

Introduction to Computational Fluid Dynamics

Fluid Mechanics and Heat Transfer. Basic equations.

Continuity (Mass Conservation)

$$\text{div}(\vec{v}) = 0$$

incompressible

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) = 0$$

Momentum Equation (Navier-Stokes equations)

Incompressible viscous fluid ($\mu = \text{constant}$, $\rho = \text{constant}$)

$$\rho \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right) = \rho \vec{F} - \text{grad } p + \mu \Delta \vec{v}$$

Introduction to Computational Fluid Dynamics

Energy equation

$$\rho \frac{dE}{dt} = -p\rho \frac{d}{dt} \left(\frac{1}{\rho} \right) + \phi + \text{div}(k \text{ grad } T)$$

where E is the internal energy of a fluid particle (viscous compressible fluid)

- gas heating due to the compression

$$-p\rho \frac{d}{dt} \left(\frac{1}{\rho} \right) \underset{\text{continuity equation}}{=} -p \text{div } \vec{v}$$

- mechanical work of the viscous forces transformation in heat

$$\Phi = \frac{1}{2} \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2$$

Introduction to Computational Fluid Dynamics

By taking into account that the enthalpy of a unit of mass is $i = E + \frac{p}{\rho}$ we obtain

$$\rho \frac{di}{dt} = \frac{dp}{dt} + \phi + \text{div}(k \text{ grad } T)$$

But for a perfect gas we have

$$di = c_p dT$$

and energy equation becomes

$$\rho \frac{d}{dt}(c_p T) = \frac{dp}{dt} + \phi + \text{div}(k \text{ grad } T)$$

where

$$\frac{df}{dt} = \frac{Df}{Dt} = \frac{\partial f}{\partial t} + (\vec{v} \cdot \nabla) f \quad \frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x_1} v_1 + \frac{\partial f}{\partial x_2} v_2 + \frac{\partial f}{\partial x_3} v_3$$

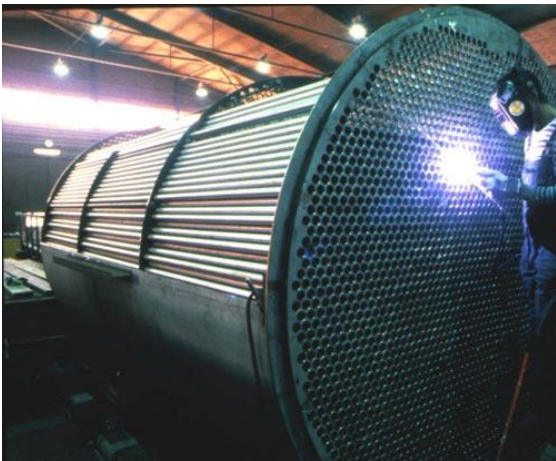
is the substantial derivative.

Introduction to Computational Fluid Dynamics

Momentum Equation (for fluid saturated porous media)

By a porous medium we mean a material consisting of a solid matrix with an interconnected void.

Porous media are present almost always in the surrounding medium, very few materials excepting fluids being non-porous.



heat exchanger



processor cooler



porous rock

Introduction to Computational Fluid Dynamics

Darcy's (law) equation (momentum equation)

$$\langle \vec{v} \rangle = -\frac{K}{\mu} \text{grad } p + \rho \vec{g}$$

where

- $\langle v \rangle$ is the average velocity (filtration velocity, superficial velocity, seepage velocity or Darcian velocity)
- $K = k\mu/\rho g$ is the permeability of the porous medium

Darcy' law expresses a linear dependence between the pressure gradient and the filtration velocity. It was reported that this linear law is not valid for large values of the pressure gradient.

Introduction to Computational Fluid Dynamics

Darcy's law extensions

Forchheimer's extension

$$\nabla p = -\frac{\mu}{K} \langle \vec{v} \rangle - \frac{c_F}{\sqrt{K}} \rho |\langle \vec{v} \rangle| \langle \vec{v} \rangle$$

where c_F is a dimensionless parameter depending on the porous medium

Brinkman's extension

$$\nabla p = -\frac{\mu}{K} \langle \vec{v} \rangle + \tilde{\mu} \Delta \langle \vec{v} \rangle$$

where $\tilde{\mu}$ is an effective viscosity

Brinkman-Forchheimer's extension

$$\nabla p = -\frac{\mu}{K} \langle \vec{v} \rangle - \frac{c_F}{\sqrt{K}} \rho |\langle \vec{v} \rangle| \langle \vec{v} \rangle + \tilde{\mu} \Delta \langle \vec{v} \rangle$$

