# Introduction to numerical simulation of fluid flows

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Winterschool April 2004, St. Petersburg (Russia)

## 1 Introduction

The central task in natural sciences is to describe reality as accurately as possible in order to better understand natural phenomena. In engineering sciences the purpose of research is to develop new products and to optimize the existing ones.

In the past there have been two approaches in science: the experimental and the theoretical. With the invention of the computer a new approach have appear: the numerical simulation.

Mathematical equations that describe the physical world with reasonable accuracy are usually so complex that analytical solutions can no longer be obtained.

**Computational Fluid Dynamics** is the analysis of systems involving fluid flow, heat transfer and associated phenomena by means of computer-based simulation. Nowadays expensive experiments are increasingly being replaced by computer simulations. Moreover, simulation enables the examination of processes that cannot be experimentally tested.

## 2 Fluids and flows

Fluids are substances that cannot resist external shear forces, even the smallest force causes deformation of a fluid particle. Although significant differences exist between liquids and gases, both types of fluids obey the same laws of motion. Fluid flow is caused by externally applied forces like pressure differences, gravity, shear, rotation and surface tension. The most important properties of fluids are density and viscosity .

A flow is **incompressible** if the fluid density (mass per unit volume) may be assumed constant. This is not only true for liquids, but also for gases if the Mach number $\mathrm{Ma} = \frac{\text{flow velocity}}{\text{sound velocity}}$ is $< 0.3$. Incompressibility is not a property of the fluid, but of the flow.

The **viscosity** of a fluid is a measure of its resistance to shear deformations. It is due to interaction between fluid molecules. As the temperature increases, the viscosities of all liquids decrease, while the viscosities of all gases increase.

In flows far from solid surfaces, the effects of viscosity are usually very small. A **inviscid (Euler) flow** cannot stick to walls and slip is possible at solid boundaries.

The **Reynolds number** is a dimensionless parameter that expresses the ratio of inertial forces to friction forces in a flow.

$$\mathrm{Re} = \frac{\rho u L}{\mu}$$

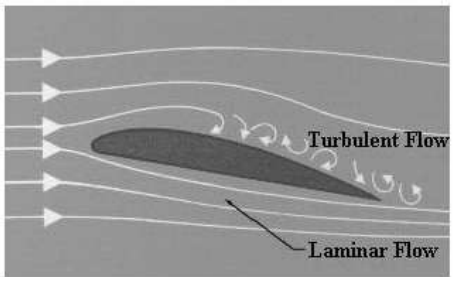
where $u$ is a characteristic velocity of the flow, $L$ is a characteristic length of the problem and $\mu$ is the dynamic viscosity.

When the flow velocity is very small, the fluid is very viscous or the geometric dimensions are very small (i.e. when the Reynolds number is small), the convective (inertial terms) in the Navier-Stokes equations play a minor role and can be neglected. The flow is then called **creeping (Stokes) flow**.

As the velocity is increased, and thus the Re, inertia becomes important but each fluid particle follows a smooth trajectory, the flow is **laminar**. Still viscosity effects dominate and are able to damp out a disturbance. Further increase in velocity may lead to instability that produces a more random type of flow called **turbulent**. Turbulent flows are unsteady, irregular, nonlinear and are characterized by the formation of eddies. At high velocities the Reynolds number is very high and viscous and turbulence effects are important in a small region near the walls, in the **boundary layer**. A finer grid is necessary to resolve the boundary layer.

Many flows of practical interest are difficult to describe exactly mathematically. These flows include turbulence, combustion or multiple phases. Since exact description is often impossible, one usually uses semi-empirical **models** to represent these phenomena.

**Lagrangian description** follows the a particle as it moves through the space. The position of a fluid particle at time t is a function of time and its




initial position.

$$\vec{r} = \vec{r}(\vec{r}_0, t) \qquad \text{where } \vec{r}(t = t_0) = \vec{r}_0$$

**Eulerian description** focus on a fixed point in space and observes fluid particles as they pass by. The velocity is expressed as a funcion of time and of the position in space at which observations are made.

$$\vec{u} = \vec{u}(\vec{r}, t)$$

Eulerian and Lagrangian points of view meet in the transport theorem (section 4).

# 3 Introduction to Numerical Methods

The equations of fluid mechanics, which were already derived about 150 years ago by Navier (1785-1836) and Stokes (1819-1903), are solvable analytically only in special cases. To obtain an approximate solution numerically, we have to use a discretization method which approximates the differential equations by a system of algebraic equations, which can then be solved on a computer.

## 3.1 Components of a numerical method

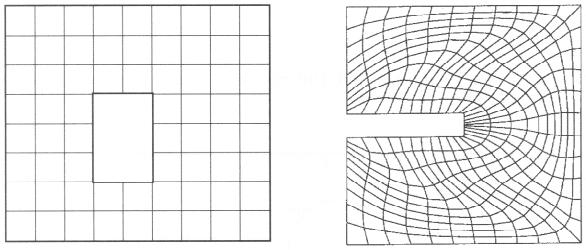
The starting point of any numerical method is the **mathematical model**, the set of partial differential equations and boundary conditions.

