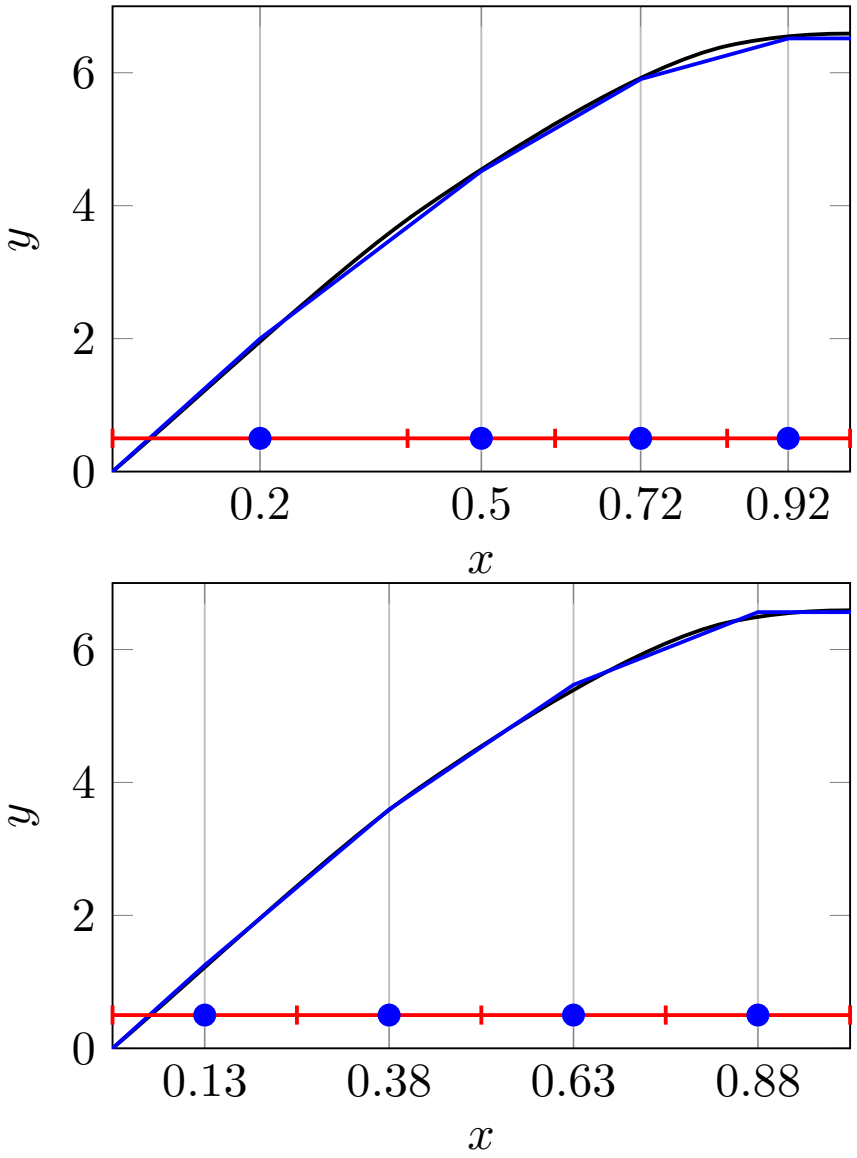
Let us consider the same ordinary differential equation

$$y''(x) + 20x = 0 \tag{318}$$

subjected to both the Dirichlet $y(0) = 0$ and Neumann $y'(1) = 0$ boundary conditions. The specific solution is now

$$y(x) = -10x\left(\frac{x^2}{3} - 1\right) \tag{319}$$

Results for nonuniform and uniform grids



Finite Element Method

Method of weighted residuals

The mathematical foundation of the finite element method is in the method of weighted residuals. Imagine ordinary differential equation

$$y''(x) + 20x = 0 \tag{320}$$

subjected to boundary conditions $y(0) = y(1) = 0$. The exact general solution of this equation is

$$y(x) = -\frac{10}{3}x^3 + C_1 x + C_2 \tag{321}$$

and a specific solution subjected to boundary conditions

$$y(x) = -\frac{10}{3}(x^3 - x) \tag{322}$$

Method of weighted residuals

The method seeks an approximate solution $\hat{y}$ in the general form

$$\hat{y}(x) = \sum_{i=1}^{N} C_i N_i(x) \tag{323}$$

where N_i are known trial functions which should be continuous and fulfilled boundary conditions. The constants C_i are unknown and they will be determined. A residual R appears when substituting approximate solution $\hat{y}$ into the differential equations

$$R(x) = \hat{y}''(x) + 20x \neq 0 \tag{324}$$

The unknown C_i constant are determined for $i = 1, \ldots N$ from

$$\int_0^1 W_i(x) R(x) \, \mathrm{d}x = 0 \tag{325}$$

Method of weighted residuals

$$\int_0^1 W_i(x) R(x)\,\mathrm{d}x = 0 \qquad i = 1, \ldots, N \tag{326}$$

Choices for the weighting functions W_i

- Collocation method $W_i(x) = \delta(x - x_i)$
- Subdomain method
  $W_i(x) = H(x - x_{i-1}) - H(x - x_i)$
- Galerkin's method $W_i(x) = N_i(x)$

$$\int_0^1 N_i(x) R(x)\,\mathrm{d}x = 0 \qquad i = 1, \ldots, N \tag{327}$$

- Least Squares Method $W_i(x) = \frac{\partial R}{\partial C_i}$

$$\int_0^1 \frac{\partial R}{\partial C_i} R(x)\,\mathrm{d}x = 0 \qquad i = 1, \ldots, N \tag{328}$$

Method of weighted residuals - example

A polynomial trial functions can be assumed

$$N(x) = x^r(x-1)^s \tag{329}$$

It is continuous and fulfils boundary conditions. Just one trial function for $r = s = 1$ is the simplest case

$$N_1(x) = x(x-1) \tag{330}$$

The approximate solution $\hat{y}(x) = \sum_{i=1}^{N} C_i N_i(x)$ where $N = 1$ takes the following form

$$\hat{y}(x) = C_1 N_1(x) = C_1(x^2 - x) \tag{331}$$

Residual may now be expressed as

$$R(x) = 2C_1 + 20x \neq 0 \tag{332}$$

Method of weighted residuals - example

The unknown constant C_1 may be determined upon integrating (Galerkin's method of weighted residuals)

$$\int_0^1 x(x-1)(2C_1+20x)\,\mathrm{d}x = 0 \tag{333}$$

This gives $-\frac{1}{3}(5+C_1)=0$ and allows to determine $C_1=-5$. The approximate solution is now

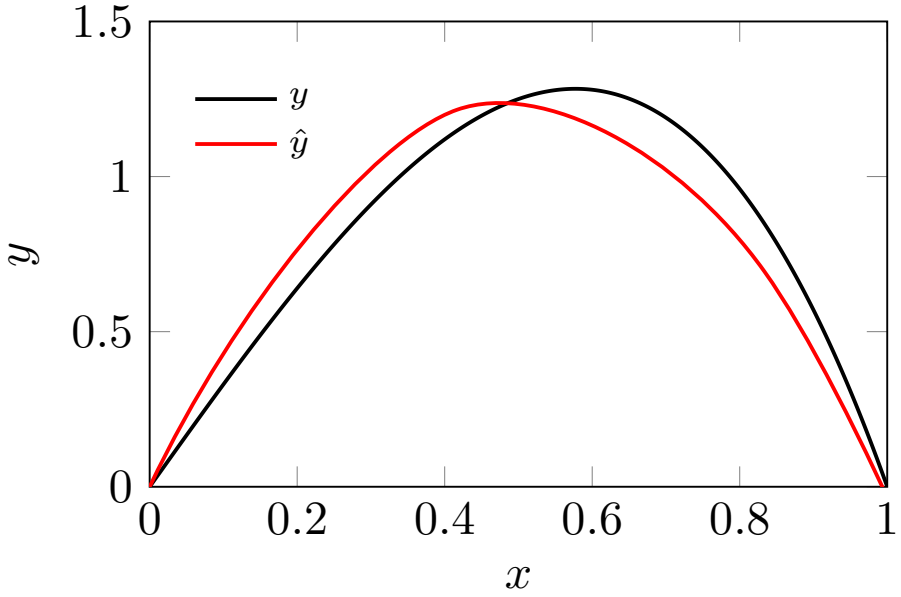
$$\hat{y}(x) = -5x(x-1) \tag{334}$$

and can be compared with the exact solution

$$y(x) = -\frac{10}{3}(x^3-x) \tag{335}$$

Method of weighted residuals - example

The simplest case with just one trial function approximates the exact solution more or less acceptably. Better agreement is possible with more than one trial functions.



Method of weighted residuals - example

The two polynomial trial functions can be assumed

$$N_1(x) = x(x-1), \quad N_2(x) = x^2(x-1) \tag{336}$$

Both are continuous and fulfil boundary conditions. The approximate solution $\hat{y}(x) = \sum_{i=1}^{N} C_i N_i(x)$ where $N = 2$ takes the following form

$$\hat{y}(x) = C_1 N_1(x) + C_2 N_2(x) = C_1(x^2 - x) + C_2(x^3 - x^2) \tag{337}$$

Residual may now be expressed as

$$R(x) = 2C_1 + 2C_2(3x - 1) + 20x \neq 0 \tag{338}$$

Method of weighted residuals - example

The unknown constants C_1, C_2 may be determined upon integrating

$$\int_0^1 x(x-1)(2C_1 + 2C_2(3x-1) + 20x)\,\mathrm{d}x = 0$$
$$\int_0^1 x^2(x-1)(2C_1 + 2C_2(3x-1) + 20x)\,\mathrm{d}x = 0$$

This gives $10 + 2C_1 + C_2 = 0$ and $1 + \frac{1}{6}C_1 + \frac{2}{15}C_2 = 0$ and allows to determine $C_1 = C_2 = -\frac{10}{3}$. The approximate solution is now

$$\hat{y}(x) = -\frac{10}{3}x(x-1)(x+1) \tag{339}$$

Method of weighted residuals - example

The case with two trial function approximates the exact solution very well. It is far better that the previous case. There is no visible difference. In fact, it is even the exact solution

$$-\frac{10}{3}x(x-1)(x+1) = -\frac{10}{3}(x^3 - x) \tag{340}$$

Method of weighted residuals - comments

- The method of weighted residuals constitutes foundation of the final element method
- The method exploits an integral formulation to minimise residual errors
- Trail functions of this method are global. It is usually difficult task to find a proper one that satisfies boundary conditions. The more dimensions the worse.

‘Element’ formulation

The approximate solution is expressed as

$$\hat{y}_e = y_j N_1(x) + y_{j+1} N_2(x) = \mathbf{N} \cdot \mathbf{y}_e \tag{341}$$

where the known local trial functions $\mathbf{N}$ and the unknown nodal values $\mathbf{y}_e$ are collected as vectors

$$\mathbf{N} = (N_1, N_2) \tag{342a}$$

$$\mathbf{y}_e = (y_j, y_{j+1}) \tag{342b}$$

The local trial functions are simply a linear interpolation

$$N_1 = \frac{x_{j+1} - x}{x_{j+1} - x_j} \quad x_j \leq x \leq x_{j+1} \tag{343a}$$

$$N_2 = \frac{x - x_j}{x_{j+1} - x_j} \quad x_j \leq x \leq x_{j+1} \tag{343b}$$

‘Element’ formulation

For each element we have the Galerkin residual condition

$$\int_{x_j}^{x_{j+1}} \mathbf{N}\, R \,\mathrm{d}x = \mathbf{0} \quad j = 1, \ldots, N \tag{344}$$

Taking under consideration our differential equation $y'' + 20x = 0$ and the approximate solution $\hat{y}_e$ it is now possible to express the residual as

$$\int_{x_j}^{x_{j+1}} \mathbf{N} \left(\frac{\mathrm{d}^2 \hat{y}_e}{\mathrm{d}x^2} + 20x \right) \mathrm{d}x = \mathbf{0} \tag{345}$$

The second derivative has to be replaced. This is due to linear nature of the trial functions.

‘Element’ formulation

Integration by parts makes it possible to replace the second derivative

$$\mathbf{N}\frac{\mathrm{d}\hat{y}_e}{\mathrm{d}x}\bigg|_{x_j}^{x_{j+1}} - \int_{x_j}^{x_{j+1}} \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\frac{\mathrm{d}\hat{y}_e}{\mathrm{d}x}\,\mathrm{d}x + \int_{x_j}^{x_{j+1}} \mathbf{N}20x\,\mathrm{d}x = \mathbf{0} \tag{346}$$

Finally, matrix form of the Galerkin residual condition for each element is now

$$\int_{x_j}^{x_{j+1}} \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\,\mathrm{d}x \cdot \mathbf{y}_e = \int_{x_j}^{x_{j+1}} \mathbf{N}20x\,\mathrm{d}x + \mathbf{N}\frac{\mathrm{d}\hat{y}_e}{\mathrm{d}x}\bigg|_{x_j}^{x_{j+1}}$$
$$j = 1, \ldots, N \tag{347}$$

Element equations

The so called 'stiffness' matrix for each element e may be introduced

$$\mathbf{K}_e = \int_{x_j}^{x_{j+1}} \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x} \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x} \, \mathrm{d}x \tag{348}$$

The above matrix is symmetric. The so called 'displacement' vector is also introduced

$$\mathbf{F}_e = \int_{x_j}^{x_{j+1}} \mathbf{N} 20x \, \mathrm{d}x + \mathbf{N} \frac{\mathrm{d}\hat{y}_e}{\mathrm{d}x} \Bigg|_{x_j}^{x_{j+1}} \tag{349}$$

The Galerkin residual condition for each element may now be written as

$$\mathbf{K}_e \cdot \mathbf{y}_e = \mathbf{F}_e \tag{350}$$

Element equations

It is possible to simplify the matrices even further. For the linear trial functions one gets the 'stiffness' matrix

$$\mathbf{K}_e = \int_{x_j}^{x_{j+1}} \begin{pmatrix} \frac{\mathrm{d}N_1}{\mathrm{d}x}\frac{\mathrm{d}N_1}{\mathrm{d}x} & \frac{\mathrm{d}N_1}{\mathrm{d}x}\frac{\mathrm{d}N_2}{\mathrm{d}x} \\ \frac{\mathrm{d}N_1}{\mathrm{d}x}\frac{\mathrm{d}N_2}{\mathrm{d}x} & \frac{\mathrm{d}N_2}{\mathrm{d}x}\frac{\mathrm{d}N_2}{\mathrm{d}x} \end{pmatrix} \mathrm{d}x = \frac{1}{x_{j+1}-x_j} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \tag{351}$$

and the 'displacement vector'

$$\mathbf{F}_e = \int_{x_j}^{x_{j+1}} \begin{pmatrix} N_1 20x \\ N_2 20x \end{pmatrix} \mathrm{d}x + \begin{pmatrix} N_1 \frac{\mathrm{d}\hat{y}_e}{\mathrm{d}x}\Big|_{x_j}^{x_{j+1}} \\ N_2 \frac{\mathrm{d}\hat{y}_e}{\mathrm{d}x}\Big|_{x_j}^{x_{j+1}} \end{pmatrix} \tag{352}$$

If the gradients are dropped, as discussed further, we have

$$\mathbf{F}_e = -\frac{10}{3}(x_j - x_{j+1}) \begin{pmatrix} 2x_j + x_{j+1} \\ x_j + 2x_{j+1} \end{pmatrix} \tag{353}$$

Element equations - example

For the interval $[0;1]$ divided equally into 3 elements we have the element matrices

$$\mathbf{K}_1 = \mathbf{K}_2 = \mathbf{K}_3 = \begin{pmatrix} 3 & -3 \\ -3 & 3 \end{pmatrix} \tag{354}$$

The global assembly process (coupling):

$$\mathbf{K} = \begin{pmatrix} K_1^{11} & K_1^{12} & 0 & 0 \\ K_1^{12} & K_1^{22} + K_2^{11} & K_2^{12} & 0 \\ 0 & K_2^{12} & K_2^{22} + K_3^{11} & K_3^{12} \\ 0 & 0 & K_3^{12} & K_3^{22} \end{pmatrix} \tag{355}$$

results in

$$\mathbf{K} = \begin{pmatrix} 3 & -3 & 0 & 0 \\ -3 & 6 & -3 & 0 \\ 0 & -3 & 6 & -3 \\ 0 & 0 & -3 & 3 \end{pmatrix} \tag{356}$$

Element equations - example

The 'displacement' vector for equally divided interval $[0;1]$ take form

$$\mathbf{F}_1 = \begin{pmatrix} \frac{10}{27} - \frac{\mathrm{d}y(0)}{\mathrm{d}x} \\ \frac{20}{27} + \frac{\mathrm{d}y(\frac{1}{3})}{\mathrm{d}x} \end{pmatrix}, \mathbf{F}_2 = \begin{pmatrix} \frac{40}{27} - \frac{\mathrm{d}y(\frac{1}{3})}{\mathrm{d}x} \\ \frac{50}{27} + \frac{\mathrm{d}y(\frac{2}{3})}{\mathrm{d}x} \end{pmatrix}, \mathbf{F}_3 = \begin{pmatrix} \frac{70}{27} - \frac{\mathrm{d}y(\frac{2}{3})}{\mathrm{d}x} \\ \frac{80}{27} + \frac{\mathrm{d}y(1)}{\mathrm{d}x} \end{pmatrix} \tag{357}$$

After the global assembly process one finally gets

$$\mathbf{F} = \begin{pmatrix} F_1^1 \\ F_1^2 + F_2^1 \\ F_2^2 + F_3^1 \\ F_3^2 \end{pmatrix} = \begin{pmatrix} \frac{10}{27} - \frac{\mathrm{d}y(0)}{\mathrm{d}x} \\ \frac{60}{27} \\ \frac{120}{27} \\ \frac{80}{27} + \frac{\mathrm{d}y(1)}{\mathrm{d}x} \end{pmatrix} \tag{358}$$

System of equations – example

The global (assembled) system of linear equations is

$$\begin{pmatrix} 3 & -3 & 0 & 0 \\ -3 & 6 & -3 & 0 \\ 0 & -3 & 6 & -3 \\ 0 & 0 & -3 & 3 \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} \frac{10}{27} - \frac{\mathrm{d}y(0)}{\mathrm{d}x} \\ \frac{60}{27} \\ \frac{120}{27} \\ \frac{80}{27} + \frac{\mathrm{d}y(1)}{\mathrm{d}x} \end{pmatrix} \quad (359)$$

It cannot, however, be solved yet. This is due to necessity of applying the global boundary conditions. These are $y_1 = y_4 = 0$. Two typical methods of applying them are discussed further.

Extracting only these equations that are related to unknown functions y_2 and y_3 for $y_1 = y_4 = 0$ results in

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & 6 & -3 & \cdot \\ \cdot & -3 & 6 & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \cdot \begin{pmatrix} \cdot \\ y_2 \\ y_3 \\ \cdot \end{pmatrix} = \begin{pmatrix} \cdot \\ \frac{60}{27} \\ \frac{120}{27} \\ \cdot \end{pmatrix} \tag{360}$$

or simpler in

$$\begin{pmatrix} 6 & -3 \\ -3 & 6 \end{pmatrix} \cdot \begin{pmatrix} y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} \frac{60}{27} \\ \frac{120}{27} \end{pmatrix} \tag{361}$$

The above system may now be solved to obtain the unknown values y_2, y_3.

Boundary conditions

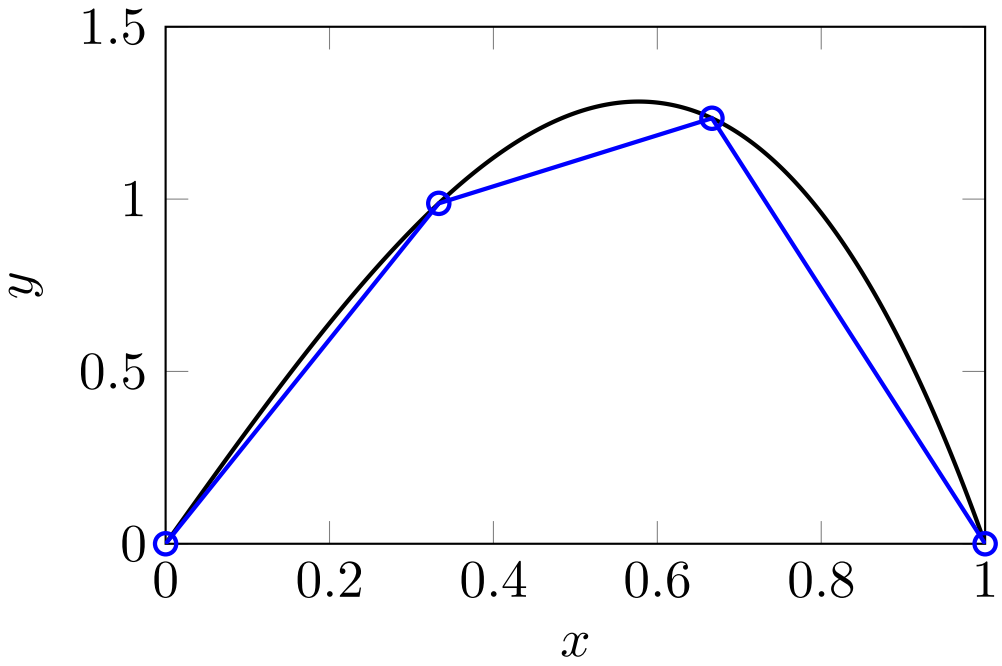
The second method does not change the layout of the matrices. However, it involves modification of specific elements by multiplying them by a 'large' number. These elements are located on the diagonal of the 'stiffness' matrix and corresponding positions of the 'displacement' vector (if non-zero)

$$\begin{pmatrix} 3\cdot 10^7 & -3 & 0 & 0 \\ -3 & 6 & -3 & 0 \\ 0 & -3 & 6 & -3 \\ 0 & 0 & -3 & 3\cdot 10^7 \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{60}{27} \\ \frac{120}{27} \\ 0 \end{pmatrix} \quad (362)$$

ODE FEM pseudocode

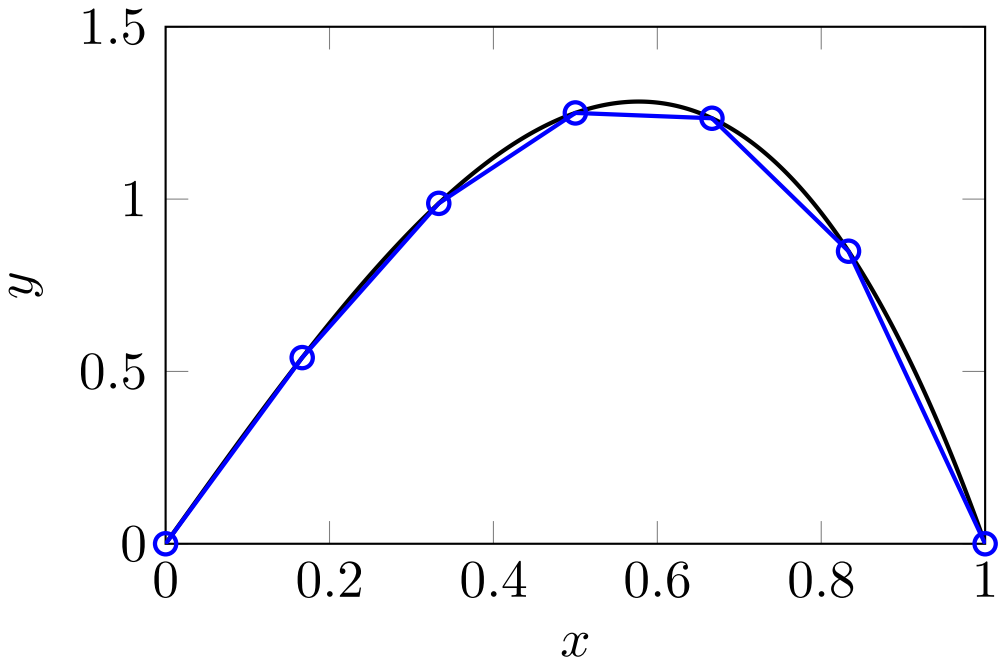
Data: Read N elements, nodes and BCs
Create global matrix $\mathbf{K}$ and vectors $\mathbf{F}$, $\mathbf{y}$;
for $e := 1$ **to** N **do**
    $\mathbf{K}_e := \int_e \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\,\mathrm{d}x$;
    $\mathbf{F}_e := \int_e \mathbf{N}20x\,\mathrm{d}x$;
    Add $\mathbf{K}_e$ to $\mathbf{K}$;
    Add $\mathbf{F}_e$ to $\mathbf{F}$;
Apply BCs;
Solve linear system $\mathbf{K}\cdot\mathbf{y} = \mathbf{F}$;

Results - ODE



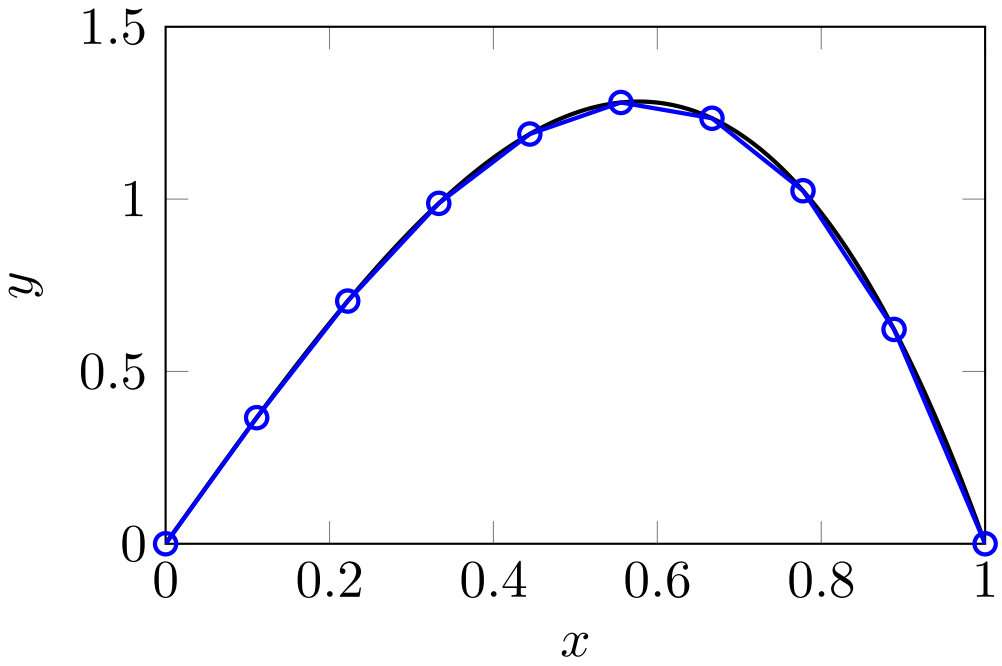
3 elements, 4 nodes

Results - ODE



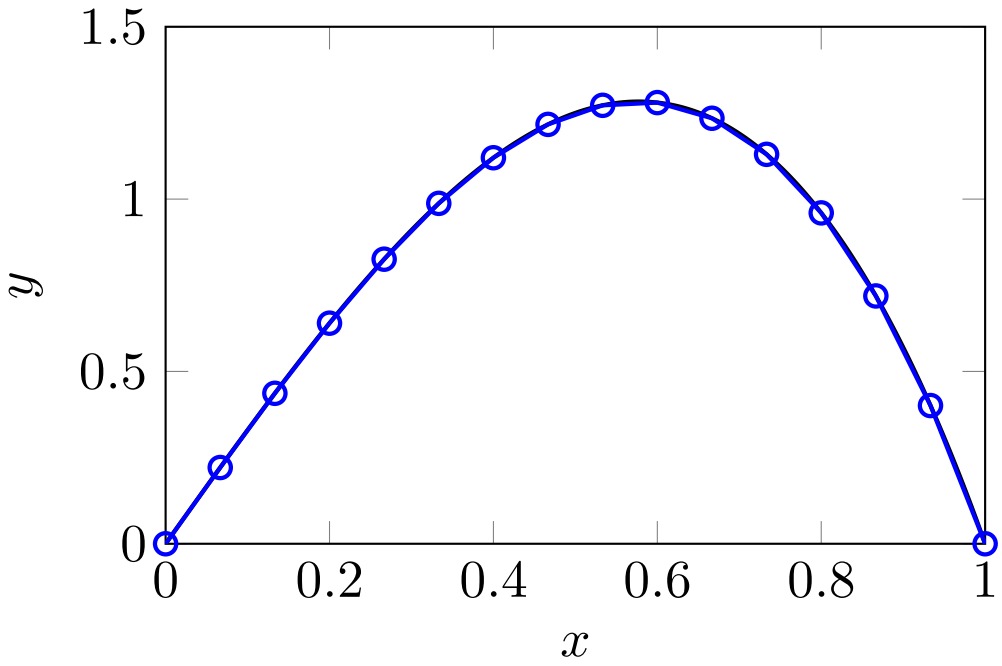
6 elements, 7 nodes

Results - ODE



9 elements, 10 nodes

Results - ODE



15 elements, 16 nodes

Linear and quadratic interpolation

Considering line equation $\hat{y}_e = a + bx$ and utilising it for two different points (x_j, y_j) and (x_{j+1}, y_{j+1}) we can get the following system of equations

$$\begin{pmatrix} y_j \\ y_{j+1} \end{pmatrix} = \begin{pmatrix} 1 & x_j \\ 1 & x_{j+1} \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} \tag{363}$$

It can be easily solved for a and b

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & x_j \\ 1 & x_{j+1} \end{pmatrix}^{-1} \cdot \begin{pmatrix} y_j \\ y_{j+1} \end{pmatrix} \tag{364}$$

