COMPUTATIONAL AERODYNAMICS (R15A2119)

COURSE FILE

IV B. Tech I Semester

(2018-2019)

Prepared By

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Department of Aeronautical Engineering

MALLA REDDY COLLEGE OF ENGINEERING & TECHNOLOGY

(Autonomous Institution – UGC, Govt. of India)

Affiliated to JNTU, Hyderabad, Approved by AICTE - Accredited by NBA & NAAC – 'A' Grade - ISO 9001:2015 Certified)
Maisammaguda, Dhulapally (Post Via. Kompally), Secunderabad – 500100, Telangana State, India.

MRCET VISION

- To become a model institution in the fields of Engineering, Technology and Management.
- To have a perfect synchronization of the ideologies of MRCET with challenging demands of International Pioneering Organizations.

MRCET MISSION

To establish a pedestal for the integral innovation, team spirit, originality and competence in the students, expose them to face the global challenges and become pioneers of Indian vision of modern society.

MRCET QUALITY POLICY.

- To pursue continual improvement of teaching learning process of Undergraduate and Post Graduate programs in Engineering & Management vigorously.
- To provide state of art infrastructure and expertise to impart the quality education.

PROGRAM OUTCOMES
(PO's)

Engineering Graduates will be able to:

1. **Engineering knowledge**: Apply the knowledge of mathematics, science, engineering fundamentals, and an engineering specialization to the solution of complex engineering problems.
2. **Problem analysis**: Identify, formulate, review research literature, and analyze complex engineering problems reaching substantiated conclusions using first principles of mathematics, natural sciences, and engineering sciences.
3. **Design / development of solutions**: Design solutions for complex engineering problems and design system components or processes that meet the specified needs with appropriate consideration for the public health and safety, and the cultural, societal, and environmental considerations.
4. **Conduct investigations of complex problems**: Use research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions.
5. **Modern tool usage**: Create, select, and apply appropriate techniques, resources, and modern engineering and IT tools including prediction and modeling to complex engineering activities with an understanding of the limitations.
6. **The engineer and society**: Apply reasoning informed by the contextual knowledge to assess societal, health, safety, legal and cultural issues and the consequent responsibilities relevant to the professional engineering practice.
7. **Environment and sustainability**: Understand the impact of the professional engineering solutions in societal and environmental contexts, and demonstrate the knowledge of, and need for sustainable development.
8. **Ethics**: Apply ethical principles and commit to professional ethics and responsibilities and norms of the engineering practice.
9. **Individual and team work**: Function effectively as an individual, and as a member or leader in diverse teams, and in multidisciplinary settings.
10. **Communication**: Communicate effectively on complex engineering activities with the engineering community and with society at large, such as, being able to comprehend and write effective reports and design documentation, make effective presentations, and give and receive clear instructions.
11. **Project management and finance**: Demonstrate knowledge and understanding of the engineering and management principles and apply these to one's own work, as a member and leader in a team, to manage projects and in multi disciplinary environments.
12. **Life- long learning**: Recognize the need for, and have the preparation and ability to engage in independent and life-long learning in the broadest context of technological change.

DEPARTMENT OF AERONAUTICAL ENGINEERING

VISION

Department of Aeronautical Engineering aims to be indispensable source in Aeronautical Engineering which has a zeal to provide the value driven platform for the students to acquire knowledge and empower themselves to shoulder higher responsibility in building a strong nation.

MISSION

The primary mission of the department is to promote engineering education and research. To strive consistently to provide quality education, keeping in pace with time and technology. Department passions to integrate the intellectual, spiritual, ethical and social development of the students for shaping them into dynamic engineers.

QUALITY POLICY STATEMENT

Impart up-to-date knowledge to the students in Aeronautical area to make them quality engineers. Make the students experience the applications on quality equipment and tools. Provide systems, resources and training opportunities to achieve continuous improvement. Maintain global standards in education, training and services.

PROGRAM EDUCATIONAL OBJECTIVES – Aeronautical Engineering

1. **PEO1 (PROFESSIONALISM & CITIZENSHIP):** To create and sustain a community of learning in which students acquire knowledge and learn to apply it professionally with due consideration for ethical, ecological and economic issues.
2. **PEO2 (TECHNICAL ACCOMPLISHMENTS):** To provide knowledge based services to satisfy the needs of society and the industry by providing hands on experience in various technologies in core field.
3. **PEO3 (INVENTION, INNOVATION AND CREATIVITY):** To make the students to design, experiment, analyze, and interpret in the core field with the help of other multi disciplinary concepts wherever applicable.
4. **PEO4 (PROFESSIONAL DEVELOPMENT):** To educate the students to disseminate research findings with good soft skills and become a successful entrepreneur.
5. **PEO5 (HUMAN RESOURCE DEVELOPMENT):** To graduate the students in building national capabilities in technology, education and research

PROGRAM SPECIFIC OUTCOMES – Aeronautical Engineering

1. To mould students to become a professional with all necessary skills, personality and sound knowledge in basic and advance technological areas.
2. To promote understanding of concepts and develop ability in design manufacture and maintenance of aircraft, aerospace vehicles and associated equipment and develop application capability of the concepts sciences to engineering design and processes.
3. Understanding the current scenario in the field of aeronautics and acquire ability to apply knowledge of engineering, science and mathematics to design and conduct experiments in the field of Aeronautical Engineering.
4. To develop leadership skills in our students necessary to shape the social, intellectual, business and technical worlds.

MALLA REDDY COLLEGE OF ENGINEERING & TECHNOLOGY

IV Year B. Tech, ANE-I Sem

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(R15A2119)COMPUTATIONAL AERODYNAMICS

Objectives:

- Application of CFD to various engineering problems.
- Understand the physics of mathematical equations governing aerodynamic flows.
- Numerical methods to solve fluid flow problems

UNIT-I - INTRODUCTION TO COMPUTATIONAL FLUID DYNAMICS

CFD – Why Computational Fluid Dynamics? What is CFD? CFD - Research tool – Design Tool, Application of CFD to various Engineering problems. Models of fluid flow- Finite Control Volume, Infinitesimal Fluid Element. substantial derivatives, divergence of Velocity.

UNIT-II - GOVERNING EQUATIONS OF FLUID DYNAMICS

The continuity equation, the momentum equation, the energy equation, physical boundary conditions. Form of Governing equation suited for CFD - Conservation form - shock fitting and shock capturing.impact of partial differential eqautions on CFD. Classification of Quasi-Linear Partial differential equation, The Eigen value method, General behavior of different classes of Partial differential equation – elliptic, parabolic and hyperbolic.

UNIT-III – DISCRETIZATION TECHNIQUES

Introduction, Finite differences and formulas for first and second derivatives, difference equations, Explicit and implicit approaches, multidimensional finite difference formulas, finite difference formulas on non-uniform grids. Basis of finite volume method- conditions on the finite volume selections- approaches - Cell-centered and cell-vertex Definition of finite volume discretization general formulation of a numerical scheme- Two dimensional finite volume method with example.

UNIT-IV - GRID GENERATION

Need for grid generation. Structured grids- Cartesian grids, stretched (compressed) grids, body fitted structured grids, Multi-block grids - overset grids with applications.

Unstructured grids- triangular/ tetrahedral cells, hybrid grids, quadrilateral/hexahedra cells. Grid Generation techniques - Delaunay triangulation, Advance font method. Surface and volume estimations, grid quality and best practice guidelines.

UNIT-V – CFD TECHNIQUES

Lax-Wendroff technique, MacCormack's technique, Crank Nicholson technique, Relaxation technique- aspects of numerical dissipation and dispersion, Alternating-Direction-Implicit (ADI) Technique. Pressure correction technique Numerical procedures- SIMPLE, SIMPLER algorithms SIMPLEC and PISO algorithms Boundary conditions for the pressure correction method. Parallel Computing.

Text Books:

1. John .D. Anderson "Computational Fluid Dynamics", McGraw Hill
2. Charles Hirsch "Numerical computation of internal and external flows" Second Edition Butterworth-Heinemann is an imprint of Elsevier

Reference Books:

1. Hoffmann, K.A: Computational Fluid Dynamics for Engineers, Engineering Education System, Austin, Tex., 1989
2. J Blazek "Computational Fluid Dynamics: Principles and Applications" Elsevier.

3. Introduction to Computational Fluid Dynamics, Chow CY, John Wiley, 1979

Outcomes:

- Solve differential equations governing fluid flow problems.
- Generation of grid according to geometry of flow.
- Application of CFD techniques for aerospace problems.

UNIT-I
INTRODUCTION TO COMPUTATIONAL FLUID DYNAMICS

What is CFD? CFD - Research tool – Design Tool

CFD – **Computational fluid dynamics** (**CFD**) is a branch of fluid mechanics that uses numerical analysis and data structures to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. With high-speed supercomputers, better solutions can be achieved. Ongoing research yields software that improves the accuracy and speed of complex simulation scenarios such as transonic or turbulent flows. Initial experimental validation of such software is performed using a wind tunnel with the final validation coming in full-scale testing, e.g. flight tests.

Why Computational Fluid Dynamics?

Analysis and Design Simulation-based design instead of “build¬ & test”

More cost effective and more rapid than EFD

CFD provides high-fidelity database for diagnosing

flow field Simulation of physical fluid phenomena that are difficult¬ for experiments Full scale simulations (e.g., ships and airplanes)

Environmental effects (wind, weather, etc.)

Hazards (e.g., explosions, radiation, pollution)

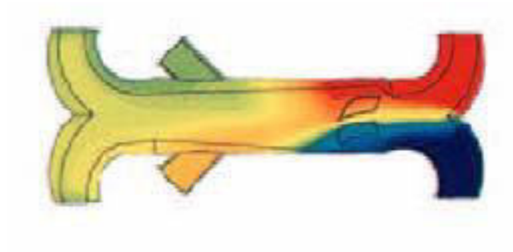
Physics (e.g., planetary boundary layer, stellar♣ evolution)

Knowledge and exploration of flow physics

Application of CFD to various Engineering problems

CFD is useful in a wide variety of applications and here we note a few to give you an idea of its use in industry. The simulations shown below have been performed using the FLUENT software. CFD can be used to simulate the flow over a vehicle. For instance, it can be used to study the interaction of propellers or rotors with the aircraft fuselage. The following figure shows the prediction of the pressure field induced by the interaction of the rotor with a helicopter fuselage in forward flight. Rotors and propellers can be represented with models of varying complexity.

The temperature distribution obtained from a CFD analysis of a mixing manifold is shown below. This mixing manifold is part of the passenger cabin ventilation system on the Boeing 767. The CFD analysis showed the effectiveness of a simpler manifold design without the need for field testing.

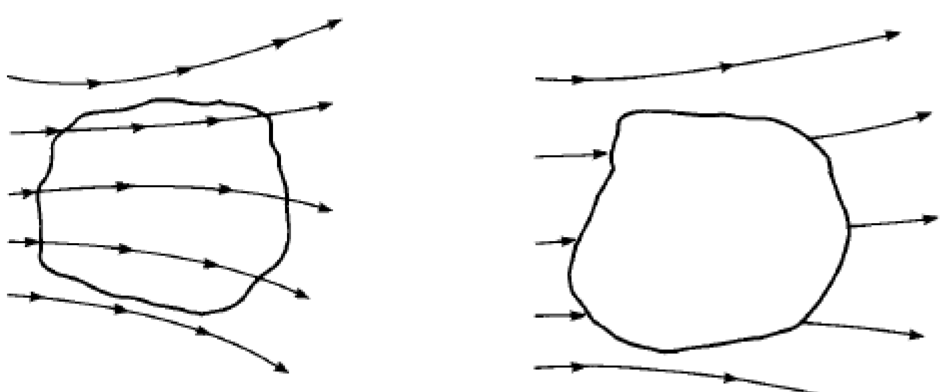


Bio-medical engineering is a rapidly growing field and uses CFD to study the circulatory and respiratory systems. The following figure shows pressure contours and a cutaway view that reveals velocity vectors in a blood pump that assumes the role of heart in open-heart surgery.

CFD is attractive to industry since it is more cost-effective than physical testing. However, one must note that complex flow simulations are challenging and error- prone and it takes a lot of engineering expertise to obtain validated solutions.

Models of fluid flow- Finite Control Volume,

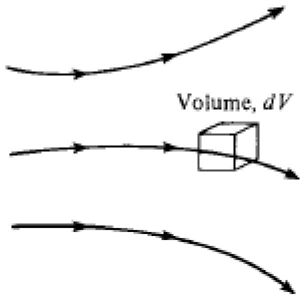
A **control volume** is a mathematical abstraction employed in the process of creating mathematical models of physical processes. In an inertial frame of reference, it is a volume fixed in space or moving with constant flow velocity through which the continuum (gas, liquid or solid) flows. The surface enclosing the control volume is referred to as the **control surface**.



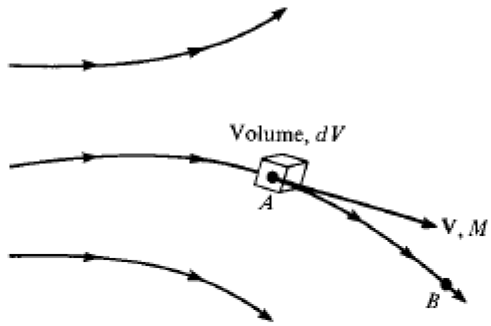
Finite control volume fixed in space with the fluid moving through it.

Finite control volume moving with the fluid such that the same fluid particles are always in the same control volume

Infinitesimal Fluid Element.



Infinitesimal fluid element fixed in space with the fluid moving through it



Infinitesimal fluid element moving along a streamline with the velocity **V** equal to the flow velocity at each point

Substantial derivative

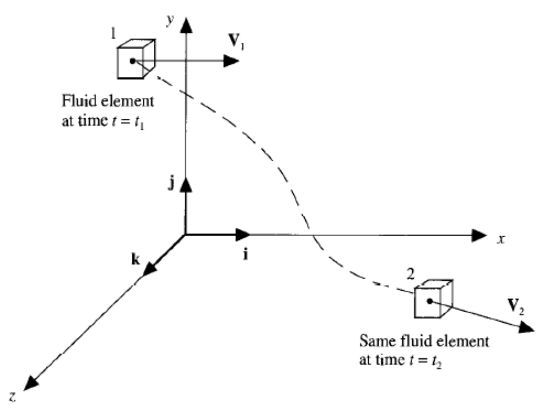
The substantial derivative has a physical meaning: the rate of change of a quantity (mass, energy, momentum) as experienced by an observer that is moving along with the flow. The observations made by a moving observer are affected by the stationary time-rate-of-change of the property (∂f/∂t), but what is observed also depends on where the observer goes as it floats along with the flow (v · ∇f). If the flow takes the observer into a region where, for example, the local energy is higher, then the observed amount of energy will be higher due to this change in location. The rate of change from the point of view of an observer floating along with a flow appears naturally in the equations of change.

$$V=u\mathbf{i}+v\mathbf{j}+w\mathbf{k}$$

Where the x,y,z components of velocity are given as

$$u=u(x,y,z,t)$$
$$v=v(x,y,z,t)$$
$$w=w(x,y,z,t)$$

Thus it is unsteady flow where u,v,w are functions of space and time. Similarly consider density ρ= ρ(x,y,z,t)



At time t_1, the fluid element is located at point 1 and later it is moved to point 2 in time t_2.
Expanding density by using taylor series about point 1 as follows:

$$\rho_2 = \rho_1 + \left(\frac{\partial \rho}{\partial x}\right)_1 (x_2 - x_1) + \left(\frac{\partial \rho}{\partial y}\right)_1 (y_2 - y_1) + \left(\frac{\partial \rho}{\partial z}\right)_1 (z_2 - z_1) + \left(\frac{\partial \rho}{\partial t}\right)_1 (t_2 - t_1) + \text{(higher-order terms)}$$