After selecting the mathematical model, one has to choose a suitable **discretization method**. The most important are: finite differences (FD), finite volume (FV) and finite element (FE) methods.

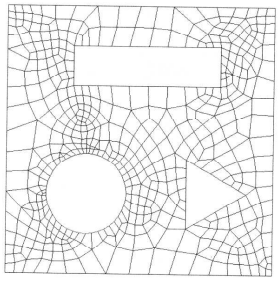
The discrete locations at which the variables are to be calculated are define by the numerical **grid**, which is essentially a discrete representation of the geometric domain on which the problem is to be solved. It divides

the solution domain into a finite number of subdomains. Different types of grids are:

- structured grid: A structured mesh is defined as a mesh where all the nodes have the same number of elements around it. This makes that the matrix of algebraic eq system has a regular structure. There is a large number of efficient solvers applicable only to structured grids. Disadvantages: only for geometrically simple domains. Difficult to control distribution of grid points.



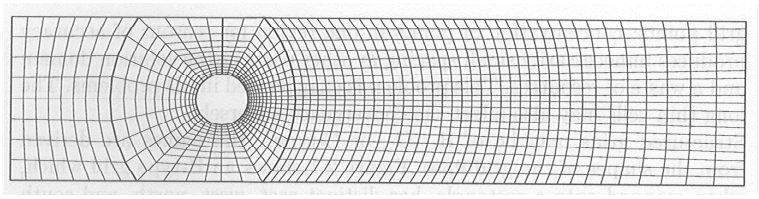
- unstructured grid: For very complex geometries, can fit arbitrary boundaries. Grids made of triangles or quadrilaterals in 2D, and tetrahedra or hexahedra in 3D are the most often used. Such grids can be generated automatically by existing algorithms. Disadvantage: irregularity of the data structure. The solvers for the algebraic equation system are usually slower than those for structured grids.



- block-structured grid: Structured grid inside each block, but the order of blocks is irregular.

## 3.2 Properties of numerical methods

**Consistency** The discretization should become exact as the grid spacing tends to zero. The difference between the discretized equation and the



exact one is called *truncation error*. For a method to be *consistent*, the truncation error must become zero when the mesh spacing $\Delta t \to 0$ and/or $\Delta x_i \to 0$. If the most important term of the truncation error is proportional to $(\Delta x)^n$ or $(\Delta t)^n$ the method is of n-th order. $n > 0$ is required for consistency.

Even if the approximations are consistent, it does not necessarily mean that the approximated solution will become the exact solution in the limit of small step size. For this to happen, the method has to be stable also.

**Stability** A numerical method is stable if does not magnify the errors that appear during the process. For temporal problems, stability guarantees that the method produces a bounded solution whenever the exact solution is also bounded.

**Convergence** A numerical method is convergent if the discrete solution tends to the exact one as the grid spacing tends to zero.

For linear initial value problems, the *Lax equivalence theorem* states:

Consistency + Stability $\Longleftrightarrow$ Convergence

For non-linear problems the stability and convergence of a method are difficult to demonstrate. Therefore convergence is ususally checked using numerical experiments, i.e. repeating the calculation on a series of successively refined grids. If the method is stable and if all approximations used in the discretization process are consistent, we usually find that the solution does converge to a *grid-independent solution*.

**Conservation** Since the equations to be solved are conservation laws, the numerical scheme should also respect these laws. This means that, at steady state and in the absence of sources, the amount of a conserved quantity leaving a closed volume is equal to the amount entering that volume.

If the strong conservation form of equations and a finite volume method are used, this is guaranteed for each individual control volume and for the domain as a whole.

**Accuracy** Numerical solutions of fluid flow are only approximate solutions. In addition to the errors that might be introduced in the development of the solution algorithm, in programming or setting up the boundary conditions, numerical solutions always include three kinds of systematic errors:

- Modeling errors: difference between the actual flow and the exact solution of the mathematical model
- Discretization errors: difference between the exact solution of the conservation equations and the exact solution of the algebraic system of equations obtained by discretizing these equations
- Iteration errors: difference between the iterative and exact solutions of the algebraic equation systems.

# 4 Mathematical description of flows

The governing equations of fluid flow represent mathematical statements of the **conservation laws** of physics:

- The mass of fluid is conserved.
- The rate of change of momentum equals the sum of the forces applied on a fluid particle (Newton's second law).
- The rate of change of energy is equal to the sum of the rate of heat addition and to the rate of work done on a fluid particle (first law of thermodynamics).

The fluid will be regarded as a continuum and the behaviour of the fluid will be described in terms of macroscopic properties, such as velocity, pressure, density and temperature.