Keeping in mind that $\hat{y}_e = \mathbf{N} \cdot \mathbf{y}_e$ where $\mathbf{N} = (N_1, N_2)$ and $\mathbf{y}_e = (y_j, y_{j+1})$ we can utilise the solution for a and b to get

$$\hat{y}_e = a + bx = \frac{x_{j+1} - x}{x_{j+1} - x_j} y_j + \frac{x - x_j}{x_{j+1} - x_j} y_{j+1} = N_1 y_j + N_2 y_{j+1} \tag{365}$$

Linear and quadratic interpolation

Introducing L_1 and L_2 for a one-dimensional element

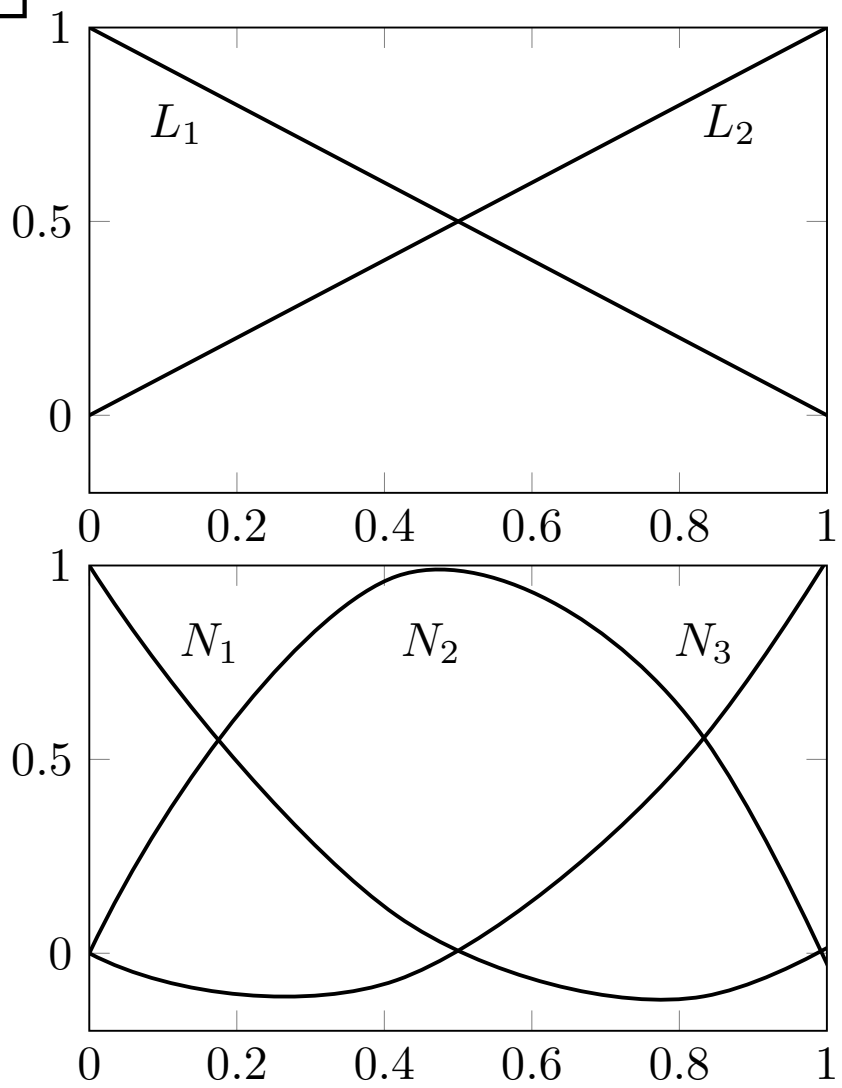
$$L_1 = N_1 = \frac{x_{j+1} - x}{x_{j+1} - x_j} \tag{366a}$$

$$L_2 = N_2 = \frac{x - x_j}{x_{j+1} - x_j} \tag{366b}$$

one can formulate similar system of equation for quadratic interpolation $\hat{y}_e = a + bx + cx^2$ through the points (x_j, y_j), $(x_{j+\frac{1}{2}}, y_{j+\frac{1}{2}})$ and (x_{j+1}, y_{j+1})

$$\begin{pmatrix} y_j \\ y_{j+\frac{1}{2}} \\ y_{j+1} \end{pmatrix} = \begin{pmatrix} 1 & x_j & x_j^2 \\ 1 & x_{j+\frac{1}{2}} & x_{j+\frac{1}{2}}^2 \\ 1 & x_{j+1} & x_{j+1}^2 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} \tag{367}$$

Linear and quadratic interpolation



The quadratic trial functions can be also expressed in terms of linear trial functions

$$N_1 = L_1 (2L_1 - 1),$$
$$N_2 = 4L_1 L_2,$$
$$N_3 = L_2 (2L_2 - 1)$$

Quadratic interpolation

The 'stiffness' matrix for each element e may now be calculated as

$$\mathbf{K}_e = \int_{x_j}^{x_{j+1}} \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x}\,\mathrm{d}x = \frac{1}{3(x_{j+1}-x_j)}\begin{pmatrix} 7 & -8 & 1 \\ -8 & 16 & -8 \\ 1 & -8 & 7 \end{pmatrix} \tag{369}$$

The 'displacement' vector is now

$$\mathbf{F}_e = \int_{x_j}^{x_{j+1}} \mathbf{N}20x\,\mathrm{d}x = \frac{10}{3}(x_{j+1}-x_j)\begin{pmatrix} x_j \\ 2(x_j+x_{j+1}) \\ x_{j+1} \end{pmatrix} \tag{370}$$

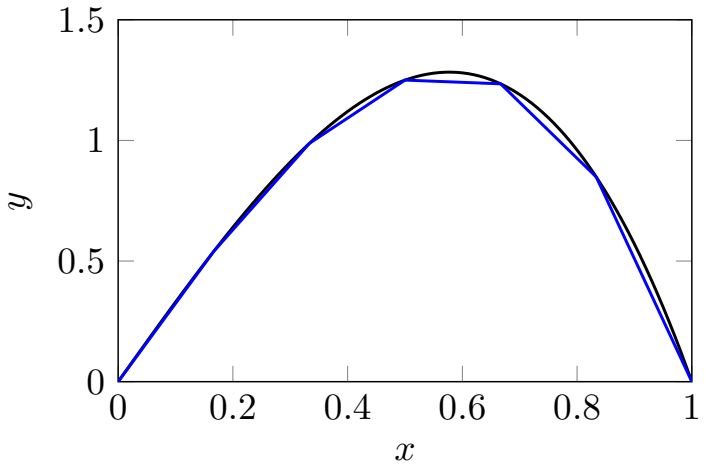
The Galerkin residual condition for each element is the same as previously

$$\mathbf{K}_e \cdot \mathbf{y}_e = \mathbf{F}_e \tag{371}$$

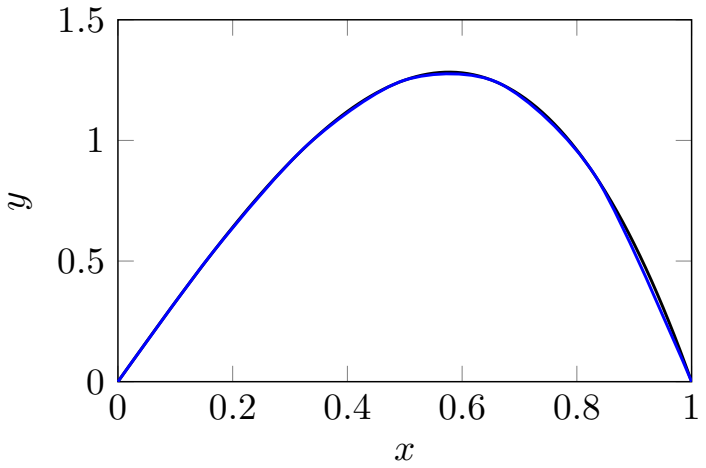
ODE quadratic FEM pseudocode

Data: Read N linear elements, n nodes and BCs
Insert midpoints $x_{j+\frac{1}{2}} := \frac{x_j + x_{j+1}}{2}$;
$n := 2n - 1$;
Create global matrix $\mathbf{K}$ and vectors $\mathbf{F}$, $\mathbf{y}$;
for $e := 1$ **to** N **do**
    $\mathbf{K}_e := \int_e \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x} \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}x} \, \mathrm{d}x$;
    $\mathbf{F}_e := \int_e \mathbf{N} 20x \, \mathrm{d}x$;
    Add $\mathbf{K}_e$ to $\mathbf{K}$;
    Add $\mathbf{F}_e$ to $\mathbf{F}$;
Apply BCs;
Solve linear system $\mathbf{K} \cdot \mathbf{y} = \mathbf{F}$;

ODE - linear vs quadratic interpolation



6 elements, 7 nodes.



3 elements, 7 nodes.

The generalised p-norm is given by

$$\|f\|_p = \left(\int_L |f(x)|^p \, \mathrm{d}x \right)^{\frac{1}{p}} \tag{372}$$

where for $p = 2$ we have a special case

$$\|f\|_2 = \sqrt{\int_L f^2(x) \, \mathrm{d}x} \tag{373}$$

The error $E = y - \hat{y}$ of a finite element solution $\hat{y}$ may now be defined by means of 2-norm. It may take the following form

$$\|E'\|_2^2 \leq C \sum_{e=1}^{N} r_e^2 \tag{374}$$

Mesh refinement

The element residue r_e is defined as

$$r_e = |L_e| \, \|f + \hat{y}_e''\|_2 \tag{375}$$

but due to the linear form of trial functions $N_i'' = 0$ it is true that $\hat{y}_e'' = 0$. This means that the element residue is $r_e = |L_e| \, \|f\|_2$ and solution error

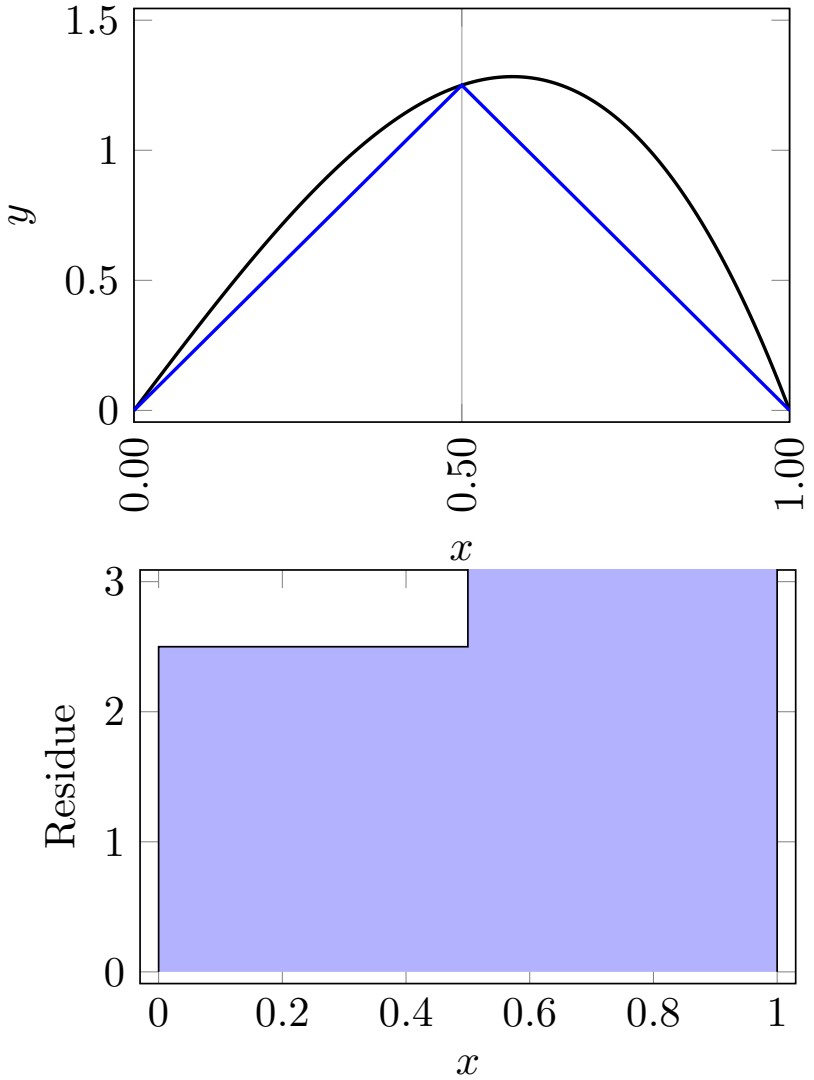
$$\|E'\|_2^2 \leq C \sum_{e=1}^{N} |L_e|^2 \|f\|_2^2 \tag{376}$$

Element's length is $|L_e| = x_{j+1} - x_j$ and utilising the trapezoidal rule we can express the element residue as

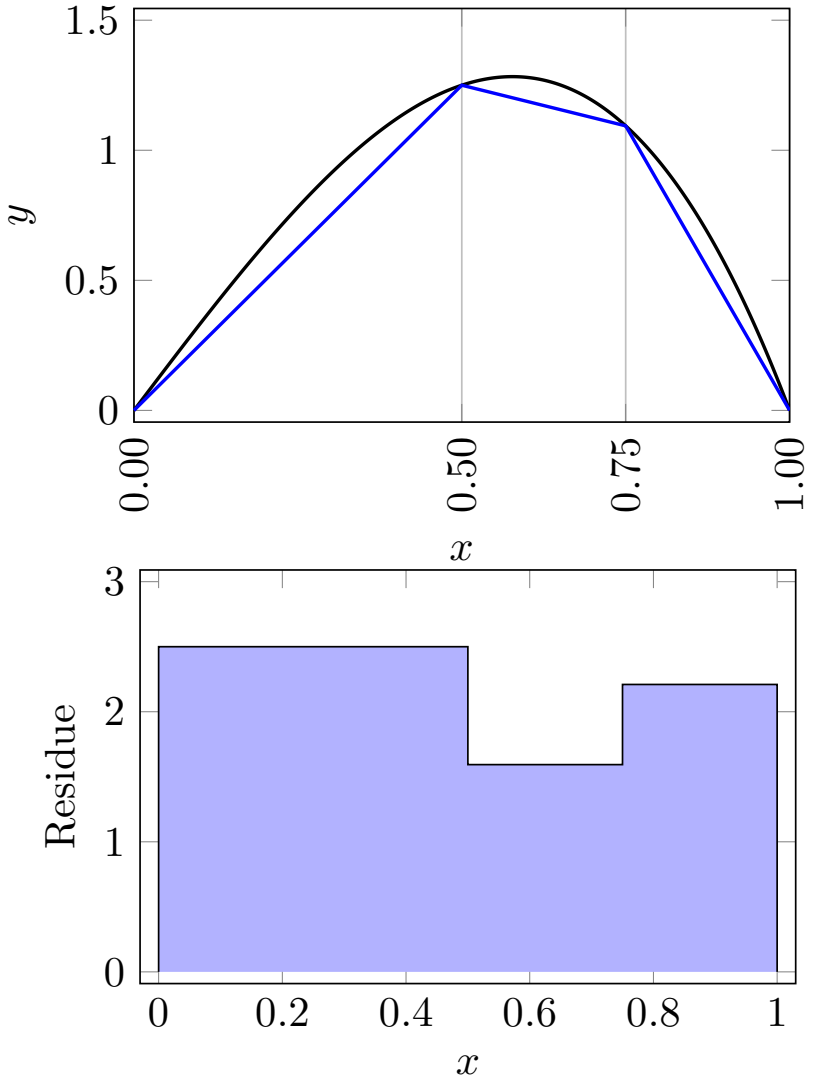
$$r_e = |L_e| \sqrt{\int_{L_e} f(x)^2 \, \mathrm{d}x} \approx (x_{j+1} - x_j)^{\frac{3}{2}} \sqrt{\frac{f_j^2 + f_{j+1}^2}{2}} \tag{377}$$

The above approximation is used for mesh refinement.

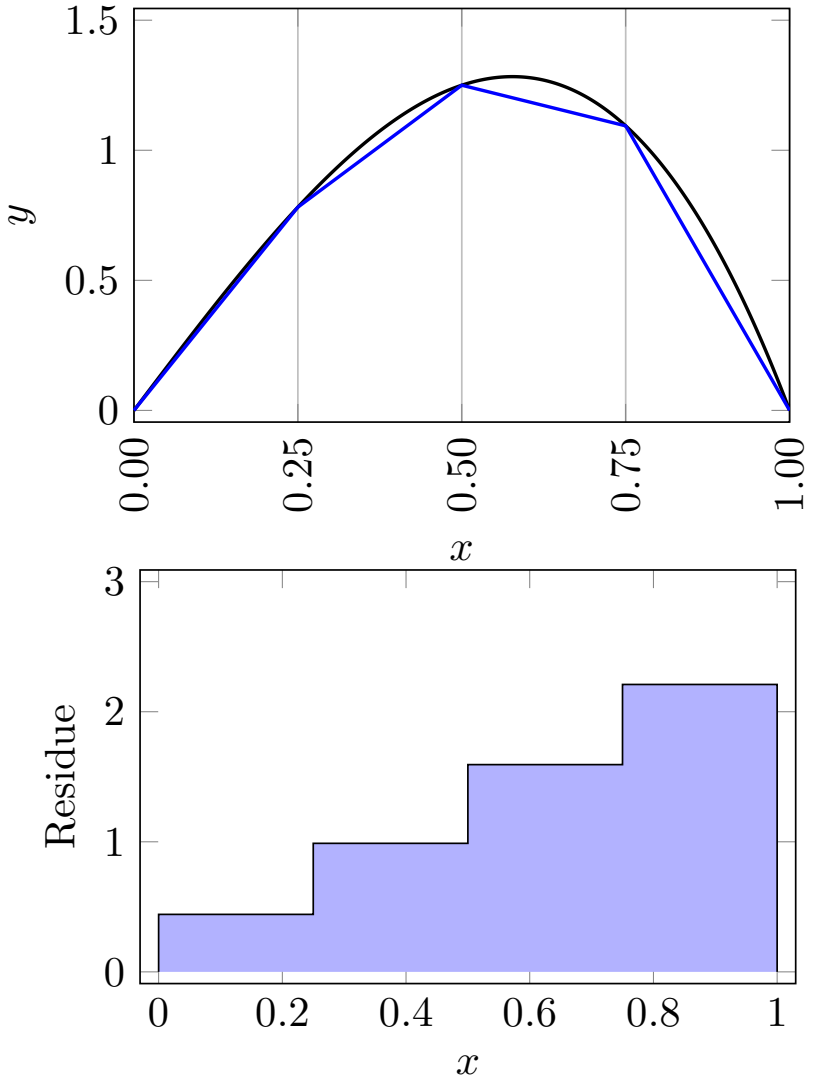
Mesh refinement - results



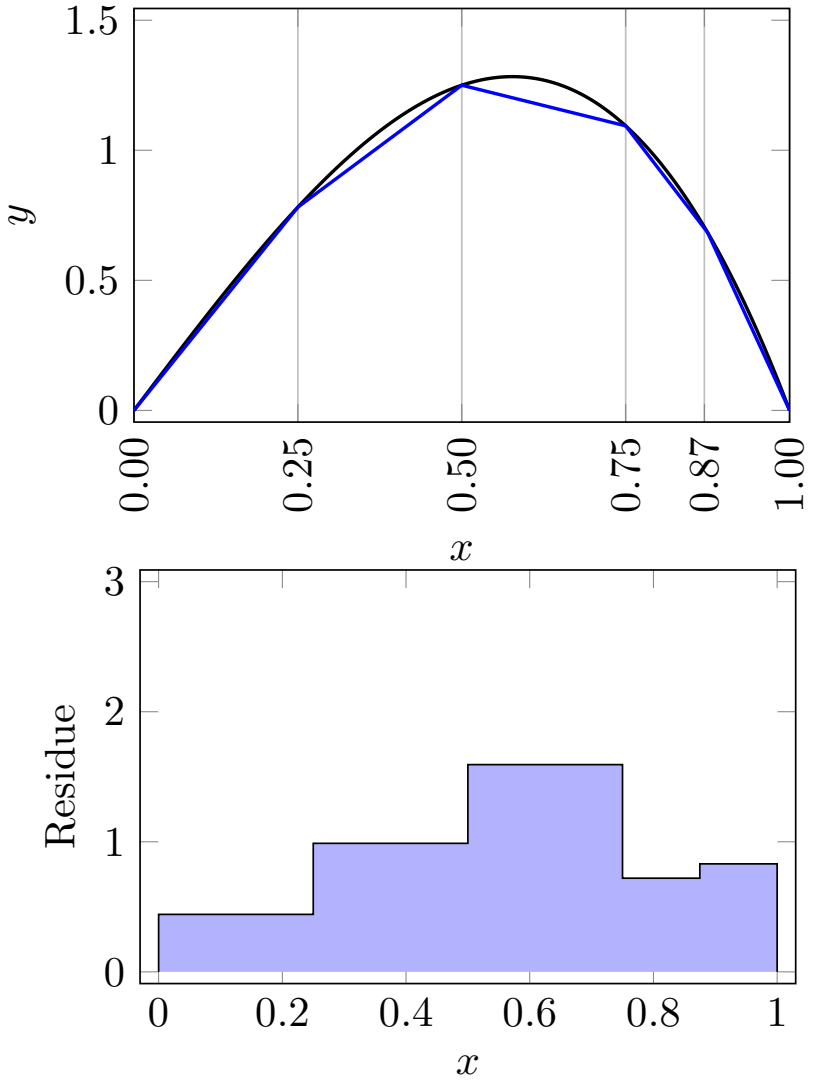
Mesh refinement - results



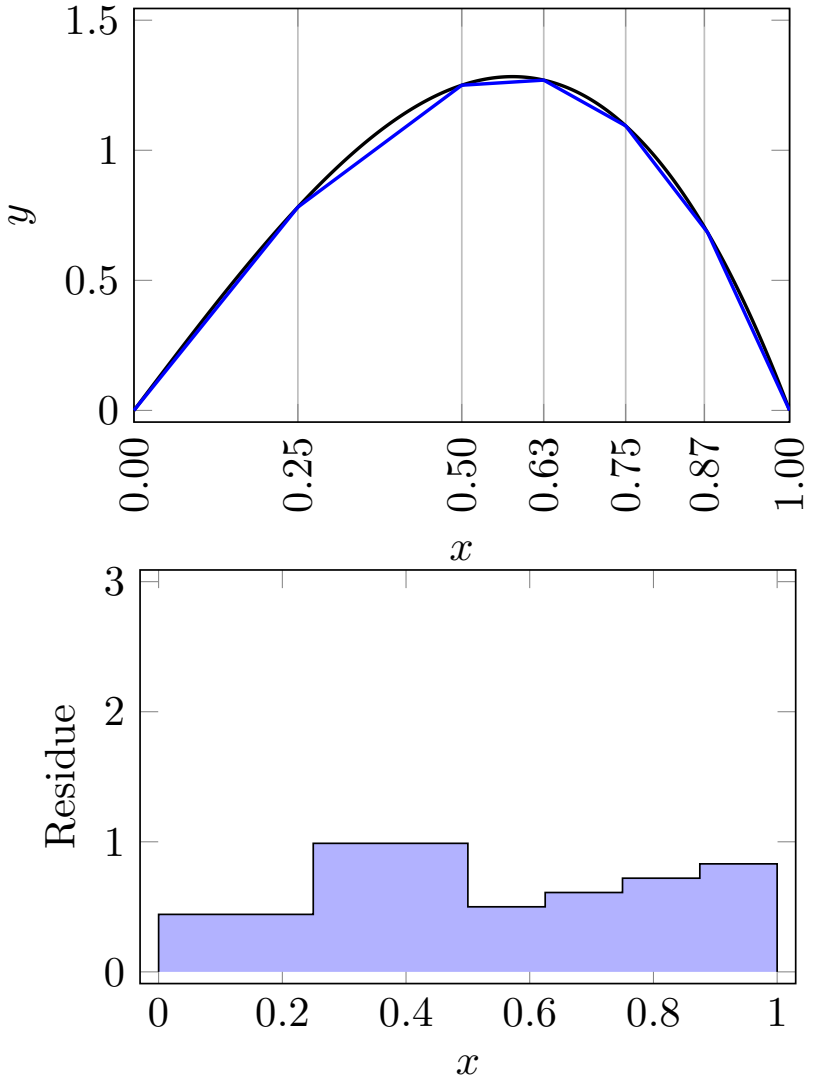
Mesh refinement - results



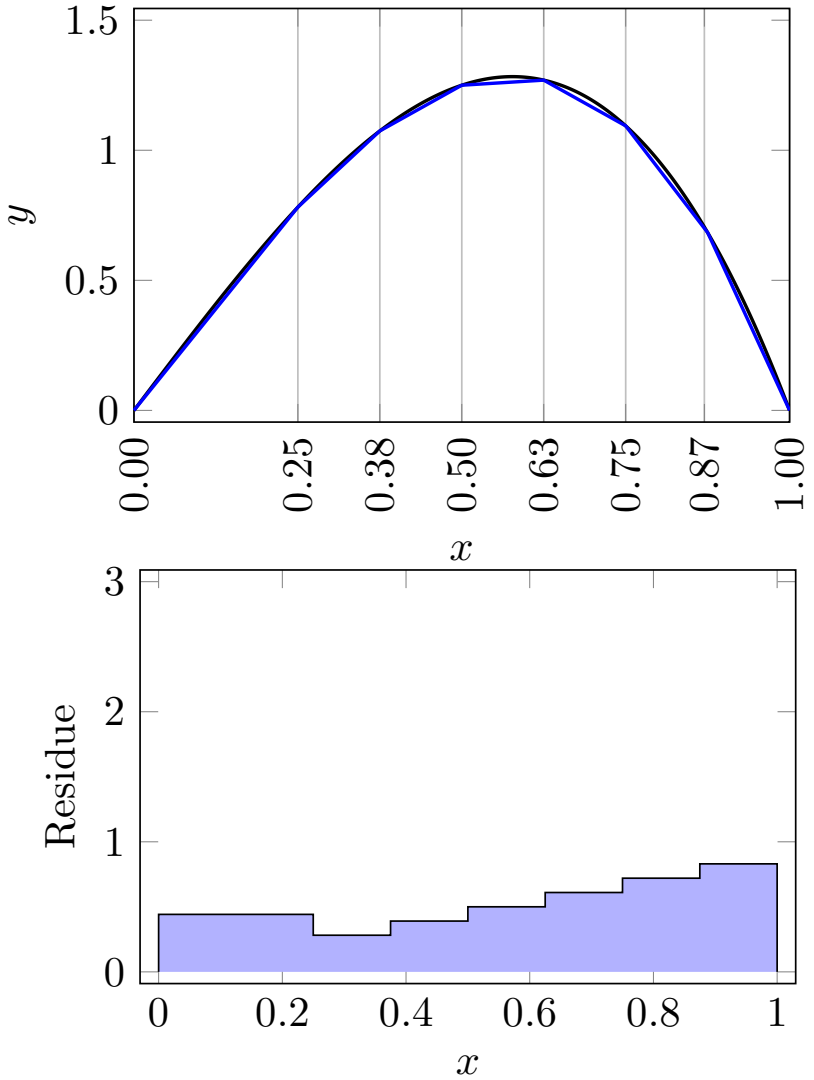
Mesh refinement - results



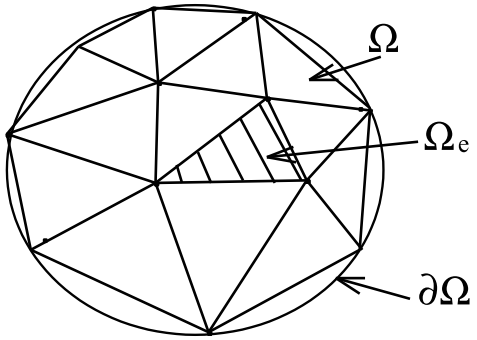
Mesh refinement - results



Mesh refinement - results



FEM for Poisson equation



Let the two dimensional form of the Poisson equation on Ω

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = -a \qquad (378)$$

be subjected to the Dirichlet boundary condition $U(x, y) = 0$ for every $(x, y) \in \partial\Omega$. It is true that

$$\iint_\Omega f(x, y)\,\mathrm{d}x\,\mathrm{d}y = \sum_e \iint_{\Omega_e} f(x, y)\,\mathrm{d}x\,\mathrm{d}y \qquad (379)$$

‘Element’ formulation

The approximate solution is expressed as

$$\hat{U}_e = \mathbf{N} \cdot \mathbf{U}_e \tag{380}$$

where the known local trial functions $\mathbf{N}$ and the unknown nodal values U_e are

$$\mathbf{N} = (N_1, N_2, N_3) \tag{381a}$$
$$\mathbf{U}_e = (U_1, U_2, U_3) \tag{381b}$$

For each element we have the Galerkin residual condition

$$\iint_{\Omega_e} \mathbf{N}\, R \, \mathrm{d}x = \mathbf{0} \tag{382}$$

‘Element’ formulation

Taking under consideration Poisson equation and the approximate solution $\hat{U}_e$ it is now possible to express the residual as

$$\iint_{\Omega_e} \mathbf{N} \left(\frac{\partial^2 \hat{U}_e}{\partial x^2} + \frac{\partial^2 \hat{U}_e}{\partial y^2} + a \right) \mathrm{d}x \, \mathrm{d}y = \mathbf{0} \qquad (383)$$

The second derivative has to be replaced (due to linear nature of the trial functions). This can be done by means of Green’s first identity

$$\iint_S \left(\psi \frac{\partial^2 \varphi}{\partial x^2} + \psi \frac{\partial^2 \varphi}{\partial y^2} \right) \mathrm{d}x \, \mathrm{d}y = \int_{\partial S} \psi \frac{\partial \varphi}{\partial n} \, \mathrm{d}L - \iint_S \left(\frac{\partial \psi}{\partial x} \frac{\partial \varphi}{\partial x} + \frac{\partial \psi}{\partial y} \frac{\partial \varphi}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \qquad (384)$$

‘Element’ formulation

Integration by means of Green’s identity makes it possible to replace the second derivative

$$\iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \hat{U}_e}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \hat{U}_e}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y - \int_{\partial \Omega_e} \mathbf{N} \frac{\partial \hat{U}_e}{\partial n} \mathrm{d}L - \iint_{\Omega_e} \mathbf{N} a \, \mathrm{d}x \, \mathrm{d}y = \mathbf{0} \quad (385)$$

The matrix form of the Galerkin residual condition for each element can now be expressed

$$\iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \cdot \mathbf{U}_e = \iint_{\Omega_e} \mathbf{N} a \, \mathrm{d}x \, \mathrm{d}y \quad (386)$$

Element equation

Introducing the 'stiffness' matrix for each element e

$$\mathbf{K}_e = \iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \tag{387}$$

and the 'displacement' vector

$$\mathbf{F}_e = \iint_{\Omega_e} \mathbf{N} a \, \mathrm{d}x \, \mathrm{d}y \tag{388}$$

one may obtain the Galerkin residual condition for each element in the form

$$\mathbf{K}_e \cdot \mathbf{U}_e = \mathbf{F}_e \tag{389}$$

Element equation

The expanded version of the 'stiffness' matrix is

$$\mathbf{K}_e = \iint_{\Omega_e} \begin{pmatrix} \frac{\partial N_1}{\partial x}\frac{\partial N_1}{\partial x} + \frac{\partial N_1}{\partial y}\frac{\partial N_1}{\partial y} & \frac{\partial N_1}{\partial x}\frac{\partial N_2}{\partial x} + \frac{\partial N_1}{\partial y}\frac{\partial N_2}{\partial y} & \frac{\partial N_1}{\partial x}\frac{\partial N_3}{\partial x} + \frac{\partial N_1}{\partial y}\frac{\partial N_3}{\partial y} \\ \frac{\partial N_1}{\partial x}\frac{\partial N_2}{\partial x} + \frac{\partial N_1}{\partial y}\frac{\partial N_2}{\partial y} & \frac{\partial N_2}{\partial x}\frac{\partial N_2}{\partial x} + \frac{\partial N_2}{\partial y}\frac{\partial N_2}{\partial y} & \frac{\partial N_2}{\partial x}\frac{\partial N_3}{\partial x} + \frac{\partial N_2}{\partial y}\frac{\partial N_3}{\partial y} \\ \frac{\partial N_1}{\partial x}\frac{\partial N_3}{\partial x} + \frac{\partial N_1}{\partial y}\frac{\partial N_3}{\partial y} & \frac{\partial N_2}{\partial x}\frac{\partial N_3}{\partial x} + \frac{\partial N_2}{\partial y}\frac{\partial N_3}{\partial y} & \frac{\partial N_3}{\partial x}\frac{\partial N_3}{\partial x} + \frac{\partial N_3}{\partial y}\frac{\partial N_3}{\partial y} \end{pmatrix} \mathrm{d}x\,\mathrm{d}y \tag{390}$$

Similarly, the same for the 'displacement' vector

$$\mathbf{F}_e = a \iint_{\Omega_e} \begin{pmatrix} N_1 \\ N_2 \\ N_3 \end{pmatrix} \mathrm{d}x\,\mathrm{d}y \tag{391}$$

The actual form of matrices depends on the trial functions. Linear form of these are discussed further.