Introduction to Computational Fluid Dynamics

Energy equation for porous media

$$(\rho c_p)_m \frac{\partial \langle T \rangle}{\partial t} + (\rho c_p)_{fluid} \langle \vec{v} \rangle \nabla \langle T \rangle = \nabla (k_e \nabla \langle T \rangle)$$

where

$$(\rho c_p)_m = \phi (\rho c_p)_{fluid} + (1 - \phi) (\rho c_p)_{solid}$$

$$k_e = \phi k_{fluid} + (1 - \phi) k_{solid}$$

Introduction to Computational Fluid Dynamics

Bouyancy driven flow¹

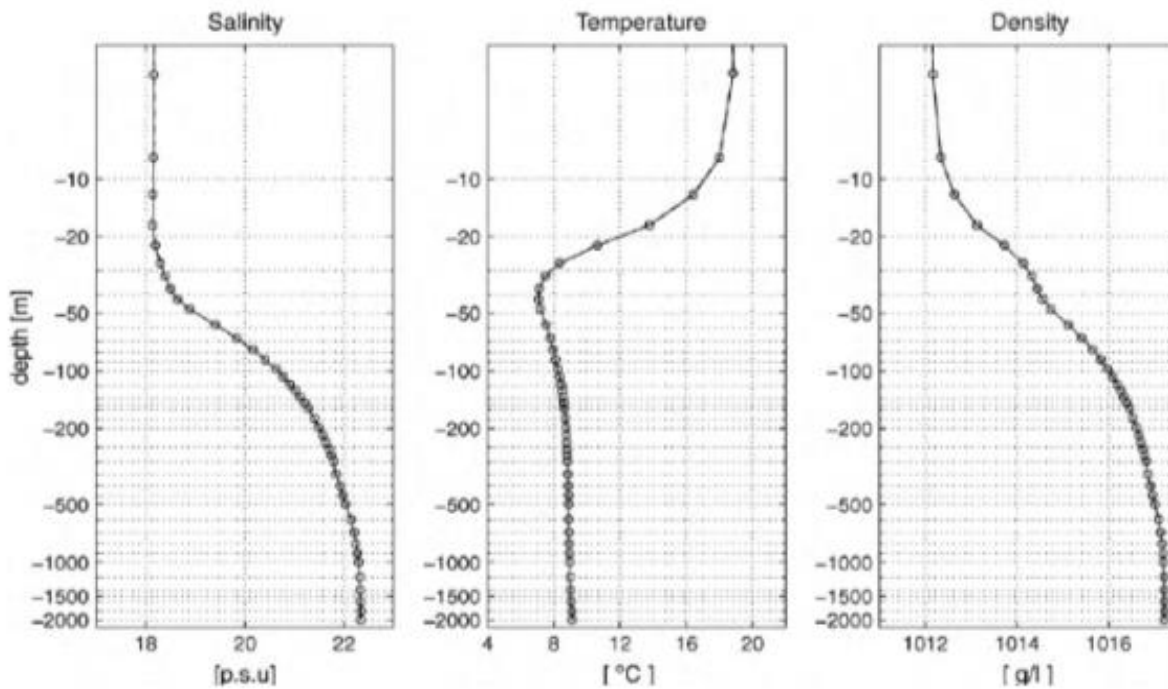
- There exists a large class of fluid flows in which the motion is caused by buoyancy in the fluid.
- Buoyancy is the force experienced in a fluid due to a variation of density in the presence of a gravitational field. According to the definition of an incompressible fluid, variations in the density normally mean that the fluid is compressible, rather than incompressible.
- For many of the fluid flows of the type mentioned above, the density variation is important only in the body-force term of the momentum equations. In all other places in which the density appears in the governing equations, the variation of density leads to an insignificant effect.
- Buoyancy results in a force acting on the fluid, and the fluid would accelerate continuously if it were not for the existence of the viscous forces.
- The situation depicted above occurs in natural convection.

¹ I.G. Currie, Fundamental Mechanics of Fluids, 3rd ed., Marcel Dekker, New York, 2003

Introduction to Computational Fluid Dynamics

Generally, density is a function of temperature and concentration

$$\rho = \rho(T, c)$$



Black Sea salinity, temperature
and density
(Ecological Modelling, 221,
2010, p. 2287-2301)

Introduction to Computational Fluid Dynamics

Boussinesq's approximation

$$(\rho - \rho_{ref}) = \rho\beta_T(T_{ref} - T) + \rho\beta_S(C_{ref} - C)$$

$$\beta_T = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p, \quad \beta_S = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial C} \right)_{p,T}$$

Momentum

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho g \beta (T - T_0) \mathbf{e}_z$$

Introduction to Computational Fluid Dynamics

Dimensionless equations

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

$$\rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = \rho F_x - \frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

$$\rho \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) = \rho F_y - \frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right)$$

$$\rho \left(\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = \rho F_z - \frac{\partial p}{\partial z} + \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \Phi + q (= 0)$$

$$\Phi = \mu \left[2 \left(\frac{\partial u}{\partial x} \right)^2 + 2 \left(\frac{\partial v}{\partial x} \right)^2 + 2 \left(\frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 \right]$$