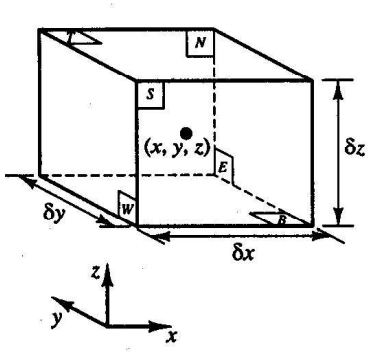
The *Reynolds transport theorem* establishes a relationship between the Lagrangian (fluid particle tracking) description and the Eulerian (fluid element control) description. This relationship is necessary for developing conservation laws in fluid mechanics, where the latter description is the most natural, because Newton's second law and the laws of thermodynamics are formulated from a Lagrangian point of view.

Transport theorem. For a differentiable scalar function $f : \Omega_t \times [0, t_{end}] \to R$, it holds that

$$\frac{d}{dt}\int_{\Omega_t} f(\vec{x},t)\,d\vec{x} = \int_{CV}\left[\frac{\partial f}{\partial t} + \mathrm{div}(f\vec{u})\right]d\vec{x},$$

where $CV = \Omega_t$ at time $t$ and $\Omega_t$ is the volume of fluid that moves with the flow and consists permanently of the same fluid particles.

We consider a small element of fluid. The six faces are labelled N (North), S (South), E (East), W (West), T (Top) and B (Bottom).




A systematic account of changes in the mass, momentum and energy of the fluid element due to fluid flow across its boundaries and due to the action of sources inside the element, leads to the fluid flow equations.

## 4.1 Rates of change following a fluid particle and for a fluid element

Let $\phi$ be a fluid property. The **total (or substantive) derivative** of $\phi$ with respect to time *following a fluid particle* is

$$\begin{aligned}\frac{D\phi}{Dt} &= \frac{\partial\phi}{\partial t} + \frac{\partial\phi}{\partial x}\frac{dx}{dt} + \frac{\partial\phi}{\partial y}\frac{dy}{dt} + \frac{\partial\phi}{\partial z}\frac{dz}{dt}\\ &= \frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z}\\ &= \frac{\partial\phi}{\partial t} + \vec{u}\cdot\mathrm{grad}\phi\end{aligned}$$

The most usefull forms of conservation laws for fluid flow computation are concerned with changes of a flow property for a fluid element which is fixed in space.

The relationship between the total derivative of $\rho\phi$, which follows a fluid particle, and the rate of change of $\rho\phi$ for a fluid element is, by transport theorem:

$$\begin{aligned}\rho\frac{D\phi}{Dt} &= \rho\left[\frac{\partial\phi}{\partial t}+\vec{u}\cdot\text{grad}\phi\right]=\rho\left[\frac{\partial\phi}{\partial t}+\text{div}(\phi\vec{u})\right]-\phi\left[\frac{\partial\rho}{\partial t}+\text{div}(\rho\vec{u})\right]\\ &= \frac{\partial\rho\phi}{\partial t}+\text{div}(\rho\phi\vec{u})\end{aligned}$$

The term $\frac{\partial\rho}{\partial t}+\text{div}(\rho\vec{u})$ is equal zero by conservation of mass.

Rate of increase of $\phi$ for a fluid particle = Rate of increase of $\phi$ of fluid element + Net rate of flow of $\phi$ out of fluid element

## 4.2 Navier-Stokes equations. Conservative form of the governing equations. Transport equation.

The conservative (or divergence) form of the governing equations of the time-dependent 3d fluid flow and heat transfer of a compressible newtonian fluid is:

| | |
|---|---|
| Mass (continuity eq) | $\frac{\partial\rho}{\partial t}+\text{div}(\rho\vec{u})=0$ |
| x-momentum | $\frac{\partial\rho u}{\partial t}+\text{div}(\rho u\vec{u})=-\frac{\partial p}{\partial x}+\text{div}(\mu\text{grad}u)+q_x$ |
| y-momentum | $\frac{\partial\rho v}{\partial t}+\text{div}(\rho v\vec{u})=-\frac{\partial p}{\partial y}+\text{div}(\mu\text{grad}v)+q_y$ |
| z-momentum | $\frac{\partial\rho w}{\partial t}+\text{div}(\rho w\vec{u})=-\frac{\partial p}{\partial z}+\text{div}(\mu\text{grad}w)+q_z$ |
| Internal energy | $\frac{\partial\rho i}{\partial t}+\text{div}(\rho i\vec{u})=-p\text{div}\vec{u}+\text{div}(k\text{grad}T)+\Phi+q_i$ |

where $i$ is the internal energy, $\vec{q}$ is the momentum source and $\Phi$ the dissipation function.

These equations are non-linear, coupled and difficult to solve. It is difficult to prove by the existing mathematical tools that a unique solution exists for particular boundary conditions.

There are significant commonalities between the various equations. The general conservative form of all fluid flow equations for the variable $\phi$ can be written as:

$$\frac{\partial\rho\phi}{\partial t}+\text{div}(\rho\phi\vec{u})=\text{div}(\Gamma\text{grad}\phi)+q_\phi \tag{1}$$

where $\Gamma$ is a diffusion coefficient.