Linear trial function

Considering plane equation

$$\hat{U}_e = a + bx + cy \tag{392}$$

one can formulate the following system of equations

$$U_1 = a + bx_i + cy_i \tag{393a}$$
$$U_2 = a + bx_j + cy_j \tag{393b}$$
$$U_3 = a + bx_k + cy_k \tag{393c}$$

for three different points (x_i, y_i), (x_j, y_j), (x_k, y_k).
Solving these for a, b and c results in

$$\hat{U}_e = \frac{U_1}{2S_e}(a_i + b_i x + c_i y) + \frac{U_2}{2S_e}(a_j + b_j x + c_j y) + \frac{U_3}{2S_e}(a_k + b_k x + c_k y) \tag{394}$$

Linear trial function

The linear trial functions then are

$$N_1 = \frac{1}{2S_e}(a_i + b_i x + c_i y) \tag{395a}$$

$$N_2 = \frac{1}{2S_e}(a_j + b_j x + c_j y) \tag{395b}$$

$$N_3 = \frac{1}{2S_e}(a_k + b_k x + c_k y) \tag{395c}$$

where

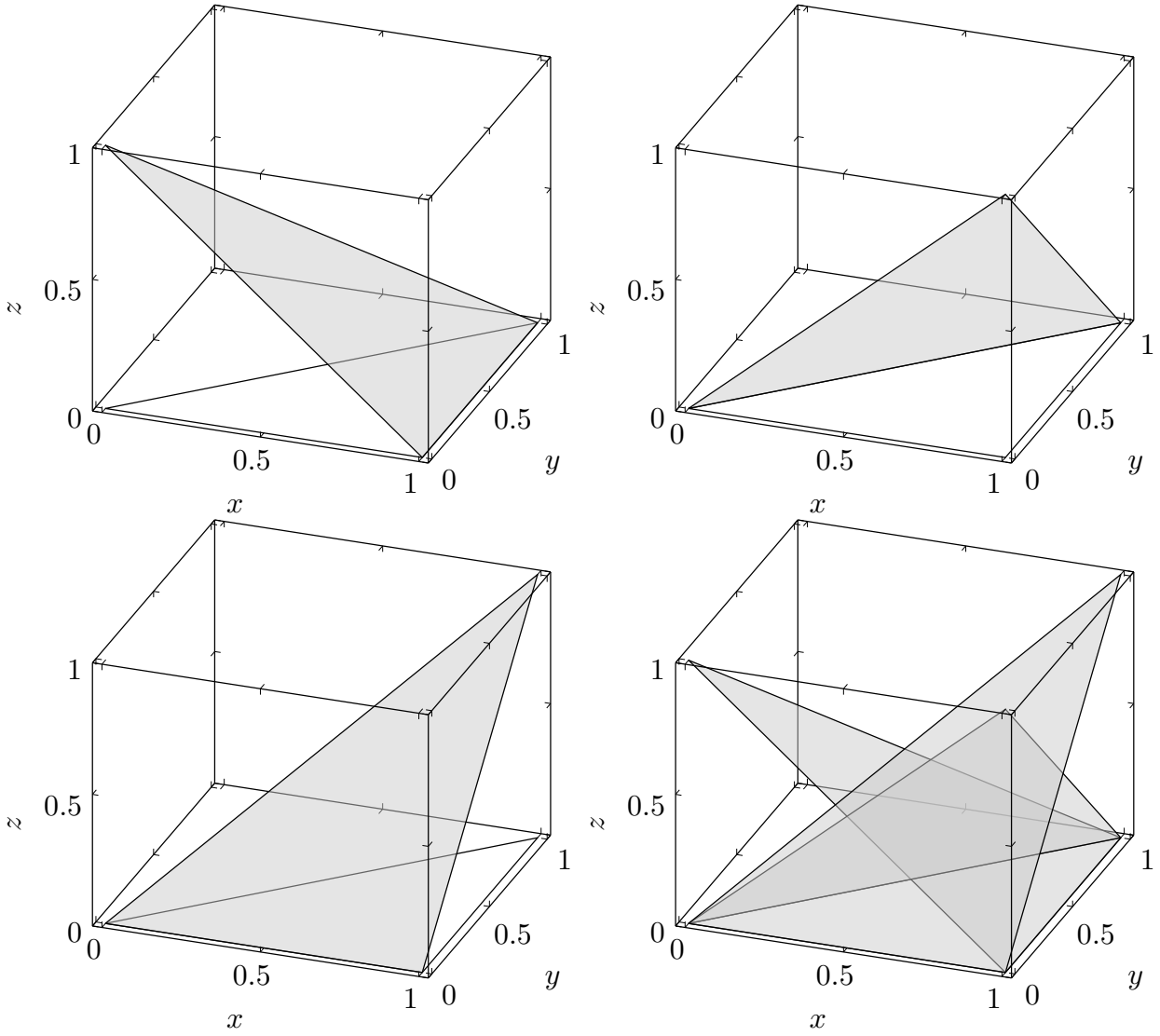
$$a_i = x_j y_k - x_k y_j; a_j = x_k y_i - x_i y_k; a_k = x_i y_j - x_j y_i;$$

$$b_i = y_j - y_k; b_j = y_k - y_i; b_k = y_i - y_j;$$

$$c_i = x_k - x_j; c_j = x_i - x_k; c_k = x_j - x_i;$$

$$S_e = \frac{1}{2}|c_k b_j - c_j b_k|$$

Linear interpolation



Integrals and derivatives

Now it is possible to calculate necessary derivatives appearing in the 'stiffness' matrix

$$\frac{\partial N_1}{\partial x} = \frac{b_i}{2S_e}, \quad \frac{\partial N_2}{\partial x} = \frac{b_j}{2S_e}, \quad \frac{\partial N_3}{\partial x} = \frac{b_k}{2S_e}, \tag{397a}$$

$$\frac{\partial N_1}{\partial y} = \frac{c_i}{2S_e}, \quad \frac{\partial N_2}{\partial y} = \frac{c_j}{2S_e}, \quad \frac{\partial N_3}{\partial y} = \frac{c_k}{2S_e} \tag{397b}$$

The same concerns integrals appearing in the 'displacement' vector

$$\iint_{S_e} N_1^\alpha N_2^\beta N_3^\gamma \,\mathrm{d}x\,\mathrm{d}y = 2S_e \frac{\alpha!\beta!\gamma!}{(\alpha+\beta+\gamma+2)!} \tag{397c}$$

Element equation

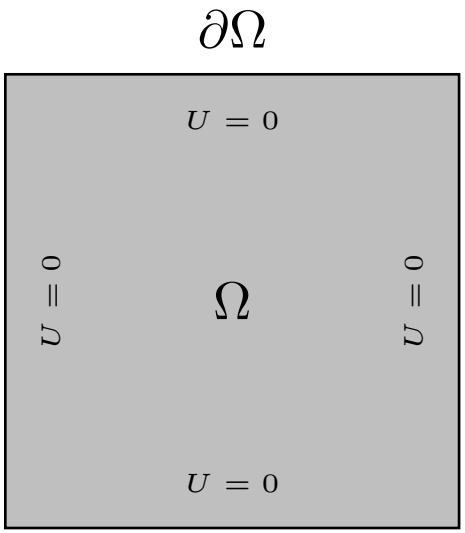
Now it is possible to simplify the matrices even further. For the linear trial functions one gets the 'stiffness' matrix

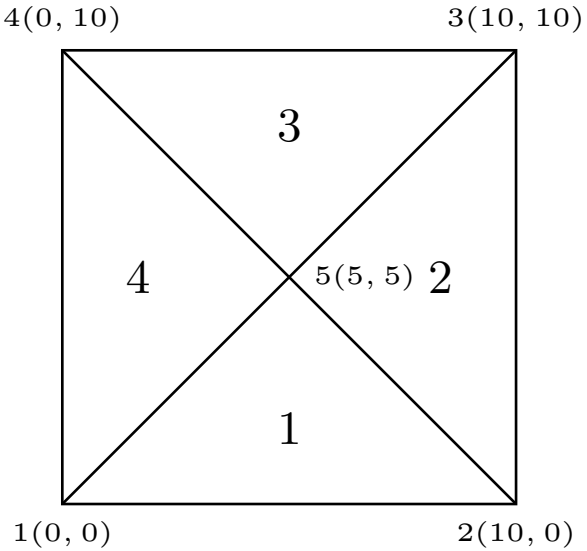
$$\mathbf{K}_e = \frac{1}{4S_e} \begin{pmatrix} b_i^2 + c_i^2 & b_i b_j + c_i c_j & b_i b_k + c_i c_k \\ b_i b_j + c_i c_j & b_j^2 + c_j^2 & b_j b_k + c_j c_k \\ b_i b_k + c_i c_k & b_j b_k + c_j c_k & b_k^2 + c_k^2 \end{pmatrix} \tag{398}$$

and the 'displacement vector'

$$\mathbf{F}_e = \frac{S_e}{3} \begin{pmatrix} a \\ a \\ a \end{pmatrix} \tag{399}$$

Four element example





Global matrix

The global assembly process (coupling) for the considered four element case:

$$\mathbf{K}=\begin{pmatrix} K_1^{11}+K_4^{11} & K_1^{12} & 0 & K_4^{12} & K_1^{13}+K_4^{13} \\ K_1^{12} & K_1^{22}+K_2^{11} & K_2^{12} & 0 & K_1^{23}+K_2^{13} \\ 0 & K_2^{12} & K_2^{22}+K_3^{11} & K_3^{12} & K_2^{23}+K_3^{13} \\ K_4^{12} & 0 & K_3^{12} & K_3^{22}+K_4^{22} & K_3^{23}+K_4^{23} \\ K_1^{13}+K_4^{13} & K_1^{23}+K_2^{13} & K_2^{23}+K_3^{13} & K_3^{23}+K_4^{23} & K_1^{33}+K_2^{33}+K_3^{33}+K_4^{33} \end{pmatrix} \tag{400}$$

The element matrices are identical

$$\mathbf{K}_1=\mathbf{K}_2=\mathbf{K}_3=\mathbf{K}_4=\frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ -1 & -1 & 2 \end{pmatrix} \tag{401}$$

Finally, the global 'stiffness' matrix is

$$\mathbf{K}=\begin{pmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & -1 & -1 & -1 & 4 \end{pmatrix} \tag{402}$$

Global vector

The 'displacement' element vector for the considered four elements

$$\mathbf{F}_1 = \mathbf{F}_2 = \mathbf{F}_3 = \mathbf{F}_4 = \frac{25}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \tag{403}$$

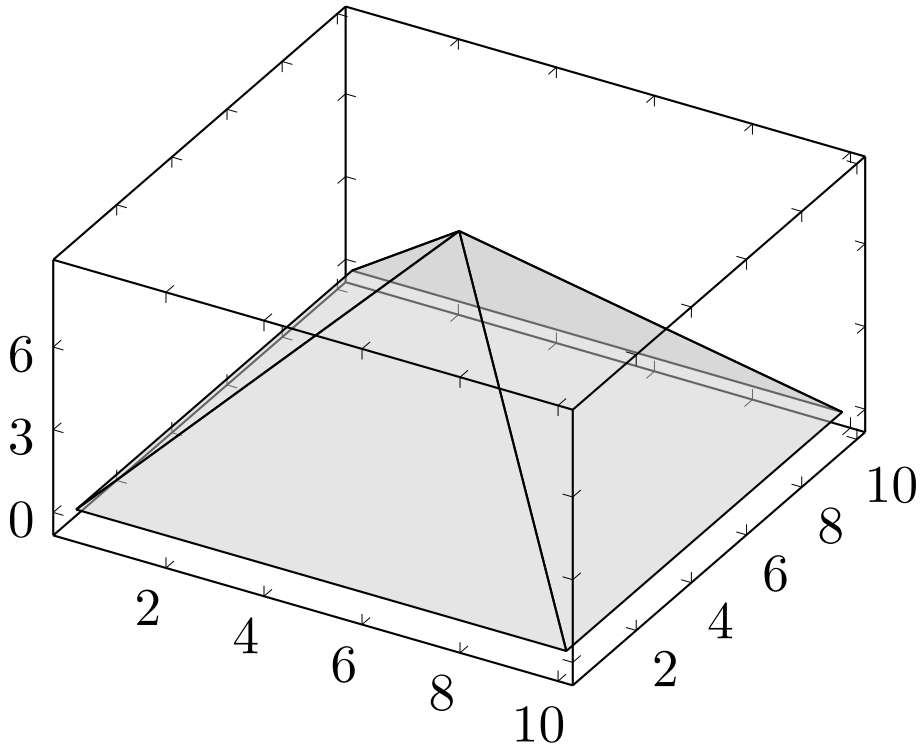
After the global assembly process one finally gets

$$\mathbf{F} = \begin{pmatrix} F_1^1 + F_4^1 \\ F_1^2 + F_2^1 \\ F_2^2 + F_3^1 \\ F_3^2 + F_4^2 \\ F_1^3 + F_2^3 + F_3^3 + F_4^3 \end{pmatrix} = \frac{50}{3}\begin{pmatrix}1\\1\\1\\1\\2\end{pmatrix} \tag{404}$$

Poisson FEM pseudocode

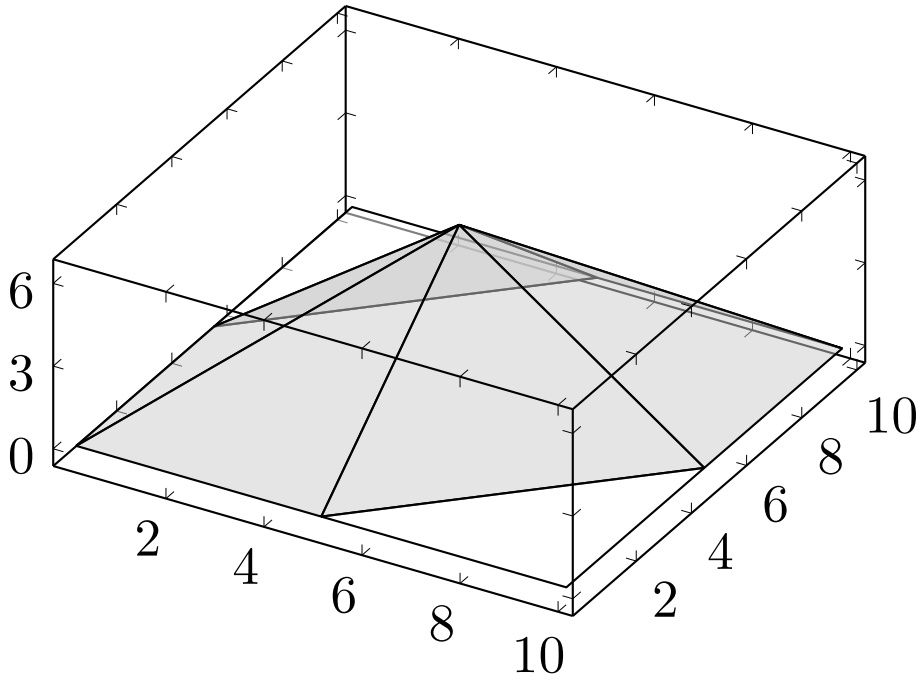
Data: Read N elements, nodes and BCs
Create global matrix $\mathbf{K}$ and vectors $\mathbf{F}$, $\mathbf{y}$;
for $e := 1$ **to** N **do**
  $\mathbf{K}_e := \iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y$;
  $\mathbf{F}_e := \iint_{\Omega_e} \mathbf{N} a \, \mathrm{d}x \, \mathrm{d}y$;
  Add $\mathbf{K}_e$ to $\mathbf{K}$;
  Add $\mathbf{F}_e$ to $\mathbf{F}$;
Apply BCs;
Solve linear system $\mathbf{K} \cdot \mathbf{y} = \mathbf{F}$;

Results - PDE



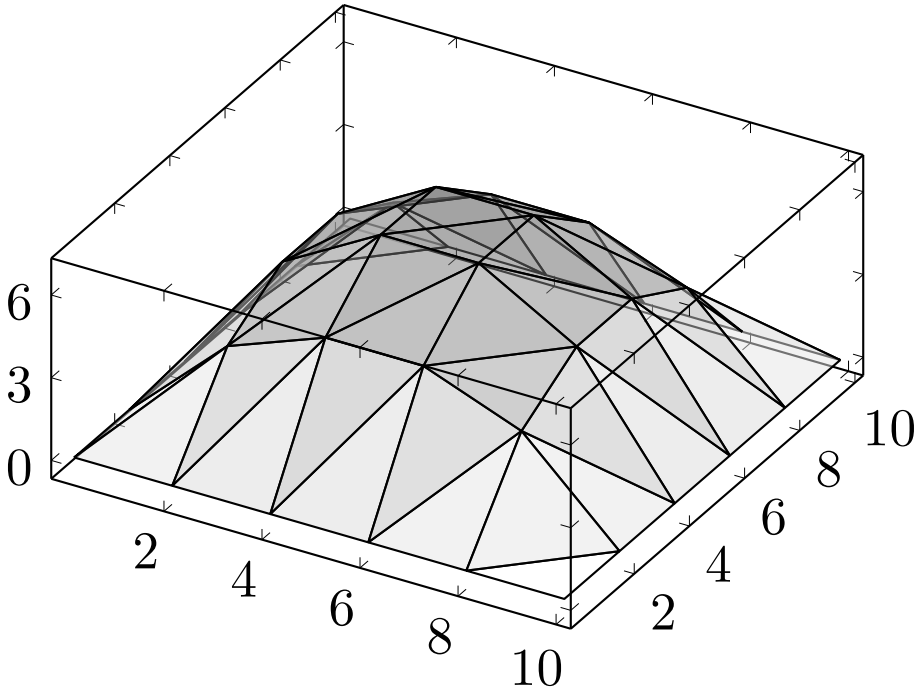
4 elements, 5 nodes

Results - PDE



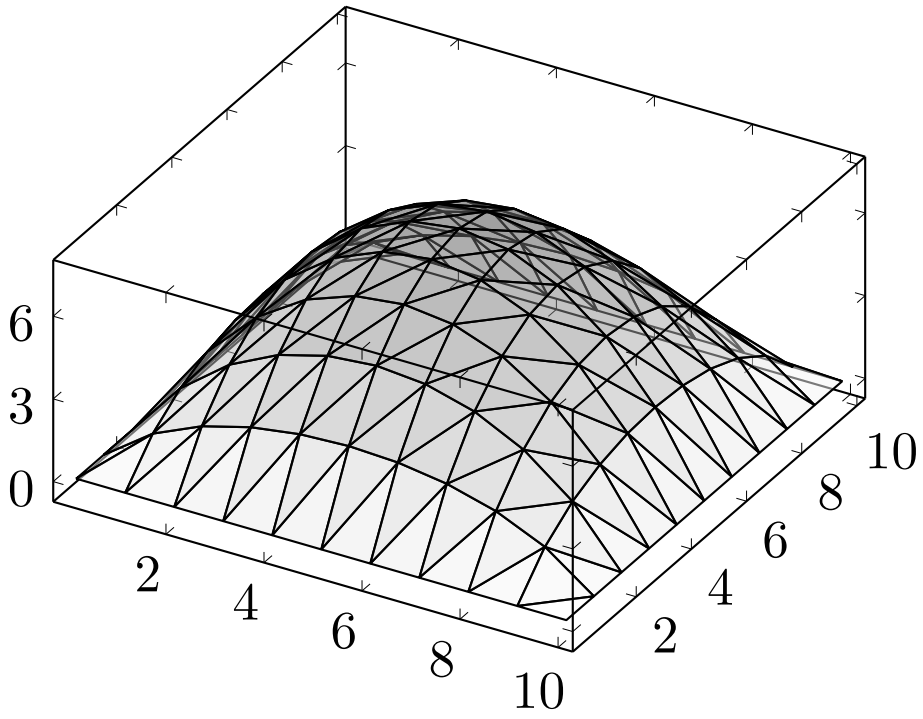
8 elements, 9 nodes

Results - PDE



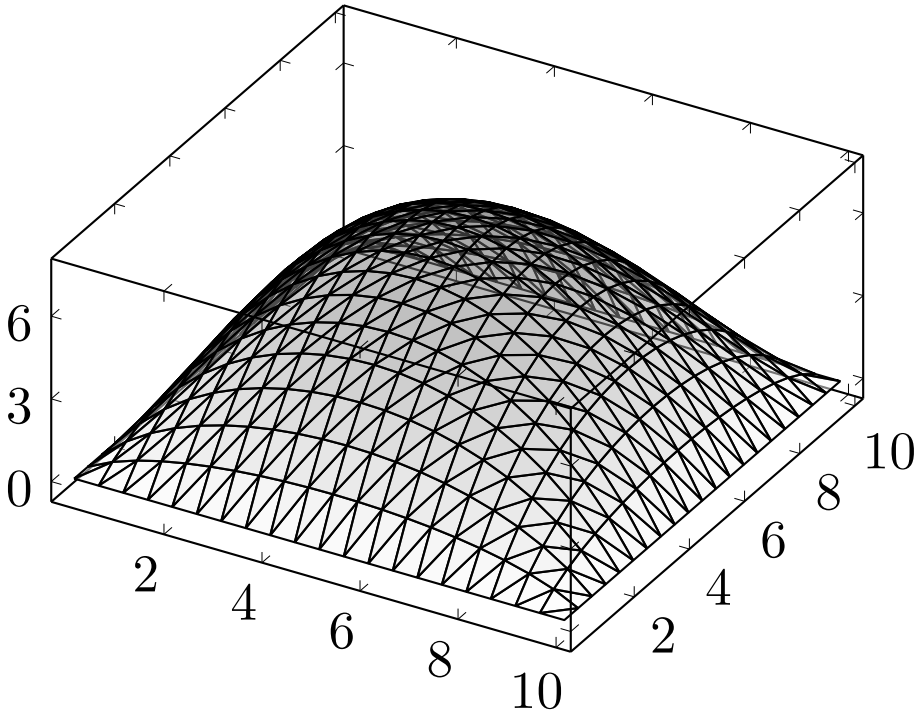
50 elements, 36 nodes

Results - PDE



200 elements, 121 nodes

Results - PDE



800 elements, 441 nodes

FEM for Laplace equation

Let the two dimensional form of Laplace equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0 \tag{405}$$

or $\nabla^2 \varphi = 0$ on Ω be subjected to both boundary conditions on $\partial\Omega$:

- Neumann

$$\frac{\partial \varphi}{\partial n} = \hat{\boldsymbol{n}} \cdot \nabla \varphi = \hat{\boldsymbol{n}} \cdot (U_x, U_y) = n_x U_x + n_y U_y = -f_N$$

- Dirichlet (as previously)

$$\varphi = \text{const} = f_D \tag{406}$$

‘Element’ formulation

As previously, FEM formulation for Poisson equation subjected to Dirichlet and Neumann BCs is

$$\iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \hat{U}_e}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \hat{U}_e}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y$$

$$- \int_{\partial\Omega_e} \mathbf{N} \frac{\partial \hat{U}_e}{\partial n} \, \mathrm{d}L - \iint_{\Omega_e} \mathbf{N} a \, \mathrm{d}x \, \mathrm{d}y = \mathbf{0} \quad (407)$$

- Poisson $\nabla^2 \varphi = -a$ with Dirichlet BC

$$\iint\limits_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \cdot \mathbf{U}_e = \iint_{\Omega_e} \mathbf{N} a \, \mathrm{d}x \, \mathrm{d}y \quad (408)$$

- Laplace $\nabla^2 \varphi = 0$ with Dirichlet + Neumann BC

$$\iint\limits_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \cdot \boldsymbol{\varphi}_e = - \int_{\partial\Omega_e} \mathbf{N} f_N \, \mathrm{d}L \quad (409)$$

Element equation

Introducing the 'stiffness' matrix as previously for each element e

$$\mathbf{K}_e = \iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \tag{410}$$

and the 'displacement' vector

$$\mathbf{F}_e = - \int_{\partial \Omega_e} \mathbf{N} f_N \, \mathrm{d}L \tag{411}$$

one may obtain the Galerkin residual condition for each element in the form

$$\mathbf{K}_e \cdot \boldsymbol{\varphi}_e = \mathbf{F}_e. \tag{412}$$

Element equation

The expanded version of the 'stiffness' matrix look the same as previously but the 'displacement' vector is now

$$\mathbf{F}_e = f_N \int_{\partial\Omega_e} \mathbf{N}\,\mathrm{d}L = -\frac{1}{2}|L| f_N \mathbf{1} \tag{413}$$

The vector $\mathbf{1}$ may take of the three following forms

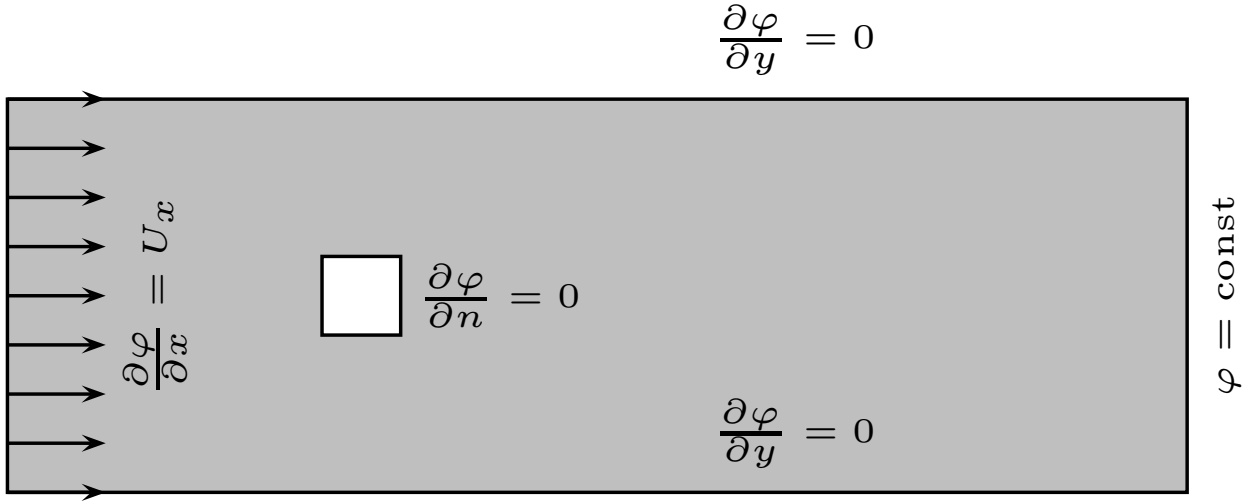
$$\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \tag{414}$$

$|L|$ stands for element side length.