Introduction to Computational Fluid Dynamics

We introduce further the dimensionless variables

$$\tau = \frac{t}{t_0}, \quad X = \frac{x}{L}, \quad Y = \frac{y}{L}, \quad Z = \frac{z}{L}, \quad U = \frac{u}{U_0}, \quad V = \frac{v}{U_0}, \quad W = \frac{w}{U_0}, \quad \vec{F}' = \frac{\vec{F}}{g}, \quad P = \frac{p}{p_0}, \quad \theta = \frac{T - T_0}{\Delta T}$$

into the governing equations

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial \tau} (U U_0) \frac{\partial \tau}{\partial t} = \frac{U_0}{t_0} \frac{\partial U}{\partial \tau}, \quad \frac{\partial u}{\partial x} = \frac{\partial}{\partial X} (U U_0) \frac{\partial X}{\partial x} = \frac{U_0}{L} \frac{\partial U}{\partial X},$$

$$\frac{\partial p}{\partial x} = \frac{\partial}{\partial X} (P p_0) \frac{\partial X}{\partial x} = \frac{p_0}{L} \frac{\partial P}{\partial X},$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) = \frac{\partial}{\partial x} \left(\frac{U_0}{L} \frac{\partial U}{\partial X} \right) = \frac{U_0}{L} \frac{\partial^2 U}{\partial X^2} \frac{\partial X}{\partial x} = \frac{U_0}{L^2} \frac{\partial^2 U}{\partial X^2}$$

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial \tau} (\theta \cdot \Delta T + T_0) \frac{\partial \tau}{\partial t} = \frac{\Delta T}{t_0} \frac{\partial \theta}{\partial \tau}, \quad \frac{\partial T}{\partial x} = \frac{\partial}{\partial X} (\theta \cdot \Delta T + T_0) \frac{\partial X}{\partial x} = \frac{\Delta T}{L} \frac{\partial \theta}{\partial X}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial x} \left(\frac{\Delta T}{L} \frac{\partial \theta}{\partial X} \right) = \frac{\Delta T}{L} \frac{\partial^2 \theta}{\partial X^2} \frac{\partial X}{\partial x} = \frac{\Delta T}{L^2} \frac{\partial^2 \theta}{\partial X^2}$$

Introduction to Computational Fluid Dynamics

and we obtain the dimensionless equations

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} + \frac{\partial W}{\partial Z} = 0$$

$$\frac{L}{t_0 U_0} \frac{\partial U}{\partial \tau} + U \frac{\partial U}{\partial X} + V \frac{\partial V}{\partial Y} + W \frac{\partial W}{\partial Z} = \frac{gL}{U_0^2} F'_x - \frac{p_0}{\rho U_0^2} \frac{\partial P}{\partial X} + \frac{\nu}{U_0 L} \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} + \frac{\partial^2 U}{\partial Z^2} \right)$$

$$\frac{L}{t_0 U_0} \frac{\partial \theta}{\partial \tau} + U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} + W \frac{\partial \theta}{\partial Z} = \frac{\left(\frac{k}{\rho c_p} \right) / \nu}{U_0 L / \nu} \left(\frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} + \frac{\partial^2 \theta}{\partial Z^2} \right) + \frac{\mu U_0}{\rho c_p L \Delta T} \phi$$

Introduction to Computational Fluid Dynamics

Dimensionless numbers

A. Strouhal number

The Strouhal number (St) is a dimensionless number describing oscillating flow mechanisms:

$$St = \frac{L}{t_0 U_0} = \frac{\omega L}{U_0} = \frac{\text{oscillation}}{\text{average velocity}}$$

B. Froude number

The Froude number (Fr) is a dimensionless number defined as the ratio of the flow inertia to the external field (the latter in many applications simply due to gravity).

In naval architecture the Froude number is a very significant figure used to determine the resistance of a partially submerged object moving through water, and permits the comparison of similar objects of different sizes, because the wave pattern generated is similar at the same Froude number only.

$$Fr = \frac{U_0}{\sqrt{gL}}$$

Introduction to Computational Fluid Dynamics

C. Euler number

It expresses the relationship between a local pressure drop e.g. over a restriction and the kinetic energy per volume, and is used to characterize losses in the flow, where a perfect frictionless flow corresponds to an Euler number of 1.

$$Eu = \frac{p_0}{\rho U_0^2}$$

Usually, we take $p_0 = \rho U_0^2$ and we obtain $Eu = 1$.

D. Reynolds number

$$Re = \frac{U_0 L}{\nu} = \frac{\rho U_0 L}{\mu}$$

The Reynolds number is defined as the ratio of inertial forces to viscous forces and consequently quantifies the relative importance of these two types of forces for given flow conditions.

- laminar flow occurs at low Reynolds numbers, where viscous forces are dominant, and is characterized by smooth, constant fluid motion;
- turbulent flow occurs at high Reynolds numbers and is dominated by inertial forces, which tend to produce chaotic eddies, vortices and other flow instabilities.

Introduction to Computational Fluid Dynamics

E. Prandtl number

$$Pr = \frac{c_p \mu}{k} = \frac{\mu / \rho}{k / \rho c_p} = \frac{\nu}{\alpha}$$

It is the ratio of momentum diffusivity to thermal diffusivity. The Prandtl number contains no such length scale in its definition and is dependent only on the fluid and the fluid state. As such, the Prandtl number is often found in property tables alongside other properties such as viscosity and thermal conductivity.