Rate of increase of $\phi$ of fluid element + Net rate of flow of $\phi$ out of fluid element (convection) = Rate of increase of $\phi$ due to diffusion + Rate of increase of $\phi$ due to sources

Equation (1) is the **transport equation for property** $\phi$ and is used as starting point in the finite volume method. By setting $\phi$ equal to 1, $u$, $v$, $w$ and $i$, and selecting appropiate values for the coefficient $\Gamma$ and the source terms we obtain the partial differential equations for mass, momentum and energy conservation.

Integration of equation (1) over a control volume CV yields

$$\int_{CV} \frac{\partial \rho\phi}{\partial t}\, dV + \int_{CV} \mathrm{div}(\rho\phi\vec{u})\, dV = \int_{CV} \mathrm{div}(\Gamma \mathrm{grad}\phi)\, dV + \int_{CV} q_\phi\, dV \quad (2)$$

The volume integrals in the convective term (second on the left hand side) and in the diffusion term (first on the right hand side) are rewritten as integrals over the bounding surface of the control volume by using Gauss divergence theorem:

$$\int_{CV} \mathrm{div}(\vec{a})\, dV = \int_S \vec{a} \cdot \vec{n}\, dS$$

Then

$$\int_{CV} \frac{\partial \rho\phi}{\partial t}\, dV + \int_S (\rho\phi\vec{u}) \cdot \vec{n}\, dS = \int_S (\Gamma \mathrm{grad}\phi) \cdot \vec{n}\, dS + \int_{CV} q_\phi\, dV \quad (3)$$

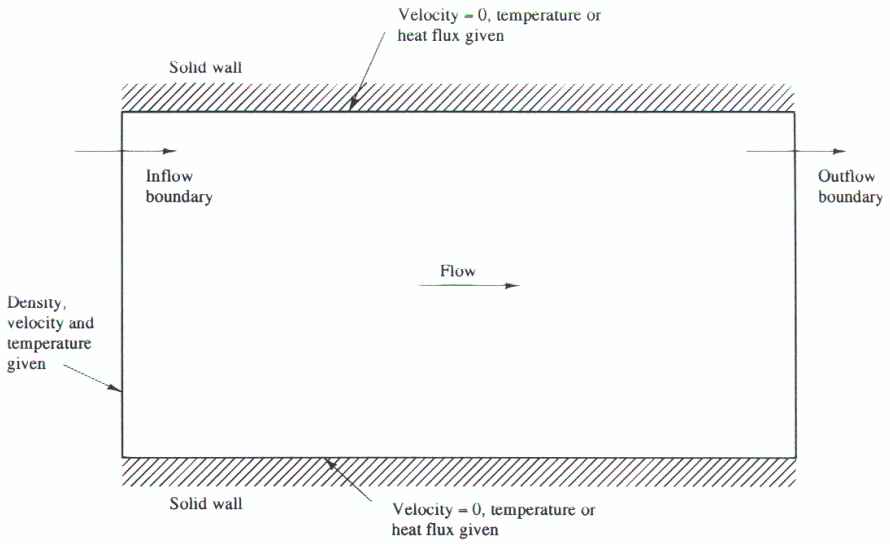
In steady state problems $\frac{\partial()}{\partial t} = 0$. This leads to the integrated form of the steady transport equation

$$\int_S (\rho\phi\vec{u}) \cdot \vec{n}\, dS = \int_S (\Gamma \mathrm{grad}\phi) \cdot \vec{n}\, dS + \int_{CV} q_\phi\, dV$$

### 4.3 Boundary conditions

Possible boundary conditions:

- Wall: No fluid penetrates the boundary, i.e. convective flux is zero. There are two types of wall condition: no-slip (fluid is at rest at the wall) or free-slip (no frictional loses at the boundary).
- Inflow (inlet)condition: Convective flux is prescribed.
- Outflow (outlet) condition: Convective flux independent of the coordinate normal to the boundary.
- Symmetry bc: $\frac{\partial \phi}{\partial n} = 0$
- Periodic bc: $\phi_1 = \phi_2$

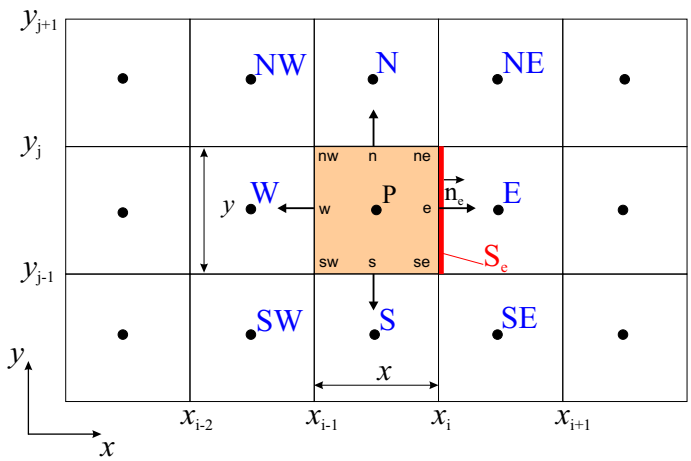



## 5 Finite Volume Method

We will consider the generic conservation equation for a scalar quantity $\phi$ and assume that the velocity field and all fluid properties are known. The Finite Volume Method begins with the integral form of this equation:

$$\int_S (\rho\phi\vec{u}) \cdot \vec{n}\, dS = \int_S (\Gamma \mathrm{grad}\phi) \cdot \vec{n}\, dS + \int_{CV} q_\phi\, dV \tag{4}$$