Laplace FEM pseudocode

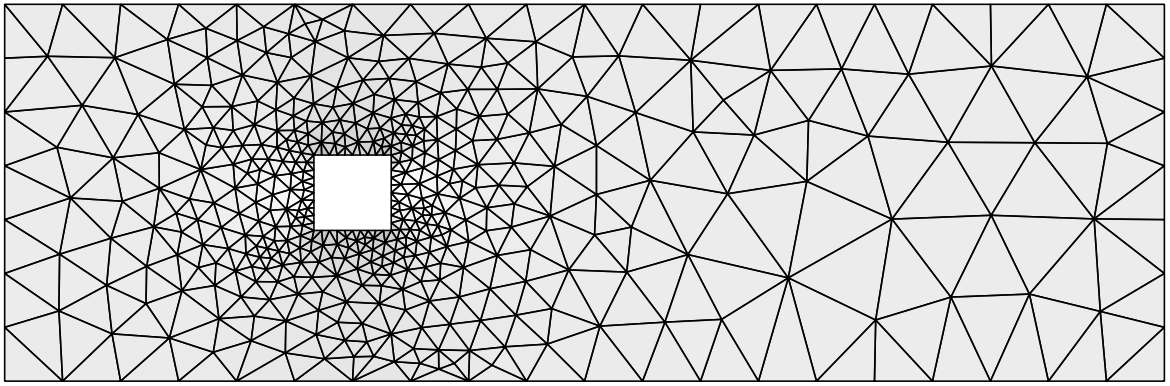
Data: Read N elements, nodes and BCs
Create global matrix $\mathbf{K}$ and vectors $\mathbf{F}$, $\mathbf{y}$;
for $e := 1$ **to** N **do**
  $\mathbf{K}_e := \iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y$;
  $\mathbf{F}_e := - \int_{\partial \Omega_e} \mathbf{N} f_N \, \mathrm{d}L$;
  Add $\mathbf{K}_e$ to $\mathbf{K}$;
  Add $\mathbf{F}_e$ to $\mathbf{F}$;
Apply BCs;
Solve linear system $\mathbf{K} \cdot \mathbf{y} = \mathbf{F}$;

Geometry and mesh - Laplace equation

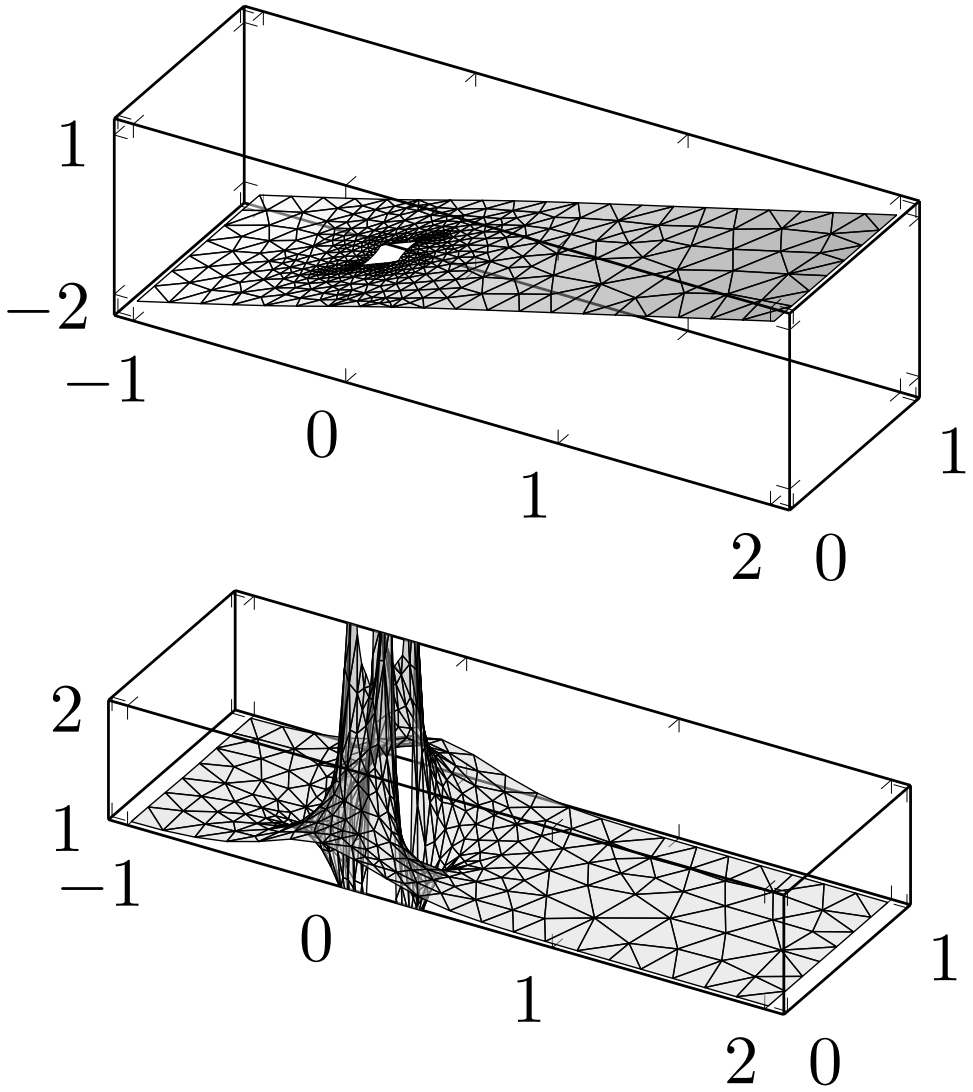


456

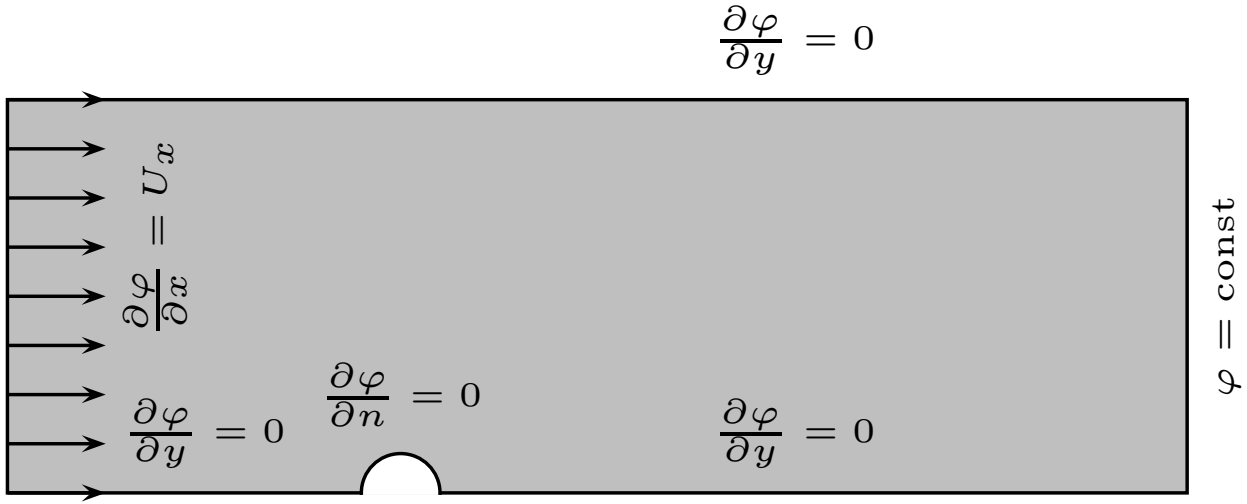
nodes and 818 elements



Results - Laplace equation

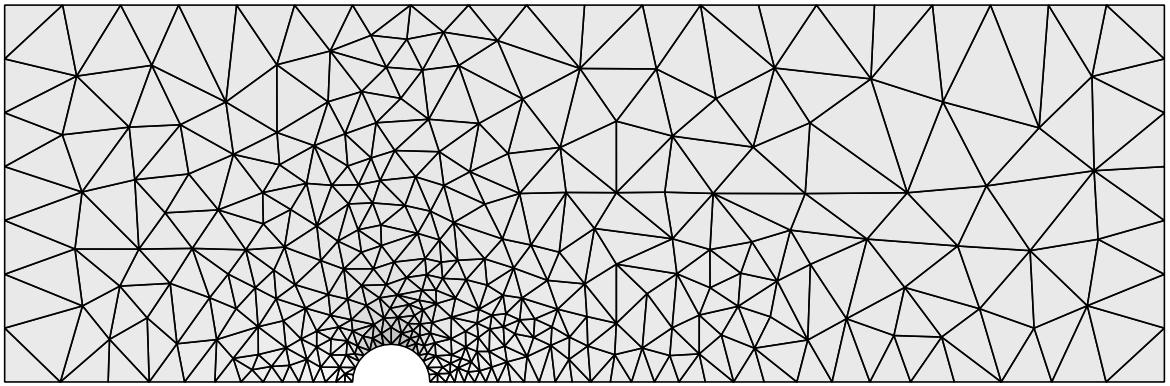


Geometry and mesh - Laplace equation

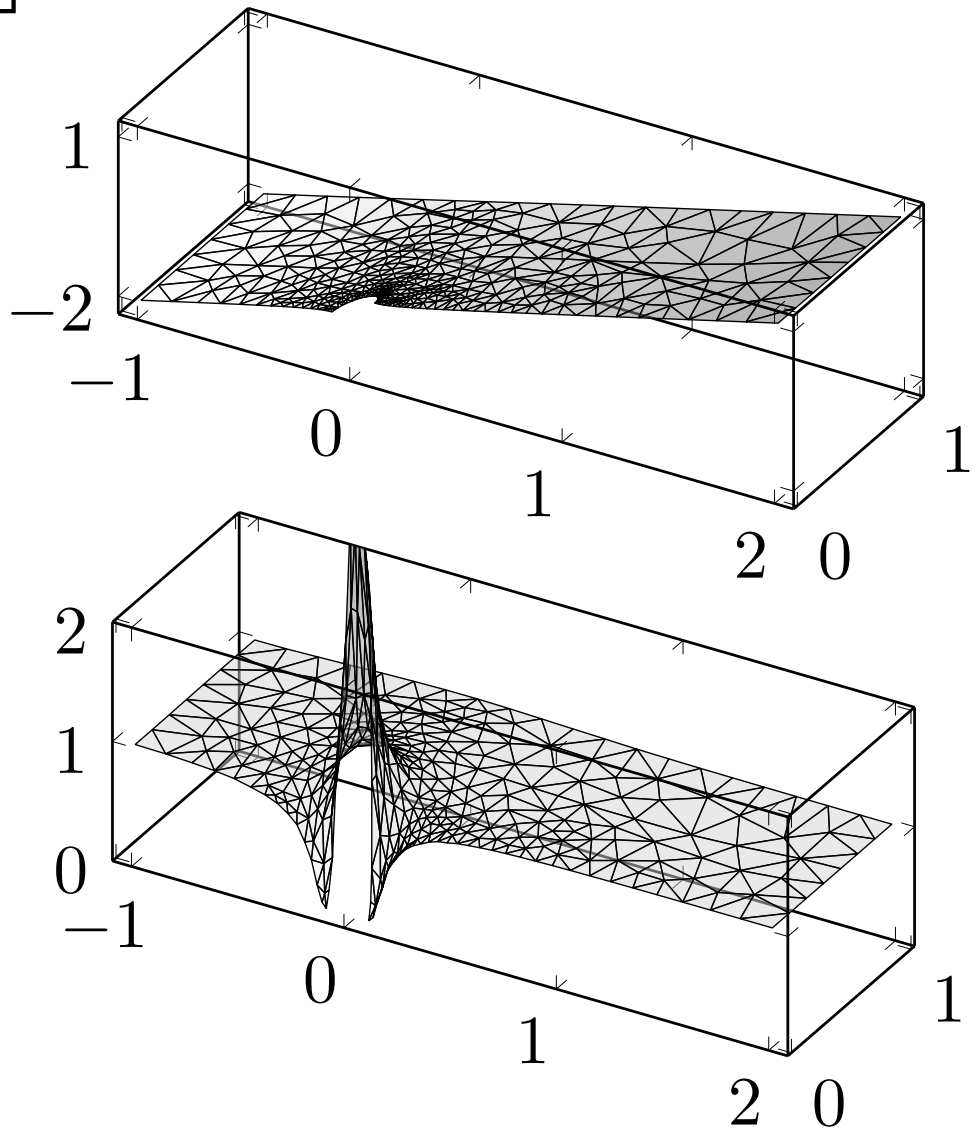


351

nodes and 607 elements



Results - Laplace equation



Creeping flow – Stokes equations

$$\mathrm{Re} \ll 1 \tag{415}$$

$$\mathbf{0} = \rho\mathbf{g} - \nabla p + \mu\nabla^2\mathbf{u} \tag{416a}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{416b}$$

$$0 = \rho g_x - \frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2}\right) \tag{417a}$$

$$0 = \rho g_y - \frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2}\right) \tag{417b}$$

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0 \tag{417c}$$

FEM formulation

The approximate solution is expressed as

$$\hat{u}_e = \mathbf{N} \cdot \mathbf{u}_e \tag{418}$$

where the quadratic trial functions $\mathbf{N}$ and the unknown nodal values u_e are

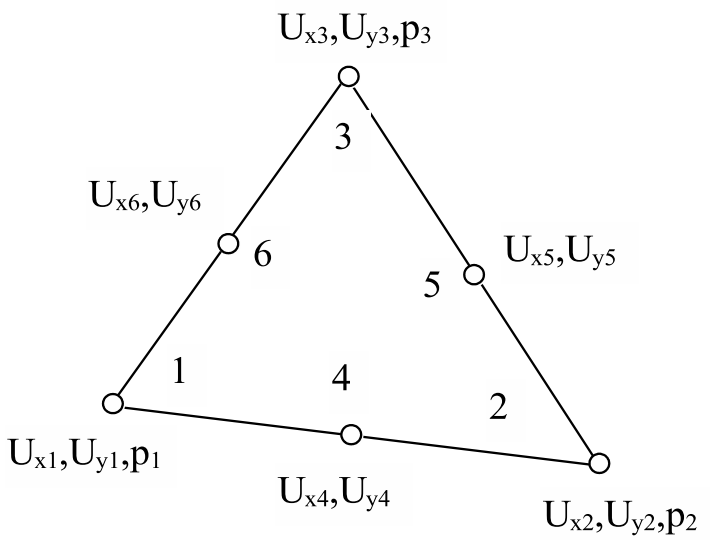
$$\mathbf{N} = (N_1, N_2, N_3, N_4, N_5, N_6) \tag{419a}$$

$$\mathbf{u}_e = (U_1, U_2, U_3, U_4, U_5, U_6) \tag{419b}$$

For each element we have the Galerkin residual condition

$$\iint_{\Omega_e} \mathbf{N}\, R \, \mathrm{d}x = \mathbf{0} \tag{420}$$

Quadratic interpolation



The quadratic trial functions can be expressed in terms of linear trial functions

$$N_1 = L_1 (2L_1 - 1)$$
$$N_2 = L_2 (2L_2 - 1)$$
$$N_3 = L_3 (2L_3 - 1)$$
$$N_4 = 4L_1 L_2$$
$$N_5 = 4L_2 L_3$$
$$N_6 = 4L_1 L_3$$

Momentum conservation equation

The Galerkin residual condition

$$\iint_{\Omega_e} \mathbf{N} \left(\rho g_x - \frac{\partial \hat{p}_e}{\partial x} + \mu \left(\frac{\partial^2 \hat{u}_{xe}}{\partial x^2} + \frac{\partial^2 \hat{u}_{xe}}{\partial y^2} \right) \right) \mathrm{d}x \, \mathrm{d}y = \mathbf{0} \tag{422}$$

by means of Green's first identity

$$\iint_S \left(\psi \frac{\partial^2 \varphi}{\partial x^2} + \psi \frac{\partial^2 \varphi}{\partial y^2} \right) \mathrm{d}x \, \mathrm{d}y = \int_{\partial S} \psi \frac{\partial \varphi}{\partial n} \, \mathrm{d}L - \iint_S \left(\frac{\partial \psi}{\partial x} \frac{\partial \varphi}{\partial x} + \frac{\partial \psi}{\partial y} \frac{\partial \varphi}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \tag{423}$$

Momentum conservation equation

is

$$\rho g_x \iint_{\Omega_e} \mathbf{N}\,\mathrm{d}x\,\mathrm{d}y - \iint_{\Omega_e} \mathbf{N}\frac{\partial \mathbf{N}}{\partial x}\,\mathrm{d}x\,\mathrm{d}y \cdot \mathbf{p}_e - \mu \iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x}\frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y}\frac{\partial \mathbf{N}}{\partial y} \right) \mathrm{d}x\,\mathrm{d}y \cdot \mathbf{u}_{xe} = \mathbf{0} \quad (424)$$

or

$$\mathbf{K}_{pxe} \cdot \mathbf{p}_e + \mathbf{K}_{xye} \cdot \mathbf{u}_{xe} = g_x \mathbf{F}_e \quad (425)$$

Similarly

$$\mathbf{K}_{pye} \cdot \mathbf{p}_e + \mathbf{K}_{xye} \cdot \mathbf{u}_{ye} = g_y \mathbf{F}_e \quad (426)$$

Momentum conservation equation

$$\mathbf{K}_{pxe} = \iint_{\Omega_e} \mathbf{N} \frac{\partial \mathbf{N}}{\partial x} \, \mathrm{d}x \, \mathrm{d}y \tag{427}$$

$$\mathbf{K}_{pye} = \iint_{\Omega_e} \mathbf{N} \frac{\partial \mathbf{N}}{\partial y} \, \mathrm{d}x \, \mathrm{d}y \tag{428}$$

$$\mathbf{K}_{xye} = \mu \iint_{\Omega_e} \left(\frac{\partial \mathbf{N}}{\partial x} \frac{\partial \mathbf{N}}{\partial x} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial \mathbf{N}}{\partial y} \right) \, \mathrm{d}x \, \mathrm{d}y \tag{429}$$

$$\mathbf{F}_e = \rho \iint_{\Omega_e} \mathbf{N} \, \mathrm{d}x \, \mathrm{d}y \tag{430}$$

Mass conservation equation

The Galerkin residual condition

$$\iint_{\Omega_e} \mathbf{N} \left(\frac{\partial \hat{u}_{xe}}{\partial x} + \frac{\partial \hat{u}_{ye}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y = \mathbf{0} \qquad (431)$$

The matrix form of the Galerkin residual condition for each element can now be expressed

$$\iint_{\Omega_e} \mathbf{N} \frac{\partial \mathbf{N}}{\partial x} \mathrm{d}x \, \mathrm{d}y \cdot \mathbf{u}_{xe} + \iint_{\Omega_e} \mathbf{N} \frac{\partial \mathbf{N}}{\partial y} \mathrm{d}x \, \mathrm{d}y \cdot \mathbf{u}_{ye} = \mathbf{0} \qquad (432)$$

or

$$\mathbf{K}_{uxe} \cdot \mathbf{u}_{xe} + \mathbf{K}_{uye} \cdot \mathbf{u}_{ye} = \mathbf{0} \qquad (433)$$

Mass conservation equation

$$\mathbf{K}_{uxe} = \iint_{\Omega_e} \mathbf{N} \frac{\partial \mathbf{N}}{\partial x} \, \mathrm{d}x \, \mathrm{d}y \tag{434}$$

$$\mathbf{K}_{uye} = \iint_{\Omega_e} \mathbf{N} \frac{\partial \mathbf{N}}{\partial y} \, \mathrm{d}x \, \mathrm{d}y \tag{435}$$

Element equations

$$\mathbf{K}_{pxe} \cdot \mathbf{p}_e + \mathbf{K}_{xye} \cdot \mathbf{u}_{xe} = g_x \mathbf{F}_e \tag{436a}$$

$$\mathbf{K}_{pye} \cdot \mathbf{p}_e + \mathbf{K}_{xye} \cdot \mathbf{u}_{ye} = g_y \mathbf{F}_e \tag{436b}$$

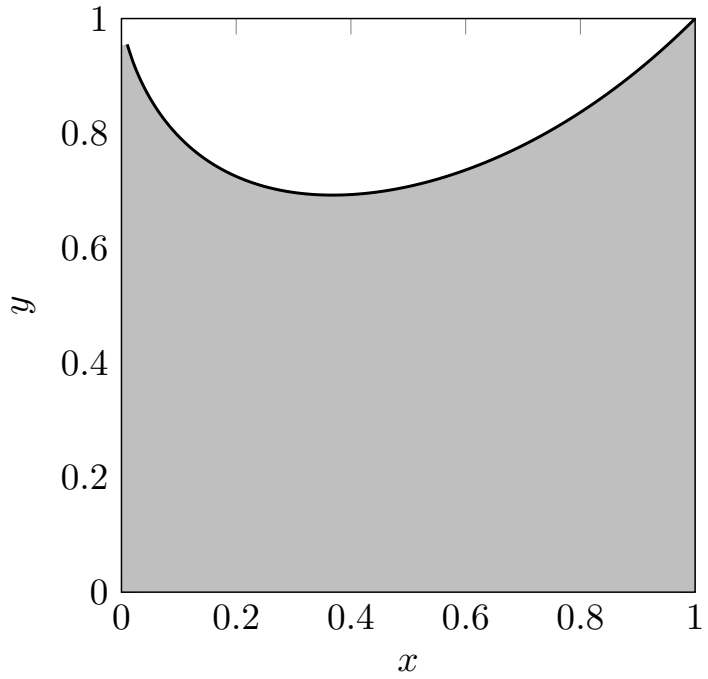
$$\mathbf{K}_{uxe} \cdot \mathbf{u}_{xe} + \mathbf{K}_{uye} \cdot \mathbf{u}_{ye} = \mathbf{0} \tag{436c}$$

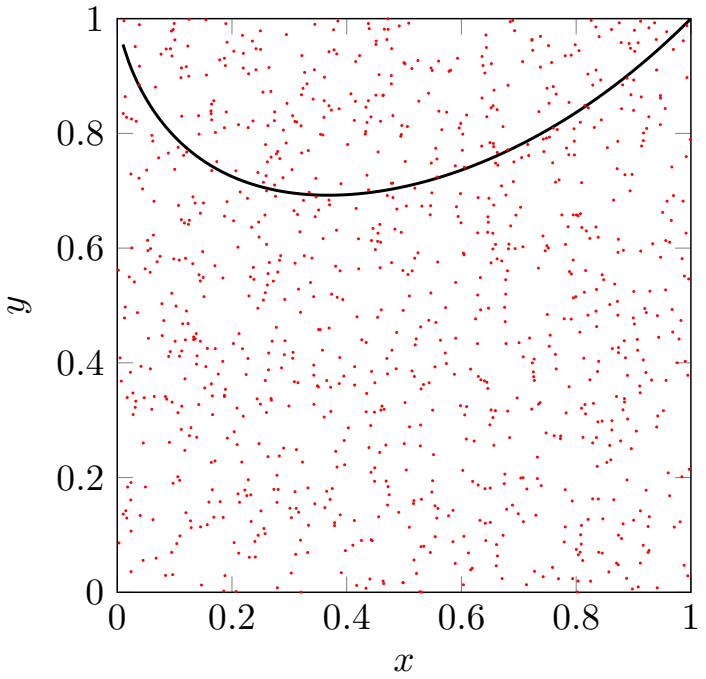
$$\begin{pmatrix} \mathbf{K}_{xye}^{6\times6} & \mathbf{0}^{6\times6} & \mathbf{K}_{pxe}^{6\times3} \\ \mathbf{0}^{6\times6} & \mathbf{K}_{xye}^{6\times6} & \mathbf{K}_{pye}^{6\times3} \\ \mathbf{K}_{uxe}^{3\times6} & \mathbf{K}_{uye}^{3\times6} & \mathbf{0}^{3\times3} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{u}_{xe}^{6\times1} \\ \mathbf{u}_{ye}^{6\times1} \\ \mathbf{p}_e^{3\times1} \end{pmatrix} = \begin{pmatrix} g_x \mathbf{F}_e^{6\times1} \\ g_y \mathbf{F}_e^{6\times1} \\ \mathbf{0}^{3\times1} \end{pmatrix} \tag{437}$$

$$\mathbf{K}_e^{15\times15} \cdot \mathbf{u}_e^{15\times1} = \mathbf{f}_e^{15\times1} \tag{438}$$

Monte Carlo Method

Monte Carlo integration





$$f(x) = x^x$$

Monte Carlo integration

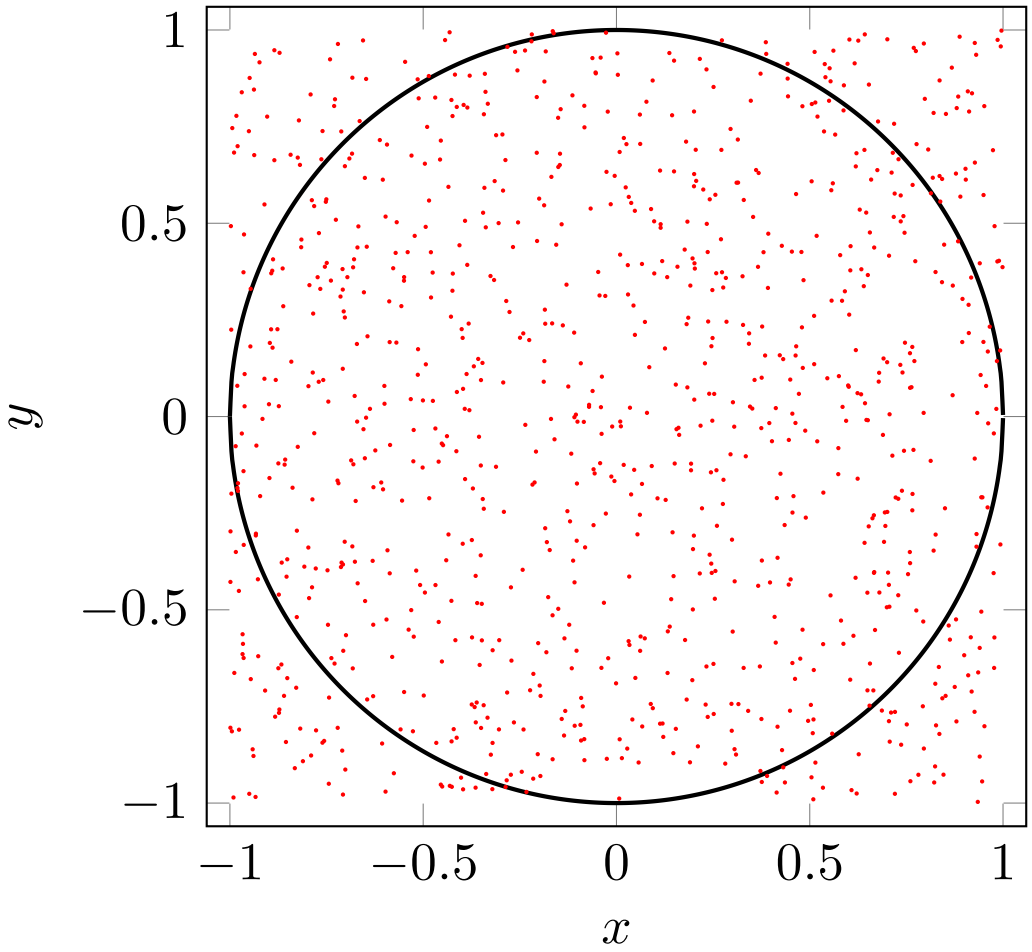
The simplest Monte Carlo integration is based on sampling uniformly distributed points $(\mathcal{U},\mathcal{U})$

$$\int_0^1 f(x)\,\mathrm{d}x \approx \frac{1}{n}\sum_{i=1}^{n} F\left(\mathcal{U},\mathcal{U}\right) \tag{439}$$

where

$$F(x,y) = \begin{cases} 1; & \text{if } f(x) \geq y \\ 0; & \text{otherwise} \end{cases} \tag{440}$$

Estimation of π



Estimation of π

The area $|D| = \pi$ of an unit circle

$$D = \left\{(x, y) : x^2 + y^2 \leq 1\right\} \tag{441}$$

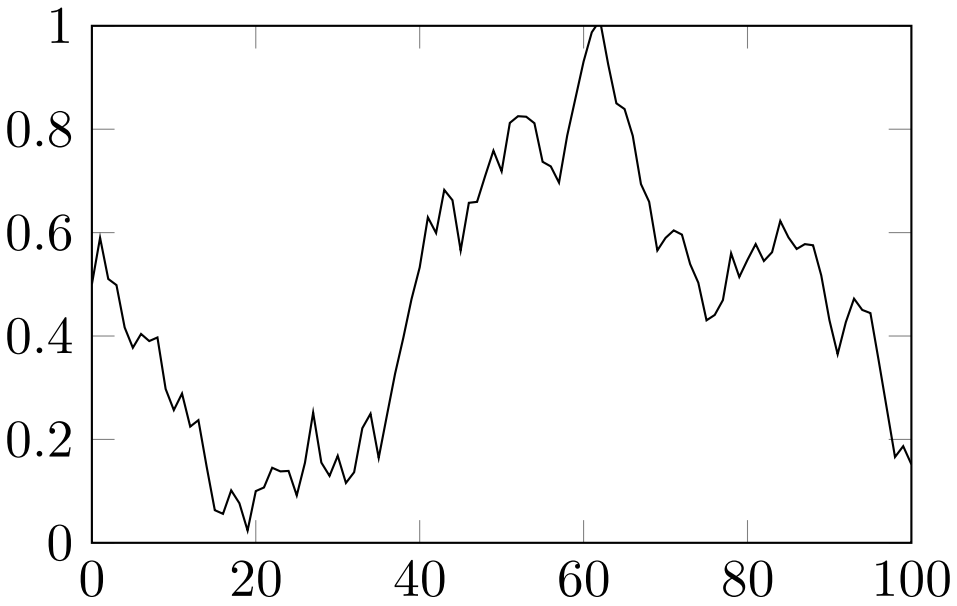
is estimated as

$$\pi = \iint_D F(x)\,\mathrm{d}x \approx \frac{4}{n}\sum_{i=1}^{n} F\left(\mathcal{U}, \mathcal{U}\right) \tag{442}$$

where

$$F(x, y) = \begin{cases} 1; & \text{if } x^2 + y^2 \leq 1 \\ 0; & \text{otherwise} \end{cases} \tag{443}$$

Wiener process and random walk 1D



Poisson equation

Poisson equation subjected to the Dirichlet boundary condition

$$\nabla^2 \phi(\mathbf{x}) = -f(\mathbf{x}); \quad \forall \mathbf{x} \in \Omega \tag{444a}$$

$$\phi(\mathbf{x}) = g(\mathbf{x}); \quad \forall \mathbf{x} \in \partial\Omega \tag{444b}$$

It can be solved as an expected value of random paths of a stochastic process

$$\phi(\mathbf{x}) = \mathrm{E}\left[g(W_\tau) + \tfrac{1}{2}\int_0^\tau f(W_t)\,\mathrm{d}t\right] \tag{445}$$

where t is a terminal time of a random walk

$$\tau = \inf\{t : W_t \in \partial\Omega\} \tag{446}$$

Poisson equation

If the Dirichlet boundary condition is $g(\mathbf{x}) = 0$ then

$$\phi(\mathbf{x}) = \tfrac{1}{2}\,\mathrm{E}\left[\int_0^\tau f(W_t)\,\mathrm{d}t\right] \tag{447}$$

We can also estimate

$$\int_0^\tau f(W_t)\,\mathrm{d}t \approx \sum_{i=1}^{m} f_i(W_\tau)\Delta t = \sum_{i=1}^{m} f_i(W_\tau)\frac{h}{V(h)} \tag{448}$$

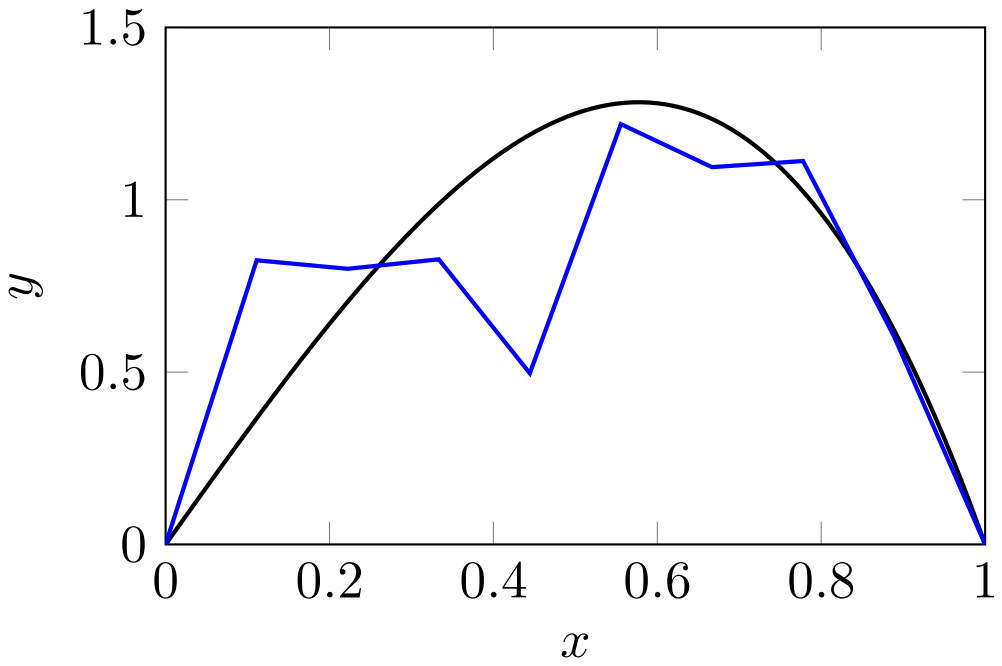
Let us consider an ordinary differential equation $y''(x) = -20x$ subjected to boundary conditions $y(0) = y(1) = 0$ (i.e. $\phi = y$, $f(x) = 20x$, $g(x) = 0$).