- gases - Pr ranges 0.7 - 1.0
- water - Pr ranges 1 - 10
- liquid metals - Pr ranges 0.001 - 0.03
- oils - Pr ranges 50 - 2000

E. Eckert number

It expresses the relationship between a flow's kinetic energy and the boundary layer enthalpy difference, and is used to characterize heat dissipation.

$$Ec = \frac{U_0^2}{c_p \Delta T}$$

Introduction to Computational Fluid Dynamics

Using the above dimensionless numbers we obtain:

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} + \frac{\partial W}{\partial Z} = 0$$

$$St \frac{\partial U}{\partial \tau} + U \frac{\partial U}{\partial X} + V \frac{\partial V}{\partial Y} + W \frac{\partial W}{\partial Z} = \frac{1}{Fr} F'_x - Eu \frac{\partial P}{\partial X} + \frac{1}{Re} \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} + \frac{\partial^2 U}{\partial Z^2} \right)$$

....

$$St \frac{\partial \theta}{\partial \tau} + U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} + W \frac{\partial \theta}{\partial Z} = \frac{1}{Re Pr} \left(\frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} + \frac{\partial^2 \theta}{\partial Z^2} \right) + \frac{Ec}{Re} \phi$$

or using differential operators

$$\nabla \cdot \vec{V} = 0 \tag{23}$$

$$St \frac{\partial \vec{V}}{\partial \tau} + (\vec{V} \cdot \nabla) \vec{V} = \frac{1}{Fr} \vec{F}' - Eu \nabla P + \frac{1}{Re} \Delta \vec{V} \tag{24}$$

$$St \frac{\partial \theta}{\partial \tau} + (\vec{V} \cdot \nabla) \theta = \frac{1}{Re Pr} \Delta \theta + \frac{Ec}{Re} \phi \tag{25}$$

Introduction to Computational Fluid Dynamics

Comments

- Dimensionless numbers allow for comparisons between very different systems and tell you how the system will behave
- Many useful relationships exist between dimensionless numbers that tell you how specific things influence the system
- When you need to solve a problem numerically, dimensionless groups help you to scale your problem.
- Analytical studies can be performed for limiting values of the dimensionless parameters

Express the governing equations in dimensionless form to:

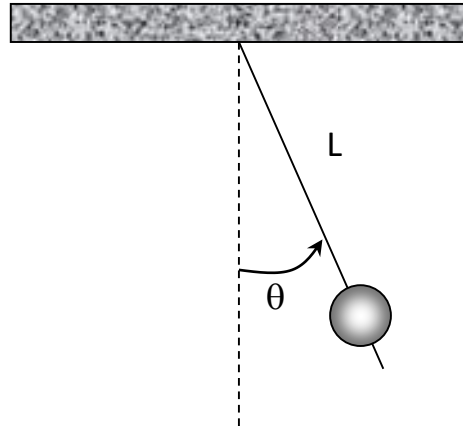
- (1) identify the governing parameters
- (2) plan experiments
- (3) guide in the presentation of experimental results and theoretical solutions

If the flow is not oscillatory, we take usually $t_0 = L/U_0$ and thus $St = 1$. If $t_0 \rightarrow \infty$ we have $St = 0$ and the flow is steady.

Introduction to Computational Fluid Dynamics

Numerical methods for initial values problems (IVP or Cauchy problem)

Pendulum



Mathematical model:

$$\frac{d^2\theta}{dt^2} + \frac{g}{L} \sin \theta = 0, \quad \theta(t_0) = \theta_0, \quad \frac{d\theta}{dt}(t_0) = \theta'_0$$

Radioactive elements decay:

$$\frac{dm}{dt} = -\lambda m, \quad m(t_0) = m_0$$

where m is the mass of the radioactive element and λ is the decay constant.

Introduction to Computational Fluid Dynamics

Theoretical aspects

The general Cauchy problem:

$$\begin{cases} y'(t) = f(t, y), & a \leq t \leq b \\ y(a) = y_a \end{cases}$$

Using numerical methods we obtain a discrete approximation of y in some points, called nodes, which form a grid (mesh).

A grid for the interval $[a, b]$ having a constant step h is:

$$a, a + h, a + 2h, \dots, a + ih, \dots, a + (N - 1)h, b$$

or

$$t_i = a + (i - 1)h, \quad i = 1, \dots, N$$

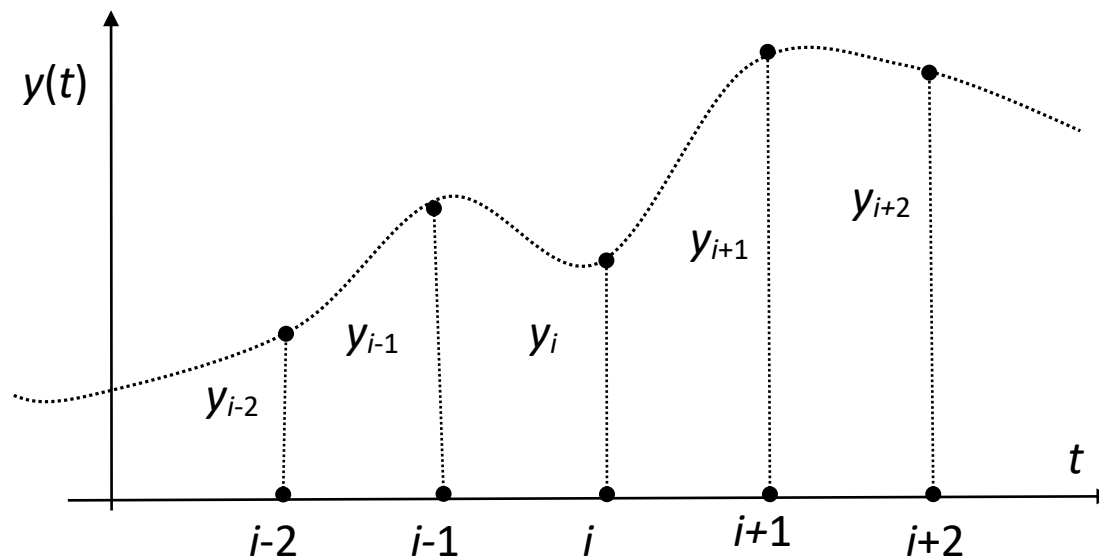
where N is the number of subintervals, and the step is constant:

$$h = (b - a)/(N - 1).$$

Introduction to Computational Fluid Dynamics

By using a numerical method we obtain the approximated discrete values

$$y(t_i) \stackrel{\text{not}}{=} y_i, \quad i = 1, \dots, N$$



Introduction to Computational Fluid Dynamics

One step methods

An example: The Euler method (Leonhard Euler-(1707 – 1783))



$$\begin{cases} y'(t) = f(t, y), & a \leq t \leq b \\ y(a) = y_a \end{cases}$$

By using a Taylor expansion (y should be of class C^2) we have:

$$y(t_{i+1}) = y(t_i + h) = y(t_i) + h y'(t_i) + \frac{h^2}{2} y''(\xi_i), \xi_i \in (t_i, t_{i+1})$$

Thus, one get:

$$y(t_{i+1}) = y(t_i) + h f(t_i, y(t_i)) + \frac{h^2}{2} y''(\xi_i)$$

By dropping the last term the Euler formula is obtained:

$$y_0 = y_a$$

$$y_{i+1} = y_i + h f(t_i, y_i), \quad i = 0, 1, \dots, N-1$$

Remark: y_{i+1} depends on y_i , t_i and h .

Introduction to Computational Fluid Dynamics

(Richard L. Burden and J. Douglas Faires , Numerical Analysis,Ninth Edition, 2011).

In Example 1 we will use an algorithm for Euler's method to approximate the solution to

$$y' = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$$

at $t = 2$. Here we will simply illustrate the steps in the technique when we have $h = 0.5$.

For this problem $f(t, y) = y - t^2 + 1$, so

$$w_0 = y(0) = 0.5;$$

$$w_1 = w_0 + 0.5 (w_0 - (0.0)^2 + 1) = 0.5 + 0.5(1.5) = 1.25;$$

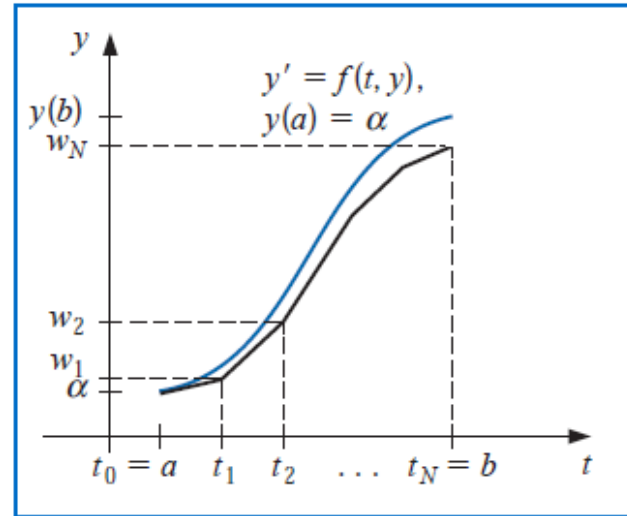
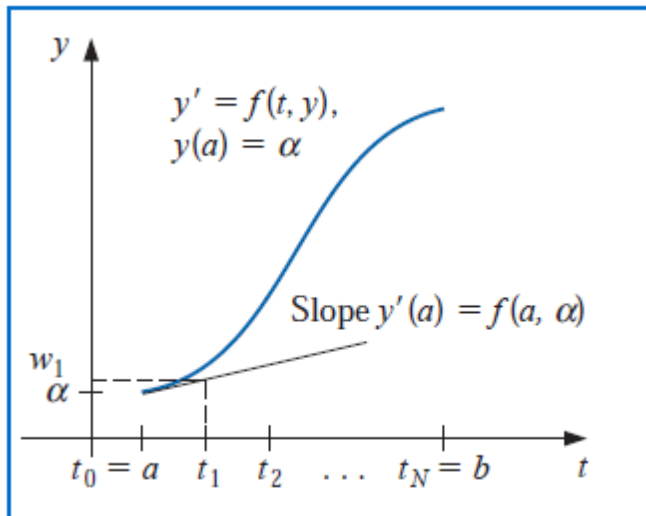
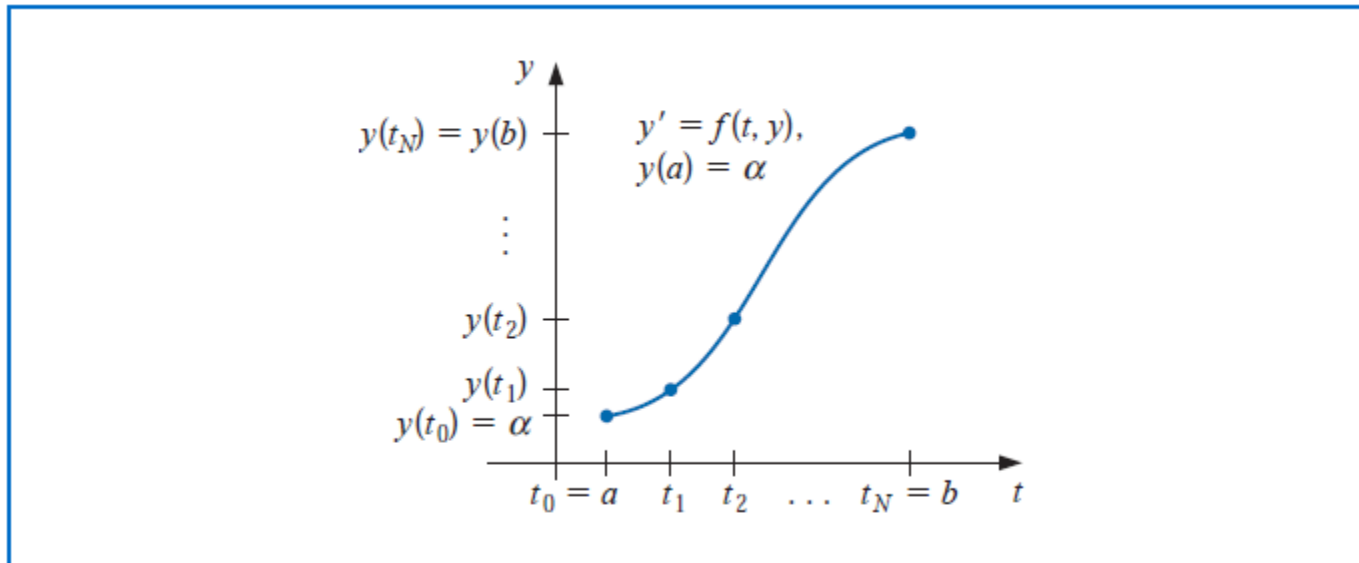
$$w_2 = w_1 + 0.5 (w_1 - (0.5)^2 + 1) = 1.25 + 0.5(2.0) = 2.25;$$