Dividing by $t_2 - t_1$ and ignoring higher-order terms, we obtain

$$\frac{\rho_2 - \rho_1}{t_2 - t_1} = \left(\frac{\partial \rho}{\partial x}\right)_1 \frac{x_2 - x_1}{t_2 - t_1} + \left(\frac{\partial \rho}{\partial y}\right)_1 \frac{y_2 - y_1}{t_2 - t_1} + \left(\frac{\partial \rho}{\partial z}\right)_1 \frac{z_2 - z_1}{t_2 - t_1} + \left(\frac{\partial \rho}{\partial t}\right)_1 \tag{2.1}$$

$$\lim_{t_2 \to t_1} \frac{\rho_2 - \rho_1}{t_2 - t_1} \equiv \frac{D\rho}{Dt}$$

Here Dρ/Dt is a symbol for the instantaneous time rate of change of density of the fluid element as it moves through point 1 whch is also called as substantial derivative.

$$\lim_{t_2 \to t_1} \frac{x_2 - x_1}{t_2 - t_1} \equiv u$$

$$\lim_{t_2 \to t_1} \frac{y_2 - y_1}{t_2 - t_1} \equiv v$$

$$\lim_{t_2 \to t_1} \frac{z_2 - z_1}{t_2 - t_1} \equiv w$$

$$\frac{D\rho}{Dt} = u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} + w\frac{\partial \rho}{\partial z} + \frac{\partial \rho}{\partial t}$$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}$$

Furthermore, in cartesian coordinates, the vector operator ∇ is defined as

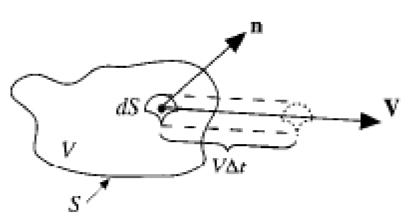
$$\nabla \equiv \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}$$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + (\mathbf{V} \cdot \nabla)$$

$$\frac{DT}{Dt} \equiv \underbrace{\frac{\partial T}{\partial t}}_{\text{Local derivative}} + \underbrace{(\mathbf{V} \cdot \nabla)}_{\text{Convective derivative}} \equiv \frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} + w\frac{\partial T}{\partial z}$$

Divergence of Velocity

Physically it is the time rate of change of the volume of a moving fluid element per unit volume.



$$\iint_S (\mathbf{V}\,\Delta t)\cdot \mathbf{dS}$$

$$\frac{D\mathscr{V}}{Dt} = \frac{1}{\Delta t}\iint_S (\mathbf{V}\cdot\Delta t)\cdot \mathbf{dS} = \iint_S \mathbf{V}\cdot \mathbf{dS}$$

$$\frac{D\mathscr{V}}{Dt} = \iiint_{\mathscr{V}} (\nabla\cdot\mathbf{V})\, d\mathscr{V}$$

$$\frac{D(\delta\mathscr{V})}{Dt} = (\nabla\cdot\mathbf{V})\,\delta\mathscr{V}$$

$$\boxed{\nabla\cdot\mathbf{V} = \frac{1}{\delta\mathscr{V}}\frac{D(\delta\mathscr{V})}{Dt}}$$

UNIT-II
GOVERNING EQUATIONS OF FLUID DYNAMICS

The continuity equation, the momentum equation, the energy equation

Continuity equation

Nonconservation form

$$\frac{D\rho}{Dt} + \rho\nabla \cdot \mathbf{V} = 0$$

Conservation form

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{V}) = 0$$

Momentum equations

Nonconservation form

x component : $$\rho\frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial\tau_{xx}}{\partial x} + \frac{\partial\tau_{yx}}{\partial y} + \frac{\partial\tau_{zx}}{\partial z} + \rho f_x$$

y component : $$\rho\frac{Dv}{Dt} = \frac{\partial p}{\partial y} + \frac{\partial\tau_{xy}}{\partial x} + \frac{\partial\tau_{yy}}{\partial y} + \frac{\partial\tau_{zy}}{\partial z} + \rho f_y$$

z component : $$\rho\frac{Dw}{Dt} = -\frac{\partial p}{\partial z} + \frac{\partial\tau_{xz}}{\partial x} + \frac{\partial\tau_{yz}}{\partial y} + \frac{\partial\tau_{zz}}{\partial z} + \rho f_z$$

Conservation form

x component:

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u\mathbf{V}) = -\frac{\partial p}{\partial x} + \frac{\partial\tau_{xx}}{\partial x} + \frac{\partial\tau_{yx}}{\partial y} + \frac{\partial\tau_{zx}}{\partial z} + \rho f_x$$

y component:

$$\frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v\mathbf{V}) = -\frac{\partial p}{\partial y} + \frac{\partial\tau_{xy}}{\partial x} + \frac{\partial\tau_{yy}}{\partial y} + \frac{\partial\tau_{zy}}{\partial z} + \rho f_y$$

z component:

$$\frac{\partial(\rho w)}{\partial t} + \nabla \cdot (\rho w\mathbf{V}) = -\frac{\partial p}{\partial z} + \frac{\partial\tau_{xz}}{\partial x} + \frac{\partial\tau_{yz}}{\partial y} + \frac{\partial\tau_{zz}}{\partial z} + \rho f_z$$

Energy equation

Nonconservation form

$$\rho\frac{D}{Dt}\left(e+\frac{V^2}{2}\right)=\rho\dot{q}+\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)$$
$$-\frac{\partial(up)}{\partial x}-\frac{\partial(vp)}{\partial y}-\frac{\partial(wp)}{\partial z}+\frac{\partial(u\tau_{xx})}{\partial x}$$
$$+\frac{\partial(u\tau_{yx})}{\partial y}+\frac{\partial(u\tau_{zx})}{\partial z}+\frac{\partial(v\tau_{xy})}{\partial x}+\frac{\partial(v\tau_{yy})}{\partial y}$$
$$+\frac{\partial(v\tau_{zy})}{\partial z}+\frac{\partial(w\tau_{xz})}{\partial x}+\frac{\partial(w\tau_{yz})}{\partial y}+\frac{\partial(w\tau_{zz})}{\partial z}+\rho\mathbf{f}\cdot\mathbf{V}\quad (2$$

Conservation form

$$\frac{\partial}{\partial t}\left[\rho\left(e+\frac{V^2}{2}\right)\right]+\nabla\cdot\left[\rho\left(e+\frac{V^2}{2}\right)\mathbf{V}\right]=\rho\dot{q}+\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)-\frac{\partial(up)}{\partial x}-\frac{\partial(vp)}{\partial y}-\frac{\partial(wp)}{\partial z}+\frac{\partial(u\tau_{xx})}{\partial x}$$
$$+\frac{\partial(u\tau_{yx})}{\partial y}+\frac{\partial(u\tau_{zx})}{\partial z}+\frac{\partial(v\tau_{xy})}{\partial x}+\frac{\partial(v\tau_{yy})}{\partial y}$$
$$+\frac{\partial(v\tau_{zy})}{\partial z}+\frac{\partial(w\tau_{xz})}{\partial x}+\frac{\partial(w\tau_{yz})}{\partial y}+\frac{\partial(w\tau_{zz})}{\partial z}+\rho\mathbf{f}\cdot\mathbf{V}\quad (2$$

physical boundary conditions

- The near wall flow is considered as laminar and the velocity varies linearly with distance from the wall
- No slip condition: u = v = 0.
- The velocity is constant along parallel to the wall and varies only in the direction normal to the wall.
- No pressure gradients in the flow direction.

Types of boundary conditions: In general, boundary conditions for any PDE can be classified into 4 major categories:

Dirichlet boundary condition: - in which the dependent variables themselves are prescribed along the domain boundary. 2) Von Neumann boundary condition: - in which the normal gradient of the dependent variables is prescribed along the boundary. 3) Robin boundary condition: - in which the boundary conditions are a linear combination of the Dirichlet and Von Neumann type. 4) Mixed boundary conditions: - in which certain portions of the boundary are defined as Dirichlet type, while others as Von Neumann type.

Shock fitting and shock capturing

In computational fluid dynamics, **shock-capturing methods** are a class of techniques for computing inviscid flows with shock waves. The computation of flow containing shock waves is an extremely difficult task because such flows result in sharp, discontinuous changes in flow variables such as pressure, temperature, density, and velocity across the shock. In shock-capturing methods, the governing equations of inviscid flows (i.e. Euler equations) are cast in conservation form and any shock waves or discontinuities are computed as part of the solution. Here, no special treatment is employed to take care of the shocks themselves, which is in contrast to the shock-fitting method, where shock waves are explicitly introduced in the solution using appropriate shock relations (Rankine–Hugoniot relations). The shock waves predicted by shock-capturing methods are generally not sharp and may be smeared over several grid elements. Also, classical shock-capturing methods have the disadvantage that unphysical oscillations (Gibbs phenomenon) may develop near strong shocks.

Impact of partial differential eqautions on CFD.

1. They are a coupled system of nonlinear partial differential equations, and hence are very difficult to solve analytically. To date, there is no general closed-form solution to these equations. (This does not mean that no general solution exists—we just have not been able to find one.)
2. For the momentum and energy equations, the difference between the non-conservation and conservation forms of the equations is just the left-hand side. The right-hand side of the equations in the two different forms is the same.
3. Note that the conservation forms of the equations contain terms on the left-hand side which include the divergence of some quantity, such as $\nabla \cdot (\rho \mathbf{V})$ or $\nabla \cdot (\rho u \mathbf{V})$. For this reason, the conservation form of the governing equations is sometimes called the *divergence form*.

Classification of Quasi-Linear Partial differential equation,

In CFD applications, computational schemes and specification of boundary conditions depend on the types of PARTIAL DIFFERENTIAL EQUATIONS. In many cases, the governing equations in fluids and heat transfer are of mixed types. For this reason, selection of computational schemes and methods to apply boundary conditions are important subjects in CFD.

Description

Partial differential equations (PDEs) in general, or the governing equations in fluid dynamics in particular, are classified into three categories:

(1) elliptic

(2) parabolic

(3) hyperbolic

Consider a system of quasi linear equations given below

$$a_1 \frac{\partial u}{\partial x} + b_1 \frac{\partial u}{\partial y} + c_1 \frac{\partial v}{\partial x} + d_1 \frac{\partial v}{\partial y} = f_1$$
$$a_2 \frac{\partial u}{\partial x} + b_2 \frac{\partial u}{\partial y} + c_2 \frac{\partial v}{\partial x} + d_2 \frac{\partial v}{\partial y} = f_2$$

Where u and

$$du = \frac{\partial u}{\partial x}\,dx + \frac{\partial u}{\partial y}\,dy$$
$$dv = \frac{\partial v}{\partial x}\,dx + \frac{\partial v}{\partial y}\,dy$$

$$\begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \begin{bmatrix} \partial u/\partial x \\ \partial u/\partial y \\ \partial v/\partial x \\ \partial v/\partial y \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ du \\ dv \end{bmatrix}$$

Let $[A]$ denote the coefficient matrix.

$$[A] \equiv \begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix}$$

Solve the above matrix for unknown like ∂u/∂x using cramer's rule. So, replacing first column of matrix [A] with constants column vector defining new mareix [B]

$$[B] = \begin{bmatrix} f_1 & b_1 & c_1 & d_1 \\ f_2 & b_2 & c_2 & d_2 \\ du & dy & 0 & 0 \\ dv & 0 & dx & dy \end{bmatrix}$$

Cramers rules give the solution for ∂u/∂xas

$$\frac{\partial u}{\partial x} = \frac{|B|}{|A|}$$
$$|A| = 0$$
$$\begin{vmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{vmatrix} = 0$$

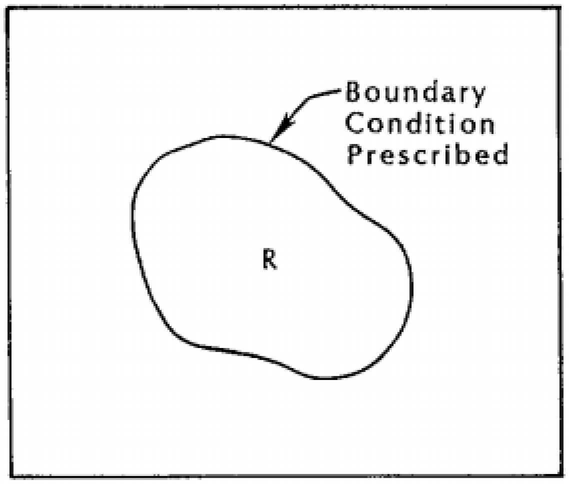
$$(a_1c_2 - a_2c_1)(dy)^2 - (a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)\,dx\,dy + (b_1d_2 - b_2d_1)(dx)^2 = 0$$

$$a = (a_1c_2 - a_2c_1)$$
$$b = -(a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)$$
$$c = (b_1d_2 - b_2d_1)$$
$$a\left(\frac{dy}{dx}\right)^2 + b\,\frac{dy}{dx} + c = 0$$
$$\frac{dy}{dx} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$
$$D = b^2 - 4ac$$

Elliptic Equations

- A PDE is elliptic in a region if ($b^2 - 4ac < 0$) at all points of the region.
- An elliptic PDE has no real characteristics but only imaginary/complex characteristics.

- A disturbance is propagated instantly in all directions within the region.
- Examples of Elliptic PDEs are Laplace equation and Poisson equation.
- The domain of solution for an elliptic PDE is a closed Region *R*.



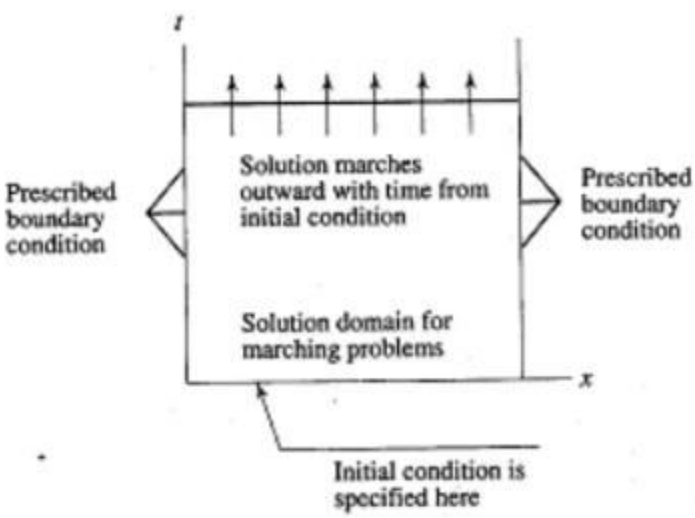
- **Boundary value problem:** Only boundary conditions are required to get the solution of elliptic equation.
- Steady state temperature distribution of a insulated solid rod.

2. Parabolic Equations

- A PDE is parabolic in a region if ($b^2 - 4ac = 0$) at all points of the region.
- Time dependent problem: Example of parabolic PDEs is unsteady heat diffusion equation.

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

- *Marching type problem*: The domain of solution for an parabolic PDE is an open Region.



- **Initial-Boundary value problems:** Initial condition and two boundary conditions are required.
- Examples: Boundary layers, jets, mixing layers, wakes, fully developed duct flows.

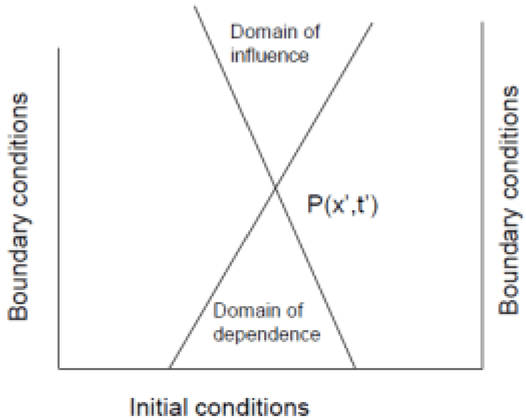
3. Hyperbolic Equations

- A PDE is hyperbolic in a region if ($b^2 - 4ac > 0$) at all points of the region.