The domain is subdivided into a finite number of small control volumes (CV) by a grid which defines the CV boundaries, not the computational nodes.



The equation (4) applies to each CV as well as to the whole domain. If we sum equations for all CVs, we obtain the global conservation equation, since surface integrals over internal CV faces cancel out.

To obtain an algebraic equation for each CV, the surface and volume integrals need to be approximated using quadrature formulae.

## 5.1 Approximation of volume integrals

The simplest approximation is the midpoint rule:

$$\int_{CV} q\,dV = \bar{q}\,\mathrm{Vol(CV)} \approx q_P\,\mathrm{Vol(CV)}$$

where $\bar{q}$ is the mean value and $q_P$ the value of $q$ at the CV center. This approximation is exact if $q$ is either constant or varies linearly within the CV; otherwise is of second order.

An approximation of higher order requires the values of $q$ at more locations that just the center. These values have to be obtained by interpolating nodal values.

For example, assuming that q is bi-quadratic ($q(x,y) = a_0 + a_1x + a_2y + a_3x^2 + a_4y^2 + a_5xy + a_6x^2y + a_7xy^2 + a_8x^2y^2$) a fourth-order approximation can be obtained by analytical integration

$$\int_{CV} q\,dV \approx \frac{\Delta x \Delta y}{36}(16q_P + 4q_s + 4q_n + 4_w + 4q_e + q_{se} + q_{sw} + q_{ne} + q_{nw})$$

Since only the value at P is available, interpolation has to be used to obtain $q$ at the other locations. It has to be a least of fourth order to retain the accuracy of the integral approximation.

## 5.2 Approximation of surface integrals

The net flux through the CV boundary is the sum of integrals over the faces:

$$\int_S f \cdot \vec{n}\,dS = \sum_k \int_{S_k} f\,dS$$

where $f$ is $f^{conv} = (\rho\phi\vec{u}) \cdot \vec{n}$ or $f^{diff} = (\Gamma \mathrm{grad}\phi) \cdot \vec{n}$.

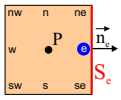
As the velocity field and the fluid properties are assumed known, the only unknown is $\phi$. If the velocity field is not known, we have a more complex problem involving non-linear coupled equations.

In what follows only a typical CV face, the east face, will be considered.

Approximation methods of the surface integral:

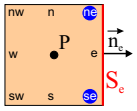
- Midpoint rule: $\mathcal{O}(\Delta x^2)$, if $f_e$ known

$$\int_{S_e} f\, dS = \bar{f}_e \cdot S_e \approx f_e \cdot S_e$$



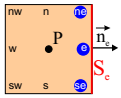

- Trapezoidal rule: $\mathcal{O}(\Delta x^2)$, if $f_{ne}$ and $f_{se}$ known

$$\int_{S_e} f\, dS \approx \frac{S_e}{2}(f_{ne} + f_{se})$$




- Simpson's rule: $\mathcal{O}(\Delta x^4)$, if $f_e$, $f_{ne}$ and $f_{se}$ known

$$\int_{S_e} f\, dS \approx \frac{S_e}{6}(f_{ne} + 4f_e + f_{se})$$




Since the values of $f$ are not known at the cell faces, they have to be obtained by interpolation.

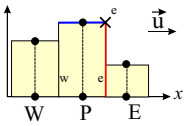
## 5.3 Interpolation

$f$ in the previous integrals represents the convective flux $f^{conv} = (\rho\phi\vec{u})\cdot\vec{n}$ or the diffusive flux $f^{diff} = (\Gamma \text{grad}\phi)\cdot\vec{n}$. Again the velocity field, $\rho$ and $\Gamma$ are assumed known at all locations. To calculate the fluxes, we need the value of $\phi$ and its gradient normal to the cell face at some locations on the CV surface. They have to be expressed in terms of nodal values by interpolation.

Different methods to approximate $\phi$ and its normal derivative at face east:

**Upwind Differencing Scheme (UDS)** Approximates $\phi_e$ by ist value at the node upstream of 'e'. It is equivalent to using a backward or forward difference approximation for the first derivative (depending on the flow direction).

$$\phi_e = \begin{cases} \phi_P & \text{if } (\vec{u}\cdot\vec{n})_e > 0 \\ \phi_E & \text{if } (\vec{u}\cdot\vec{n})_e < 0 \end{cases}$$

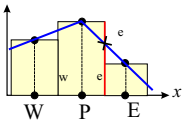



This approximation is of first order ($\mathcal{O}(\Delta x)$), unconditionally stable (it will never yield oscillatory solutions) and *numerically diffusive* (rapid

variations in the variable are smeared out, very fine grids are required to obtain accurate solutions).