$$w_3 = w_2 + 0.5 (w_2 - (1.0)^2 + 1) = 2.25 + 0.5(2.25) = 3.375;$$

and

$$y(2) \approx w_4 = w_3 + 0.5 (w_3 - (1.5)^2 + 1) = 3.375 + 0.5(2.125) = 4.4375. \quad \square$$

Introduction to Computational Fluid Dynamics



One may notice that the Euler method follows the tangent for the current node to approximate the value in the next node.

Introduction to Computational Fluid Dynamics

Same problem for $h = 0.2$ (11 nodes). Comparison with the exact values given by $y(t) = (t + 1)^2 - 0.5e^t$.

t_i	w_i	$y_i = y(t_i)$	$ y_i - w_i $
0.0	0.5000000	0.5000000	0.0000000
0.2	0.8000000	0.8292986	0.0292986
0.4	1.1520000	1.2140877	0.0620877
0.6	1.5504000	1.6489406	0.0985406
0.8	1.9884800	2.1272295	0.1387495
1.0	2.4581760	2.6408591	0.1826831
1.2	2.9498112	3.1799415	0.2301303
1.4	3.4517734	3.7324000	0.2806266
1.6	3.9501281	4.2834838	0.3333557
1.8	4.4281538	4.8151763	0.3870225
2.0	4.8657845	5.3054720	0.4396874

Introduction to Computational Fluid Dynamics

An one step method for the Cauchy problem is given by

$$y_{i+1} = y_i + h\phi(t_i, y_i, h), \quad [t, y] \in [a, b] \times \mathbf{R}^n, \quad h > 0$$
$$\phi : [a, b] \times \mathbf{R}^{n+1} \rightarrow \mathbf{R}^n$$

Considering the exact solution (in the grid points) $\tilde{y}(t_i)$ we define *the local truncation error* as follow:

$$T(t_i, y_i, h) = \frac{y_{i+1} - y_i}{h} - \frac{\tilde{y}(t_{i+1}) - \tilde{y}(t_i)}{h} = \phi(t_i, y_i, h) - \frac{\tilde{y}(t_{i+1}) - \tilde{y}(t_i)}{h}$$

(the difference between the approximation increment and the exact increment for one step)

A method ϕ is consistent if $T(t, y, h) \rightarrow 0$ uniformly when $h \rightarrow 0$ for $(t, y) \in [a, b] \times \mathbf{R}^n$.

(it is necessary that $\phi(t, y, 0) = f(t, y)$)

Introduction to Computational Fluid Dynamics

A method ϕ is of order p if

$$\|T(t, y, h)\| \leq Kh^p$$

uniformly on $[a, b] \times \mathbf{R}^n$, where $\| \cdot \|$ is a vector norm, and K is constant.