- Example of hyperbolic PDEs is wave equation.

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2}$$

- The domain of solution for an parabolic PDE is an open Region.



- Initial boundary value problem: Two Initial conditions and two boundary conditions are required.
- Solution may be discontinuous (shock waves) : steady/unsteady compressible flows at supersonic speeds.
- **Method of Characteristics:** A classical method to solve hyperbolic equations with two independent variables: Applicable to two-dimensional, steady, isentropic, adiabatic, irrotational flow of a perfect gas.

Physical Interpretation

- Consider the flow of a body having velocity **u** in a quiescent fluid.
- The movement of this body disturbs the fluid particles ahead of the body.
- The propagation speed of disturbance would be equal to speed of sound, **a**.
- The ratio of the speed of body to the speed of sound is called Mach number **M=u/a.**
- Consider the steady two-dimensional velocity potential equation:

$$(1 - M^2)\phi_{xx} + \phi_{yy} = 0$$

Now $A = (1 - M^2)$, $B = 0$ and $C = 1$

Thus, $(B^2 - 4AC = -4(1 - M^2))$

- There are three types of PDEs for the three types of flows.

1 Elliptic PDEs: Subsonic($M < 0$).

2 Parabolic PDEs: Sonic($M = 0$).

3 Hyperbolic PDEs: Supersonic($M > 0$).

The physical situations these types of equations represent can be illustrated by the flow velocity relative to the speed of sound as shown in Figure 2.1.1. Consider that the flow velocity u is the velocity of a body moving in the quiescent fluid.The movement of this body disturbs the fluid particles ahead of the body, setting off the propagation velocity equal to the speed of sound a. The ratio of these two competing speeds is defined as Mach number, **M=u/a.**

For subsonic speed, M < 1, as time t increases, the body moves a distance, ut, which is always shorter than the distance at of the sound wave (Figure 2.1.1a). The sound wave reaches the observer, prior to the arrival of the body, thus warning the observer that an object is approaching. The zones outside and inside of the circles are known as the zone of silence and zone of action, respectively.

If, on the other hand, the body travels at the speed of sound, M = 1, then the observer does not hear the body approaching him prior to the arrival of the body, as these two actions are simultaneous (Figure 2.1.lb). All circles representing the distance traveled by the sound wave are tangent to the vertical line at the position of the observer. For supersonic speed, M > 1, the velocity of the body is faster than the speed of sound (Figure 2.1.1c). The line tangent to the circles of the speed of sound, known as a Mach wave, forms the boundary between the zones of silence (outside) and action (inside). Only after the body has passed by does the observer become aware of it.

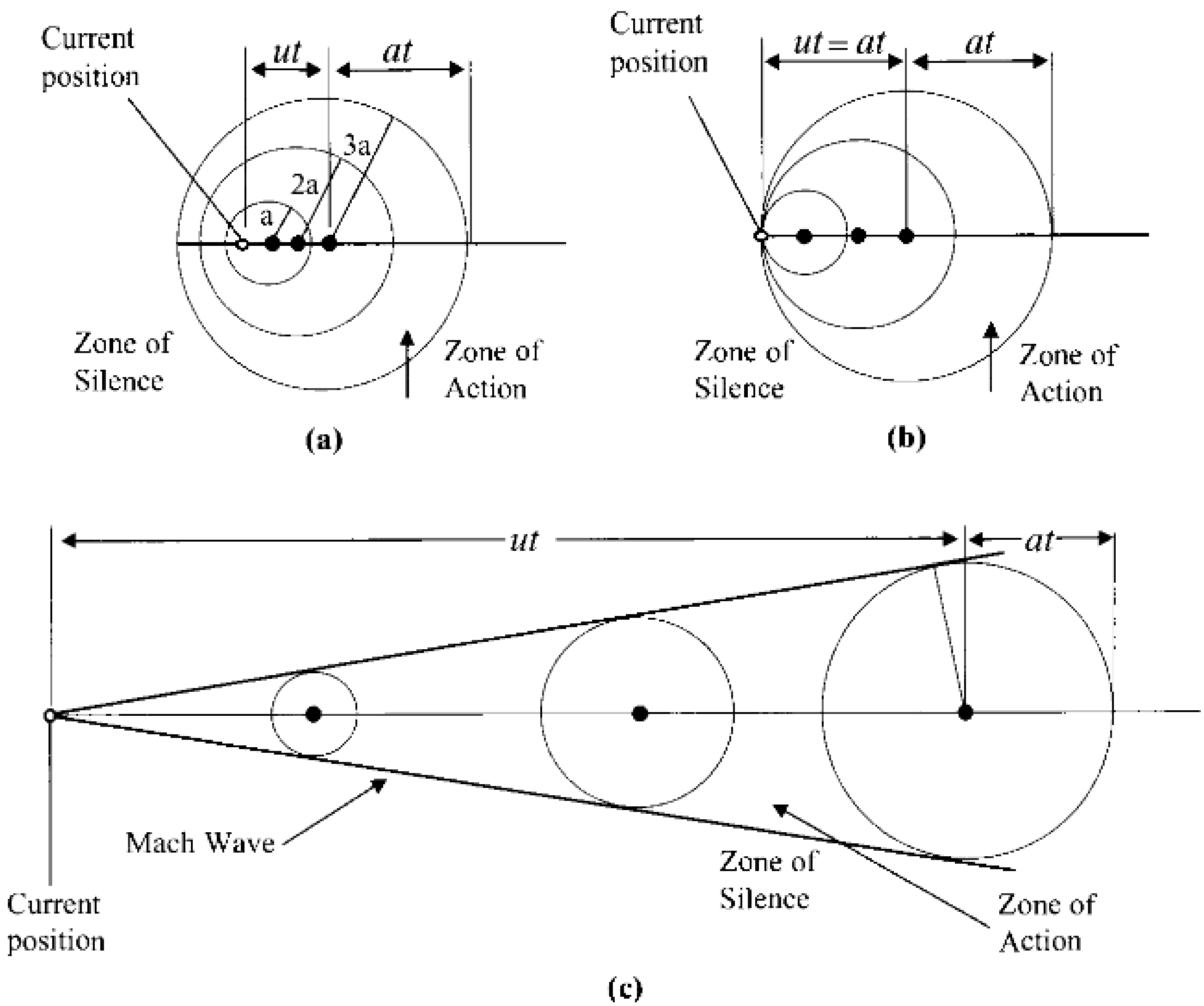


Figure 2.1.1 Subsonic, sonic, and supersonic flows. **(a)** Subsonic ($u < a$, $M < 1$). **(b)** Sonic ($u = a$, $M = 1$). **(c)** Supersonic ($u > a$, $M > 1$).

The governing equations for subsonic flow, transonic flow, and supersonic flow are classified as elliptic, parabolic, and hyperbolic, respectively. We shall elaborate on these equations below. Most of the governing equations in fluid dynamics are second order partial differential equations. For generality, let us consider the partial differential equation of the form [Sneddon, 1957] in a two-dimensional domain.

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + Fu + G = 0 \qquad (2.1.1)$$

Where the coefficients A, B, C, D, E, and F are constants or may be functions of both independent and/or dependent variables. To assure the continuity of the first derivative of u, **$u_x = \partial u/\partial x$ and $uy = \partial u/\partial y$.** We write

$$du_x = \frac{\partial u_x}{\partial x}dx + \frac{\partial u_x}{\partial y}dy = \frac{\partial^2 u}{\partial x^2}dx + \frac{\partial^2 u}{\partial x \partial y}dy \tag{2.1.2a}$$

$$du_y = \frac{\partial u_y}{\partial x}dx + \frac{\partial u_y}{\partial y}dy = \frac{\partial^2 u}{\partial x \partial y}dx + \frac{\partial^2 u}{\partial y^2}dy \tag{2.1.2b}$$

Here u forms a solution surface above or below the $x - y$ plane and the slope dy/dx representing the solution surface is defined as the characteristic curve.

Equations (2.1.1), (2.1.2a). and (2.1.2b) can be combined to form a matrix equation

$$\begin{bmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{bmatrix} = \begin{bmatrix} H \\ du_x \\ du_y \end{bmatrix} \tag{2.1.3}$$

where

$$H = -\left(D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + Fu + G \right) \tag{2.1.4}$$

Since it is possible to have discontinuities in the second order derivatives of the dependent variable along the characteristics, these derivatives are indeterminate.

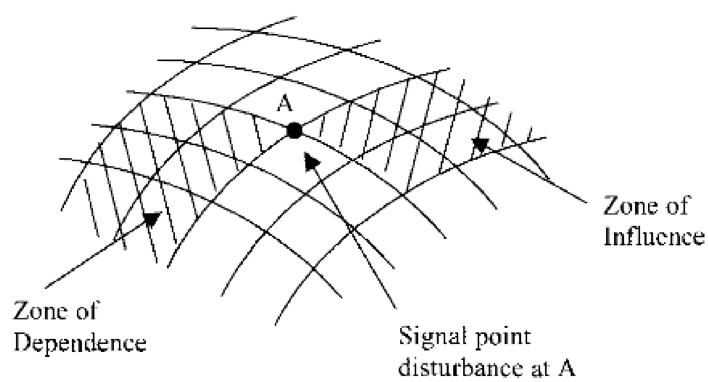


Figure 2.1.2 Propagation of disturbance and characteristics.

This happens when the determinant of the coefficient matrix in (2.1.3) is equal to zero.

$$\begin{vmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{vmatrix} = 0 \tag{2.1.5}$$

which yields

$$A\left(\frac{dy}{dx}\right)^2 - B\left(\frac{dy}{dx}\right) + C = 0 \tag{2.1.6}$$

Solving this quadratic equation yields the equation of the characteristics in physical space,

$$\frac{dy}{dx} = \frac{B \pm \sqrt{B^2 - 4AC}}{2A} \tag{2.1.7}$$

Depending on the value of $B^2 - 4AC$, characteristic curves can be real or imaginary.

For problems in which real characteristics exist, a disturbance propagates only over a finite region (Figure 2.1.2). The downstream region affected by this disturbance at point A is called the zone of influence. A signal at point A will be felt only if it originates from a finite region called the zone of dependence of point A.

The second order PDE is classified according to the sign of the expression ($B^2 - 4AC$).

(a) Elliptic if $B^2 - 4AC < 0$

In this case, the characteristics do not exist.

(b) Parabolic if $B^2 - 4AC = 0$

In this case, one set of characteristics exists.

(c) Hyperbolic if $B^2 - 4AC > 0$

In this case, two sets of characteristics exist.

Note that (2.1.1) resembles the general expression of a conic section,

$AX^2 + BXY + CY^2 + DX + EY + F = 0$ (2.1.8)

in which one can identify the following geometrical properties:

$B^2 - 4AC < 0$ ellipse

$B^2 - 4AC = 0$ parabola

$B^2 - 4AC > 0$ hyperbola

This is the origin of terms used for classification of partial differential equations.

Examples

(a) Elliptic equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{2.1.9}$$

$A = 1, \quad B = 0, \quad C = 1$

$B^2 - 4AC = -4 < 0$

(b) Parabolic equation

$$\frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2} = 0 \quad (\alpha > 0) \tag{2.1.10}$$

$A = -\alpha, \quad B = 0, \quad C = 0$

$B^2 - 4AC = 0$

(c) Hyperbolic equation

1-D First Order Wave Equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad (a > 0) \tag{2.1.11}$$

1-D Second Order Wave Equation

Differentiating (2.1.11) with respect to x and t,

$$\frac{\partial^2 u}{\partial t \partial x} + a \frac{\partial^2 u}{\partial x^2} = 0 \tag{2.1.12a}$$

$$\frac{\partial^2 u}{\partial t^2} + a \frac{\partial^2 u}{\partial t \partial x} = 0 \tag{2.1.12b}$$

Combining (2.1.12a) and (2.1.12b) yields

$$\frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} = 0 \tag{2.1.13}$$

where

$A = 1, \quad B = 0, \quad C = -a^2$

$B^2 - 4AC = 4a^2 > 0$

The Eigen value method, General behavior of different classes of Partial differential equation – elliptic, parabolic and hyperbolic.

$$a_1 \frac{\partial u}{\partial x} + b_1 \frac{\partial u}{\partial y} + c_1 \frac{\partial v}{\partial x} + d_1 \frac{\partial v}{\partial y} = 0$$

$$a_2 \frac{\partial u}{\partial x} + b_2 \frac{\partial u}{\partial y} + c_2 \frac{\partial v}{\partial x} + d_2 \frac{\partial v}{\partial y} = 0$$

Defining W as the column vector

$$W = \begin{Bmatrix} u \\ v \end{Bmatrix}$$

$$\begin{bmatrix} a_1 & c_1 \\ a_2 & c_2 \end{bmatrix} \frac{\partial W}{\partial x} + \begin{bmatrix} b_1 & d_1 \\ b_2 & d_2 \end{bmatrix} \frac{\partial W}{\partial y} = 0$$

$$[K]\frac{\partial W}{\partial x} + [M]\frac{\partial W}{\partial y} = 0$$

$$\frac{\partial W}{\partial x} + [K]^{-1}[M]\frac{\partial W}{\partial y} = 0$$

$$\frac{\partial W}{\partial x} + [N]\frac{\partial W}{\partial y} = 0$$

where by definition $[N] = [K]^{-1}[M]$.

If the eigen values are all real, the equations are hyperbolic.
If the eigen values are all complex the equations are elliptic or else they are parabolic.

WELL POSED PROBLEMS

The mathematical term **well-posed problem** stems from a definition given by Jacques Hadamard. He believed that mathematical models of physical phenomena should have the properties that:

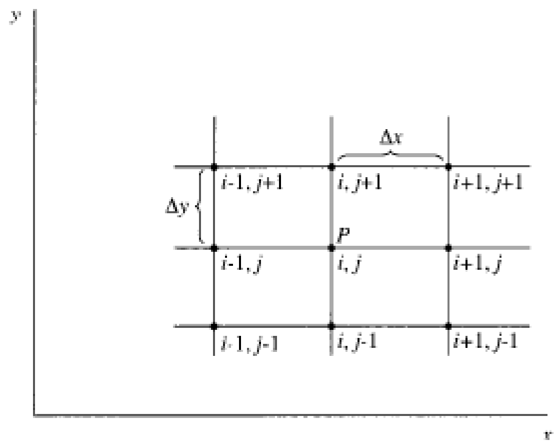
1. a solution exists,
2. the solution is unique,
3. the solution's behavior changes continuously with the initial conditions.

If the problem is well-posed, then it stands a good chance of solution on a computer using a stable algorithm. If it is not well-posed, it needs to be re-formulated for numerical treatment. Typically this involves including additional assumptions, such as smoothness of solution.

UNIT-III – DISCRETIZATION TECHNIQUES

Introduction, Finite differences

In mathematics, **finite-difference methods** (FDM) are numerical methods for solving differential equations by approximating them with difference equations, in which finite differences approximate the derivatives. FDMs are thus discretization methods.