Monte Carlo ODE pseudocode

Data: Read input variables
for $i := 1$ **to** i_{max} **do**
  if not $\mathrm{boundary}(x_i)$ **then**
    $S := 0;$
    for $k := 1$ **to** n **do**
      $I := 0;$
      $\alpha := i;$
      while not $\mathrm{boundary}(x_\alpha)$ **do**
        $\alpha := \alpha + 2\lfloor \mathcal{U}(0,1) + \frac{1}{2} \rfloor - 1;$
        $I := I + 20 f(x_\alpha);$
      $S := S + I;$
    $y_i := \frac{h^2}{2} \frac{S}{n};$

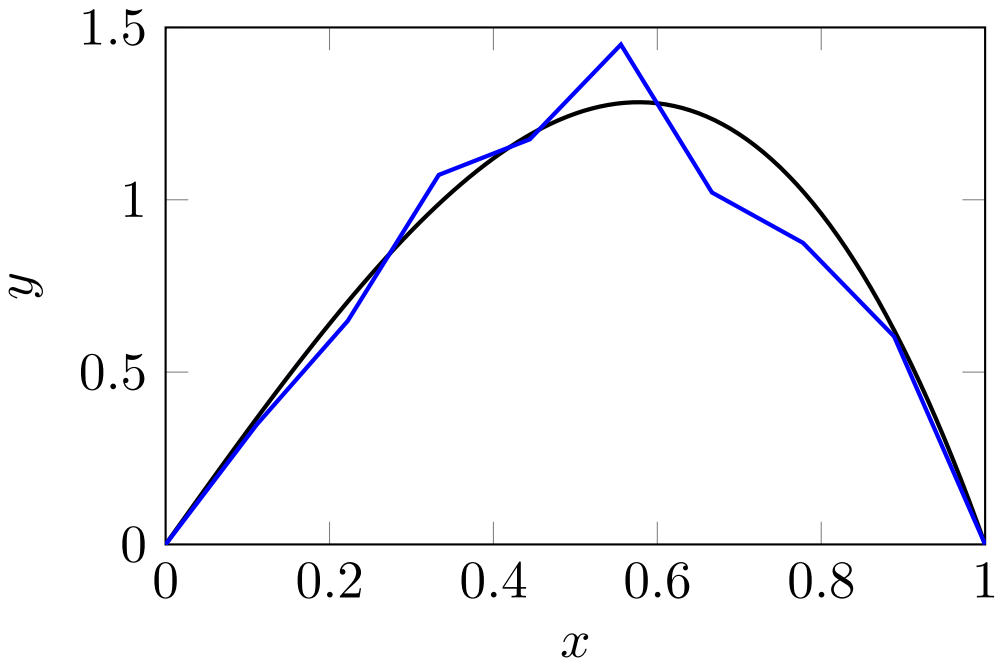
Results – ODE

$n = 10$



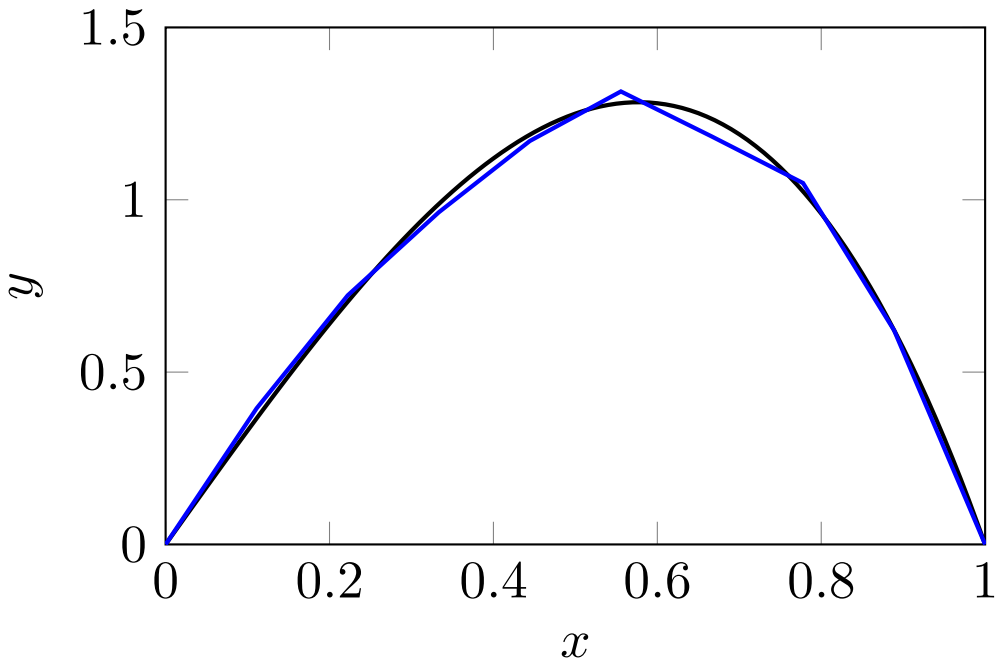
Results – ODE

$n = 100$



Results – ODE

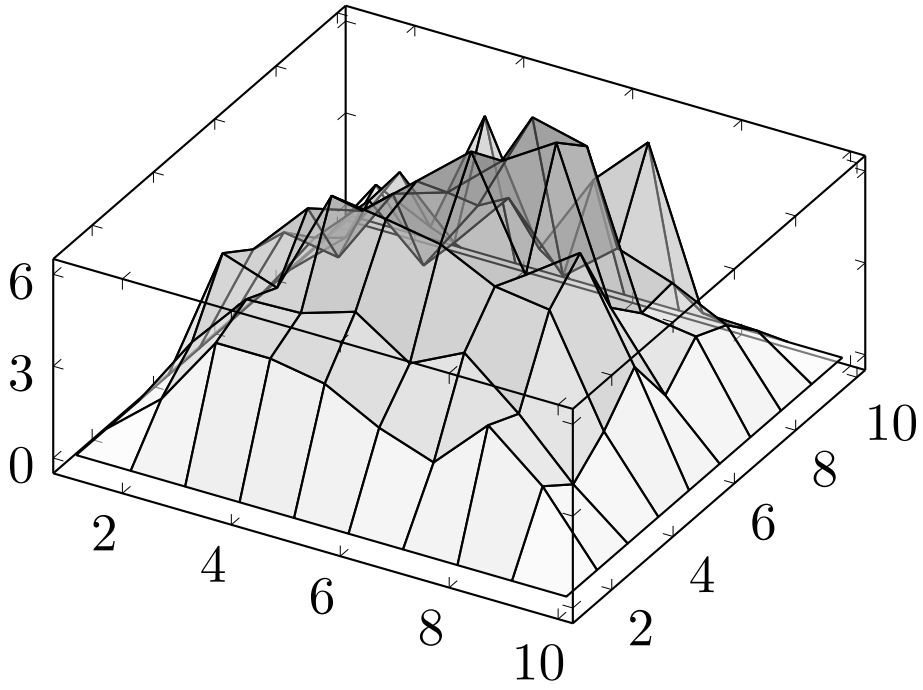
$n = 1000$



Monte Carlo Poisson pseudocode

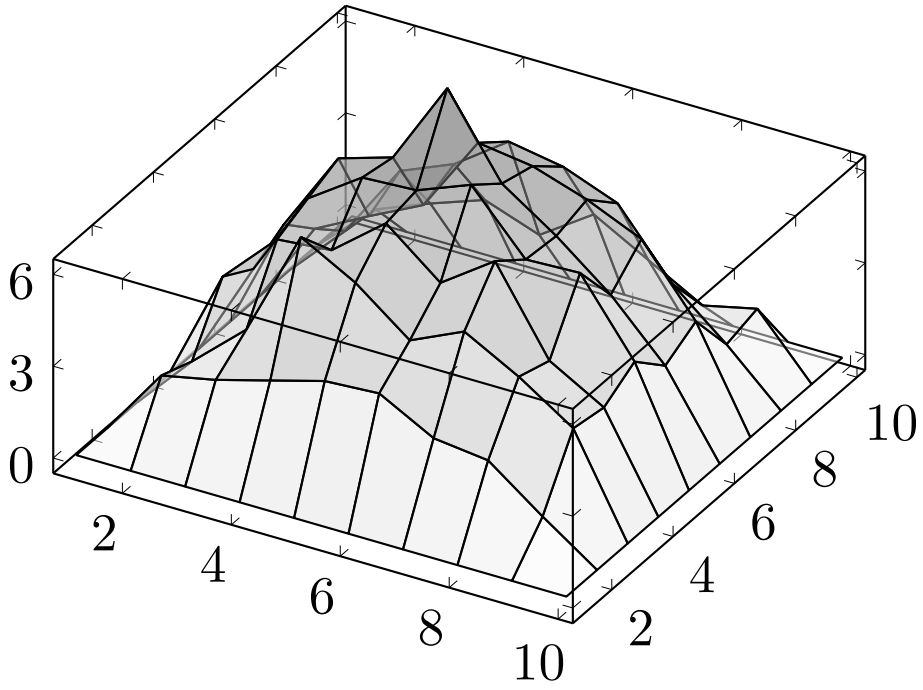
Data: Read input variables and BCs
for $i := 1$ **to** i_{max} **do**
  for $j := 1$ **to** j_{max} **do**
    if not $\mathrm{boundary}(\mathbf{x}_{ij})$ **then**
      $\tau_n := 0;$
      for $k := 1$ **to** n **do**
        $S := 0;$
        $\alpha := i;\ \beta := j;$
        while not $\mathrm{boundary}(\mathbf{x}_{\alpha\beta})$ **do**
          $\alpha := \alpha + 2\lfloor \mathcal{U}(0,1) + \frac{1}{2} \rfloor - 1;$
          $\beta := \beta + 2\lfloor \mathcal{U}(0,1) + \frac{1}{2} \rfloor - 1;$
          $S := S + 1;$
        $\tau_n := \tau_n + S;$
      $\phi_{ij} := -\frac{a\,h^2}{2}\frac{\tau_n}{n};$

Results – Poisson equation



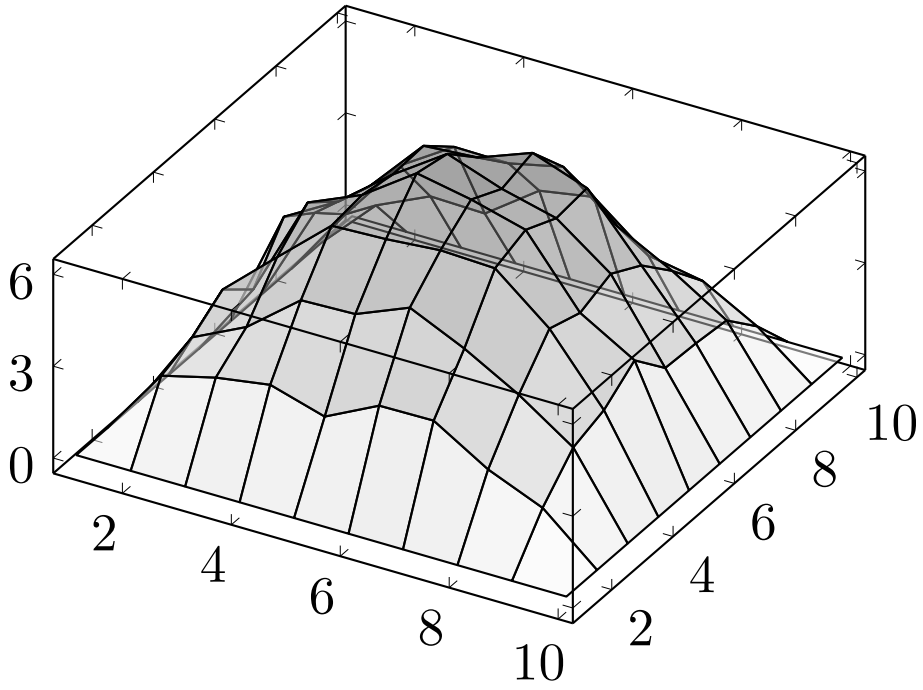
$n = 10$

Results – Poisson equation



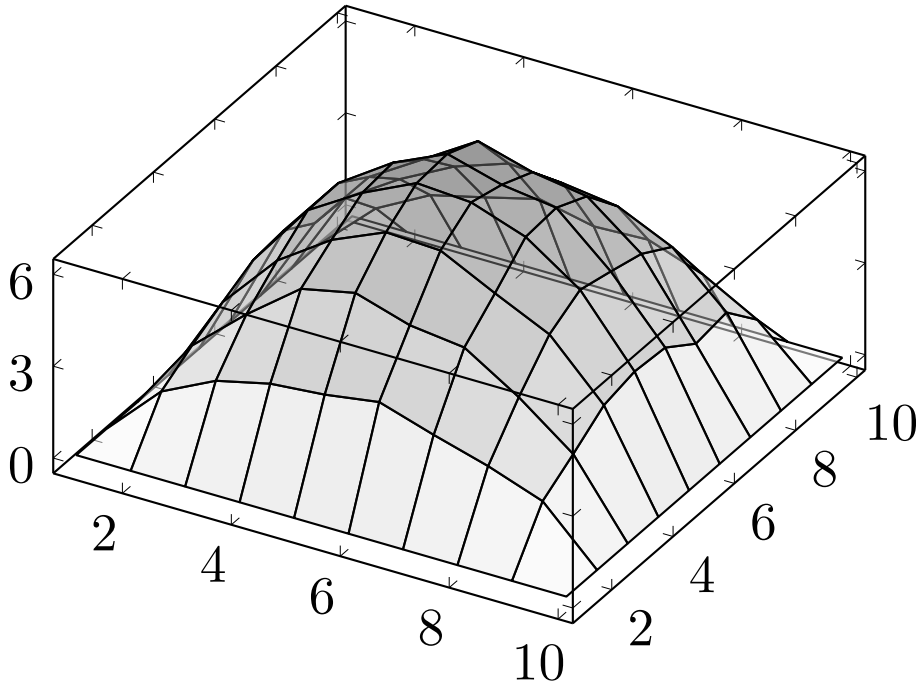
$n = 50$

Results – Poisson equation



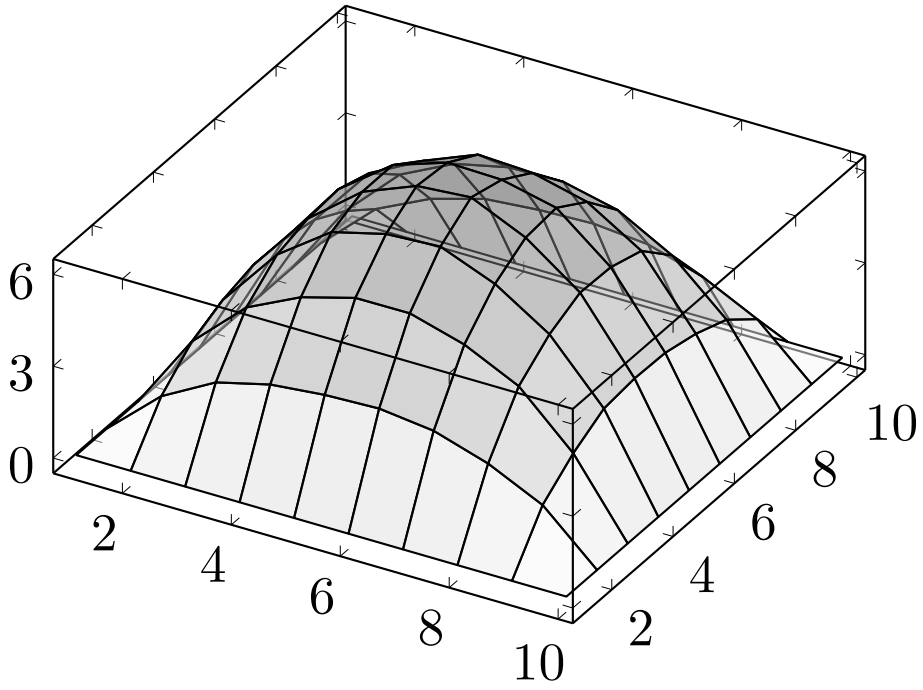
$n = 100$

Results – Poisson equation



$n = 500$

Results – Poisson equation



$n = 5000$

Lattice Boltzmann Method

Definitions and ideas

The kinetic theory of gases treats gas as a large number of small molecules. They are in constant (and random) motion and constantly collide with one another.
Knowing the position and velocity of each particle at some instant in time it would be possible to know the exact dynamical state of the whole system. The motion of particles could then be described by means of classical mechanics. This would allow for prediction of all future states of the system.
Due to the large number of molecules a statistical treatment is possible and necessary.

Assumptions

- The gas is compose of small molecules which means that the average distance separating particles is large in comparison with their size.
- Molecules are in constant and random motion
- The large number of molecules make it possible to apply statistical treatment
- Molecules have the same mass and spherical shape
- Molecules constantly and elastically collide
- The only interaction is due to collision (no other forces on one another)

Phase space and the distribution function

For N molecules we can think of *phase space* in which the coordinates consist of the position x_i, velocity vectors (v_i) and the time t. For a three dimensional case we have $6N$ dimensional phase space (three coordinates + three velocities times N molecules). The system can be described by a probability distribution function f that depends on $6N$ variables plus time t.
For a single molecule this reduces to 6 dimensional phase space (x_1, x_2, x_3, v_1, v_2, v_3). This can be treated as a statistical approach in which a system is represented by an ensemble of many copies.

Interpretation of the distribution function

The elementary volume and $\mathrm{d}V$ and product $\mathrm{d}v$ of elementary velocities are defined as

$$\mathrm{d}V = \prod_{i=1}^{D} \mathrm{d}x_i, \quad \mathrm{d}v = \prod_{i=1}^{D} \mathrm{d}v_i \tag{449}$$

where D means the physical dimension size. The distribution f that depends on $\mathbf{r}, \mathbf{v}, t$ represents the probability of finding a particular molecule mass with a given position and velocity per unit phase space.

$$\int_{\mathbb{R}^D} \int_{\mathbb{R}^D} f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}V\, \mathrm{d}v \tag{450}$$

The above integrate represents the total mass of molecules.

Continuous Boltzmann equation

If no collisions occur then the probability of finding a particular molecule mass with a given position and velocity at $(\mathbf{r}, \mathbf{v}, t)$ equals the probability at $(\mathbf{r} + \mathrm{d}\mathbf{r}, \mathbf{v} + \mathrm{d}\mathbf{v}, t + \mathrm{d}t)$

$$f(\mathbf{r} + \mathrm{d}\mathbf{r}, \mathbf{v} + \mathrm{d}\mathbf{v}, t + \mathrm{d}t)\,\mathrm{d}V\,\mathrm{d}v - f(\mathbf{r}, \mathbf{v}, t)\,\mathrm{d}V\,\mathrm{d}v = 0 \tag{451}$$

If, however, collisions take place then

$$f(\mathbf{r} + \mathrm{d}\mathbf{r}, \mathbf{v} + \mathrm{d}\mathbf{v}, t + \mathrm{d}t)\,\mathrm{d}V\,\mathrm{d}v - f(\mathbf{r}, \mathbf{v}, t)\,\mathrm{d}V\,\mathrm{d}v = \Omega(f)\,\mathrm{d}V\,\mathrm{d}v\,\mathrm{d}t \tag{452}$$

where Ω is so called collision operator. It takes under consideration collisions during $\mathrm{d}t$ interval.

Continuous Boltzmann equation

We can now expand the left hand side of the previous equation by means of Taylor's theorem

$$f(\mathbf{r} + \mathrm{d}\mathbf{r}, \mathbf{v} + \mathrm{d}\mathbf{v}, t + \mathrm{d}t) \approx$$
$$f(\mathbf{r}, \mathbf{v}, t) + \mathrm{d}\mathbf{r} \cdot \nabla f + \mathrm{d}\mathbf{v} \cdot \nabla_v f + \frac{\partial f}{\partial t}\mathrm{d}t \quad (453)$$

The two above equations give the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \nabla_v f = \Omega(f) \quad (454)$$

where $\mathbf{v} = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$ and $m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{F}$.

Collision operator

The simplification of the complicated collision operator Ω is needed. It should, however, fulfil at least two conditions:

- conservation of collision invariants φ

$$\int_{\mathbb{R}^D} \varphi \, \Omega \, \mathrm{d}v = 0 \tag{455}$$

  where collision invariants are: 1 (obvious), $\mathbf{v}$ and $\frac{1}{2}\|\mathbf{v}\|^2$.
- tendency to the Maxwell–Boltzmann distribution (relaxation to local equilibrium)

BGK approximation

The BGK (Bhatnagar–Gross–Krook) approximation is the most popular simplification of the collision operator

$$\Omega = \frac{1}{\tau}\left(f^{eq} - f\right) \tag{456}$$

It expresses relaxation to local equilibrium f^{eq} with the relaxation time τ. Both conditions are fulfilled.
The Boltzmann equations without external forces $\mathbf{F}$ is now

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f = \frac{1}{\tau}\left(f^{eq} - f\right) \tag{457}$$

Now the equation is linear! More precisely, it is a linear partial differential equation.

Maxwell–Boltzmann distribution

It is the basic law of the kinetic theory of gases. The Maxwell–Boltzmann distribution is used for molecules being not far from thermodynamic equilibrium. Other effects like quantum effects and relativistic speeds are neglected. The distribution is

$$f^{eq} = \rho \left(2\pi RT\right)^{-\frac{D}{2}} e^{-\frac{\|\mathbf{v}-\mathbf{u}\|^2}{2RT}} = \rho \left(\sqrt{2\pi} c_s\right)^{-D} e^{-\frac{\|\mathbf{c}\|^2}{2c_s^2}} \quad (458)$$

This distribution is valid for freely moving molecules without interacting with one another. The exceptions are only elastic collisions.

From Boltzmann eq. to conservation eqs

It is possible to derive the conservation laws from the Boltzmann equation. Firstly, from the interpretation of distribution function f it arises the definition of macroscopic density

$$\rho(\mathbf{r}, t) = \int_{\mathbb{R}^D} f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}v \tag{459}$$

The average value of a quantity φ is defined as

$$\langle \varphi \rangle = \frac{\int_{\mathbb{R}^D} \varphi\, f\, \mathrm{d}v}{\int_{\mathbb{R}^D} f\, \mathrm{d}v} = \frac{1}{\rho} \int_{\mathbb{R}^D} \varphi\, f\, \mathrm{d}v \tag{460}$$

The integration is carried out over velocity space.