**Central Difference Scheme (CDS)** Linear interpolation between the two nearest nodes.

$$\phi_e = \phi_E \lambda_e + \phi_P (1 - \lambda_e)$$




where the linear interpolation factor $\lambda_e$ is defined as

$$\lambda_e = \frac{x_e - x_P}{x_E - x_P}$$

This is the simplest second order scheme. It may produce oscillatory solutions.

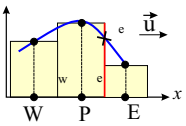
A possible approximation for the gradient (needed for the evaluation of diffusive fluxes) is

$$\left(\frac{\partial \phi}{\partial x}\right)_e \approx \frac{\phi_E - \phi_P}{x_E - x_P}$$

When the face 'e' is midway between P and E (uniform grid), the approximation is $\mathcal{O}(\Delta x^2)$, otherwise it is $\mathcal{O}(\Delta x)$.

**Quadratic Upwind Interpolation (QUICK)** To construct a parabola for interpolation three points are necessary: P, E and a third point on the upstream side (according with the nature of convection).

$$\phi_e = \begin{cases} \phi_P + g_1(\phi_E - \phi_P) + g_2(\phi_P - \phi_W) & \text{for } u_x > 0 \\ \phi_E + g_3(\phi_P - \phi_E) + g_4(\phi_E - \phi_{EE}) & \text{for } u_x < 0 \end{cases}$$




where the coefficients $g_i$ can be expressed in terms of the nodal coordinates by:

$$g_1 = \frac{(x_e - x_P)(x_e - x_W)}{(x_E - x_P)(x_E - x_W)} \qquad g_2 = \frac{(x_e - x_P)(x_E - x_P)}{(x_P - x_W)(x_E - x_W)}$$

$$g_3 = \frac{(x_e - x_E)(x_e - x_{EE})}{(x_P - x_E)(x_P - x_{EE})} \qquad g_4 = \frac{(x_e - x_E)(x_P - x_e)}{(x_E - x_{EE})(x_P - x_{EE})}$$

This quadratic interpolation is of order $\mathcal{O}(\Delta x^3)$.

## 5.4 Solution of linear equation systems

By summing all the approximated integrals we produce an algebraic equation at each control volume:

$$A_P \phi_P + \sum_l A_l \phi_l = Q_P$$

where the index $l$ runs over the neighbour nodes involved, and the system of equations for the whole domain has the matrix form

$$[A] \cdot [\phi] = [Q]$$

The matrix $A$ is always sparse.

There are mainly two types of methods for solving the system of linear algebraic equations:

**Direct methods**

- Gauss elimination
- LU decomposition
- Tridiagonal matrix algorithm (TDMA)

The number of operations for a $N \times N$ system is $O(N^3)$. It is required to store all the $N^2$ coefficients.

**Indirect or iterative methods**

- Jacobi method
- Gauss-Seidel method
- Successive over-relaxation (SOR)
- Conjugate gradient method (CG)
- Multigrid methods

Iterative methods are based on the repeated application of a relatively simple algorithm leading to a (eventual) convergence after a (sometimes large) number of repetitions. The total number of operations, typically on the order of N per iteration cycle, cannot be predicted in advance. It is not possible to guarantee convergence unless the system of equations satisfies strict criteria. The main advantage of iterative methods is that only non-zero coefficients need to be stored.

In an iterative method one guesses a solution and uses the equation to systematically improve it. If each iteration is cheap and the number of iterations is small, an iterative solver may cost less than a direct method. In CFD problems this is usually the case.

When using iterative solvers, it is important to know when to quit. The most common convergence criteria is based on the difference between two succesive iterates. The procedure is stopped when this difference is less than a pre-selected value.

The convergence behaviour of traditional iterative methods deteriorates as the grid is refined, more and more iteration steps are required to reduce the iteration error below a given tolerance. *Multigrid methods* is a new class of iterative methods for solving discrete elliptic equations. The number of iteration steps is independent of the number of unknowns, thus finer discretization no longer leads to an increase in the number of iteration steps.

## 5.5 Unsteady problems: Time discretization

Up to now we have discussed the discretization of the convective and diffusive fluxes and source terms for steady problems. For the unsteady (initial value) problem we rewrite the conservation equation in the form

$$\frac{\partial \rho\phi}{\partial t} = -\mathrm{div}(\rho\phi\vec{u}) + \mathrm{div}(\Gamma \mathrm{grad}\phi) + q_\phi = f(t,\phi(t)),\ \phi(t_0) = \phi^0$$

The convective, diffusive and source terms represented by $f(t,\phi(t))$ are discretized using finite volume method. For time integration we can use similar methods than for Initial Value problems in ODE.

$$\int_{t_n}^{t_{n+1}} \frac{\partial \rho\phi}{\partial t}\, dt = \rho(\phi^{n+1} - \phi n) = \int_{t_n}^{t_{n+1}} f(t,\phi(t))\, dt$$

The right hand side integral is evaluated numerically.