Formulas for first and second derivatives

First, assuming the function whose derivatives are to be approximated is properly-behaved, by Taylor's theorem, we can create a Taylor series expansion

If $u_{i,j}$ denotes velocity at point (I,j) then the velocity $u_{i+1,j}$ at point (i+1,j) can be expressed in terms of Taylor series expanded about point (I,j) as follows:

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots$$

Solving above equation for derivative gives

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i+1,j} - u_{i,j}}{\Delta x}}_{\text{Finite-difference representation}} \underbrace{- \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{\Delta x}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^2}{6} + \cdots}_{\text{Truncation error}}$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} \approx \frac{u_{i+1,j} - u_{i,j}}{\Delta x}$$

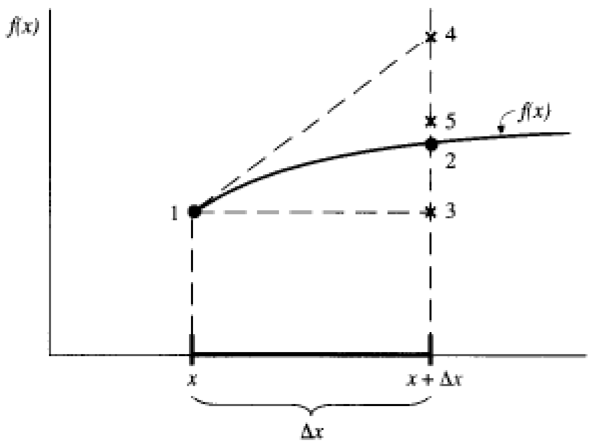
The lowest order term in truncation error involves Δx to the first power; hence the finite difference expression

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x)$$

Is called first order accurate and the symbol O(Δx) is a formal mathematical notation which represents terms of order Δx. The above equation uses information to the right of grid point (i,j) i.e it uses $u_{i+1,j}$ and $u_{i,j}$. As a result it is known as first order forward difference.

First, consider a continuous function of x, namely, $f(x)$, with all derivatives defined at x. Then, the value of f at a location $x + \Delta x$ can be estimated from a Taylor series expanded about point x, that is,

$$f(x+\Delta x) = \underbrace{f(x)}_{\substack{\text{First guess} \\ \text{(not very good)}}} + \underbrace{\frac{\partial f}{\partial x}\Delta x}_{\substack{\text{Add to capture} \\ \text{slope}}} + \underbrace{\frac{\partial^2 f}{\partial x^2}\frac{(\Delta x)^2}{2}}_{\substack{\text{Add to account} \\ \text{for curvature}}} + \cdots$$



$$f(x) = \sin\ 2\pi x$$

$$\text{At } x = 0.2: \qquad f(x) = 0.9511$$

$$\text{At } x = 0.22: \qquad f(x) = 0.9823$$

$$f(0.22) \approx f(0.2) = 0.9511$$

$$f(x+\Delta x) \approx f(x) + \frac{\partial f}{\partial x}\Delta x$$

$$f(0.22) \approx f(0.2) + 2\pi \cos\,[2\pi(0.2)](0.02)$$

$$\approx 0.9511 + 0.388 = 0.9899$$

$$f(x+\Delta x) \approx f(x) + \frac{\partial f}{\partial x}\Delta x + \frac{\partial^2 f}{\partial x^2}\frac{(\Delta x)^2}{2}$$

$$f(0.22) \approx f(0.2) + 2\pi \cos\,[2\pi(0.2)](0.02) - 4\pi^2 \sin\,[2\pi(0.2)]\frac{(0.02)^2}{2}$$

$$\approx 0.9511 + 0.0388 - 0.0075$$

$$\approx 0.9824$$

Let us now write a Taylor series expansion for $u_{i-1,j}$, expanded about $u_{i,j}$.

$$u_{i-1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j}(-\Delta x) + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{(-\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(-\Delta x)^3}{6} + \cdots$$

$$u_{i-1,j} = u_{i,j} - \left(\frac{\partial u}{\partial x}\right)_{i,j}\Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{(\Delta x)^2}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^3}{6} + \cdots$$

Solving for $(\partial u/\partial x)_{i,j}$, we obtain

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + O(\Delta x)}$$

The above equation uses information to the left of grid point (i,j) i.e it uses $u_{i-1,j}$ and $u_{i,j}$. As a result it is known as first order backward or rearward difference

In most CFD applications first order accuracy is not sufficient second order difference are obtained by subtract forward and backward differences as follows:

$$u_{i+1,j} - u_{i-1,j} = 2\left(\frac{\partial u}{\partial x}\right)_{i,j}\Delta x + 2\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^3}{6} + \cdots$$

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O(\Delta x)^2}$$

The lowest order term in truncation error involves Δx to the first power; hence the finite difference expression is of second order. The above equation uses information to the left and right of grid point (i,j) i.e it uses $u_{i+1,j}$, $u_{i-1,j}$ and $u_{i,j}$. As a result it is known as second order central difference.

Similarly the finite differences for y derivatives are given as

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \begin{cases} \dfrac{u_{i,j+1} - u_{i,j}}{\Delta y} + O(\Delta y) & \textit{Forward difference} \\ \dfrac{u_{i,j} - u_{i,j-1}}{\Delta y} + O(\Delta y) & \textit{Rearward difference} \\ \dfrac{u_{i,j+1} - u_{i,j-1}}{2\Delta y} + O(\Delta y)^2 & \textit{Central difference} \end{cases}$$

$$u_{i+1,j} + u_{i-1,j} = 2u_{i,j} + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}(\Delta x)^2 + \left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j}\frac{(\Delta x)^4}{12} + \cdots$$

Solving for $(\partial^2 u/\partial x)_{i,j}$,

$$\boxed{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + O(\Delta x)^2}$$

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} + O(\Delta y)^2$$

These are examples of second derivative finite differences are known as second differences.

For mixed derivatives

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} + \left(\frac{\partial^2 u}{\partial x\,\partial y}\right)_{i,j} \Delta x + \left(\frac{\partial^3 u}{\partial x^2\,\partial y}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^4 u}{\partial x^3\,\partial y}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} - \left(\frac{\partial^2 u}{\partial x\,\partial y}\right)_{i,j} \Delta x + \left(\frac{\partial^3 u}{\partial x^2\,\partial y}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^4 u}{\partial x^3\,\partial y}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots$$

Subtracting above two equations

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j} = 2\left(\frac{\partial^2 u}{\partial x\,\partial y}\right)_{i,j} \Delta x + \left(\frac{\partial^4 u}{\partial x^3\,\partial y}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots$$

$$\left(\frac{\partial^2 u}{\partial x\,\partial y}\right)_{i,j} = \frac{(\partial u/\partial y)_{i+1,j} - (\partial u/\partial y)_{i-1,j}}{2\Delta x} - \left(\frac{\partial^4 u}{\partial x^3\,\partial y}\right)_{i,j} \frac{(\Delta x)^2}{12} + \cdots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} + O(\Delta y)^2$$

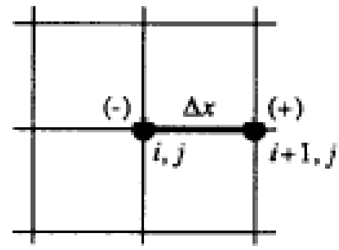
$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y} + O(\Delta y)^2$$

$$\boxed{\left(\frac{\partial^2 u}{\partial x\,\partial y}\right)_{i,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4\Delta x\,\Delta y} + O[(\Delta x)^2, (\Delta y)^2]}$$

This known as second order central difference for mixed derivative.

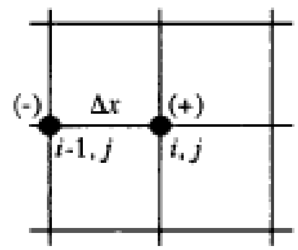
First-order forward difference with respect to x

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x}$$



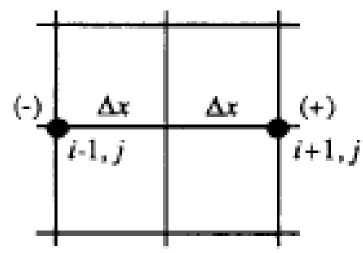
First-order rearward difference with respect to x

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x}$$



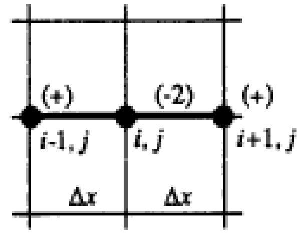
Second-order central difference with respect to x

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$



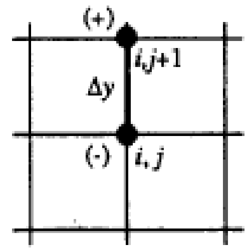
Second-order central second difference with respect to x

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$



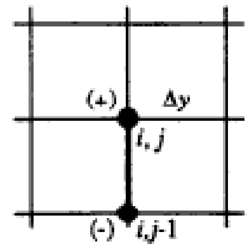
First-order forward difference with respect to y

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta y}$$



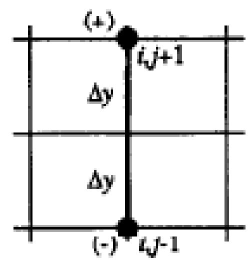
First-order rearward difference with respect to y

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \frac{u_{i,j} - u_{i,j-1}}{\Delta y}$$



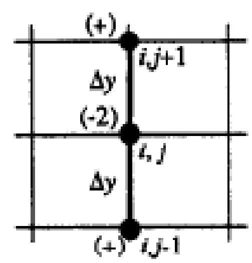
Second-order central difference with respect to y

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y}$$



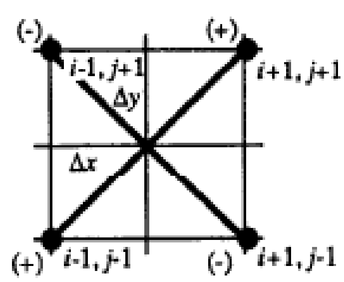
Second-order central second difference with respect to y

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2}$$



Second-order central mixed difference with respect to x and y

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{u_{i+1,j+1} + u_{i-1,j-1} - u_{i-1,j+1} - u_{i+1,j-1}}{4\Delta x\, \Delta y}$$



Difference equations

When all the partial derivatives in agiven PDE are replaced by finite difference the algebraic equation is known as difference equation.

Consider a one dimensional heat conduction equation with constant thermal diffusivity

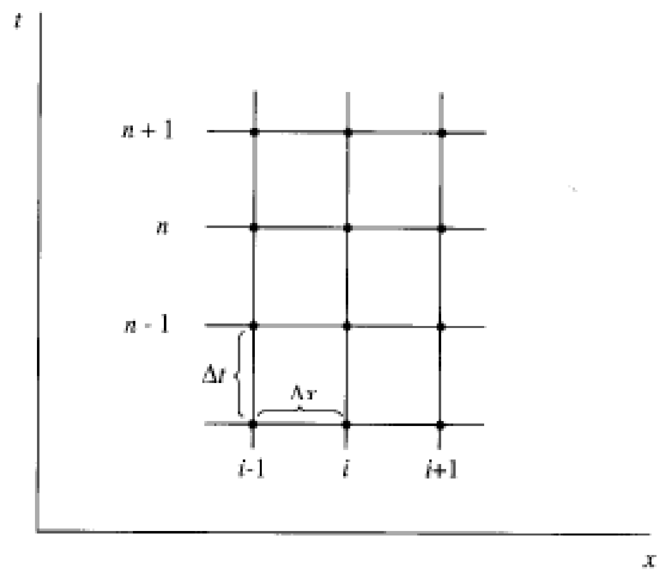
$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

This equation is parabolic in nature. So we use marching solution with respect to time. Here time is representd by prefix n to grid point.

$$\left(\frac{\partial T}{\partial t}\right)_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t} - \left(\frac{\partial^2 T}{\partial t^2}\right)_i^n \frac{\Delta t}{2} + \cdots$$

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^n = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2} - \left(\frac{\partial^4 T}{\partial x^4}\right)_i^n \frac{(\Delta x)^2}{12} + \cdots$$

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0$$



$$\overbrace{\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2}}^{\text{Partial differential equation}} = \underbrace{0 = \frac{T_i^{n+1} - T_i^n}{\Delta t} - \frac{\alpha (T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2}}_{\text{Difference equation}}$$

$$+ \underbrace{\left[-\left(\frac{\partial^2 T}{\partial t^2}\right)_i^n \frac{\Delta t}{2} + \alpha \left(\frac{\partial^4 T}{\partial x^4}\right)_i^n \frac{(\Delta x)^2}{12} + \cdots \right]}_{\text{Truncation error}}$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{\alpha(T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2}$$

The above equation is known as difference equation for one dimensional heat conduction governing equation.

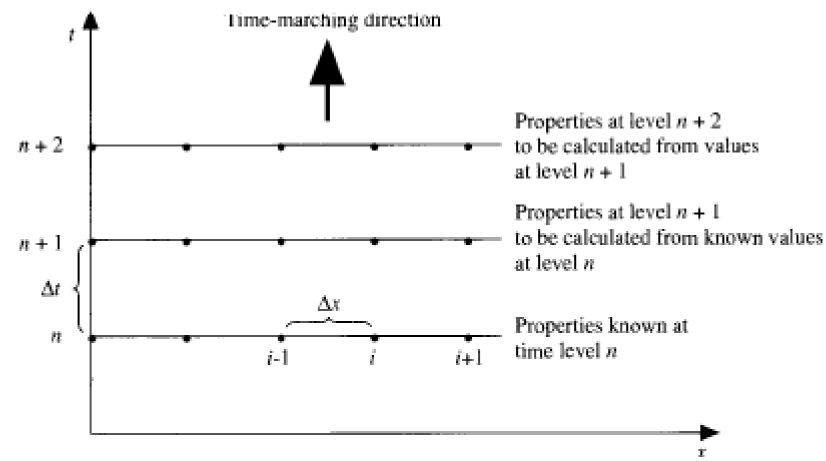
Explicit and implicit approaches

Consider the same 1D heat conduction equation

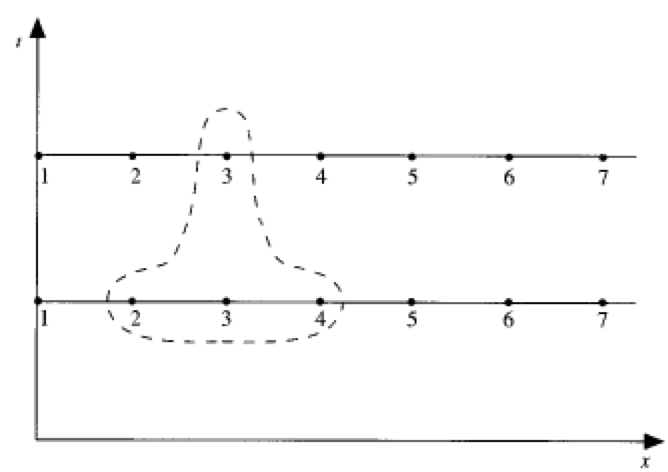
$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{\alpha(T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2}$$

With some rearrangements of above equation gives

$$T_i^{n+1} = T_i^n + \alpha \frac{\Delta t}{(\Delta x)^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$



In the above equation left hand side is unkown and all the right side terms in n level are known by boundary conditions. Thus by marching in time direction with varying n levels as shown in above figure the solution is obtained .



$$T_2^{n+1} = T_2^n + \alpha \frac{\Delta t}{(\Delta x)^2}(T_3^n - 2T_2^n + T_1^n)$$

$$T_3^{n+1} = T_3^n + \alpha \frac{\Delta t}{(\Delta x)^2}(T_4^n - 2T_3^n + T_2^n)$$

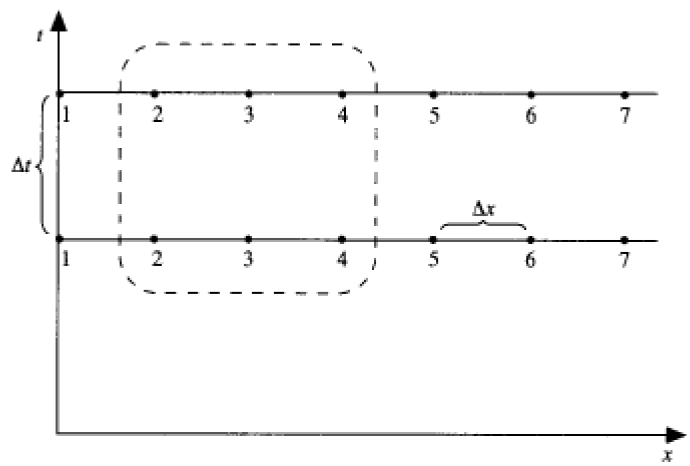
Similarly we can get for T^{n+4}, T^{n+5} and T^{n+6} . As these equations are solving for only one single unknown then it is known as explicit method.