Averaged Boltzmann equation

Multiplying the Boltzmann equation by φ and then integrating over velocity space results in

$$\int_{\mathbb{R}^D} \varphi \frac{\partial f}{\partial t} \,\mathrm{d}v + \int_{\mathbb{R}^D} \varphi\, \mathbf{v} \cdot \nabla f \,\mathrm{d}v + \int_{\mathbb{R}^D} \varphi \frac{\mathbf{F}}{m} \cdot \nabla_v f \,\mathrm{d}v = \int_{\mathbb{R}^D} \varphi\, \Omega(f) \,\mathrm{d}v \quad (461)$$

Taking advantage of the average definition the averaged Boltzmann equation may now be rewritten as

$$\frac{\partial}{\partial t} \left(\rho \langle \varphi \rangle\right) + \nabla \cdot \left(\rho \langle \varphi\, \mathbf{v} \rangle\right) - \rho \mathbf{f} \cdot \langle \nabla_v \varphi \rangle = 0 \quad (462)$$

Mass conservation equation

Substituting $\varphi = 1$ into the averaged Boltzmann equation we have

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \langle \mathbf{v} \rangle) = 0 \tag{463}$$

Comparing the above equation with the mass conservation equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{464}$$

it becomes obvious that the macroscopic velocity $\mathbf{u}$ must be

$$\mathbf{u} = \langle \mathbf{v} \rangle = \frac{1}{\rho} \int_{\mathbb{R}^D} \mathbf{v}\, f \, \mathrm{d}v \tag{465}$$

Momentum conservation equation

Substituting $\varphi \leftarrow \mathbf{v}$ into the averaged Boltzmann equation we have

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \langle \mathbf{v}\mathbf{v} \rangle) - \rho \mathbf{f} = 0 \tag{466}$$

Introducing the microscopic velocity $\mathbf{c}$ in the mean velocity frame

$$\mathbf{c}(\mathbf{r}, \mathbf{v}, t) = \mathbf{v} - \mathbf{u}(\mathbf{r}, t) \tag{467}$$

it is possible to define the stress tensor

$$\boldsymbol{\sigma} = -\rho \langle \mathbf{c}\mathbf{c} \rangle = -\int_{\mathbb{R}^D} \mathbf{c}\mathbf{c} f \, \mathrm{d}v \tag{468}$$

Now, the averaged Boltzmann equations becomes the macroscopic momentum conservation equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \rho \mathbf{f} + \nabla \cdot \boldsymbol{\sigma} \tag{469}$$

Energy conservation equation

Substituting $\varphi = \frac{1}{2}\|\mathbf{v}\|^2 \equiv \frac{1}{2}\mathbf{v}\cdot\mathbf{v}$ into the averaged Boltzmann equation we have

$$e = \frac{1}{2}\langle\|\mathbf{c}\|^2\rangle = \frac{1}{2\rho}\int_{\mathbb{R}^D}\|\mathbf{c}\|^2 f\,\mathrm{d}v \tag{470}$$

Introducing the heat vector $\mathbf{q}$ definition

$$\mathbf{q} = \frac{1}{2}\rho\langle\mathbf{c}\|\mathbf{c}\|^2\rangle = \frac{1}{2}\int_{\mathbb{R}^D}\mathbf{c}\|\mathbf{c}\|^2 f\,\mathrm{d}v \tag{471}$$

we have the macroscopic energy conservation equation

$$\frac{\partial}{\partial t}\left(\rho\left(e+\frac{1}{2}\|\mathbf{u}\|^2\right)\right)+\nabla\cdot\left(\rho\left(e+\frac{1}{2}\|\mathbf{u}\|^2\right)\mathbf{u}\right) = \rho\mathbf{f}\cdot\mathbf{u}+\nabla\cdot(\boldsymbol{\sigma}\cdot\mathbf{u}-\mathbf{q}) \tag{472}$$

Equation of state

From the definition of the stress tensor $\boldsymbol{\sigma} = -\rho\langle \mathbf{cc} \rangle$ and the internal energy $e = 2^{-1}\langle \mathbf{c} \cdot \mathbf{c} \rangle$ we have

$$\operatorname{tr}\langle \mathbf{cc} \rangle = 2e \tag{473}$$

Additionally, by means of the stress tensor we have pressure definition $p = -D^{-1} \operatorname{tr} \boldsymbol{\sigma}$. Combining these results in

$$2\rho e = pD \tag{474}$$

The above equation together with the equipartition of energy for mono-atomic gases gives the equation of state

$$p = \rho RT = \rho c_s^2 \tag{475}$$

Velocity space discretisation

The velocity space $\mathbf{v}$ is discretised into a finite set of Q velocities $\{\mathbf{v}_n\}$ where $Q = |\{\mathbf{v}_n\}|$. Discrete distributions are defined by means of the discretised velocity space

$$f_n(\mathbf{r}, t) = W_n \, f(\mathbf{r}, \mathbf{v}_n, t) \tag{476a}$$

$$f_n^{eq}(\mathbf{r}, t) = W_n \, f^{eq}(\mathbf{r}, \mathbf{v}_n, t) \tag{476b}$$

W_n are the weights of the Gaussian quadrature rule. The density may now be approximated as

$$\int_{\mathbb{R}^D} f(\mathbf{r}, \mathbf{v}, t) \, \mathrm{d}v \approx \sum_n W_n f(\mathbf{r}, \mathbf{v}_n, t) = \sum_n f_n(\mathbf{r}, t) \tag{477}$$

Discrete Boltzmann equation

The discrete distribution function f_n satisfies the discrete Boltzmann equation (with BGK approximation)

$$\frac{\partial f_n}{\partial t} + \mathbf{v}_n \cdot \nabla f_n = \frac{1}{\tau}\left(f_n^{eq} - f_n\right) \tag{478}$$

The fluid density, velocity and internal energy are now calculated from the discrete distribution function:

Quantity	Continuous	discrete
ρ	$\int_{\mathbb{R}^D} f \,\mathrm{d}v$	$\sum_n f_n$
$\rho\mathbf{u}$	$\int_{\mathbb{R}^D} \mathbf{v}\, f \,\mathrm{d}v$	$\sum_n \mathbf{v}_n f_n$
ρe	$\frac{1}{2}\int_{\mathbb{R}^D} \|\mathbf{v}-\mathbf{u}\|^2 f \,\mathrm{d}v$	$\frac{1}{2}\sum_n \|\mathbf{v}_n-\mathbf{u}\|^2 f_n$

To recover correct form of the Navier–Stokes equations the discrete velocity set has to be chosen so the following quadratures hold exactly

$$\forall_{0\leq m\leq 3} \quad \int_{\mathbb{R}^D} f^{eq} \prod_{i=0}^{m} \mathbf{v}\, \mathrm{d}v = \sum_n f_n^0 \prod_{i=0}^{m} \mathbf{v}_n \tag{479}$$

The above may be reduced to

$$I = \int_{\mathbb{R}^D} e^{-\frac{\|\mathbf{v}\|^2}{2c_s^2}} \psi(v)\, \mathrm{d}v \approx \sum_n W_n e^{-\frac{\|\mathbf{v}_n\|^2}{2c_s^2}} \psi(v_n) \tag{480}$$

where

$$W_n = e^{\frac{\|\mathbf{v}_n\|^2}{2c_s^2}} \left(\sqrt{2\pi} c_s\right)^D w_n \tag{481}$$

and

$$w_n = \pi^{-\frac{D}{2}} \prod_{i=1}^{D} \omega_i \tag{482}$$

Space discretisation

The space discretisation follows the velocity space discretisation. This means it is discretised into a lattices (D1Q3, D2Q9, D3Q27 discussed further). From the quadratures it arises speed of the model

$$c = \sqrt{3} c_s \tag{483}$$

The speed c is used for space discretisation in the following manner $\Delta x_i = c\,\Delta t$ where Δt represents time step (time space discretisation).
One may also introduce dimensionless lattice velocities

$$\mathbf{e}_n = \frac{\mathbf{v}_n}{c} \tag{484}$$

Lattice Boltzmann equation

Introducing the substantial derivative symbol $\frac{\mathrm{d}_n}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{v}_n \cdot \nabla$ makes it possible to rewrite the discretised Boltzmann equation

$$\frac{\mathrm{d}_n f_n}{\mathrm{d}t} = \frac{1}{\tau}\left(f_n^{eq} - f_n\right) \tag{485}$$

The substantial derivative is approximated by means of

$$\frac{\mathrm{d}_n f_n(\mathbf{r},t)}{\mathrm{d}t} = \frac{f_n(\mathbf{r}+\mathbf{v}_n\Delta t, t+\Delta t) - f_n(\mathbf{r},t)}{\Delta t} + \mathcal{O}\left(\Delta t\right) \tag{486}$$

From the two above one gets the Lattice Boltzmann equation

$$f_n(\mathbf{r}+\mathbf{v}_n\Delta t, t+\Delta t) - f_n(\mathbf{r},t) = \frac{1}{\hat{\tau}}\left(f_n^0(\mathbf{r},t) - f_n(\mathbf{r},t)\right) \tag{487}$$

where dimensionless collision time is $\hat{\tau} = \frac{\tau}{\Delta t}$.

Equations

Continuous Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \Omega(f) \tag{488}$$

Continuous Boltzmann equation with BGK approximation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \frac{1}{\tau} \left(f^{eq} - f \right) \tag{489}$$

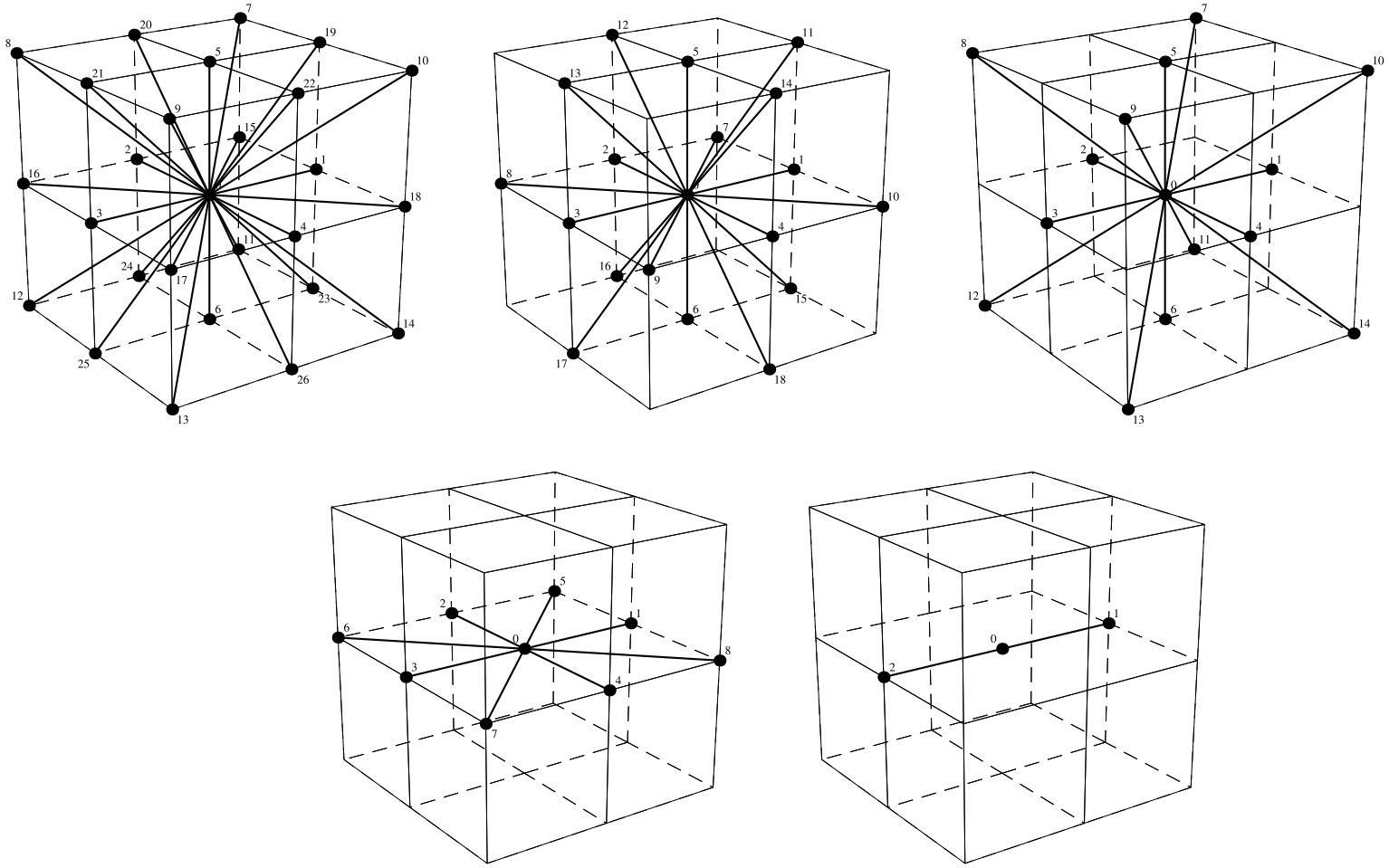
Discrete Boltzmann equation

$$\frac{\partial f_n}{\partial t} + \mathbf{v}_n \cdot \nabla f_n = \frac{1}{\tau} \left(f_n^{eq} - f_n \right) \tag{490}$$

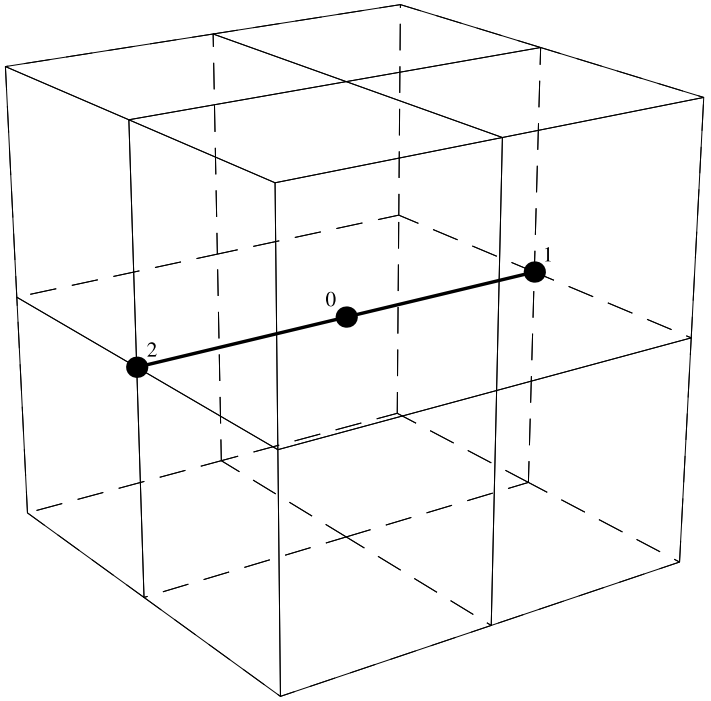
Lattice Boltzmann equation

$$f_n(\mathbf{r} + \mathbf{v}_n \Delta t, t + \Delta t) - f_n(\mathbf{r}, t) = \frac{1}{\hat{\tau}} \left(f_n^0(\mathbf{r}, t) - f_n(\mathbf{r}, t) \right) \tag{491}$$

Typical lattices

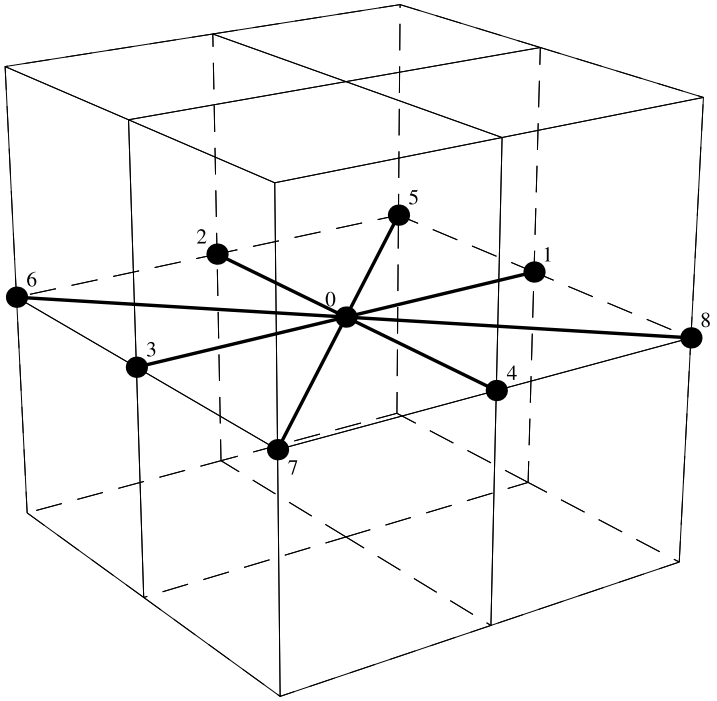


D1Q3 lattice



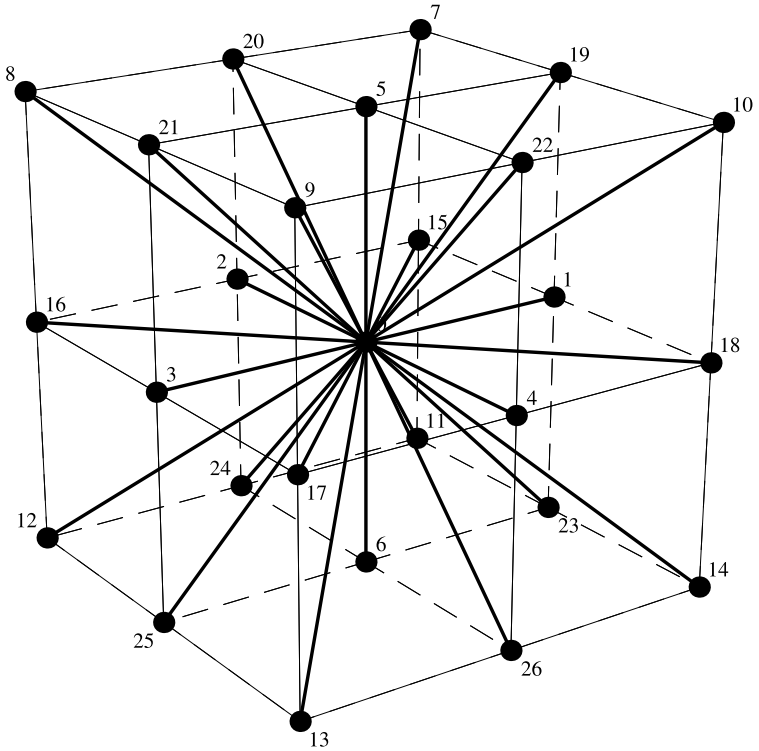
$$w_n = \begin{cases} \frac{2}{3}, & n = 0; \\ \frac{1}{6}, & n \in \{1, 2\}. \end{cases}$$

D2Q9 lattice



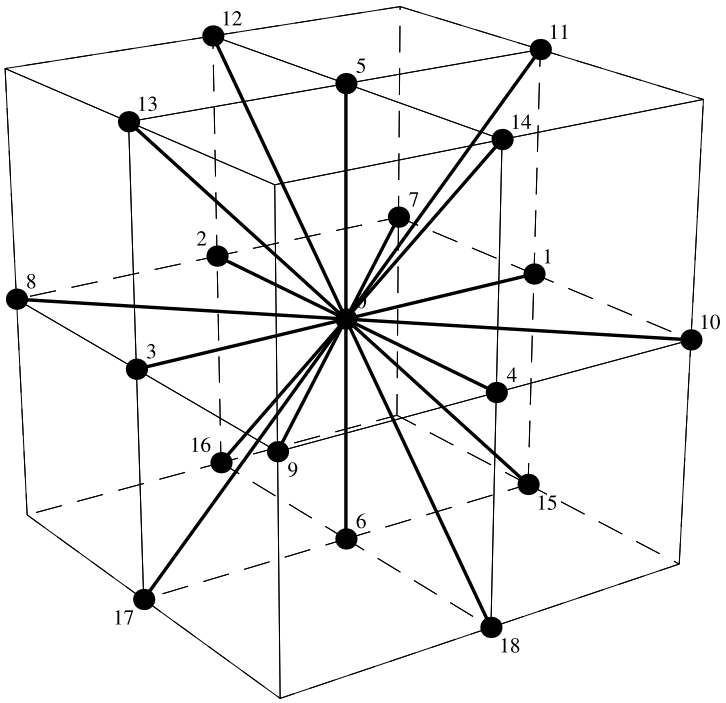
$$w_n = \begin{cases} \frac{4}{9}, & n = 0; \\ \frac{1}{9}, & n \in \{1, \ldots, 4\}; \\ \frac{1}{36}, & n \in \{5, \ldots, 8\}. \end{cases}$$

D3Q27 lattice



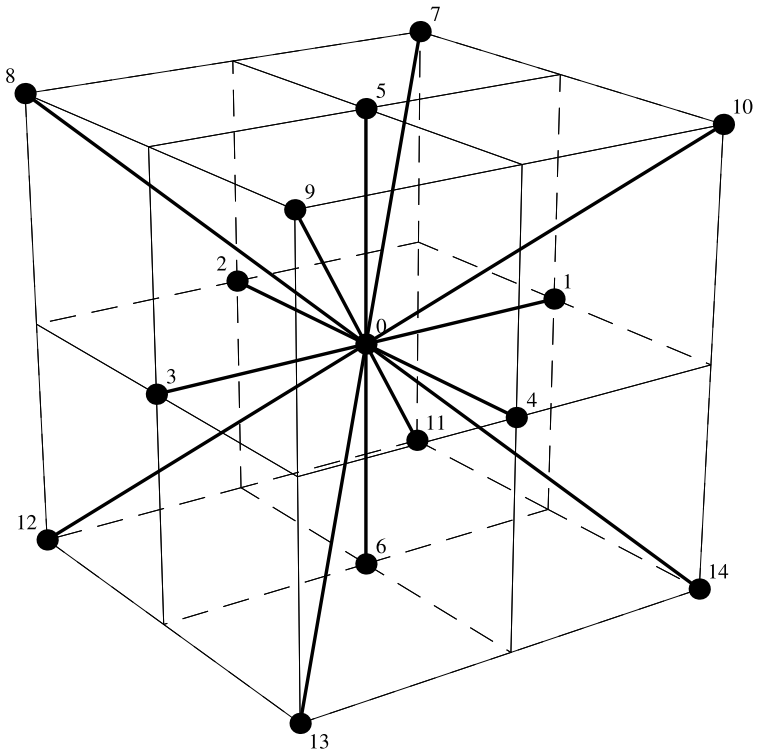
$$w_n = \begin{cases} \frac{8}{27}, & n = 0; \\ \frac{2}{27}, & n \in \{1, \ldots, 6\}; \\ \frac{1}{54}, & n \in \{15, \ldots, 26\}; \\ \frac{1}{216}, & n \in \{7, \ldots, 14\}; \end{cases}$$

D3Q19 lattice



$$w_n = \begin{cases} \frac{1}{3}, & n = 0; \\ \frac{2}{18}, & n \in \{1, \ldots, 6\}; \\ \frac{1}{36}, & n \in \{7, \ldots, 18\}; \end{cases}$$

D3Q15 lattice



$$w_n = \begin{cases} \frac{2}{9}, & n = 0; \\ \frac{1}{9}, & n \in \{1, \ldots, 6\}; \\ \frac{1}{72}, & n \in \{7, \ldots, 14\}; \end{cases}$$

Expansion of the Maxwell–Boltzmann distribution

The Maxwell–Boltzmann distribution can be rearranged

$$f^{eq} = \rho \left(\sqrt{2\pi} c_s\right)^{-D} e^{-\frac{\|\mathbf{v}\|^2}{2c_s^2}} e^{-\left(\frac{\|\mathbf{u}\|^2}{2c_s^2} - \frac{\mathbf{v}\cdot\mathbf{u}}{c_s^2}\right)} \tag{492}$$

Now f^{eq} can be expanded into a Taylor series in terms of the fluid velocity

$$f^0 = \rho \left(\sqrt{2\pi} c_s\right)^{-D} e^{-\frac{\|\mathbf{v}\|^2}{2c_s^2}} \left(1 + \frac{\mathbf{v}\cdot\mathbf{u}}{c_s^2} + \frac{(\mathbf{v}\cdot\mathbf{u})^2}{2c_s^4} - \frac{\|\mathbf{u}\|^2}{2c_s^2}\right) \tag{493}$$

This is valid for low Mach numbers

$$f^{eq} = f^0 + \mathcal{O}\left(\frac{\|\mathbf{u}\|^3}{c_s^3}\right) = f^0 + \mathcal{O}\left(\mathrm{Ma}^3\right) \tag{494}$$

Discrete Maxwell–Boltzmann distribution

The discrete equilibrium distribution is defined by means of the discretised velocity space

$$f_n^0(\mathbf{r}, t) = W_n f^0(\mathbf{r}, \mathbf{v}_n, t) \tag{495}$$

where weights are

$$W_n = e^{\frac{\|\mathbf{v}_n\|^2}{2c_s^2}} \left(\sqrt{2\pi} c_s\right)^D w_n \tag{496}$$

Together with the Taylor expansion for low Mach numbers we have

$$f_n^0 = w_n \rho \left(1 + \frac{\mathbf{v}_n \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{v}_n \cdot \mathbf{u})^2}{2c_s^4} - \frac{\|\mathbf{u}\|^2}{2c_s^2}\right) \tag{497}$$

Streaming and collision

The Lattice Boltzmann equation

$$f_n(\mathbf{r} + \mathbf{v}_n \Delta t, t + \Delta t) = f_n(\mathbf{r}, t) + \frac{1}{\hat{\tau}} \left(f_n^0(\mathbf{r}, t) - f_n(\mathbf{r}, t) \right) \tag{498}$$

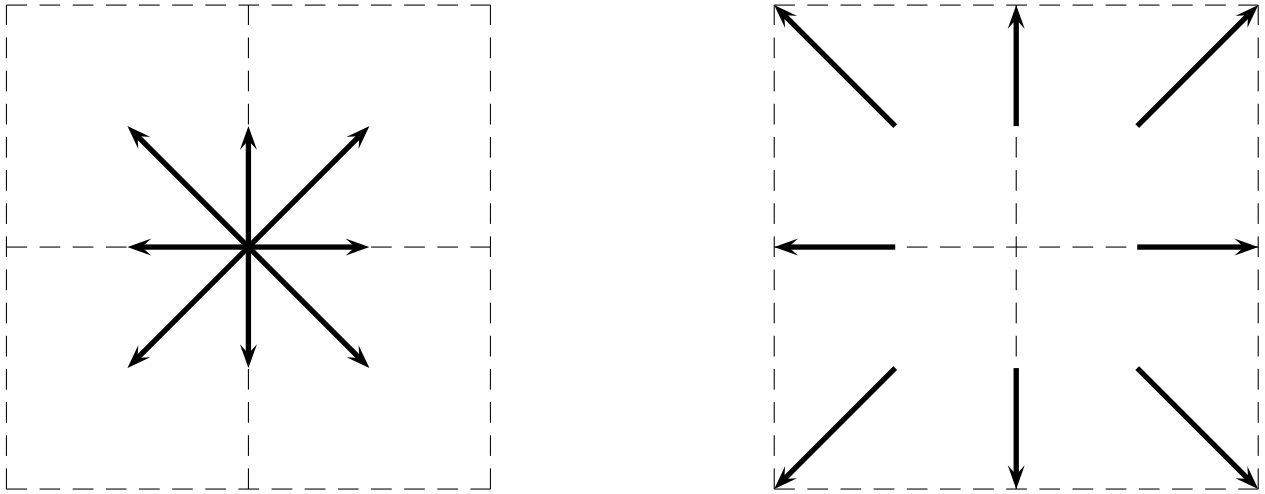
The collision step

$$f_n^t(\mathbf{r}, t + \Delta t) = f_n(\mathbf{r}, t) + \frac{1}{\hat{\tau}} \left(f_n^0(\mathbf{r}, t) - f_n(\mathbf{r}, t) \right) \tag{499}$$

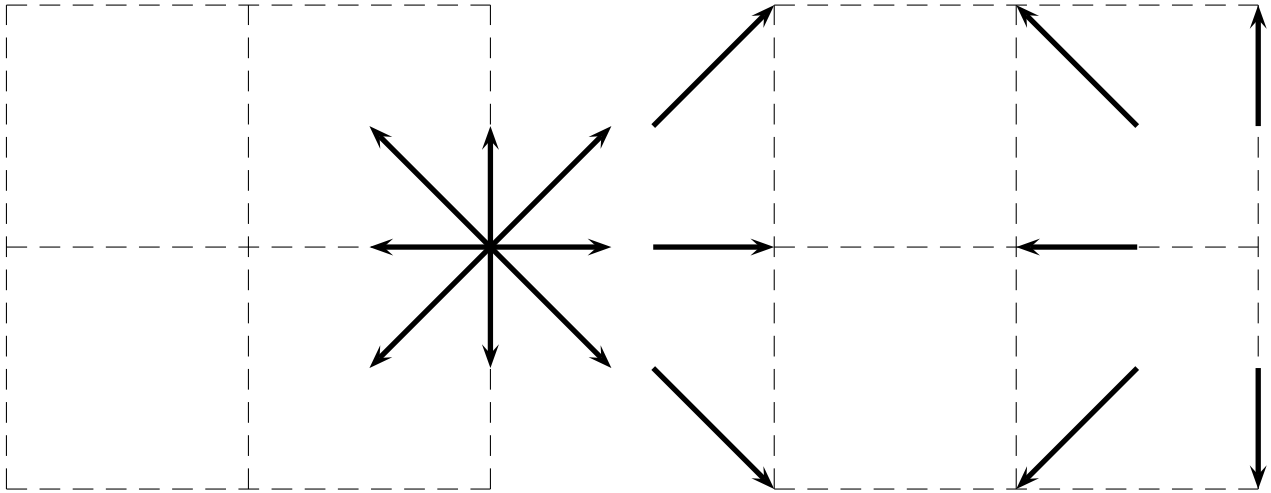
The streaming step

$$f_n(\mathbf{r} + \mathbf{v}_n \Delta t, t + \Delta t) = f_n^t(\mathbf{r}, t + \Delta t) \tag{500}$$

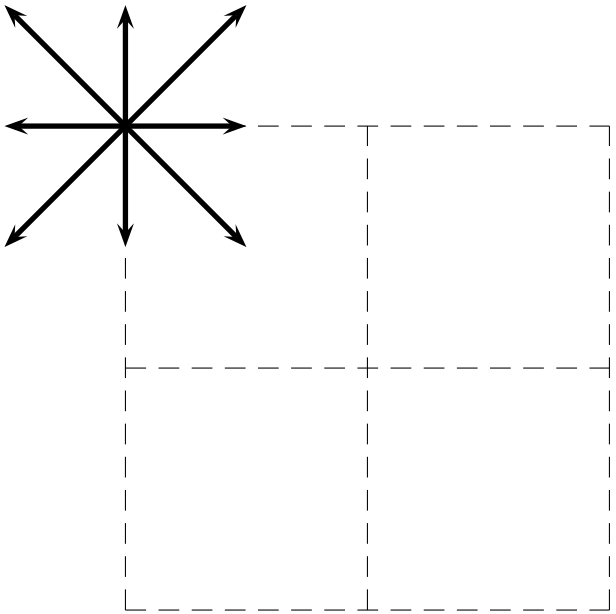
Streaming

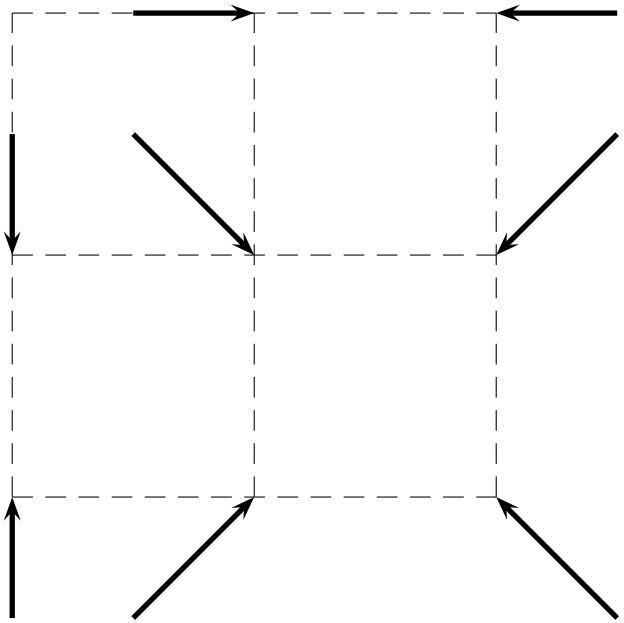


Streaming



Streaming





LBM pseudocode

$k := 0;$

repeat

$R := 0;$

$\rho := \sum_n f_n;$

$\mathbf{u} := \frac{1}{\rho} \sum_n \mathbf{v}_n f_n;$

Calculate residue;

$f_n^0 := w_n \rho \left(1 + \frac{\mathbf{v}_n \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{v}_n \cdot \mathbf{u})^2}{2c_s^4} - \frac{\|\mathbf{u}\|^2}{2c_s^2} \right);$

$f_n^t(\mathbf{r}, t + \Delta t) := f_n(\mathbf{r}, t) + \frac{1}{\hat{\tau}} \left(f_n^0(\mathbf{r}, t) - f_n(\mathbf{r}, t) \right);$

Apply Bounceback;

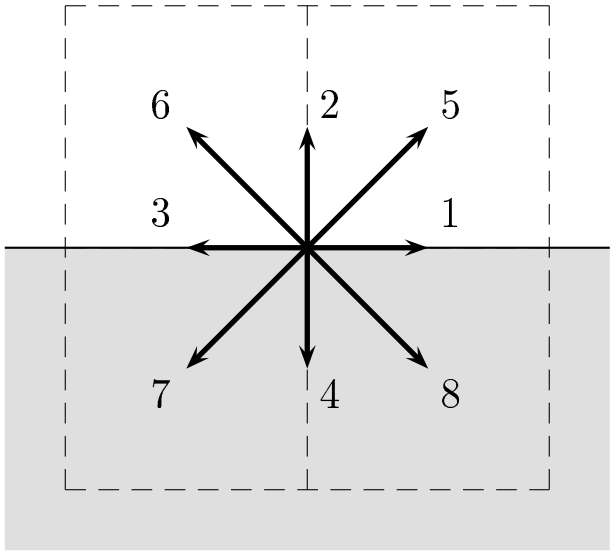
$f_n(\mathbf{r} + \mathbf{v}_n \Delta t, t + \Delta t) := f_n^t(\mathbf{r}, t + \Delta t);$

Apply other BCs;

$k := k + 1;$

until $k < k_{max}$ **and** $R > R_{min}$;

Boundary conditions



$$f_5^t = f_7^t \tag{501a}$$

$$f_2^t = f_4^t \tag{501b}$$

$$f_6^t = f_8^t \tag{501c}$$

Chapman–Enskog expansion

The Navier–Stokes equations can be recovered from the Lattice Boltzmann equation

$$\frac{\partial}{\partial t}\left(\rho\mathbf{u}\right) + \nabla\cdot\left(\rho\mathbf{u}\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u} \tag{502}$$

through the Chapman–Enskog expansion (multi-scale analysis). The expansion of the discrete Maxwell–Boltzmann distribution is used

$$f_n^0 = w_n\rho\left(1 + \frac{\mathbf{v}_n\cdot\mathbf{u}}{c_s^2} + \frac{\left(\mathbf{v}_n\cdot\mathbf{u}\right)^2}{2c_s^4} - \frac{\|\mathbf{u}\|^2}{2c_s^2}\right) \tag{503}$$

The first RHS term is responsible for ∇p, the second for $\nabla^2\mathbf{u}$, the last two terms are related to $\rho\mathbf{u}\mathbf{u}$.