Examples of methods for time integration:

- Explicit or forward Euler method: order $\mathcal{O}(\Delta t)$,

  $\phi^{n+1} = \phi^n + f(t_n,\phi^n)\cdot\Delta t$

- Implicit or backward Euler method: order $\mathcal{O}(\Delta t)$,

  $\phi^{n+1} = \phi^n + f(t_{n+1},\phi^{n+1})\cdot\Delta t$

- Leapfrog method (midpoint rule): explicit, order $\mathcal{O}(\Delta t^2)$,

  $\phi^{n+1} = \phi^{n-1} + f(t_n,\phi^n)\cdot 2\Delta t$

- Crank-Nicolson method (trapezoidal rule): implicit, order $\mathcal{O}(\Delta t^2)$,

  $$\phi^{n+1} = \phi^n + \tfrac{1}{2}\left[f(t_n, \phi^n) + f(t_{n+1}, \phi^{n+1})\right] \cdot \Delta t$$

Time integration methods are classified in:

- **Explicit**: solution values at time $t_{n+1}$ are computed from the values of $f$ at time $t_n$, i.e. all fluxes and source terms are evaluated using known values at time $t_n$.

  Advantages:

  - direct computation without solving a system of equations
  - easy to programm and parallelize
  - few number of operations per time step

  Disadvantage: strong conditions on the time step for stability

- **Implicit**: $f$ is evaluated at time $t_{n+1}$, i.e. all fluxes and source terms are evaluated in terms of the unknown variable values at the new time $t_{n+1}$.

  Advantage: much larger time steps possible, always stable.

  Disadvantages:

  - every time step require the solution of a system of equations
  - more number of operations
  - difficult to programm and parallelize

## 5.6 Coupling of pressure and velocity

Up to now we have assumed that the velocity field was known. This is in general not the case.

Transport equations for each velocity component (momentum equation) can be derived from the general transport equation by replacing $\phi$ by $u$, $v$ and $w$. The velocity field must also satisfy the continuity equation.

x-momentum equation

$$\frac{\partial}{\partial x}(\rho u u) + \frac{\partial}{\partial y}(\rho v u) = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) - \frac{\partial p}{\partial x} + q_u$$

y-momentum equation

$$\frac{\partial}{\partial x}(\rho u v) + \frac{\partial}{\partial y}(\rho v v) = \frac{\partial}{\partial x}\left(\mu \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial y}\right) - \frac{\partial p}{\partial y} + q_v$$

Continuity equation

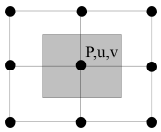
$$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0$$

The convective terms of the momentum equation are non-linear. All three equation are coupled because every velocity component appears in each momentum equation and the continuity equation. The most complex issue to be solved is the role played by the pressure. It appears in both moment equation but there is no equation for the pressure.

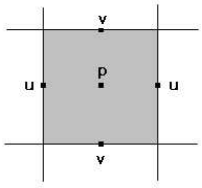
If the flow is compressible, the continuity equation may be used as a transport equation for density and the energy equation for the temperature. The pressure may than be obtained from the density and temperature by using the equation of state $p = p(\rho, t)$. If the flow is incompressible, the density is constant and not related with the pressure. In this case coupling between pressure and velocity introduces a constraint on the solution of the flow field: if the correct pressure field is applied in the momentum equation the resulting velocity field should satisfy continuity.

Different variable arrangements can be chosen on the grid:

- **Colocated grid**
  - Node for pressure and velocity components at the CV center.
  - Same CV for all variables.
  - Possible oscillations of pressure.




- **Staggered grid**
  Advantages:
  - The different unknown variables are located at different grid nodes. Pressure located in the cell centers, velocities at cell faces.
  - Strong coupling between the velocities and pressure helps to avoid oscillations.




Other staggering method is the Arbitrary Lagrangian-Eulerian (ALE).

### 5.7 Summary

The Finite Volume Method uses the integral form of the conservation equations as starting point. The domain is subdivided into a finite number of contiguous control volumes (CV) and the conservation equations are applied to each CV. At the centroid of each CV lies a computational node a which the variable values are to be calculated. Interpolation is used to express variable values at the CV surface in terms of the nodal values. Surface and volume integrals are approximated using quadrature formulae. As a result, one obtains an algebraic equation for each CV, in which a number of neighbour nodal values appear.

The FVM can use any type of grid, so it is suitable for complex geometries. The method is conservative by construction. But FV methods of higher order than second are very difficult to develop in 3D.

The FVM satisfies conservation automatically.