For a given PDE we can write n number of difference equations with various methods like the following

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{\frac{1}{2}(T_{i+1}^{n+1} + T_{i+1}^n) + \frac{1}{2}(-2T_i^{n+1} - 2T_i^n) + \frac{1}{2}(T_{i-1}^{n+1} + T_{i-1}^n)}{(\Delta x)^2}$$

The above finite difference method is known as Crank Nicholoson form.

In the above both left and right handside terms are unknowns i.e. n+1 level terms. So to obtain the solution for a equation with more than one unknown it requires equations equal to number of unknowns. Thus solving simulkataneous euqtions or unknowns is known as implicit method.



$$\frac{\alpha\,\Delta t}{2(\Delta x)^2} T_{i-1}^{n+1} - \left[1 + \frac{\alpha\,\Delta t}{(\Delta x)^2}\right] T_i^{n+1} + \frac{\alpha\,\Delta t}{2(\Delta x)^2} T_{i+1}^{n+1}$$

$$= -T_i^n - \frac{\alpha\,\Delta t}{2(\Delta t)^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

$$A = \frac{\alpha\,\Delta t}{2(\Delta x)^2}$$

$$B = 1 + \frac{\alpha\,\Delta t}{(\Delta x)^2}$$

$$K_i = -T_i^n - \frac{\alpha\,\Delta t}{2(\Delta x)^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

$$AT_{i-1}^{n+1} - BT_i^{n+1} + AT_{i+1}^{n+1} = K_i$$

At grid point 2 : $AT_1 - BT_2 + AT_3 = K_2$

$$-BT_2 + AT_3 = K_2 - AT_1$$

At grid point 3 : $AT_2 - BT_3 + AT_4 = K_3$

At grid point 4 : $AT_3 - BT_4 + AT_5 = K_4$

At grid point 5 : $AT_4 - BT_5 + AT_6 = K_5$

At grid point 6 : $AT_5 - BT_6 + AT_7 = K_6$

$$AT_5 - BT_6 = K_6 - AT_7 = K'_6$$

$$\begin{bmatrix} B & A & 0 & 0 & 0 \\ A & -B & A & 0 & 0 \\ 0 & A & -B & A & 0 \\ 0 & 0 & A & -B & A \\ 0 & 0 & 0 & A & -B \end{bmatrix} \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} K'_2 \\ K_3 \\ K_4 \\ K_5 \\ K'_6 \end{bmatrix}$$

1. To obtain a steady state solution by means of assuming some arbitrary initial conditions for a flow field, and then calculating the flow in steps of time, going out to a sufficiently large number of time steps until a final steady-state flow is approached at large values of time. In this situation, the final steady state is the desired result, and the time marching is simply a means to that end. The solution to the supersonic blunt body problem is a case in point, as discussed in Sec.

Explicit approach

Advantage: Relatively simple to set up and program.

Disadvantage: In terms of our above example, for a given Δx, Δt must be less than some limit imposed by stability constraints. In some cases, Δt must be very small to maintain stability; this can result in long computer running times to make calculations over a given interval of t.

Implicit approach

Advantage: Stability can be maintained over much larger values of Δt, hence using considerable fewer time steps to make calculations over a given interval of t. This results in less computer time.

Disadvantage: More complicated to set up and program.

Disadvantage	Since massive matrix manipulations are usually required at each time step, the computer time per time step is much larger than in the explicit approach.
Disadvantage	Since large Δt can be taken, the truncation error is large, and the use of implicit methods to follow the exact transients (time variations of the independent variable) may not be as accurate as an explicit approach. However, for a time-dependent solution in which the steady state is the desired result, this relative timewise inaccuracy is not important.

Basis of finite volume method-

The **finite volume method** (**FVM**) is a method for representing and evaluating partial differential equations in the form of algebraic equations [LeVeque, 2002; Toro, 1999]. Similar to the finite difference method or finite element method, values are calculated at discrete places on a meshed geometry. "Finite volume" refers to the small volume surrounding each node point on a mesh. In the finite volume method, volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem. These terms are then evaluated as fluxes at the surfaces of each finite volume. Because the flux entering a given volume is identical to that leaving the adjacent volume, these methods are conservative. Another advantage of the finite volume method is that it is easily formulated to allow for unstructured meshes. The method is used in many computational fluid dynamics packages.

4

Finite-Volume Methods

Finite-volume methods (FVM) – sometimes also called box methods – are mainly employed for the numerical solution of problems in fluid mechanics, where they were introduced in the 1970s by McDonald, MacCormack, and Paullay. However, the application of the FVM is not limited to flow problems. An important property of finite-volume methods is that the balance principles, which are the basis for the mathematical modelling of continuum mechanical problems, per definition, also are fulfilled for the discrete equations (conservativity). In this chapter we will discuss the most important basics of finite-volume discretizations applied to continuum mechanical problems. For clarity in the presentation of the essential principles we will restrict ourselves mainly to the two-dimensional case.

4.1 General Methodology

In general, the FVM involves the following steps:

(1) Decomposition of the problem domain into control volumes.
(2) Formulation of integral balance equations for each control volume.
(3) Approximation of integrals by numerical integration.
(4) Approximation of function values and derivatives by interpolation with nodal values.
(5) Assembling and solution of discrete algebraic system.

In the following we will outline in detail the individual steps (the solution of algebraic systems will be the topic of Chap. 7). We will do this by example for the general stationary transport equation (see Sect. 2.3.2)

$$\frac{\partial}{\partial x_i}\left(\rho v_i \phi - \alpha \frac{\partial \phi}{\partial x_i}\right) = f \tag{4.1}$$

for some problem domain Ω. We remark that a generalization of the FVM to other types of equations as given in Chap. 2 is straightforward (in Chap. 10 this will be done for the Navier-Stokes equations).

The starting point for a finite-volume discretization is a decomposition of the problem domain Ω into a finite number of subdomains V_i $(i = 1, \ldots, N)$, called *control volumes* (CVs), and related nodes where the unknown variables are to be computed. The union of all CVs should cover the whole problem domain. In general, the CVs also may overlap, but since this results in unnecessary complications we consider here the non-overlapping case only. Since finally each CV gives one equation for computing the nodal values, their final number (i.e., after the incorporation of boundary conditions) should be equal to the number of CVs. Usually, the CVs and the nodes are defined on the basis of a numerical grid, which, for instance, is generated with one of the techniques described in Chap. 3. In order to keep the usual terminology of the FVM, we always talk of volumes (and their surfaces), although strictly speaking this is only correct for the three-dimensional case.

For one-dimensional problems the CVs are subintervals of the problem interval and the nodes can be the midpoints or the edges of the subintervals (see Fig. 4.1).

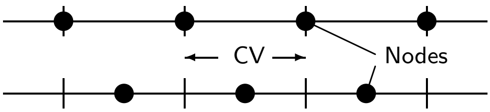


Fig. 4.1. Definitions of CVs and edge (top) and cell-oriented (bottom) arrangement of nodes for one-dimensional grids

In the two-dimensional case, in principle, the CVs can be arbitrary polygons. For quadrilateral grids the CVs usually are chosen identically with the grid cells. The nodes can be defined as the vertices or the centers of the CVs (see Fig. 4.2), often called edge or cell-centered approaches, respectively. For triangular grids, in principle, one could do it similarily, i.e., the triangles define the CVs and the nodes can be the vertices or the centers of the triangles. However, in this case other CV definitions are usually employed. One approach is closely related to the Delaunay triangulation discussed in Sect. 3.4.2. Here, the nodes are chosen as the vertices of the triangles and the CVs are defined as the polygons formed by the perpendicular bisectors of the sides of the surrounding triangles (see Fig. 4.3). These polygons are known as *Voronoi polygons* and in the case of convex problems domains and non-obtuse triangles there is a one-to-one correspondance to a Delaunay triangulation with its "nice" properties. However, this approach may fail for arbitrary triangulations. Another more general approach is to define a polygonal CV by joining the centroids and the midpoints of the edges of the triangles surrounding a node leading to the so-called *Donald polygons* (see Fig. 4.4).

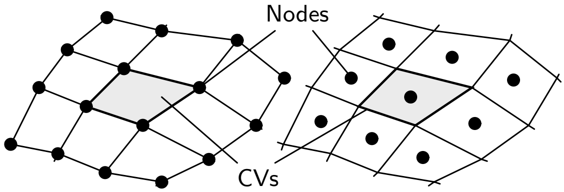


Fig. 4.2. Edge-oriented (left) and cell-oriented (right) arrangements of nodes for quadrilateral grids

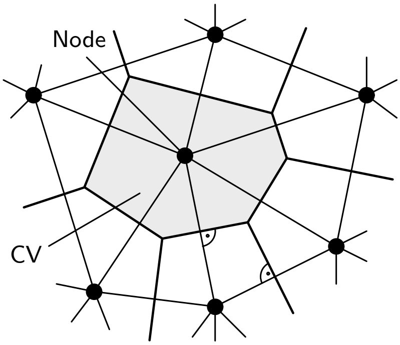


Fig. 4.3. Definition of CVs and nodes for triangular grids with Voronoi polygons

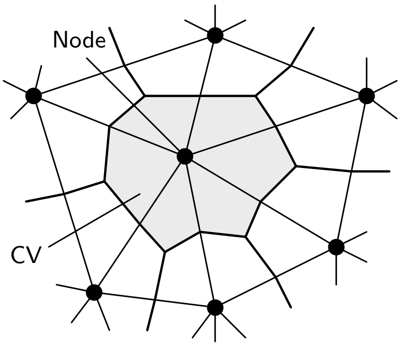


Fig. 4.4. Definition of CVs and nodes for triangular grids with Donald polygons

For three-dimensional problems on the basis of hexahedral or tetrahedral grids similar techniques as in the two-dimensional case can be applied (see, e.g., [26]).

After having defined the CVs, the balance equations describing the problem are formulated in integral form for each CV. Normally, these equations are directly available from the corresponding continuum mechanical conservation laws (applied to a CV), but they can also be derived by integration from the corresponding differential equations. By integration of (4.1) over an arbitrary control volume V and application of the Gauß integral theorem, one obtains:

$$\int_S \left(\rho v_i \phi - \alpha \frac{\partial \phi}{\partial x_i} \right) n_i \, \mathrm{d}S = \int_V f \, \mathrm{d}V \, , \tag{4.2}$$

where S is the surface of the CV and n_i are the components of the unit normal vector to the surface. The integral balance equation (4.2) constitutes the starting point for the further discretization of the considered problem with an FVM.

As an example we consider quadrilateral CVs with a cell-oriented arrangement of nodes (a generalization to arbitrary polygons poses no principal difficulties). For a general quadrilateral CV we use the notations of the distinguished points (midpoint, midpoints of faces, and edge points) and the unit normal vectors according to the so-called compass notation as indicated in Fig. 4.5. The midpoints of the directly neighboring CVs we denote – again in compass notation – with capital letters S, SE, etc. (see Fig. 4.6).

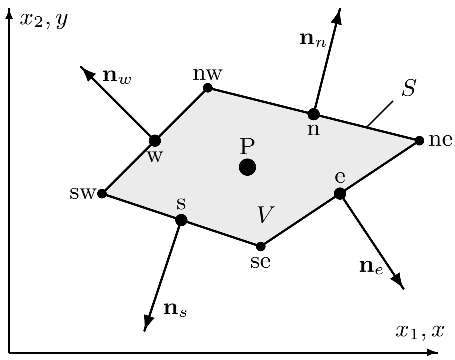


Fig. 4.5. Quadrilateral control volume with notations

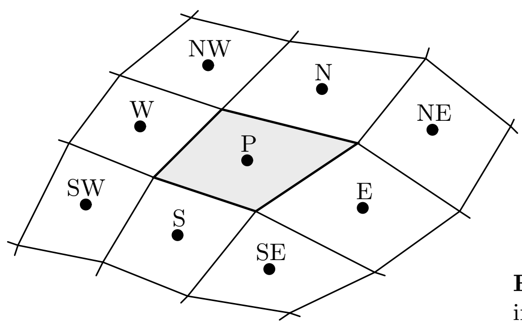


Fig. 4.6. Notations for neighboring control volumes

The surface integral in (4.2) can be split into the sum of the four surface integrals over the cell faces S_c ($c = \mathrm{e}, \mathrm{w}, \mathrm{n}, \mathrm{s}$) of the CV, such that the balance equation (4.2) can be written equivalently in the form

$$\sum_c \int_{S_c} \left(\rho v_i \phi - \alpha \frac{\partial \phi}{\partial x_i} \right) n_{ci} \, \mathrm{d}S_c = \int_V f \, \mathrm{d}V \, . \tag{4.3}$$

The expression (4.3) represents a balance equation for the convective and diffusive fluxes F_c^{C} and F_c^{D} through the CV faces, respectively, with

$$F_c^{\mathrm{C}} = \int_{S_c} (\rho v_i \phi)\, n_{ci}\, \mathrm{d}S_c \quad \text{and} \quad F_c^{\mathrm{D}} = -\int_{S_c} \left(\alpha \frac{\partial \phi}{\partial x_i} \right) n_{ci}\, \mathrm{d}S_c\, .$$

For the face S_{e}, for instance, the unit normal vector $\mathbf{n}_{\mathrm{e}} = (n_{\mathrm{e}1}, n_{\mathrm{e}2})$ is defined by the following (geometric) conditions:

$$(\mathbf{x}_{\mathrm{ne}} - \mathbf{x}_{\mathrm{se}}) \cdot \mathbf{n}_{\mathrm{e}} = 0 \quad \text{und} \quad |\mathbf{n}_{\mathrm{e}}| = \sqrt{n_{\mathrm{e}1}^2 + n_{\mathrm{e}2}^2} = 1\, .$$

From this one obtains the representation

$$\mathbf{n}_{\mathrm{e}} = \frac{(y_{\mathrm{ne}} - y_{\mathrm{se}})}{\delta S_{\mathrm{e}}}\, \mathbf{e}_1 - \frac{(x_{\mathrm{ne}} - x_{\mathrm{se}})}{\delta S_{\mathrm{e}}}\, \mathbf{e}_2\ , \tag{4.4}$$

where

$$\delta S_{\mathrm{e}} = |\mathbf{x}_{\mathrm{ne}} - \mathbf{x}_{\mathrm{se}}| = \sqrt{(x_{\mathrm{ne}} - x_{\mathrm{se}})^2 + (y_{\mathrm{ne}} - y_{\mathrm{se}})^2}$$

denotes the length of the face S_{e}. Analogous relations result for the other CV faces.

For neighboring CVs with a common face the absolute value of the total flux $F_{\mathrm{c}} = F_{\mathrm{c}}^{\mathrm{C}} + F_{\mathrm{c}}^{\mathrm{D}}$ through this face is identical, but the sign differs. For instance, for the CV around point P the flux F_{e} is equal to the flux $-F_{\mathrm{w}}$ for the CV around point E (since $(\mathbf{n}_{\mathrm{e}})_{\mathrm{P}} = -(\mathbf{n}_{\mathrm{w}})_{\mathrm{E}}$). This is exploited for the implementation of the method in order to avoid on the one hand a double computation for the fluxes and on the other hand to ensure that the corresponding absolute fluxes really are equal (important for conservativity, see Sect. 8.1.4). In the case of quadrilateral CVs the computation can be organized in such a way that, starting from a CV face at the boundary of the problem domain, for instance, only F_{e} und F_{n} have to be computed.

It should be noted that up to this point we haven't introduced any approximation, i.e., the flux balance (4.3) is still exact. The actual discretization now mainly consists in the approximation of the surface integrals and the volume integral in (4.3) by suitable averages of the corresponding integrands at the CV faces. Afterwards, these have to be put into proper relation to the unknown function values in the nodes.