Simplifications

Knowing the structure of the discrete Maxwell–Boltzmann distribution we can now drop the nonlinear terms

$$f_n^0 = w_n \rho \left(1 + \frac{\mathbf{v}_n \cdot \mathbf{u}}{c_s^2} \right) \tag{504}$$

to recover Stokes equations

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} \tag{505}$$

For both cases the dynamic viscosity is defined as

$$\mu = \rho \left(\hat{\tau} - \frac{1}{2} \right) c_s^2 \Delta t \tag{506}$$

Smoothed Particle Hydrodynamics

Properties

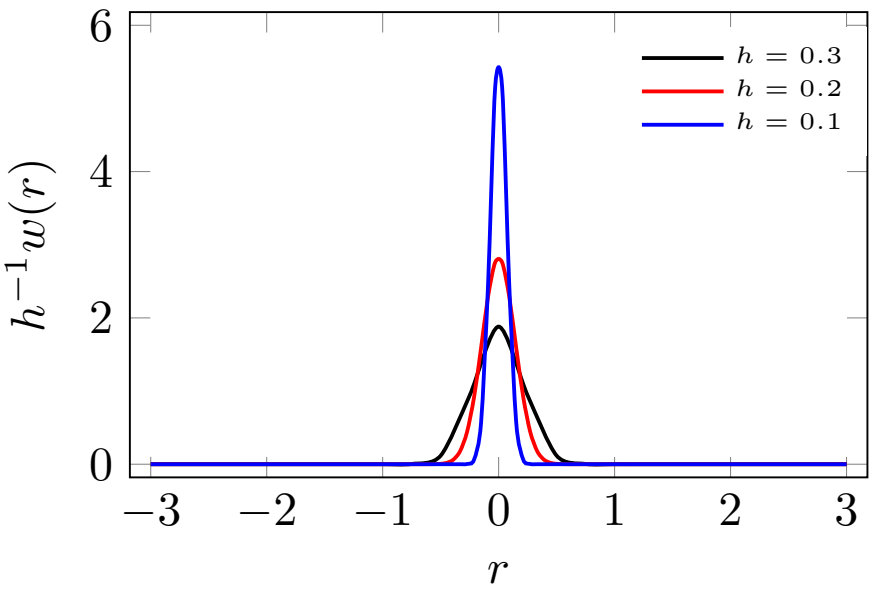
- the flow domain is divided into a set of particles,
- the particles are assigned a mass and velocity,
- Lagrangian description of motion is utilised,
- properties of a particle are calculated as summations over all the neighbouring particles (smoothed as an average),
- SPH can be classified as meshfree method,
- takes advantage of the integral representation and approximation of a function.

Integral representation of a function

The basis of SPH method is the integral representation of a function f where δ is the Dirac delta

$$f(\mathbf{x}) = \iiint_{\Omega} f(\mathbf{x}')\,\delta(\mathbf{x}-\mathbf{x}')\,\mathrm{d}V' \tag{507}$$

$$w(r) := \sigma e^{-r^2}$$



Smoothing kernel

If the Dirac delta is replaced in the integral (exact) representation of a function

$$f(\mathbf{x}) = \iiint_{\Omega} f(\mathbf{x}')\,\delta(\mathbf{x}-\mathbf{x}')\,\mathrm{d}V' \tag{508}$$

by a smoothing function (smoothing kernel) W, the following approximation of a function is obtained

$$f(\mathbf{x}) \approx \iiint_{\Omega} f(\mathbf{x}')\,W(\mathbf{x}-\mathbf{x}',h)\,\mathrm{d}V' \tag{509}$$

where h is the smoothing length.

Smoothing kernel – properties

- normalisation condition

$$\iiint_{\Omega} W(\mathbf{x}-\mathbf{x}',h)\,\mathrm{d}V' = 1 \tag{510}$$

- approaching to Dirac delta property

$$\lim_{h\to 0} W(\mathbf{x}-\mathbf{x}',h) = \delta(\mathbf{x}-\mathbf{x}') \tag{511}$$

- symmetry condition – symmetric property

$$W(\mathbf{x}-\mathbf{x}',h) = W(\mathbf{x}'-\mathbf{x},h) \tag{512}$$

Smoothing kernel – properties

- compact support condition

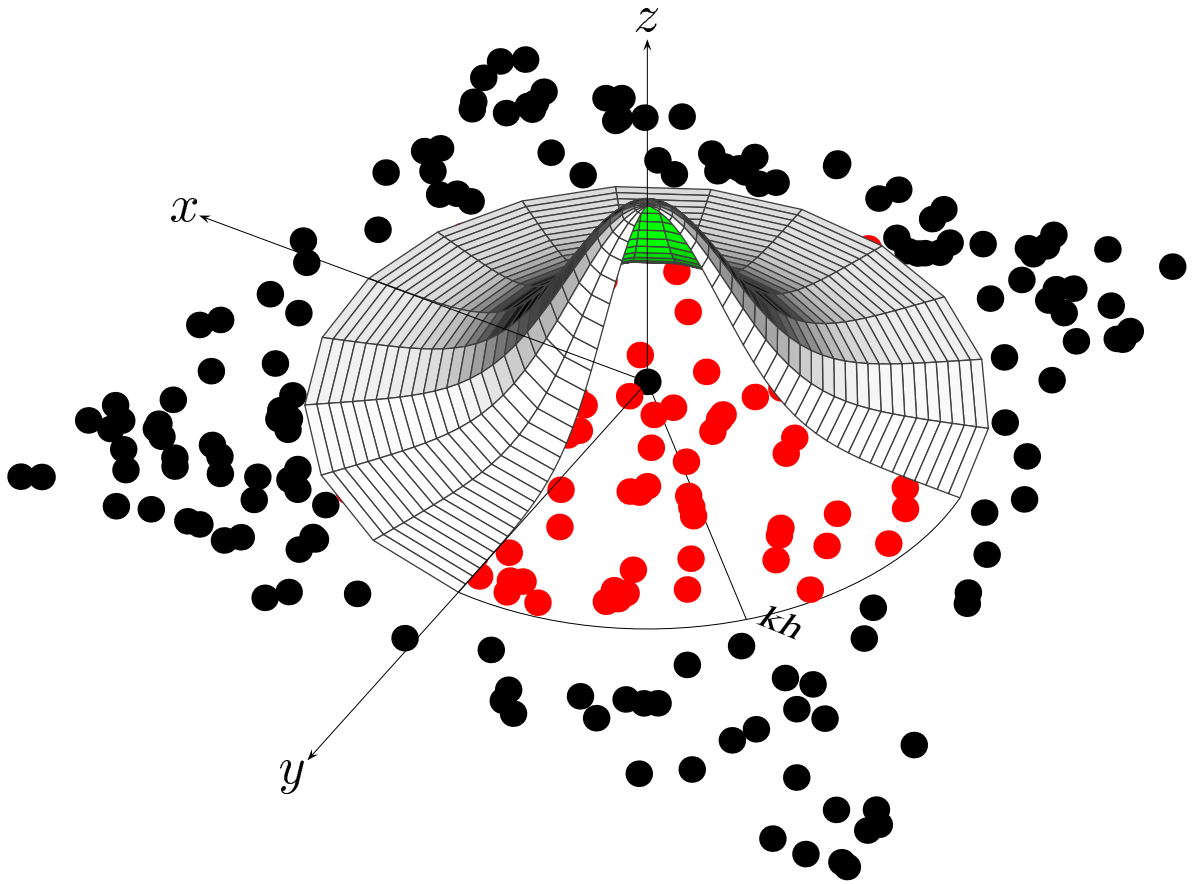
$$\forall_{\|\mathbf{x}-\mathbf{x}'\|>kh} W(\mathbf{x}-\mathbf{x}', h) = 0 \tag{513}$$

- positivity

$$W(\mathbf{x}-\mathbf{x}', h) \geq 0 \tag{514}$$

- monotonically decreasing W as h increase – decay property,
- smoothness (continues and differentiable W) up to the second order at least.

Smoothing kernel



Smoothing kernel

There are many forms of W. To simplify the notation, the following substitutions are adopted

$$W(\mathbf{x}-\mathbf{x}',h) = W\left(\frac{\|\mathbf{x}-\mathbf{x}'\|}{h}\right) = W(r) = \frac{w(r)}{h^D} \quad (515)$$

where r is the relative distance (related to the smoothing length h). Therefore, the kernel W decomposes into the kernel w relative to h^D. Thus, w has the same properties as W, but is dimensionless and simpler to analyse and write.

Gaussian kernel

The Gaussian smoothing kernel is given by

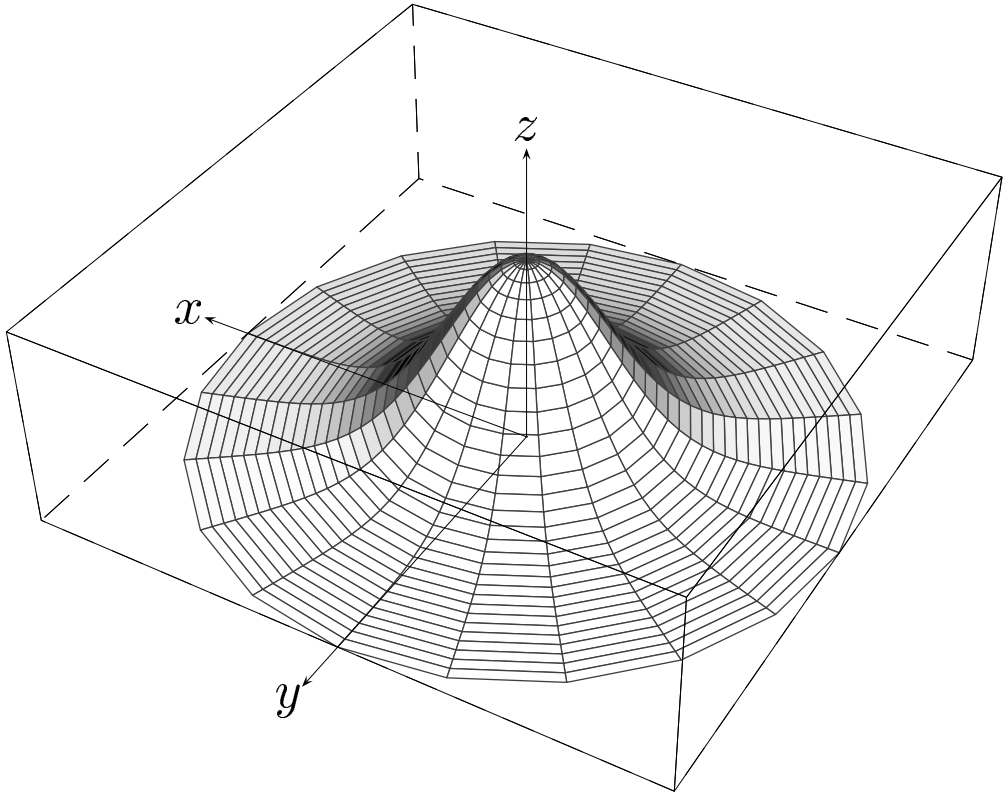
$$w(r) = \sigma e^{-r^2}, \quad r \in [0; \infty[\tag{516}$$

The value of the normalization coefficient σ, depending on the dimension of the space D, is

$$\sigma = \pi^{-D/2} \tag{517}$$

The Gaussian kernel fulfils the conditions of normalisation, symmetry, positivity and decay property. What is more, the Gaussian kernel is also smooth (continuous with derivatives). The compactness condition is not met. Approaches to the Dirac delta as $h \to 0$.

Gaussian kernel



Super Gaussian kernel

$$w(r) = \left(\frac{D}{2} + 1 - r^2 \right) \sigma e^{-r^2}, \quad r \in [0; \infty[\tag{518}$$

where

$$\sigma = \pi^{-D/2} \tag{519}$$

Similar to original Gaussian kernel but lacks positivity!

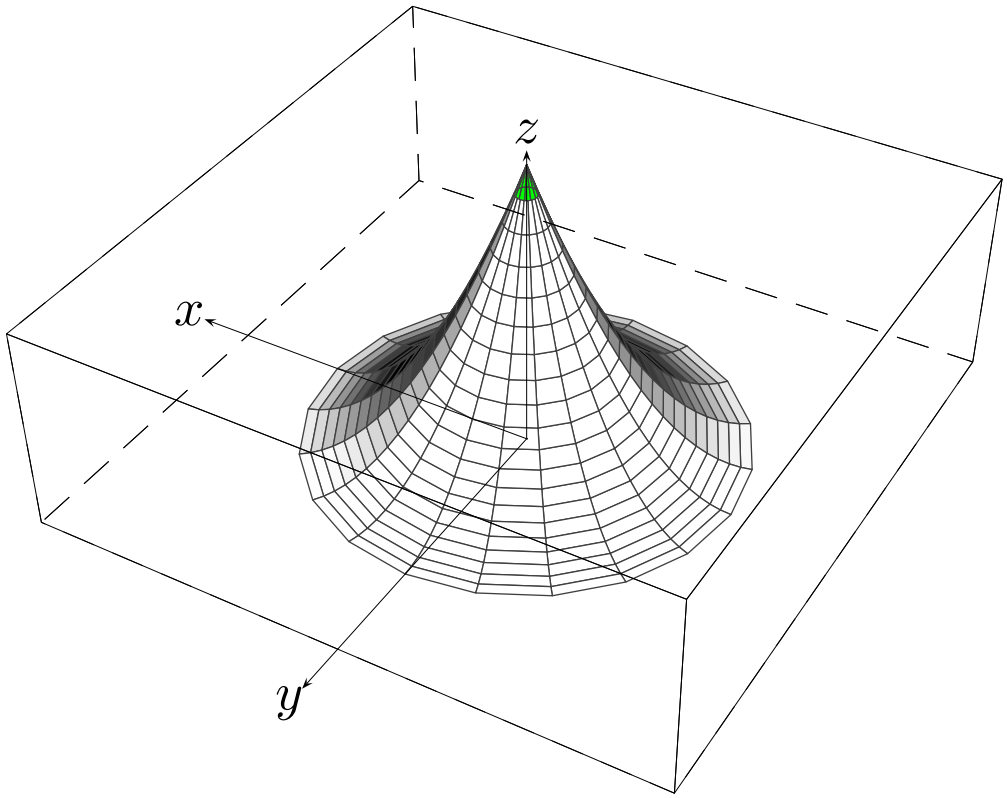
Quadratic kernel

$$w(r) = \sigma \begin{cases} (2-r)^2, & r \in [0;2[, \\ 0, & r \in [2;\infty[\end{cases} \tag{520}$$

where $\sigma = \frac{3}{16}$ for $D = 1$, $\sigma = \frac{3}{8\pi}$ for $D = 2$, $\sigma = \frac{15}{64\pi}$ for $D = 3$.

However, w is continues but w' is only piecewise linear and w'' is discontinues!

Quadratic kernel



Cubic kernel

$$w(r) = \sigma \begin{cases} \frac{1}{4}(2-r)^3 - (1-r)^3, & r \in [0;1[, \\ \frac{1}{4}(2-r)^3, & r \in [1;2[, \\ 0, & r \in [2;\infty[\end{cases} \tag{521}$$

where $\sigma = \frac{2}{3}$ for $D = 1$, $\sigma = \frac{10}{7\pi}$ for $D = 2$, $\sigma = \frac{1}{\pi}$ for $D = 3$.

However, w, w' are continues but w'' is only piecewise linear.

Quadratic kernel

$$w(r) = \sigma \begin{cases} \left(\frac{5}{2} - r\right)^4 - 5\left(\frac{3}{2} - r\right)^4 + 10\left(\frac{1}{2} - r\right)^4, & r \in [0; \frac{1}{2}[, \\ \left(\frac{5}{2} - r\right)^4 - 5\left(\frac{3}{2} - r\right)^4, & r \in [\frac{1}{2}; \frac{3}{2}[, \\ \left(\frac{5}{2} - r\right)^4, & r \in [\frac{3}{2}; \frac{5}{2}[, \\ 0 & r \in [\frac{5}{2}; \infty[\end{cases} \tag{522}$$

where $\sigma = \frac{1}{24}$ for $D = 1$, $\sigma = \frac{96}{1199\pi}$ for $D = 2$, $\sigma = \frac{1}{20\pi}$ for $D = 3$.

This time w, w' and w'' are continuous.

Approximation of a function

The approximation of a function comes directly from the integral representation of the function

$$f(\mathbf{x}) \approx \iiint_{\Omega} f(\mathbf{x}')\, W(\mathbf{x}-\mathbf{x}', h)\, \mathrm{d}V' \tag{523}$$

when discretising the integral by means of a finite sum

$$f(\mathbf{x}) \approx \sum_{j} f(\mathbf{x}_j)\, W(\mathbf{x}-\mathbf{x}_j, h) \Delta |V_j| \tag{524}$$

Elementary volume is $\Delta |V_j| = \frac{m_j}{\rho_j}$ so

$$f(\mathbf{x}) \approx \sum_{j} \frac{m_j}{\rho_j} f(\mathbf{x}_j)\, W(\mathbf{x}-\mathbf{x}_j, h) \tag{525}$$

Approximation of a function

The function $f(\mathbf{x}_j)$ is related to the particles j inside the smoothing kernel of the W approximation. Thus, the approximation

$$f(\mathbf{x}) \approx \sum_j \frac{m_j}{\rho_j} f(\mathbf{x}_j)\, W(\mathbf{x} - \mathbf{x}_j, h) \tag{526}$$

is a discrete approximation of the continuous function f at any point $\mathbf{x}$ that belongs to the area Ω. If the value of the function f is to be calculated at the point $\mathbf{x}_i$, then

$$f(\mathbf{x}_i) \approx \sum_j \frac{m_j}{\rho_j} f(\mathbf{x}_j)\, W(\mathbf{x}_i - \mathbf{x}_j, h) = \sum_j \frac{m_j}{\rho_j} f(\mathbf{x}_j)\, W_{ij} \tag{527}$$

where W_{ij} means $W(\mathbf{x}_i - \mathbf{x}_j, h)$.

Approximation of a gradient

The gradient of the function f relative to the $\mathbf{x}$ coordinates is obtained from the integral representation of the function

$$\nabla f(\mathbf{x}) \approx \iiint_{\Omega} f(\mathbf{x}') \nabla W(\mathbf{x} - \mathbf{x}', h) \, \mathrm{d}V' \tag{528}$$

By discretising the integral, we have a gradient at $\mathbf{x}_i$

$$\nabla f(\mathbf{x}_i) \approx \sum_j \frac{m_j}{\rho_j} f(\mathbf{x}_j) \nabla_i W_{ij} \tag{529}$$

Spatial differentiation is performed on the known form of the smoothing kernel W.

Better approximation of a gradient

$$\nabla f(\mathbf{x}_i) \approx \sum_j \frac{m_j}{\rho_j} \left(f(\mathbf{x}_j) - f(\mathbf{x}_i) \right) \nabla_i W_{ij} \qquad (530)$$

gives exact 0 for constant f.

$$\nabla f(\mathbf{x}_i) \approx \rho_i \sum_j m_j \left(\frac{f(\mathbf{x}_i)}{\rho_i^2} + \frac{f(\mathbf{x}_j)}{\rho_j^2} \right) \nabla_i W_{ij} \qquad (531)$$

is symmetric for i and j.

Approximation of a divergence

The divergence approximation of the vector $\mathbf{f}$ is similar to the gradient approximation. This is because the divergence operator is computed relative to the $\mathbf{x}$ coordinates

$$\nabla \cdot \mathbf{f}(\mathbf{x}) \approx \iiint_{\Omega} \mathbf{f}(\mathbf{x}') \cdot \nabla W(\mathbf{x} - \mathbf{x}', h) \, \mathrm{d}V' \qquad (532)$$

The simplest approximation of divergence is obtained by discretising the above integral

$$\nabla \cdot \mathbf{f}(\mathbf{x}_i) \approx \sum_j \frac{m_j}{\rho_j} \mathbf{f}(\mathbf{x}_j) \cdot \nabla_i W_{ij} \qquad (533)$$

Better approximation of a divergence

$$\nabla \cdot \mathbf{f}(\mathbf{x}_i) \approx \sum_j \frac{m_j}{\rho_j} \left(\mathbf{f}(\mathbf{x}_j) - \mathbf{f}(\mathbf{x}_i)\right) \cdot \nabla_i W_{ij} \qquad (534)$$

gives exact 0 for constant $\mathbf{f}$.

$$\nabla \cdot \mathbf{f}(\mathbf{x}_i) \approx \rho_i \sum_j m_j \left(\frac{\mathbf{f}(\mathbf{x}_i)}{\rho_i^2} + \frac{\mathbf{f}(\mathbf{x}_j)}{\rho_j^2}\right) \cdot \nabla_i W_{ij} \qquad (535)$$

is symmetric for i and j.

Approximation of a Laplacian

The Laplacian approximation of a scalar can be represented by the same method as in the case of the gradient

$$\nabla^2 f(\mathbf{x}) \approx \iiint_{\Omega} f(\mathbf{x}') \nabla^2 W(\mathbf{x} - \mathbf{x}', h) \, \mathrm{d}V' \qquad (536)$$

The simplest approximation of the Laplacian is obtained by discretizing the above integral

$$\nabla^2 f(\mathbf{x}_i) \approx \sum_j \frac{m_j}{\rho_j} f(\mathbf{x}_j) \nabla_i^2 W_{ij} \qquad (537)$$

Better approximation of a Laplacian

$$\nu\nabla^2\mathbf{u}_i = \frac{\mu}{\rho}\nabla\cdot\nabla\mathbf{u}_i \approx \mu\sum_j \frac{m_j}{\rho_i\rho_j}\mathbf{u}_j\nabla_i^2 W_{ij} \tag{538}$$

$$\nu\nabla^2\mathbf{u}_i = \frac{\mu}{\rho}\nabla\cdot\nabla\mathbf{u}_i \approx -\mu\sum_j \frac{m_j}{\rho_i\rho_j}\left(\mathbf{u}_i-\mathbf{u}_j\right)\nabla_i^2 W_{ij} \tag{539}$$

$$\begin{aligned}\nabla\cdot\left(\nu_i\nabla\mathbf{u}_i\right) &= \frac{1}{\rho}\nabla\cdot\left(\mu_i\nabla\mathbf{u}_i\right)\\ &\approx \sum_j \frac{(\mu_i+\mu_j)m_j\,\mathbf{u}_{ij}}{\rho_i\rho_j}\frac{\mathbf{x}_{ij}\cdot\nabla_i W_{ij}}{r_{ij}^2+0.01h^2}\end{aligned} \tag{540}$$

Mass conservation equation in SPH

The mass conservation equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \mathbf{u} \tag{541}$$

is approximated using the velocity divergence approximation

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_j \frac{m_j}{\rho_j} \mathbf{u}_j \cdot \nabla_i W_{ij} \tag{542}$$

In most cases, a function approximation is used, assuming $f = \rho$. Therefore

$$\rho_i = \sum_j m_j W_{ij} \tag{543}$$

Momentum conservation equation in SPH

The momentum conservation equation in its most general form, taking into account the mass forces from gravity $\mathbf{g}$, is written as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{g} + \frac{1}{\rho}\nabla \cdot \boldsymbol{\sigma} \tag{544}$$

The approximation of this equation in the SPH method can be obtained by means of the divergence approximation

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t} = \mathbf{g}_i + \frac{1}{\rho_i}\sum_j \frac{m_j}{\rho_j}\boldsymbol{\sigma}_j \cdot \nabla_i W_{ij} \tag{545}$$

Navier–Stokes equation in SPH

In the approximation of the Navier–Stokes equation in the SPH method, particular types of forces are distinguished: forces from the pressure gradient $\mathbf{f}_{pi}$ and forces related to viscosity $\mathbf{f}_{\mu i}$. The equation of motion then has the following form

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t} = \mathbf{g}_i - \mathbf{f}_{pi} + \mathbf{f}_{\mu i} \tag{546}$$

Assuming the following notation for each type of force together with the gravity acceleration $\mathbf{g}$ in the form $\mathbf{f}_i = \mathbf{g}_i - \mathbf{f}_{pi} + \mathbf{f}_{\mu i}$, the equation of motion can be presented in a form that occurs in other Lagrangian methods

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t} = \mathbf{f}_i \tag{547}$$

Equation of state in SPH

The determination of pressure in the SPH method involves the use of an artificial equation of state in which pressure is explicitly related to density. One possible form for such an equation could be

$$p = p_0 + B\left(\left(\frac{\rho}{\rho_0}\right)^{\gamma} - 1\right) \tag{548}$$

In this case, it is referred to as a weakly compressible fluid. The γ exponent is usually taken as $\gamma \approx 7$, and ρ_0 is the reference fluid density. Often, due to simplicity, $p_0 = 0$ is assumed.