Some examples of commercial CFD codes are: CFX, Phoenics, Fluent and Flow3d.

## 6 Turbulent flows

Most flow encountered in practice are turbulent. In contrast to laminar flow problems, numerical simulation of turbulent flows cannot be carried out by simply discretizing the governing equations and solving them in certain grid. This is caused by the fact that turbulence is essentially three dimensional and contains many length scales simultaneously. With increasing Reynolds number the length scales of the smallest eddies in the flow become smaller and smaller. Consequently, the amount of computational ressources necessary to describe all the length scales that occur, increases with the Reynolds number. Even the largest supercomputer do not have (yet) the require speed and memory capacity to handle this amount of data, except for turbulent flow with relative low Re.

In order to compute all significant structures (motions) of a turbulent flow, the domain on which the computation is performed must be at least as large as the largest eddy, and the grid must be as fine as the smallest eddy.

Computational methods to simulate turbulent flows:

- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- Reynolds Averaged Navier-Stokes Models (RANS)

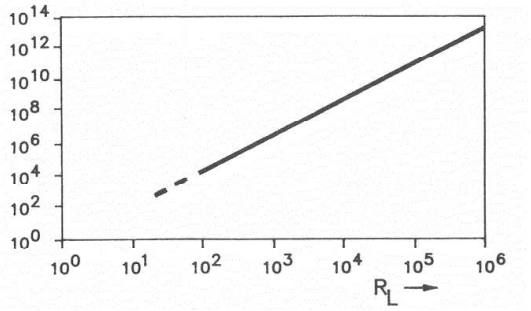
## 6.1 Direct Numerical Simulation (DNS)

The most accurate approach to turbulence simulation is to solve the NS eq without averaging. This so-called direct simulation does not assume any modelling, it discretize and solve de NS eq on a grid sufficiently fine for resolving all motions occurring in the turbulent flow. The computed flow field obtained is equivalent to a laboratory experiment. The characteristic length scale for the smallest eddies is given by the Kolmogorov scale $\eta$. The relation between $\eta$ and the length scale $L$ of the largest eddies is given by:

$$\frac{L}{\eta} \sim (\mathrm{Re}_L)^{\frac{3}{4}}$$

where $\mathrm{Re}_L$ is the Reynolds number with respect to $L$. If the dimensions of the mean flow field are of the order $L^3$ and the sizes h of the grid elements are about equal to $\eta$, then the number of elements $n_{elem}$ needed to discretize the flow field is

$$n_{elem} \sim (\mathrm{Re}_L)^{\frac{9}{4}}$$



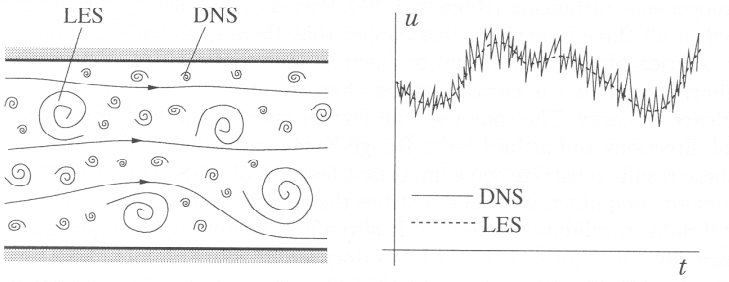

In industrial applications such as aerodynamic investigations of automobiles or aircraft, typical Reynolds numbers are $10^6$ and above. Hence, solving these type of problems properly using DNS would require over $10^13$ grid points. Neither existing parallel computers nor computers of the near future can supply the storage space or the necessary CPU performance demanded by such a simulation.

## 6.2 Large Eddy Simulation (LES)

Only the large eddies (or resolvable scale motions) are calculated, whereas the small eddies (subgrid-scale motions) are modelled by a closure assumption.

| Properties of the large eddies: | Properties of small eddies: |
|---|---|
| - produced from the mean flow | - produced by large eddies |
| - transport mass, momentum, energy | - dissipative |
| - flow dependent | - almost universal |
| - anisotropic | - nearly isotropic |
| - hard to model | - easier to model |

The flow dependent large eddies are directly affected by the boundary conditions. They are therefore the most difficult ones to model. LES avoids this problem by explicit computation of these motions. Since the small eddies dissipate energy from the large ones, a so-called subgrid-scale (SGS) model is needed that take into account this physical energy cascade process. The sizes of the grid elements, and thereby the distinction between large and small eddies, has to be chosen to be small enough for the unresolved subgrid-scale motions to behave statistically in a nearly isotropic manner. If this is the case, the SGS motions can be modelled independently of the flow geometry.




### 6.3 Reynolds Averaged Navier-Stokes Models (RANS)

Each unknown variable is decomposed in a mean and a fluctuation part, $\phi = \bar{\phi} + \phi'$. This decomposition is substituted in the NS eqs and then the eqs are averaged over time. The nonlinearity of these eqs gives rise to new terms, the set of eqs is not closed, turbulence models are necessary.

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