4.2 Approximation of Surface and Volume Integrals

We start with the approximation of the surface integrals in (4.3), which for a cell-centered variable arrangement suitably is carried out in two steps:

(1) Approximation of the surface integrals (fluxes) by values on the CV faces.

(2) Approximation of the variable values at the CV faces by node values.

As an example let us consider the approximation of the surface integral

$$\int_{S_e} w_i n_{ei} \, dS_e$$

over the face S_e of a CV for a general integrand function $\mathbf{w} = (w_1(\mathbf{x}), w_2(\mathbf{x}))$ (the other faces can be treated in a completely analogous way).

The integral can be approximated in different ways by involving more or less values of the integrand at the CV face. The simplest possibility is an approximation by just using the midpoint of the face:

$$\int_{S_e} w_i n_{ei} \, dS_e \approx g_e \, \delta S_e \, , \tag{4.5}$$

where we denote with $g_e = w_{ei} n_{ei}$ the normal component of $\mathbf{w}$ at the location e. With this, one obtains an approximation of 2nd order (with respect to the face length δS_e) for the surface integral, which can be checked by means of a Taylor series expansion (Exercise 4.1). The integration formula (4.5) corresponds to the *midpoint rule* known from numerical integration.

Other common integration formulas, that can be employed for such approximations are, for instance, the *trapezoidal rule* and the *Simpson rule*. The corresponding formulas are summarized in Table 4.1 with their respective orders (with respect to δS_e).

Table 4.1. Approximations for surface integrals over the face S_e

Name	Formula	Order
Midpoint rule	$\delta S_e g_e$	2
Trapezoidal rule	$\delta S_e (g_{ne} + g_{se})/2$	2
Simpson rule	$\delta S_e (g_{ne} + 4g_e + g_{se})/6$	4

For instance, by applying the midpoint rule for the approximation of the convective and diffusive fluxes through the CV faces in (4.3), we obtain the approximations:

$$F_c^C \approx \underbrace{\rho v_i n_{ci} \delta S_c}_{\dot{m}_c} \phi_c \quad \text{and} \quad F_c^D \approx -\alpha n_{ci} \delta S_c \left(\frac{\partial \phi}{\partial x_i} \right)_c ,$$

where, for simplicity, we have assumed that v_i, ρ, and α are constant across the CV. $\dot{m}_c$ denotes the mass flux through the face S_c. Inserting the definition of the normal vector, we obtain, for instance, for the convective flux through the face S_e, the approximation

$$F_e^C \approx \dot{m}_e \phi_e = \rho[v_1(y_{ne} - y_{se}) - v_2(x_{ne} - x_{se})] .$$

Before we turn to the further discretization of the fluxes, we first deal with the approximation of the volume integral in (4.3), which normally also is carried out by means of numerical integration. The assumption that the value f_P of f in the CV center represents an average value over the CV leads to the two-dimensional midpoint rule:

$$\int_V f \, dV \approx f_P \, \delta V ,$$

where δV denotes the volume of the CV, which for a quadrilateral CV is given by

$$\delta V = \frac{1}{2} |(x_{se} - x_{nw})(y_{ne} - y_{sw}) - (x_{ne} - x_{sw})(y_{se} - y_{nw})| .$$

An overview of the most common two-dimensional integration formulas for Cartesian CVs with the corresponding error order (with respect to δV) is given in Fig. 4.7 showing a schematical representation with the corresponding location of integration points and weighting factors. As a formula this means, e.g., in the case of the Simpson rule, an approximation of the form:

$$\int_V f \, dV \approx \frac{\delta V}{36}(16 f_P + 4 f_e + 4 f_w + 4 f_n + 4 f_s + f_{ne} + f_{se} + f_{ne} + f_{se}) .$$

It should be noted that the formulas for the two-dimensional numerical integration can be used to approximate the surface integrals occurring in three-dimensional applications. For three-dimensional volume integrals analogous integration formulas as for the two-dimensional case are available.

In summary, by applying the midpoint rule (to which we will retrict ourselves) we now have the following approximation for the balance equation (4.3):

$$\underbrace{\sum_c \dot{m}_c \phi_c}_{\text{conv. fluxes}} - \underbrace{\sum_c \alpha n_{ci} \, \delta S_c \left(\frac{\partial \phi}{\partial x_i} \right)_c}_{\text{diff. fluxes}} = \underbrace{f_P \, \delta V}_{\text{source}}. \tag{4.6}$$

In the next step it is necessary to approximate the function values and derivatives of ϕ at the CV faces occurring in the convective and diffusive flux expressions, respectively, by variable values in the nodes (here the CV centers). In order to clearly outline the essential principles, we will first explain the corresponding approaches for a two-dimensional Cartesian CV as indicated in Fig. 4.8. In this case the unit normal vectors $\mathbf{n}_c$ along the CV faces are given by

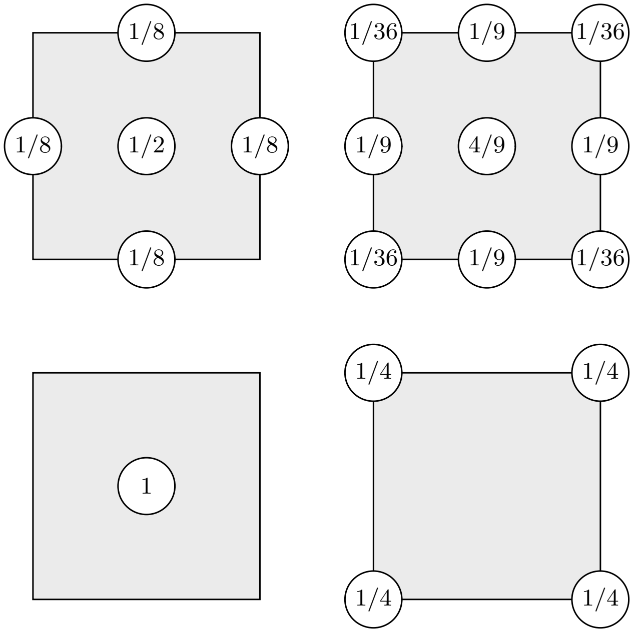


Fig. 4.7. Schematic representation of numerical integration formulas for two-dimensional volume integrals over a Cartesian CV

$$\mathbf{n}_\mathrm{e} = \mathbf{e}_1\,, \quad \mathbf{n}_\mathrm{w} = -\mathbf{e}_1\,, \quad \mathbf{n}_\mathrm{n} = \mathbf{e}_2\,, \quad \mathbf{n}_\mathrm{s} = -\mathbf{e}_2$$

and the expressions for the mass fluxes through the CV faces simplify to

$$\dot{m}_\mathrm{e} = \rho v_1(y_\mathrm{n} - y_\mathrm{s})\,, \quad \dot{m}_\mathrm{n} = \rho v_2(x_\mathrm{e} - x_\mathrm{w})\,,$$
$$\dot{m}_\mathrm{w} = \rho v_1(y_\mathrm{s} - y_\mathrm{n})\,, \quad \dot{m}_\mathrm{s} = \rho v_2(x_\mathrm{w} - x_\mathrm{e})\,.$$

Particularities that arise due to non-Cartesian grids will be considered in Sect. 4.5.

4.3 Discretization of Convective Fluxes

For the further approximation of the convective fluxes F_c^C, it is necessary to approximate ϕ_c by variable values in the CV centers. In general, this involves using neighboring nodal values ϕ_E, ϕ_P, ... of ϕ_c. The methods most frequently employed in practice for the approximation will be explained in the following, where we can restrict ourselves to one-dimensional considerations for the face S_e, since the other faces and the second (or third) spatial dimension can be treated in a fully analogous way. Traditionally, the corresponding approximations are called differencing techniques, since they result

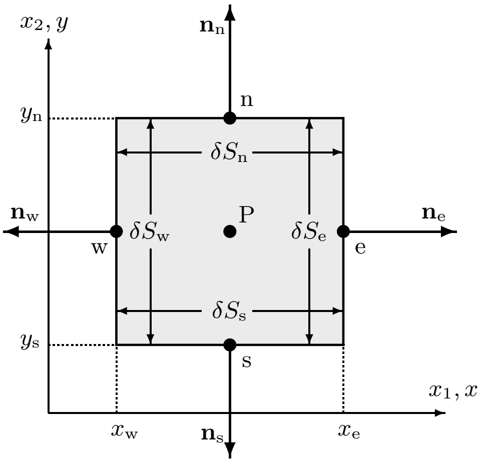


Fig. 4.8. Cartesian control volume with notations

in formulas analogous to finite-difference methods. Strictly speaking, these are interpolation techniques.

4.3.1 Central Differences

For the *central differencing scheme (CDS)* ϕ_e is approximated by linear interpolation with the values in the neighboring nodes P und E (see Fig. 4.9):

$$\phi_\mathrm{e} \approx \gamma_\mathrm{e}\phi_\mathrm{E} + (1-\gamma_\mathrm{e})\phi_\mathrm{P}\,. \tag{4.7}$$

The interpolation factor γ_e is defined by

$$\gamma_\mathrm{e} = \frac{x_\mathrm{e} - x_\mathrm{P}}{x_\mathrm{E} - x_\mathrm{P}}\,.$$

The approximation (4.7) has, for an equidistant grid as well as for a non-equidistant grid, an interpolation error of 2nd order. This can be seen from a Taylor series expansion of ϕ around the point x_P:

$$\phi(x) = \phi_\mathrm{P} + (x - x_\mathrm{P})\left(\frac{\partial\phi}{\partial x}\right)_\mathrm{P} + \frac{(x-x_\mathrm{P})^2}{2}\left(\frac{\partial^2\phi}{\partial x^2}\right)_\mathrm{P} + T_\mathrm{H}\,,$$

where T_H denotes the terms of higher order. Evaluating this series at the locations x_e and x_E and taking the difference leads to the relation

$$\phi_\mathrm{e} = \gamma_\mathrm{e}\phi_\mathrm{E} + (1-\gamma_\mathrm{e})\phi_\mathrm{P} - \frac{(x_\mathrm{e}-x_\mathrm{P})(x_\mathrm{E}-x_\mathrm{e})}{2}\left(\frac{\partial^2\phi}{\partial x^2}\right)_\mathrm{P} + T_\mathrm{H}\,,$$

which shows that the leading error term depends quadratically on the grid spacing.

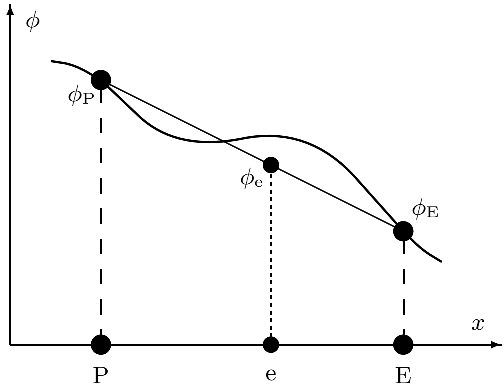


Fig. 4.9. Approximation of ϕ_e with CDS method

By involving additional grid points, central differencing schemes of higher order can be defined. For instance, an approximation of 4th order for an equidistant grid is given by

$$\phi_e = \frac{1}{48}(-3\phi_{EE} + 27\phi_E + 27\phi_P - 3\phi_W)\,,$$

where EE denotes the "east" neighboring point of E (see Fig. 4.11). Note that an application of this formula only makes sense if it is used together with an integration formula of 4th order, e.g., the Simpson rule. Only in this case is the total approximation of the convective flux also of 4th order.

When using central differencing approximations unphysical oscillations may appear in the numerical solution (the reasons for this problem will be discussed in detail in Sect. 8.1). Therefore, one often uses so-called *upwind approximations*, which are not sensitive or less sensitive to this problem. The principal idea of these methods is to make the interpolation dependent on the direction of the velocity vector. Doing so, one exploits the transport property of convection processes, which means that the convective transport of ϕ only takes place "downstream". In the following we will discuss two of the most important upwind techniques.

4.3.2 Upwind Techniques

The simplest upwind method results if ϕ is approximated by a step function. Here, ϕ_e is determined depending on the direction of the mass flux as follows (see Fig. 4.10):

$$\phi_e = \phi_P\,, \quad \text{if } \dot{m}_e > 0\,,$$
$$\phi_e = \phi_E\,, \quad \text{if } \dot{m}_e < 0\,.$$

This method is called *upwind differencing scheme (UDS)*. A Taylor series expansion of ϕ around the point x_P, evaluated at the point x_e, gives:

$$\phi_e = \phi_P + (x_e - x_P)\left(\frac{\partial \phi}{\partial x}\right)_P + \frac{(x_e - x_P)^2}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_P + T_H \, .$$

This shows that the UDS method (independent of the grid) has an interpolation error of 1st order. The leading error term in the resulting approximation of the convective flux F_e^C becomes

$$\underbrace{\dot{m}_e(x_e - x_P)}_{\alpha_{num}}\left(\frac{\partial \phi}{\partial x}\right)_P \, .$$

The error caused by this is called *artificial* or *numerical diffusion*, since the error term can be interpreted as a diffusive flux. The coefficient α_{num} is a measure for the amount of the numerical diffusion. If the transport direction is nearly perpendicular to the CV face, the approximation of the convective fluxes resulting with the UDS method is comparably good (the derivative $(\partial \phi / \partial x)_P$ is then small). Otherwise the approximation can be quite inaccurate and for large mass fluxes (i.e., large velocities) it can then be necessary to employ very fine grids (i.e., $x_e - x_P$ very small) for the computation in order to achieve a solution with an adequate accuracy. The disadvantage of the relatively poor accuracy is confronted by the advantage that the UDS method leads to an unconditionally bounded solution algorithm. We will discuss this aspect in more detail in Sect. 8.1.5.

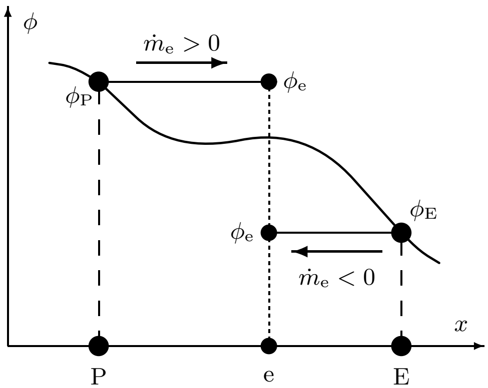


Fig. 4.10. Mass flux dependent approximation of ϕ_e with UDS method

An upwind approximation frequently employed in practice is the quadratic upwind interpolation, which in the literature is known as the QUICK method (Quadratic Upwind Interpolation for Convective Kinematics). Here, a quadratic polynomial is fitted through the two neighboring points P and E, and a third point, which is located upstream (W or EE depending on the flow direction). Evaluating this polynomial at point e one obtains the approximation (see also Fig. 4.11):

$$\phi_e = a_1\phi_E - a_2\phi_W + (1 - a_1 + a_2)\phi_P\,, \quad \text{if } \dot{m}_e > 0\,,$$
$$\phi_e = b_1\phi_P - b_2\phi_{EE} + (1 - b_1 + b_2)\phi_E\,, \quad \text{if } \dot{m}_e < 0\,,$$

where

$$a_1 = \frac{(2-\gamma_w)\gamma_e^2}{1+\gamma_e-\gamma_w}\,, \qquad a_2 = \frac{(1-\gamma_e)(1-\gamma_w)^2}{1+\gamma_e-\gamma_w}\,,$$
$$b_1 = \frac{(1+\gamma_w)(1-\gamma_e)^2}{1+\gamma_{ee}-\gamma_e}\,, \quad b_2 = \frac{\gamma_{ee}^2\gamma_e}{1+\gamma_{ee}-\gamma_e}\,.$$

For an equidistant grid one has:

$$a_1 = \frac{3}{8}\,, \quad a_2 = \frac{1}{8}\,, \quad b_1 = \frac{3}{8}\,, \quad b_2 = \frac{1}{8}\,.$$

In this case the QUICK method possesses an interpolation error of 3rd order. However, if it is used together with numerical integration of only 2nd order the overall flux approximation also is only of 2nd order, but it is somewhat more accurate than with the CDS method.