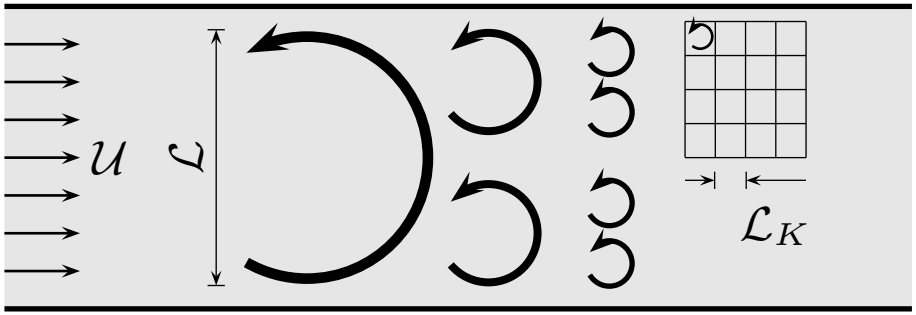
SPH pseudocode

$t := 0$;
foreach *i* **do**
  Generate $\mathbf{x}_i(0)$, $\mathbf{u}_i(0)$, $\rho_i(0)$, $h_i(0)$;
foreach *i* **do**
  $\mathbf{f}_i^0 := \mathbf{f}_i := \mathbf{g}_i - \mathbf{f}_{pi} + \mathbf{f}_{\mu i}$;
repeat
  foreach *i* **do**
    Find $\mathcal{N}_i$;
    Calculate ρ_i, p_i;
  foreach *i* **do**
    Calculate $\mathbf{f}_{pi}$, $\mathbf{f}_{\mu i}$;
  foreach *i* **do**
    Calculate new $\mathbf{x}_i$, $\mathbf{u}_i$;
    Apply BCs;
  $t := t + \Delta t$;
until $t < t_{max}$;

Turbulence modelling

Turbulence features

- Irregularity
- Unsteadiness
- 3-D in terms of space and vortex structures
- Diffusivity
- Dissipation
- Energy cascade
- Need for constant energy supply



Kolmogorov scales

Kolmogorov scales are the smallest vorticity scales where nearly the whole dissipation takes place. There are three scales, for velocity $\mathcal{U}_K = (\nu\varepsilon)^{1/4}$, length $\mathcal{L}_K = \left(\nu^3\varepsilon^{-1}\right)^{1/4}$ and time $t_K = \left(\nu\varepsilon^{-1}\right)^{1/2}$.
The Reynolds number for these scales

$$\mathrm{Re}_K = \frac{\mathcal{U}_K\mathcal{L}_K}{\nu} = \frac{(\nu\varepsilon)^{1/4}\left(\nu^3\varepsilon^{-1}\right)^{1/4}}{\nu} = 1 \qquad (549)$$

It means that at this level the inertial forces are of the same order as the viscous forces.
The dissipation intensity of the kinetic energy of fluctuation can also be estimated in terms of a length scale for large scale motion (vorticity) as

Kolmogorov scales

$$\varepsilon \sim \frac{\mathcal{U}^2}{t} = \frac{\mathcal{U}^2}{\mathcal{L}/\mathcal{U}} = \frac{\mathcal{U}^3}{\mathcal{L}} \tag{550}$$

It means that the energy $\mathcal{U}^2$ of the large scales is dissipated proportionally to time $\mathcal{L}/\mathcal{U}$. Substituting the dissipation in equation for $\mathcal{L}_K$ with that for ε we have

$$\mathcal{L}_K = \left(\frac{\nu^3 \mathcal{L}}{\mathcal{U}^3}\right)^{1/4} \tag{551}$$

Introducing a Reynolds number for large scales $\mathrm{Re}_{\mathcal{L}} = \frac{\mathcal{U}\mathcal{L}}{\nu}$ it is possible to find a relation for the ratio of length scales by means of this Reynolds number in the form of

$$\frac{\mathcal{L}}{\mathcal{L}_K} \sim \left(\frac{\mathcal{U}^3}{\nu^3 \mathcal{L}}\right)^{1/4} \mathcal{L} = \left(\frac{\mathcal{U}\mathcal{L}}{\nu}\right)^{3/4} = \mathrm{Re}_{\mathcal{L}}^{3/4} \tag{552}$$

Mesh size

The ratio of length scales, as a function of the Reynolds number is

$$\frac{\mathcal{L}}{\mathcal{L}_K} \sim \mathrm{Re}_{\mathcal{L}}^{3/4} \tag{553}$$

A three dimensional mesh (number of nodes) is then proportional to

$$\left(\frac{\mathcal{L}}{\mathcal{L}_K}\right)^3 \sim \mathrm{Re}_{\mathcal{L}}^{9/4} \tag{554}$$

If, for instance, $\mathrm{Re} = 10^4$ then

$$\left(\frac{\mathcal{L}}{\mathcal{L}_K}\right)^3 \sim 10^9 \tag{555}$$

Calculation time

A minimal number of time steps $\Delta t \leq \mathcal{L}_K/\mathcal{U}$ of a simulation time t can be estimated by means of $\mathcal{L}_K$

$$\frac{t}{\Delta t} = \frac{t}{\mathcal{L}_K/\mathcal{U}} = \frac{t}{\mathcal{L}/\mathcal{U}}\mathrm{Re}^{3/4} \tag{556}$$

The necessary number of operations equals a number of nodes times a number of time steps

$$\left(\frac{\mathcal{L}}{\mathcal{L}_K}\right)^3 \frac{t}{\Delta t} = \frac{t}{\mathcal{L}/\mathcal{U}}\mathrm{Re}^3 \tag{557}$$

Calculation time

The computation time equals a number of necessary operations times a number of evaluations per operation (e.g. 10^3) over a CPU performance expressed in e.g. TFLOPS $= 10^{12}\,\mathrm{s}^{-1}$

$$\frac{10^3}{10^{12}}\left(\frac{\mathcal{L}}{\mathcal{L}_K}\right)^3\frac{t}{\Delta t}=\frac{10^3}{10^{12}}\frac{t}{\mathcal{L}/\mathcal{U}}\mathrm{Re}^3 \quad \mathrm{s} \tag{558}$$

For instance, if the time of a numerical simulation is $t = 10\mathcal{L}/\mathcal{U}$ then the following CPU time is estimated

$$\frac{10^3}{10^{12}}\left(\frac{\mathcal{L}}{\mathcal{L}_K}\right)^3\frac{t}{\Delta t}=\frac{10^4\,\mathrm{Re}^3}{10^{12}} \quad \mathrm{s} \tag{559}$$

Calculation time

Estimated 1 teraFLOPS CPU time is

$$\frac{10^3}{10^{12}}\left(\frac{\mathcal{L}}{\mathcal{L}_K}\right)^3\frac{t}{\Delta t}=\frac{10^4\,\mathrm{Re}^3}{10^{12}}\quad\mathrm{s}\tag{560}$$

for $\mathrm{Re}=10^3$ it takes 10 second,
for $\mathrm{Re}=10^4$ it takes 3 hours,
for $\mathrm{Re}=10^5$ it takes 115 days,
for $\mathrm{Re}=10^6$ it takes 327 years...

only for a short period of simulated time

$$t=10\mathcal{L}/\mathcal{U}\tag{561}$$

Performance

CPU	@	TFLOPS†
i3 M380	2.53 GHz x 2(4)	0.017
i7 930	2.80 GHz x 4(8)	0.034
i7 870	2.93 GHz x 4(8)	0.041
i7 2670QM	2.20 GHz x 4(8)	0.064
i5 1035G1	1.00 GHz x 4(8)	0.132
i7 10700T	2.00 GHz x 8(16)	0.257
i7 6850K	3.60 GHz x 6(12)	0.284
2 x Xeon Gold 5120	2.20 GHz x 28	0.673

†Intel® LINPACK Benchmark for Linux

Some classical experiments

- Reynolds experiment (Reynolds number Re)

$$\mathrm{Re} = \frac{uL}{\nu} \tag{562}$$

- Taylor instability or vortices (Taylor number Ta)

$$\mathrm{Ta} = \frac{\omega R_1}{\nu^2} \left(R_2 - R_1\right)^3 \tag{563}$$

- Rayleigh-Bénard instability (Rayleigh number Ra)

$$\mathrm{Ra} = \frac{g\beta h^3}{\nu\alpha} \left(T_b - T_u\right) \tag{564}$$

Turbulence glossary

- DNS – Direct Numerical Simulation
- LES – Large Eddy Simulation
- RANS – Reynolds Averaged Navier–Stokes
- RAS – Reynolds Averaged Simulation
- URANS – Unsteady Reynolds Averaged Navier–Stokes
- URAS – Unsteady Reynolds Averaged Simulation
- DES – Detached Eddy Simulation
- SST – Shear Stress Transport
- RNG – ReNormalisation Group
- EARSM – Explicit Algebraic Reynolds Stress Models
- RST – Reynolds Stress Transport

Turbulence modelling

- DNS
- LES
- DES
- URAS/RAS
  - Models based on the Boussinesq hypothesis (0-eq, 1-eq, 2-eq models)
  - Models which do not take advantage of the Boussinesq hypothesis
    - RST models
    - EARSM

Decompositions and averages

Decomposition

$$f(\mathbf{r},t) = \bar{f}(\mathbf{r}) + f'(\mathbf{r},t) \tag{565}$$

- Realisations $\bar{f}(\mathbf{r}) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f_i(\mathbf{r},t)$
- Time $\bar{f}_\tau(\mathbf{r}) = \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau f(\mathbf{r},t)\,\mathrm{d}t$
- Time $\bar{f}_t(\mathbf{r},t) = \frac{1}{\Delta t} \int_t^{t+\Delta t} f(\mathbf{r},t)\,\mathrm{d}t$
- Spatial $\bar{f}_V(\mathbf{r},t) = \frac{1}{|V|} \iiint_V f(\mathbf{r},t)\,\mathrm{d}V$

Comments

In practice it is usually enough to know what the average velocity is (not the fluctuation). The velocity vector field is be decomposed into average and fluctuation components $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$. The time of averaging Δt should be chosen to be greater than the fluctuation range and smaller than the function that is going to be averaged. The averaging process of the Navier–Stokes equation introduces a number of new unknown functions.

- Averaged mass conservation equation

$$\nabla \cdot \bar{\mathbf{u}} = 0 \tag{566}$$

- Averaged Navier–Stokes equation

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = \bar{\mathbf{f}} - \nabla \bar{p}_k + \nu \nabla^2 \bar{\mathbf{u}} - \nabla \cdot \overline{\mathbf{u}'\mathbf{u}'} \tag{567}$$

Reynolds stress tensor $\mathbf{R} = -\overline{\mathbf{u}'\mathbf{u}'}$ and the total stress tensor $\bar{\boldsymbol{\sigma}} = -\bar{p}\boldsymbol{\delta} + 2\mu\bar{\mathbf{D}} + \rho\mathbf{R}$ makes it possible to obtain the averaged momentum equation

$$\rho \frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = \rho\bar{\mathbf{f}} + \nabla \cdot \bar{\boldsymbol{\sigma}} \tag{568}$$

- Averaged Fourier–Kirchhoff equation

$$c_v \left(\frac{\partial(\rho \bar{T})}{\partial t} + \nabla \cdot \left(\rho \bar{T} \bar{\mathbf{u}} \right) \right) = 2\mu \bar{\mathbf{D}}^2 + \nabla \cdot (\lambda \nabla \bar{T}) - c_v \nabla \cdot \left(\rho \overline{T' \mathbf{u}'} \right) + \rho \varepsilon \quad (569)$$

The averaging process of the Navier–Stokes equation introduces six unknown (because of the symmetry) components of the Reynolds stress tensor. The averaged Fourier–Kirchhoff equations gives a further three of the vector $\overline{T' \mathbf{u}'}$.

Comments

It is important to realise that the closure of system of the mass conservation and Navier–Stokes equations has been lost. Further modelling is required.
Formulating additional relationships for unknown functions to achieve closure of equations is called turbulence modelling. Any additional closure equation must fulfil a few basic criteria such as coordinate invariance. This is fulfilled by proper tensor formulation of the exact and modelled equations. Another criterion is called realisability meaning that a solution must be physical.
Practically, however, it is difficult to achieve all these requirements. This is because some parts of the exact transport equations are modelled or even dropped.

Closure

There are two main approaches to achieve closure. The models may be divided between those which assume the eddy viscosity hypothesis and those which do not

- Models not assuming the eddy viscosity hypothesis
  - Reynolds stress transport equation
  - Algebraic stress tensor models
- Boussinesq hypothesis assumed

Reynolds stress transport equation

$$\frac{\partial \mathbf{R}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\mathbf{R}) = -\nabla \bar{\mathbf{u}} \cdot (\mathbf{R}^{\mathrm{T}} + \mathbf{R}) + \nabla \cdot \left(\left(C k^2 \varepsilon^{-1} + \nu \right) \nabla \mathbf{R} \right) - \mathbf{\Pi} + \tfrac{2}{3} \varepsilon \boldsymbol{\delta} \quad (570)$$

The left hand side represents unsteadiness and convection. On the right hand side the two first terms represent production. The two terms under divergence are responsible for diffusion.
The right hand side fourth term is the second unknown tensor $\mathbf{\Pi}$ need to be modelled. The last right hand side term $\frac{2}{3}\rho\varepsilon\boldsymbol{\delta}$ is the so called dissipation tensor for isotropic turbulence.

Algebraic stress tensor models

Without using the eddy viscosity hypothesis two transport equations for k and a second variable are formulated. Instead of the linear Boussinesq hypothesis – algebraic, non-linear relationships are formulated between the stress anisotropy tensor $\mathbf{a}$ and the average flow properties. The tensor $\mathbf{a}$ is related to the Reynolds stress tensor by:

$$\mathbf{a} = \frac{\mathbf{R}}{k} - \frac{2}{3}\boldsymbol{\delta} \tag{571}$$

Typically, relationships depend on average strain rate and spin tensors

$$\mathbf{a} = f(\bar{\mathbf{D}}, \bar{\boldsymbol{\Omega}}) \tag{572}$$

Boussinesq hypothesis

The turbulence stresses is related to the mean flow $R_{xy} = \mu_t \frac{\partial \bar{U}_x}{\partial y}$. This linear relationship is

$$\mathbf{R} = a_0 \boldsymbol{\delta} + 2\nu_t \bar{\mathbf{D}} \tag{573}$$

The trace of this relations allows to find a constant $-2k = 3a_0$ which gives

$$\mathbf{R} = -\tfrac{2}{3} k \boldsymbol{\delta} + 2\nu_t \bar{\mathbf{D}} \tag{574}$$

The Reynolds equation becomes

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = \bar{\mathbf{f}} - \nabla p_e + \nabla \cdot \left(2\nu_e \bar{\mathbf{D}}\right) \tag{575}$$

where $\nu_e = \nu_t + \nu$, $p_e = \bar{p}_k + \frac{2}{3}k$.

Eddy diffusivity hypothesis

The eddy diffusivity hypothesis is introduced by direct analogy with the eddy viscosity hypothesis. It reduces the number of unknown functions in the Fourier–Kirchhoff equation $-c_v \rho \overline{T' \mathbf{u}'} = \lambda_t \nabla \bar{T}$.
The Fourier–Kirchhoff equation then becomes

$$c_v \left(\frac{\partial(\rho \bar{T})}{\partial t} + \nabla \cdot \left(\rho \bar{T} \bar{\mathbf{u}} \right) \right) = 2\mu \bar{\mathbf{D}}^2 + \nabla \cdot \left(\lambda_e \nabla \bar{T} \right) + \rho \varepsilon \tag{576}$$

where λ_t can be estimated by means of the turbulent Prandtl number $\lambda_t = \frac{\mu_t c_v}{\mathrm{Pr}_t}$. Effective conductivity is introduced by means of the definition
$\lambda_e = \lambda_t + \lambda = \frac{\mu_t c_v}{\mathrm{Pr}_t} + \lambda$.

Trace of RST equation

Calculating the trace of the Reynolds stress transport equation

$$\frac{\partial \mathbf{R}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\mathbf{R}) = -\nabla \bar{\mathbf{u}} \cdot (\mathbf{R}^{\mathrm{T}} + \mathbf{R}) + \nabla \cdot \left(\left(C k^2 \varepsilon^{-1} + \nu \right) \nabla \mathbf{R} \right) - \mathbf{\Pi} + \frac{2}{3} \varepsilon \boldsymbol{\delta} \quad (577)$$

results in kinetic energy k transport equation which is used in the preceding one- and two-equation turbulence models $\mathrm{tr}\,\mathbf{R} = -2k$ for $\nu_t = C_\mu k^2 \varepsilon^{-1}$.
The traces of $\mathbf{\Pi}$ by definition $\mathrm{tr}\,\mathbf{\Pi} = 0$ and the transport equation for k takes the following form

$$\frac{\partial k}{\partial t} + \nabla \cdot (\rho k \bar{\mathbf{u}}) = \nabla \bar{\mathbf{u}} : \mathbf{R} + \nabla \cdot \left(\left(\nu_t \sigma_k^{-1} + \nu \right) \nabla k \right) - \varepsilon \quad (578)$$

Zero-equation model

Zero k and ε are assumed. It allows the Boussinesq equation to be reduced to $\mathbf{R} = 2\nu_t \bar{\mathbf{D}}$.
Eddy viscosity μ_t is modelled by means of the Prandtl–Kolmogorov hypothesis. This hypothesis comes directly from dimensionless analysis $\nu_t = c\mathcal{U}\mathcal{L}$.
The velocity scale $\mathcal{U}$ is often approximated by means of the maximal velocity $|\bar{\mathbf{u}}|_{max}$ and length scale $\mathcal{L}$ by the volume of the flow domain $|V|$ by $\mathcal{U} \sim |\bar{\mathbf{u}}|_{max}$, $\mathcal{L} \sim \sqrt[3]{|V|}$.
The Boussinesq hypothesis takes the following form

$$\mathbf{R} = C\sqrt[3]{|V|}|\bar{\mathbf{u}}|_{max}\bar{\mathbf{D}} \tag{579}$$

No new unknown functions! However, zero-equation models are not as accurate but they are robust (first approximation for more complex models).

One-equation model

One transport equation for k is introduced

$$\frac{\mathrm{d}k}{\mathrm{d}t} = \nabla\bar{\mathbf{u}} : \mathbf{R} + \nabla \cdot \left(\left(\nu_t \sigma_k^{-1} + \nu\right) \nabla k\right) - \varepsilon \qquad (580)$$

where 'production' $\nabla\bar{\mathbf{u}} : \mathbf{R} = 2\nu_t \bar{\mathbf{D}}^2$. According to Prandtl–Kolmogorov hypothesis $\mathcal{U} = \sqrt{k}$ and $\varepsilon \sim \frac{\mathcal{U}^3}{\mathcal{L}}$ so $\varepsilon = k^{3/2}\mathcal{L}^{-1}$. Finally, the k transport equation arrives

$$\frac{\mathrm{d}k}{\mathrm{d}t} = 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\nu_t \sigma_k^{-1} + \nu\right) \nabla k\right) - k^{3/2}\mathcal{L}^{-1} \qquad (581)$$

where eddy viscosity is estimated as $\nu_t = \sqrt{k}\mathcal{L}$ by means of another Prandtl hypothesis.

Two-equation k-ε model

Two additional equations have to be formulated. The first, for the kinetic energy k, comes from the Reynolds stress transport equation

$$\frac{\mathrm{d}k}{\mathrm{d}t} = 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_k} + \nu \right) \nabla k \right) - \varepsilon \qquad (582)$$

and that for the dissipation ε is analogous to it

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = C_{\varepsilon 1} \frac{\varepsilon}{k} 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_\varepsilon} + \nu \right) \nabla \varepsilon \right) - C_{\varepsilon 2} \frac{\varepsilon^2}{k} \qquad (583)$$

Both of them are transport equations for a scalar function. The eddy viscosity depends on both k and ε and is postulated, as previously, to have the form $\nu_t = C_\nu \frac{k^2}{\varepsilon}$.

Comments

The five constants in equations are empirical, that is, should be deduced from experiment for a specific geometry. This 'standard' set is given by

$$\sigma_k = 1,\ \sigma_\varepsilon = 1.3,$$
$$C_\mu = 0.09,\ C_{\varepsilon 1} = 1.44,\ C_{\varepsilon 2} = 1.92 \quad (584)$$

Two-equation k-ω model

The turbulent frequency ω is proportional to the ratio of dissipation and kinetic energy $\omega \sim \frac{\varepsilon}{k}$ and using the constant C_μ, they are then related by $\varepsilon = C_\mu k\omega$. The eddy viscosity takes the form $\nu_t = \frac{k}{\omega}$. The two transport equations take the following form

$$\frac{\mathrm{d}k}{\mathrm{d}t} = 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_{k1}} + \nu \right) \nabla k \right) - C_\mu k\omega \quad (585)$$

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = \alpha_1 \frac{\omega}{k} 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_{\omega 1}} + \nu \right) \nabla \omega \right) - \beta_1 \omega^2 \quad (586)$$

This 'standard' set is constant is $\sigma_{k1} = 2$, $\sigma_{\omega 1} = 2$, $C_\mu = 0.09$, $\alpha_1 = \frac{5}{9}$, $\beta_1 = \frac{3}{40}$.

Two equations SST model

The shear stress model combines the k-ω model near the wall with the k-ε far from it. Firstly, the k-ε model has to be transformed to the k-ω formulation by means of relation $\varepsilon = C_\mu k\omega$. This results in

$$\frac{\mathrm{d}k}{\mathrm{d}t} = 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_{k2}} + \nu \right) \nabla k \right) - C_\mu k\omega \quad (587)$$

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = \alpha_2 \frac{\omega}{k} 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_{\omega 2}} + \nu \right) \nabla \omega \right) - \beta_2 \omega^2 + 2\frac{\omega}{\sigma_{\omega 2}} \nabla k \cdot \nabla \omega \quad (588)$$

Additional cross-diffusion terms now appear. The 'standard' set of constants is different from that for the original k-ε $\sigma_{k2} = 1$, $\sigma_{\omega 2} = 0.856$, $C_\mu = 0.09$, $\alpha_2 = 0.44$, $\beta_2 = 0.0828$.

Two equations SST model

Secondly, the equations for the k-ω model are multiplied by a blending function F_1 and the transformed k-ε equations by $(1 - F_1)$. The equations then are added. This results in

$$\frac{\mathrm{d}k}{\mathrm{d}t} = 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_{k3}} + \nu \right) \nabla k \right) - C_\mu k\omega \quad (589)$$

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = \alpha_3 \frac{\omega}{k} 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\frac{\nu_t}{\sigma_{\omega 3}} + \nu \right) \nabla \omega \right) - \beta_3 \omega^2 + (1 - F_1) \frac{2}{\omega} \sigma_{\omega 3} \nabla k \cdot \nabla \omega \quad (590)$$

Constants marked with the subscript '3', namely σ_{k3}, $\sigma_{\omega 3}$, α_3, β_3 are linear combinations of constants from the component models $C_3 = F_1 C_1 + (1 - F_1) C_2$.

Additional passive transport equation

The additional variable transport equation may be added to the closed system after averaging, as

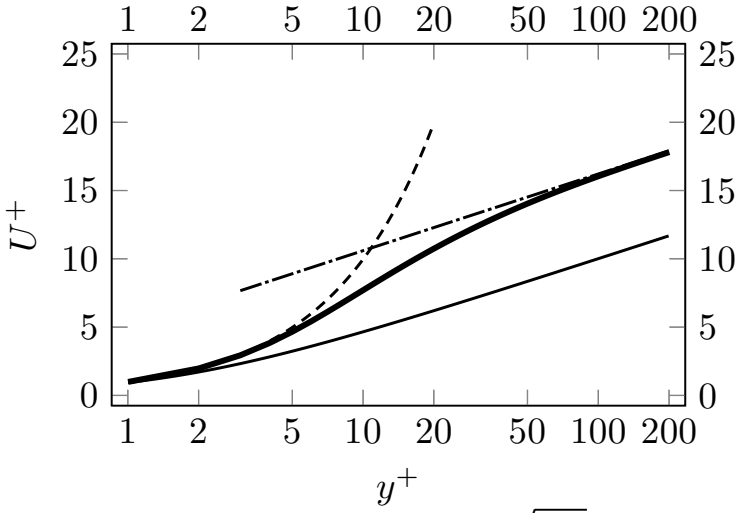
$$\frac{\partial \bar{f}}{\partial t} + \nabla \cdot \left(\bar{f} \bar{\mathbf{u}} \right) = -\nabla \cdot \left(\overline{f' \mathbf{u}'} \right) - \nabla \cdot \bar{\mathbf{k}} + \bar{S}_f \qquad (591)$$

The first term of the right hand side can be modelled by means of the eddy diffusivity hypothesis and the turbulent diffusivity coefficient Γ, $-\overline{f' \mathbf{u}'} = \Gamma \nabla \bar{f}$ and the additional transport equation takes the form

$$\frac{\partial \bar{f}}{\partial t} + \nabla \cdot \left(\bar{f} \bar{\mathbf{u}} \right) = \nabla \cdot \left(\left(\frac{\nu_t}{\mathrm{Sc}_t} + D \right) \nabla \bar{f} \right) + \bar{S}_f \qquad (592)$$

where the turbulent diffusivity coefficient Γ may be represented as a function of the eddy viscosity and the turbulent Schmidt number $\Gamma = \frac{\nu_t}{\mathrm{Sc}_t}$ where $\mathrm{Sc} = \frac{\nu}{D}$.

Turbulent boundary layer



Friction velocity $U_\tau = \sqrt{\frac{\bar{\tau}_0}{\rho}}$

Characteristic length $l = \frac{\nu}{U_\tau}$

dimensionless distance $y^+ = \frac{y}{l}$

dimensionless velocity $U^+ = \frac{\bar{U}_x}{U_\tau}$

- $y^+ < 11$ laminar sublayer
- $5 < y^+ < 30$ buffer region
- $11 < y^+ < 250$ turbulent sublayer (log-law layer)
- $y^+ < 250$ inner turbulent boundary layer
- $y^+ > 250$ outer turbulent boundary layer

LES

Filtration of the N–S equations is associated with LES method. Small scales are removed by means of filtering

$$\bar{f}(\mathbf{r},t) = \iiint_{\mathbb{R}^3} \int_{-\infty}^{+\infty} f(\mathbf{r}'',t'')G(\mathbf{r}-\mathbf{r}'',t-t'')\,\mathrm{d}t''\,\mathrm{d}V'' \tag{593}$$

where G is a filter. Typically it is a product

$$G(\mathbf{r}-\mathbf{r}'',t-t'') = G_t(t-t'')\prod_{i=1}^{3} G_{vi}(x_i - x_i'') \tag{594}$$

For $G_t(t-t'') = \tau^{-1}\mathrm{H}(t'')$ and $G_{vi}(x_i - x_i'') = \delta(x_i - x_i'')$ we have time average $\bar{f}_\tau(\mathbf{r}) = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau f(\mathbf{r},t)\,\mathrm{d}t$.

Filtration of the N–S equations results in

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = \bar{\mathbf{f}} - \nabla p_k + \nabla \cdot \left(2\nu \bar{\mathbf{D}} + \boldsymbol{\tau}\right) \qquad (595)$$

where Leonard's decomposition $\boldsymbol{\tau} = -\mathbf{L} - \mathbf{C} - \mathbf{R}$

$$\mathbf{L} = \overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}}, \ \mathbf{C} = \overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}, \ \mathbf{R} = \overline{\mathbf{u}'\mathbf{u}'} \qquad (596)$$

represents the cross stress tensor $\mathbf{C}$ (interactions between large and small scales), Reynolds subgrid tensor $\mathbf{R}$ (interactions among subgrid scales) and Leonard tensor $\mathbf{L}$ (interactions among the large scales).
For $\mathbf{L} = \mathbf{0}$ and $\mathbf{C} = \mathbf{0}$ we have Reynolds equations.

LES

Subgrid stress tensor need to be modelled

$$\boldsymbol{\tau} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}} \tag{597}$$

Boussinesq like hypothesis assumed

$$\boldsymbol{\tau} = -\tfrac{2}{3}k_{sgs}\boldsymbol{\delta} + 2\nu_{sgs}\bar{\mathbf{D}} \tag{598}$$

Filtered Navier–Stokes equation

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\nabla p_e + \nabla \cdot \left(2(\nu + \nu_{sgs})\bar{\mathbf{D}}\right) \tag{599}$$

Most popular SGS LES models

- zero-equation
  - Smagorinsky
  - WALE (Wall-Adapting Local Eddy-viscosity)
- one-equation k_{sgs}

Smagorinsky – the simplest model. The SGS eddy viscosity is modelled as

$$\nu_{sgs} = C_k \Delta \sqrt{k_{sgs}} \tag{600}$$

where Δ is the filter width.
The SGS kinetic energy is modelled by means of an algebraic equation – zero-equation model

$$k_{sgs} = C_k C_\varepsilon^{-1} \Delta^2 \bar{\mathbf{D}}^2 \tag{601}$$

Finally, the SGS ν_t is

$$\nu_{sgs} = C_S \Delta^2 \sqrt{2\bar{\mathbf{D}}^2} \tag{602}$$

WALE (Wall-Adapting Local Eddy-viscosity)
The SGS kinetic energy is modelled by means of an algebraic equation – zero-equation model

$$k_{sgs} = \frac{C_w^4 \Delta^2}{C_k^2} \frac{\left(\bar{\mathbf{S}}{:}\bar{\mathbf{S}}\right)^3}{\left(\left(\bar{\mathbf{D}}{:}\bar{\mathbf{D}}\right)^{\frac{5}{2}} + \left(\bar{\mathbf{S}}{:}\bar{\mathbf{S}}\right)^{\frac{5}{4}}\right)^2} \tag{603}$$

where

$$\bar{\mathbf{S}} = \tfrac{1}{2}\left(\nabla\mathbf{u}\cdot\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\cdot(\nabla\mathbf{u})^{\mathrm{T}}\right) \tag{604}$$

One-equation k_{sgs} – one transport (differential) equation is introduced by direct analogy with the one-equation RAS k transport equation

$$\frac{\mathrm{d}k_{sgs}}{\mathrm{d}t} = 2\nu_{sgs}\bar{\mathbf{D}}^2 + \nabla\cdot\left(\left(\nu+\nu_{sgs}\right)\nabla k_{sgs}\right) - C_\varepsilon k_{sgs}^{\frac{3}{2}}\Delta^{-1} \tag{605}$$

The reduced version of the above

$$2\nu_{sgs}\bar{\mathbf{D}}^2 = -C_\varepsilon k_{sgs}^{\frac{3}{2}}\Delta^{-1} \tag{606}$$

leads to Smagorinsky model.

DES

DES is a combination of LES and RAS. RAS is used near the wall and LES is used when the mesh if fine enough (far from the wall). DES modification is introduce by means of DES length scale

$$\tilde{d} = \min\left(C_{DES}\Delta, \mathcal{L}\right) \tag{607}$$

in the k transport equation

$$\frac{\mathrm{d}k}{\mathrm{d}t} = 2\nu_t \bar{\mathbf{D}}^2 + \nabla \cdot \left(\left(\nu + \nu_t \sigma_k^{-1}\right) \nabla k\right) - C_\varepsilon k^{\frac{3}{2}} \tilde{d}^{-1} \tag{608}$$

References

List of references

[1] Ferziger J.H., Perić M., *Computational Methods for Fluid Dynamics*, Springer-Verlag, Berlin, 2002

[2] Groot R. D., Warren P. B., *Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation*, The Journal of Chemical Physics, 107, pp 4423–4435, 1997

[3] Jasak H., *Error analysis and estimation for the finite volume method with applications to fluid flows*, PhD Thesis, 1996

[4] Monaghan J. J., *Smoothed Particle Hydrodynamics*, Annual Review of Astronomy and Astrophysics, 30, pp 543–574, 1992

[5] Pope S. B., *Turbulent Flows*, Cambridge University Press, Cambridge, 2000

[6] Succi S., *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford University Press, Oxford, 2001

[7] Tesch K., *Fluid Mechanics*, Wyd. PG, 2008 (in Polish)

[8] Tesch K., *Numerical Fluid Mechanics*, Wyd. PG, 2021 (in Polish)

[9] Wilcox D. C., *Turbulence Modeling for CFD*, DCW Industries, California, 1994

[10] Zienkiewicz O. C., Taylor R. L., *The Finite Element Method*, Butterworth–Heinemann, Oxford, 2000