We may use the following notation:

$$T(t, y, h) = O(h^p), \quad h \rightarrow 0$$

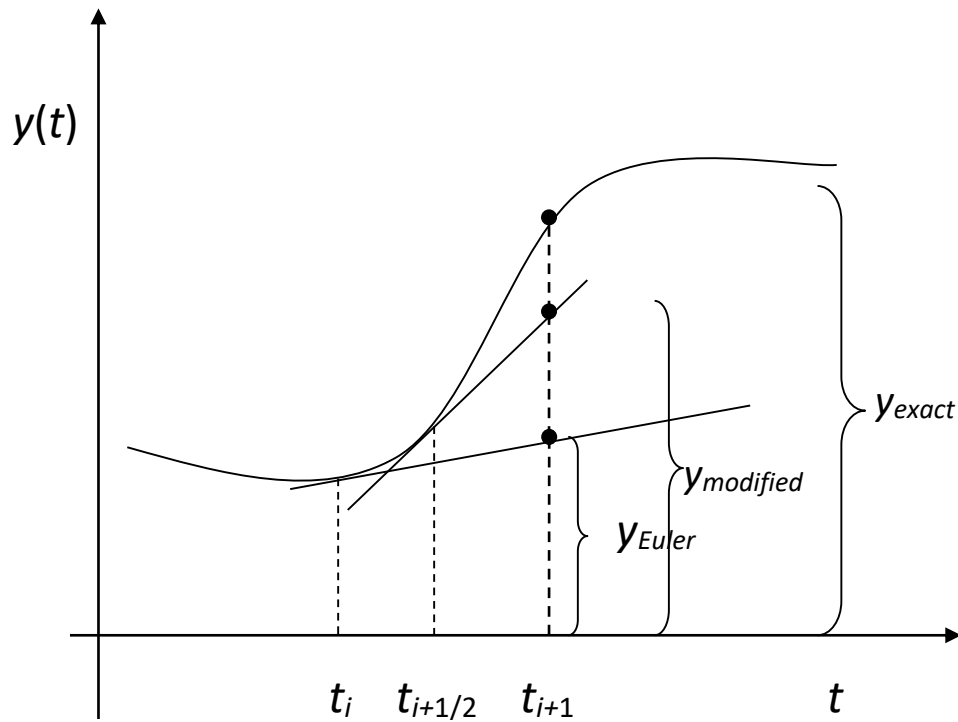
(for $p > 1$ the method is consistent).

It can be shown that Euler method is a method of order one, $O(h)$.

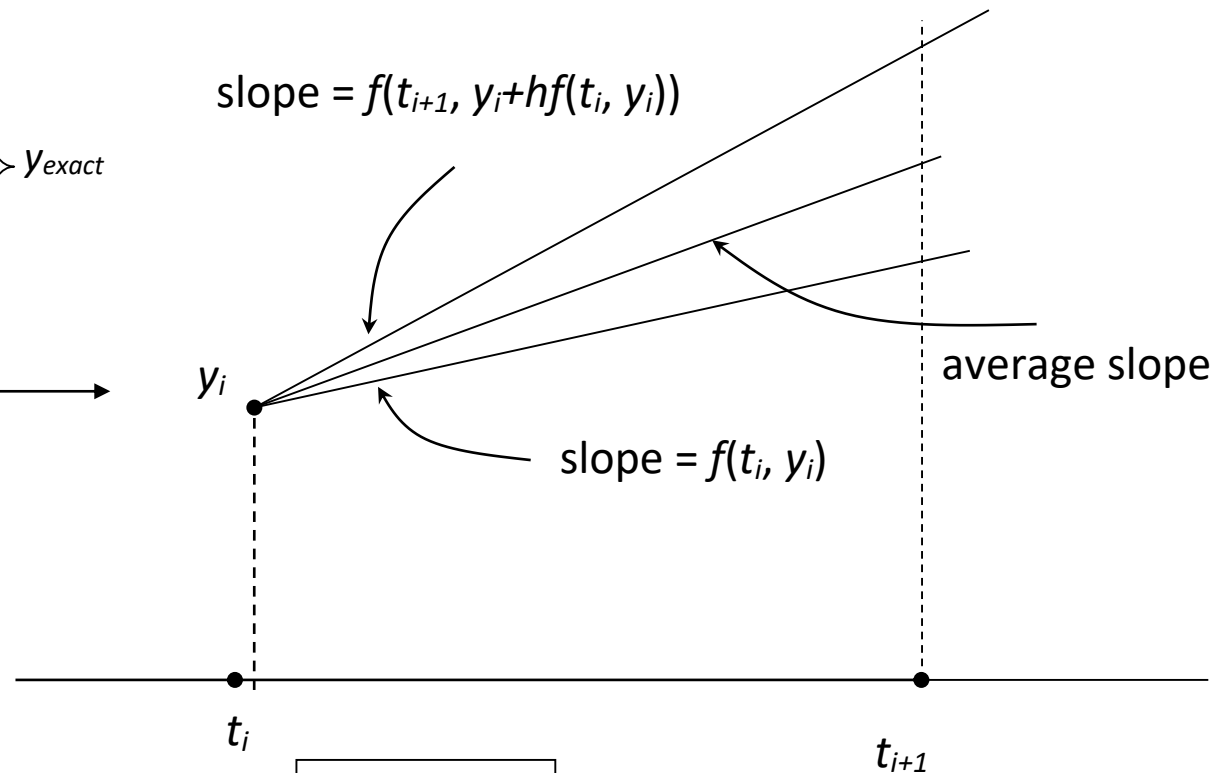
Introduction to Computational Fluid Dynamics