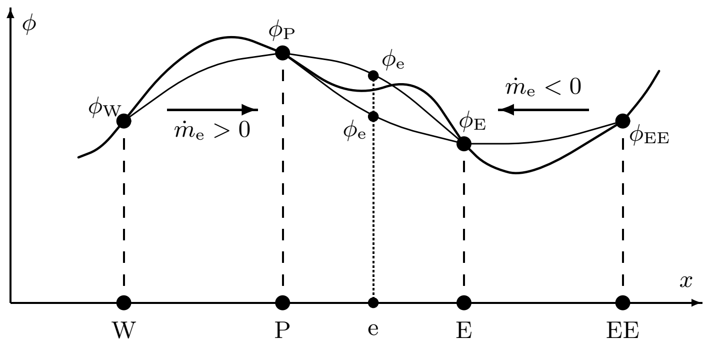


Fig. 4.11. Mass flux dependent approximation of ϕ_e with QUICK method

Before we turn to the discretization of the diffusive fluxes, we will point to a special technique for the treatment of convective fluxes, which is frequently employed for transport equations.

4.3.3 Flux-Blending Technique

The principal idea of *flux-blending*, which goes back to Khosla und Rubin (1974), is to mix different approximations for the convective flux. In this way one attempts to combine the advantages of an accurate approximation of a higher order scheme with the better robustness and boundedness properties of a lower order scheme (mostly the UDS method).

To explain the method we again consider exemplarily the face S_e of a CV. The corresponding approximations for ϕ_e in the convective flux F_e^C for the two methods to be combined are denoted by ϕ_e^{ML} and ϕ_e^{MH}, where ML and MH are the lower and higher order methods, respectively. The approximation for the combined method reads:

$$\phi_{\mathrm{e}} \approx (1-\beta)\phi_{\mathrm{e}}^{\mathrm{ML}} + \beta\phi_{\mathrm{e}}^{\mathrm{MH}} = \phi_{\mathrm{e}}^{\mathrm{ML}} + \underbrace{\beta(\phi_{\mathrm{e}}^{\mathrm{MH}} - \phi_{\mathrm{e}}^{\mathrm{ML}})}_{b_\beta^{\phi,\mathrm{e}}} . \tag{4.8}$$

From (4.8) for $\beta=0$ and $\beta=1$ the methods ML and MH, respectively, result. However, it is possible to choose for β any other value between 0 and 1, allowing to control the portions of the corresponding methods according to the needs of the underlying problem. However, due to the loss in accuracy, values $\beta < 1$ should be selected only if with $\beta = 1$ on the given grid no "reasonable" solution can be obtained (see Sect. 8.1.5) and a finer grid is not possible due to limitations in memory or computing time.

Also, if $\beta = 1$ (i.e., the higher order method) is employed, it can be beneficial to use the splitting according to (4.8) in order to treat the term $b_\beta^{\phi,\mathrm{e}}$ "explicitly" in combination with an iterative solver. This means that this term is computed with (known) values of ϕ from the preceding iteration and added to the source term. This may lead to a more stable iterative solution procedure, since this (probably critical) term then makes no contribution to the system matrix, which becomes more diagonally dominant. It should be pointed out that this modification has no influence on the converged solution, which is identical to that obtained with the higher order method MH alone. We will discuss this approach in some more detail at the end of Sect. 7.1.4.

4.4 Discretization of Diffusive Fluxes

For the approximation of diffusive fluxes it is necessary to approximate the values of the normal derivative of ϕ at the CV faces by nodal values in the CV centers. For the east face S_{e} of the CV, which we will again consider exemplarily, one has to approximate (in the Cartesian case) the derivative $(\partial\phi/\partial x)_{\mathrm{e}}$. For this, difference formulas as they are common in the framework of the finite-difference method can be used (see, e.g., [9]).

The simplest approximation one obtains when using a central differencing formula

$$\left(\frac{\partial \phi}{\partial x}\right)_{\mathrm{e}} \approx \frac{\phi_{\mathrm{E}} - \phi_{\mathrm{P}}}{x_{\mathrm{E}} - x_{\mathrm{P}}}, \tag{4.9}$$

which is equivalent to the assumption that ϕ is a linear function between the points x_{P} and x_{E} (see Fig. 4.12). For the discussion of the error of this approximation, we consider the difference of the Taylor series expansion around x_{e} at the locations x_{P} and x_{E}:

$$\left(\frac{\partial \phi}{\partial x}\right)_{\mathrm{e}} = \frac{\phi_{\mathrm{E}} - \phi_{\mathrm{P}}}{x_{\mathrm{E}} - x_{\mathrm{P}}} + \frac{(x_{\mathrm{e}} - x_{\mathrm{P}})^2 - (x_{\mathrm{E}} - x_{\mathrm{e}})^2}{2(x_{\mathrm{E}} - x_{\mathrm{P}})} \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{\mathrm{e}} - \frac{(x_{\mathrm{e}} - x_{\mathrm{P}})^3 + (x_{\mathrm{E}} - x_{\mathrm{e}})^3}{6(x_{\mathrm{E}} - x_{\mathrm{P}})} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{\mathrm{e}} + T_{\mathrm{H}} .$$

One can observe that for an equidistant grid an error of 2nd order results, since in this case the coefficient in front of the second derivative is zero. In the case of non-equidistant grids, one obtains by a simple algebraic rearrangement that this leading error term is proportional to the grid spacing and the expansion rate ξ_{e} of neighboring grid spacings:

$$\frac{(1 - \xi_{\mathrm{e}})(x_{\mathrm{e}} - x_{\mathrm{P}})}{2} \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{\mathrm{e}} \quad \text{with} \quad \xi_{\mathrm{e}} = \frac{x_{\mathrm{E}} - x_{\mathrm{e}}}{x_{\mathrm{e}} - x_{\mathrm{P}}} .$$

This means that the portion of the 1st order error term gets larger the more the expansion rate deviates from 1. This aspect should be taken into account in the grid generation such that neighboring CVs do not differ that much in the corresponding dimensions (see also Sect. 8.3).

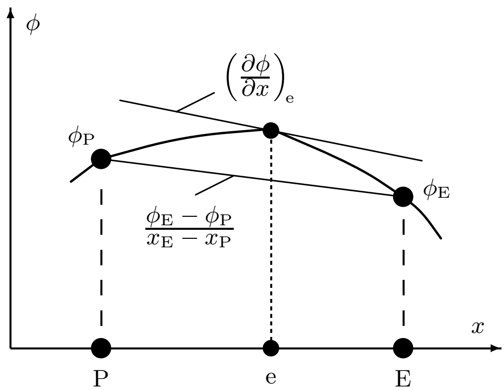


Fig. 4.12. Central differencing formula for approximation of 1st derivative at CV face

One obtains a 4th order approximation of the derivative at the CV face for an equidistant grid by

$$\left(\frac{\partial \phi}{\partial x}\right)_{\mathrm{e}} \approx \frac{1}{24\Delta x}(\phi_{\mathrm{W}} - 27\phi_{\mathrm{P}} + 27\phi_{\mathrm{E}} - \phi_{\mathrm{EE}}) , \tag{4.10}$$

which, for instance, can be used together with the Simpson rule to obtain an overall approximation for the diffusive flux of 4th order.

Although principally there are also other possibilities for approximating the derivatives (e.g., forward or backward differencing formulas), in practice almost only central differencing formulas are employed, which possess the best accuracy for a given number of grid points involved in the discretization. Problems with boundedness, as for the convective fluxes, do not exist. Thus, there is no reason to use less accurate approximations. For CVs located at the boundary of the problem domain, it might be necessary to employ forward or backward differencing formulas because there are no grid points beyond the boundary (see Sect. 4.7).

4.5 Non-Cartesian Grids

The previous considerations with respect to the discretization of the convective and diffusive fluxes were confined to the case of Cartesian grids. In this section we will discuss necessary modifications for general (quadrilateral) CVs.

For the convective fluxes, simple generalizations of the schemes introduced in Sect. 4.3 (e.g., UDS, CDS, QUICK, ...) can be employed for the approximation of ϕ_c. For instance, a corresponding CDS approximation for ϕ_e reads:

$$\phi_\mathrm{e} \approx \frac{|\mathbf{x}_{\tilde{\mathrm{e}}} - \mathbf{x}_\mathrm{P}|}{|\mathbf{x}_\mathrm{E} - \mathbf{x}_\mathrm{P}|}\,\phi_\mathrm{E} + \frac{|\mathbf{x}_\mathrm{E} - \mathbf{x}_{\tilde{\mathrm{e}}}|}{|\mathbf{x}_\mathrm{E} - \mathbf{x}_\mathrm{P}|}\,\phi_\mathrm{P}\,, \tag{4.11}$$

where $\mathbf{x}_{\tilde{\mathrm{e}}}$ is the intersection of the connnecting line of the points P and E with the (probably extended) CV face S_e (see Fig. 4.13). For the convective flux through S_e this results in the following approximation:

$$F_\mathrm{e}^\mathrm{C} \approx \frac{\dot{m}_\mathrm{e}}{|\mathbf{x}_\mathrm{E} - \mathbf{x}_\mathrm{P}|}\left(|\mathbf{x}_{\tilde{\mathrm{e}}} - \mathbf{x}_\mathrm{P}|\phi_\mathrm{E} + |\mathbf{x}_\mathrm{E} - \mathbf{x}_{\tilde{\mathrm{e}}}|\phi_\mathrm{P}\right)\,.$$

When the grid at the corresponding face has a "kink", an additional error results because the points $\mathbf{x}_{\tilde{\mathrm{e}}}$ and $\mathbf{x}_\mathrm{e}$ do not coincide (see Fig. 4.13). This aspect should be taken into account for the grid generation (see also Sect. 8.3).

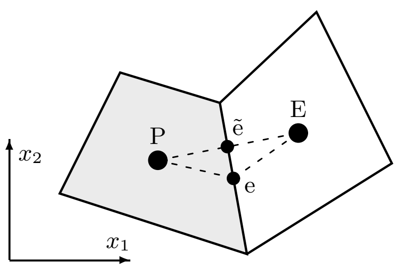


Fig. 4.13. Central difference approximation of convective fluxes for non-Cartesian control volumes

Let us turn to the approximation of the diffusive fluxes, for which farther reaching distinctions to the Cartesian case arise as for the convective fluxes. Here, for the required approximation of the normal derivative of ϕ in the center of the CV face there are a variety of different possibilities, depending on the directions in which the derivative is approximated, the locations where the appearing derivatives are evaluated, and the node values which are used for the interpolation. As an example we will give here one variant and consider only the CV face S_e.

Since along the normal direction in general there are no nodal points, the normal derivative has to be expressed by derivatives along other suitable directions. For this we use here the coordinates $\tilde{\xi}$ and $\tilde{\eta}$ defined according to Fig. 4.14. The direction $\tilde{\xi}$ is determined by the connecting line between points P and E, and the direction $\tilde{\eta}$ is determined by the direction of the CV face. Note that $\tilde{\xi}$ and $\tilde{\eta}$, because of a distortion of the grid, can deviate from the directions ξ und η, which are defined by the connecting lines of P with the CV face centers e and n. The larger these deviations are, the larger the discretization error becomes. This is another aspect that has to be taken into account when generating the grid (see also Sect. 8.3).

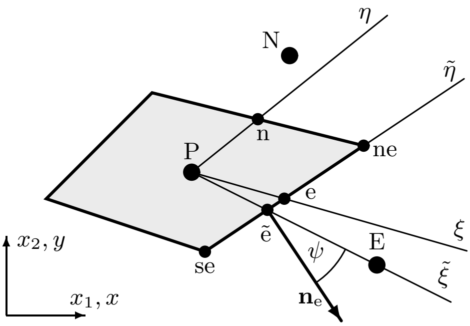


Fig. 4.14. Approximation of diffusive fluxes for non-Cartesian control volumes

A coordinate transformation $(x, y) \rightarrow (\tilde{\xi}, \tilde{\eta})$ results for the normal derivative in the following representation:

$$\frac{\partial \phi}{\partial x} n_{e1} + \frac{\partial \phi}{\partial y} n_{e2} = \frac{1}{J} \left[\left(\frac{\partial y}{\partial \tilde{\eta}} n_{e1} - \frac{\partial x}{\partial \tilde{\eta}} n_{e2} \right) \frac{\partial \phi}{\partial \tilde{\xi}} + \left(\frac{\partial x}{\partial \tilde{\xi}} n_{e2} - \frac{\partial y}{\partial \tilde{\xi}} n_{e1} \right) \frac{\partial \phi}{\partial \tilde{\eta}} \right] \quad (4.12)$$

with the Jacobi determinant

$$J = \frac{\partial x}{\partial \tilde{\xi}} \frac{\partial y}{\partial \tilde{\eta}} - \frac{\partial y}{\partial \tilde{\xi}} \frac{\partial x}{\partial \tilde{\eta}} .$$

The metric quantities can be approximated according to

$$\frac{\partial \mathbf{x}}{\partial \tilde{\xi}} \approx \frac{\mathbf{x}_E - \mathbf{x}_P}{|\mathbf{x}_E - \mathbf{x}_P|} \quad \text{and} \quad \frac{\partial \mathbf{x}}{\partial \tilde{\eta}} \approx \frac{\mathbf{x}_{ne} - \mathbf{x}_{se}}{\delta S_e} , \quad (4.13)$$

which results for the Jacobi determinant in the approximation

$$J_e \approx \frac{(x_E - x_P)(y_{ne} - y_{se}) - (y_E - y_P)(x_{ne} - x_{se})}{|\mathbf{x}_E - \mathbf{x}_P| \, \delta S_e} = \cos \psi ,$$

where ψ denotes the angle between the direction $\tilde{\xi}$ and $\mathbf{n}_e$ (see Fig. 4.14). ψ is a measure for the deviation of the grid from orthogonality ($\psi = 0$ for an orthogonal grid).

The derivatives with respect to $\tilde{\xi}$ and $\tilde{\eta}$ in (4.12) can be approximated in the usual way with a finite-difference formula. For example, the use of a central difference of 2nd order gives:

$$\frac{\partial \phi}{\partial \tilde{\xi}} \approx \frac{\phi_E - \phi_P}{|\mathbf{x}_E - \mathbf{x}_P|} \quad \text{and} \quad \frac{\partial \phi}{\partial \tilde{\eta}} \approx \frac{\phi_{ne} - \phi_{se}}{\delta S_e} \,. \tag{4.14}$$

Inserting the approximations (4.13) and (4.14) into (4.12) and using the component representation (4.4) of the unit normal vector $\mathbf{n}_e$ we finally obtain the following approximation for the diffusive flux through the CV face S_e:

$$F_e^D \approx D_e(\phi_E - \phi_P) + N_e(\phi_{ne} - \phi_{se}) \tag{4.15}$$

with

$$D_e = \frac{\alpha\left[(y_{ne} - y_{se})^2 + (x_{ne} - x_{se})^2\right]}{(x_{ne} - x_{se})(y_E - y_P) - (y_{ne} - y_{se})(x_E - x_P)} \,, \tag{4.16}$$

$$N_e = \frac{\alpha\left[(y_{ne} - y_{se})(y_E - y_P) + (x_{ne} - x_{se})(x_E - x_P)\right]}{(y_{ne} - y_{se})(x_E - x_P) - (x_{ne} - x_{se})(y_E - y_P)} \,. \tag{4.17}$$

The coefficient N_e represents the portion that arise due to the non-orthogonality of the grid. If the grid is orthogonal, $\mathbf{n}_e$ and $\mathbf{x}_E - \mathbf{x}_P$ have the same direction such that $N_e = 0$. The coefficient N_e (and the corresponding values for the other CV faces) should be kept as small as possible (see als Sect. 8.3).