Improved Euler methods

evaluation of the tangent is made in an intermediary point of the interval $[t_i, t_{i+1}]$



Modified Euler



Heun

Introduction to Computational Fluid Dynamics

-evaluation in the middle of $[t_i, t_{i+1}]$, $t_{i+1/2} = t_i + \frac{1}{2}h$ ^{not}

$$y(t_{i+1}) = y(t_i) + h f\left(t_{i+1/2}, y_{i+1/2}\right) = y(t_i) + h f\left(t_i + \frac{1}{2}h, \underbrace{y_i + \frac{1}{2}hf(t_i, y_i)}_{\text{Euler}}\right)$$

$$y(t_{i+1}) = y(t_i) + h f\left(t_i + \frac{1}{2}h, \underbrace{y_i + \frac{1}{2}hf(t_i, y_i)}_{K_1(t_i, y_i)}\right)$$

$K_2(t_i, y_i, h)$

$$K_1(t_i, y_i) = f(t_i, y_i)$$

$$K_2(t_i, y_i, h) = f\left(t_i + \frac{1}{2}h, y_i + \frac{1}{2}hK_1\right)$$

$$y_{i+1} = y_i + hK_2$$

modified Euler method

$$K_1(t_i, y_i) = f(t_i, y_i)$$

$$K_2(t_i, y_i, h) = f(t_i + h, y_i + hK_1)$$

$$y_{i+1} = y_i + \frac{1}{2}h(K_1 + K_2)$$

Heun's method (trapezoidal rule)

Introduction to Computational Fluid Dynamics

Runge-Kutta type methods

evaluation in intermediary points of $[t_i, t_{i+1}]$



Carl David Tolmé Runge
(1856 – 1927)



Martin Wilhelm Kutta
(1867 – 1944)

Standard Runge-Kutta method

$$y_{i+1} = y_i + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$

$$K_1 = f(t_i, y_i)$$

$$K_2 = f\left(t_i + \frac{1}{2}h, y_i + \frac{1}{2}hK_1\right)$$

$$K_3 = f\left(t_i + \frac{1}{2}h, y_i + \frac{1}{2}hK_2\right)$$

$$K_4 = f(t_i + h, y_i + hK_3)$$

Introduction to Computational Fluid Dynamics

Matlab solvers for Cauchy problems (ODE)

Syntax

```
[t, Y] = solver(odefun, tspan, y0, options, p1, p2, ...)
```

or

```
sol = solver(odefun, [t0 tf], y0...)
```

where solver can be

ode45, ode23, ode113, ode15s, ode23s, ode23t or ode23tb.

Input parameters (selection)

odefun – right hand member of the Cauchy problem

tspan –integration interval.

y0– initial value

options – solver options.

Introduction to Computational Fluid Dynamics

Output parameters:

`t` – column vector of time points;

`y` – solution array

`sol` – solution structure

<code>sol.x</code>	Steps chosen by the solver.
<code>sol.y</code>	Each column <code>sol.y(:, i)</code> contains the solution at <code>sol.x(i)</code> .
<code>sol.solver</code>	Solver name.

Introduction to Computational Fluid Dynamics

Solver	Problem Type	Order of Accuracy	When to Use
ode45	Nonstiff	Medium	Most of the time. This should be the first solver you try.
ode23	Nonstiff	Low	For problems with crude error tolerances or for solving moderately stiff problems.
ode113	Nonstiff	Low to high	For problems with stringent error tolerances or for solving computationally intensive problems.
ode15s	Stiff	Low to medium	If ode45 is slow because the problem is stiff.
ode23s	Stiff	Low	If using crude error tolerances to solve stiff systems and the mass matrix is constant.
ode23t	Moderately Stiff	Low	For moderately stiff problems if you need a solution without numerical damping.
ode23tb	Stiff	Low	If using crude error tolerances to solve stiff systems.

Introduction to Computational Fluid Dynamics

Example: Solve pendulum equation using ode45:

$$\frac{d^2\theta}{dt^2} + \frac{g}{L}\sin\theta = 0, \quad \theta(0) = 0, \quad \frac{d\theta}{dt}(0) = 0.1$$

We note $y_1 = \theta$ and rewrite the system in the form

$$\frac{dy_1}{dt} = y_2;$$

$$\frac{dy_2}{dt} = -\frac{g}{L}\sin y_1$$

$$y_1(0) = 0; \quad \frac{dy_1}{dt}(0) = 0.1$$

```
function dy=fPendul(t,y,flag,g,L)
dy=[y(2); -g/L*sin(y(1))];
```

Introduction to Computational Fluid Dynamics

```
%pendulum equation
a=0;b=pi/2;%integration interval
g=9.8;%accelaration due to the gravity
L=0.1;%length of the pendulum
y0=[0,0.1];%initial conditions
options=odeset('RelTol',1e-8);%modify the options
%use the solver
[t,y]=ode45('fPendul',[a,b],y0,options,g,L)
plot(t,y(:,1));
```