The values for ϕ_{ne} and ϕ_{se} in (4.15) can be approximated, for instance, by linear interpolation of four neighboring nodal values:

$$\phi_{ne} = \frac{\gamma_P\phi_P + \gamma_E\phi_E + \gamma_N\phi_N + \gamma_{NE}\phi_{NE}}{\gamma_P + \gamma_E + \gamma_N + \gamma_{NE}}$$

with suitable interpolation factors γ_P, γ_E, γ_N, and γ_{NE} (see Fig. 4.15).

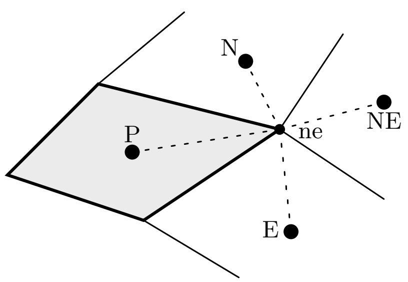


Fig. 4.15. Interpolation of values in CV edges for discretization of diffusive fluxes for non-Cartesian CV

4.6 Discrete Transport Equation

Let us now return to our example of the general two-dimensional transport equation (4.3) and apply the approximation techniques introduced in the preceding sections to it.

We employ exemplarily the midpoint rule for the integral approximations, the UDS method for the convective flux, and the CDS method for the diffusive flux. Additionally, we assume that we have velocity components $v_1, v_2 > 0$ and that the grid is a Cartesian one. With these assumptions one obtains the following approximation of the balance equation (4.3):

$$\begin{aligned}
&\left(\rho v_1 \phi_\mathrm{P} - \alpha \frac{\phi_\mathrm{E} - \phi_\mathrm{P}}{x_\mathrm{E} - x_\mathrm{P}}\right)(y_\mathrm{n} - y_\mathrm{s}) \\
&- \left(\rho v_1 \phi_\mathrm{W} - \alpha \frac{\phi_\mathrm{P} - \phi_\mathrm{W}}{x_\mathrm{P} - x_\mathrm{W}}\right)(y_\mathrm{n} - y_\mathrm{s}) \\
&+ \left(\rho v_2 \phi_\mathrm{P} - \alpha \frac{\phi_\mathrm{N} - \phi_\mathrm{P}}{y_\mathrm{N} - y_\mathrm{P}}\right)(x_\mathrm{e} - x_\mathrm{w}) \\
&- \left(\rho v_2 \phi_\mathrm{S} - \alpha \frac{\phi_\mathrm{P} - \phi_\mathrm{S}}{y_\mathrm{P} - y_\mathrm{S}}\right)(x_\mathrm{e} - x_\mathrm{w}) = f_\mathrm{P}(y_\mathrm{n} - y_\mathrm{s})(x_\mathrm{e} - x_\mathrm{w}) \,.
\end{aligned}$$

A simple rearrangement gives a relation of the form

$$a_\mathrm{P}\phi_\mathrm{P} = a_\mathrm{E}\phi_\mathrm{E} + a_\mathrm{W}\phi_\mathrm{W} + a_\mathrm{N}\phi_\mathrm{N} + a_\mathrm{S}\phi_\mathrm{S} + b_\mathrm{P} \tag{4.18}$$

with the coefficients

$$\begin{aligned}
a_\mathrm{E} &= \frac{\alpha}{(x_\mathrm{E} - x_\mathrm{P})(x_\mathrm{e} - x_\mathrm{w})} \,, \\
a_\mathrm{W} &= \frac{\rho v_1}{x_\mathrm{e} - x_\mathrm{w}} + \frac{\alpha}{(x_\mathrm{P} - x_\mathrm{W})(x_\mathrm{e} - x_\mathrm{w})} \,, \\
a_\mathrm{N} &= \frac{\alpha}{(y_\mathrm{N} - y_P)(y_\mathrm{n} - y_\mathrm{s})} \,, \\
a_\mathrm{S} &= \frac{\rho v_2}{y_\mathrm{n} - y_\mathrm{s}} + \frac{\alpha}{(y_\mathrm{P} - y_\mathrm{S})(y_\mathrm{n} - y_\mathrm{s})} \,, \\
a_\mathrm{P} &= \frac{\rho v_1}{x_\mathrm{e} - x_\mathrm{w}} + \frac{\alpha(x_\mathrm{E} - x_\mathrm{W})}{(x_\mathrm{P} - x_\mathrm{W})(x_\mathrm{E} - x_\mathrm{P})(x_\mathrm{e} - x_\mathrm{w})} + \\
&\quad \frac{\rho v_2}{y_\mathrm{n} - y_\mathrm{s}} + \frac{\alpha(y_\mathrm{N} - y_\mathrm{S})}{(y_\mathrm{P} - y_\mathrm{S})(y_\mathrm{N} - y_\mathrm{P})(y_\mathrm{n} - y_\mathrm{s})} \,, \\
b_\mathrm{P} &= f_\mathrm{P} \,.
\end{aligned}$$

If the grid is equidistant in each spatial direction (with grid spacings Δx and Δy), the coefficients become:

$$a_\mathrm{E} = \frac{\alpha}{\Delta x^2}\,, \quad a_\mathrm{W} = \frac{\rho v_1}{\Delta x} + \frac{\alpha}{\Delta x^2}\,, \quad a_\mathrm{N} = \frac{\alpha}{\Delta y^2}\,, \quad a_\mathrm{S} = \frac{\rho v_2}{\Delta y} + \frac{\alpha}{\Delta y^2}\,,$$

$$a_\mathrm{P} = \frac{\rho v_1}{\Delta x} + \frac{2\alpha}{\Delta x^2} + \frac{\rho v_2}{\Delta y} + \frac{2\alpha}{\Delta y^2}\,, \quad b_\mathrm{P} = f_\mathrm{P}\,.$$

In this particular case (4.18) coincides with a discretization that would result from a corresponding finite-difference method (for general grids this normally is not the case).

It can be seen that – independent from the grid employed – one has for the coefficients in (4.18) the relation

$$a_{\mathrm{P}} = a_{\mathrm{E}} + a_{\mathrm{W}} + a_{\mathrm{N}} + a_{\mathrm{S}} \,.$$

This is characteristic for finite-volume discretizations and expresses the conservativity of the method. We will return to this important property in Sect. 8.1.4.

Equation (4.18) is valid in this form for all CVs, which are not located at the boundary of the problem domain. For boundary CVs the approximation (4.18) includes nodal values outside the problem domain, such that they require a special treatment depending on the given type of boundary condition.

4.7 Treatment of Boundary Conditions

We consider the three boundary condition types that most frequently occur for the considered type of problems (see Chap. 2): a prescibed variable value, a prescibed flux, and a symmetry boundary. For an explanation of the implementation of such conditions into a finite-volume method, we consider as an example a Cartesian CV at the west boundary (see Fig. 4.16) for the transport equation (4.3). Correspondingly modified approaches for the non-Cartesian case or for other types of equations can be formulated analogously (for this see also Sect. 10.4).

Let us start with the case of a prescribed boundary value $\phi_{\mathrm{w}} = \phi^0$. For the convective flux at the boundary one has the approximation:

$$F_{\mathrm{w}}^{\mathrm{C}} \approx \dot{m}_{\mathrm{w}} \phi_{\mathrm{w}} = \dot{m}_{\mathrm{w}} \phi^0 \,.$$

With this the approximation of $F_{\mathrm{w}}^{\mathrm{C}}$ is known (the mass flux $\dot{m}_{\mathrm{w}}$ at the boundary is also known) and can simply be introduced in the balance equation (4.6). This results in an additional contribution to the source term b_{P}.

The diffusive flux through the boundary is determined with the same approach as in the interior of the domain (see (4.18)). Analogously to (4.9) the derivative at the boundary can be approximated as follows:

$$\left(\frac{\partial \phi}{\partial x}\right)_{\mathrm{w}} \approx \frac{\phi_{\mathrm{P}} - \phi_{\mathrm{w}}}{x_{\mathrm{P}} - x_{\mathrm{w}}} = \frac{\phi_{\mathrm{P}} - \phi^0}{x_{\mathrm{P}} - x_{\mathrm{w}}} \,. \tag{4.19}$$

This corresponds to a forward difference formula of 1st order. Of course, it is also possible to apply more elaborate formulas of higher order. However, since the distance between the boundary point w and the point P is smaller than the distance between two inner points (half as much for an equidistant grid, see Fig. 4.16), a lower order approximation at the boundary usually does not influence the overall accuracy that much.

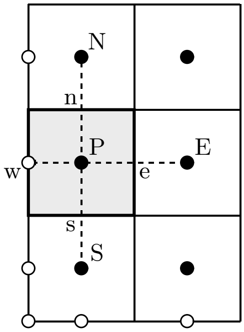


Fig. 4.16. Cartesian boundary CV at west boundary with notations

In summary, one has for the considered boundary CV a relation of the form (4.18) with the modified coefficients:

$$\begin{aligned} a_{\mathrm{W}} &= 0\,, \\ a_{\mathrm{P}} &= \frac{\rho v_1}{x_{\mathrm{e}} - x_{\mathrm{w}}} + \frac{\alpha(x_{\mathrm{E}} - x_{\mathrm{w}})}{(x_{\mathrm{P}} - x_{\mathrm{w}})(x_{\mathrm{E}} - x_{\mathrm{P}})(x_{\mathrm{e}} - x_{\mathrm{w}})} + \\ &\quad \frac{\rho v_2}{y_{\mathrm{n}} - y_{\mathrm{s}}} + \frac{\alpha(y_{\mathrm{N}} - y_{\mathrm{S}})}{(y_{\mathrm{P}} - y_{\mathrm{S}})(y_{\mathrm{N}} - y_{\mathrm{P}})(y_{\mathrm{n}} - y_{\mathrm{s}})}\,, \\ b_{\mathrm{P}} &= f_{\mathrm{P}} + \left[\frac{\rho v_1}{x_{\mathrm{e}} - x_{\mathrm{w}}} + \frac{\alpha}{(x_{\mathrm{P}} - x_{\mathrm{w}})(x_{\mathrm{e}} - x_{\mathrm{w}})}\right]\phi^0. \end{aligned}$$

All other coefficients are computed as for a CV in the interior of the problem domain.

Let us now consider the case where the flux $F_{\mathrm{w}} = F^0$ is prescribed at the west boundary. The flux through the CV face is obtained by dividing F^0 through the length of the face $x_{\mathrm{e}} - x_{\mathrm{w}}$. The resulting value is introduced in (4.6) as total flux and the modified coefficients for the boundary CV become:

$$\begin{aligned} a_{\mathrm{W}} &= 0\,, \\ a_{\mathrm{P}} &= \frac{\rho v_1}{x_{\mathrm{e}} - x_{\mathrm{w}}} + \frac{\alpha}{(x_{\mathrm{E}} - x_{\mathrm{P}})(x_{\mathrm{e}} - x_{\mathrm{w}})} + \\ &\quad \frac{\rho v_2}{y_{\mathrm{n}} - y_{\mathrm{s}}} + \frac{\alpha(y_{\mathrm{N}} - y_{\mathrm{S}})}{(y_{\mathrm{P}} - y_{\mathrm{S}})(y_{\mathrm{N}} - y_{\mathrm{P}})(y_{\mathrm{n}} - y_{\mathrm{s}})}\,, \\ b_{\mathrm{P}} &= f_{\mathrm{P}} + \frac{F^0}{x_{\mathrm{e}} - x_{\mathrm{w}}}\,. \end{aligned}$$

All other coefficients remain unchanged.

Sometimes it is possible to exploit symmetries of a problem in order to downsize the problem domain to save computing time or get a higher accuracy (with a finer grid) with the same computational effort. In such cases one has to consider symmetry planes or symmetry lines at the corresponding problem boundary. In this case one has the boundary condition:

$$\frac{\partial \phi}{\partial x_i} n_i = 0 . \tag{4.20}$$

From this condition it follows that the diffusive flux through the symmetry boundary is zero (see (4.18)). Since also the normal component of the velocity vector has to be zero at a symmetry boundary (i.e., $v_i n_i = 0$), the mass flux and, therefore, the convective flux through the boundary is zero. Thus, in the balance equation (4.6) the total flux through the corresponding CV face can be set to zero. For the boundary CV in Fig. 4.16 this results in the following modified coefficients:

$$\begin{aligned} a_\mathrm{W} &= 0 , \\ a_\mathrm{P} &= \frac{\rho v_1}{x_\mathrm{e} - x_\mathrm{w}} + \frac{\alpha}{(x_\mathrm{E} - x_\mathrm{P})(x_\mathrm{e} - x_\mathrm{w})} + \\ & \quad \frac{\rho v_2}{y_\mathrm{n} - y_\mathrm{s}} + \frac{\alpha (y_\mathrm{N} - y_\mathrm{S})}{(y_\mathrm{P} - y_\mathrm{S})(y_\mathrm{N} - y_\mathrm{P})(y_\mathrm{n} - y_\mathrm{s})} . \end{aligned}$$

If required, the (unknown) variable value at the boundary can be determined by a finite-difference approximation of the boundary condition (4.20). In the considered case, for instance, with a forward difference formula (cp. (4.19)) one simply obtains $\phi_\mathrm{w} = \phi_\mathrm{P}$.

As with all other discretization techniques, the algebraic system of equations resulting from a finite-volume discretization has a unique solution only if the boundary conditions at all boundaries of the problem domain are taken into account (e.g., as outlined above). Otherwise there would be more unknowns than equations.

4.8 Algebraic System of Equations

As exemplarily outlined in Sect. 4.6 for the general scalar transport equation, a finite-volume discretization for each CV results in an algebraic equation of the form:

$$a_\mathrm{P} \phi_\mathrm{P} - \sum_c a_c \phi_c = b_\mathrm{P} ,$$

where the index c runs over all neighboring points that are involved in the approximation as a result of the discretization scheme employed. Globally, i.e., for all control volumes V_i $(i = 1, \ldots, N)$ of the problem domain, this gives a linear system of N equations

$$a_P^i \phi_P^i - \sum_c a_c^i \phi_c^i = b_P^i \quad \text{for all} \quad i = 1, \ldots, N \tag{4.21}$$

for the N unknown nodal values ϕ_P^i in the CV centers.

After introducing a corresponding numbering of the CVs (or nodal values), in the case of a Cartesian grid the system (4.21) has a fully analogous structure that also would result from a finite-difference approximation. To illustrate this, we consider first the one-dimensional case. Let the problem domain be the interval $[0, L]$, which we divide into N not necessarily equidistant CVs (subintervals) (see Fig 4.17).

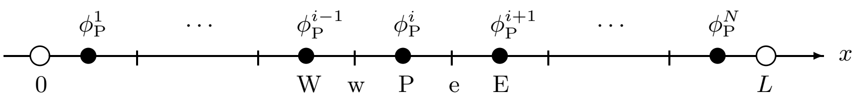


Fig. 4.17. Arrangement of CVs and nodes for 1-D transport problem

Using the second-order central differencing scheme, the discrete equations have the form:

$$a_P^i \phi_P^i - a_E^i \phi_E^i - a_W^i \phi_W^i = b_P^i \,. \tag{4.22}$$

With the usual lexicographical numbering of the nodal values as given in Fig. 4.17 one has:

$$\begin{aligned} \phi_W^i &= \phi_P^{i-1} \quad \text{for all} \ \ i = 2, \ldots, N \,, \\ \phi_E^i &= \phi_P^{i+1} \quad \text{for all} \ \ i = 1, \ldots, N-1 \,. \end{aligned}$$

Thus, the result is a linear system of equations which can be represented in matrix form as follows:

$$\underbrace{\begin{bmatrix} a_P^1 & -a_E^1 & & & & & \\ -a_W^2 & a_P^2 & -a_E^2 & & 0 & & \\ & \cdot & \cdot & \cdot & & & \\ & & -a_W^i & a_P^i & -a_E^i & & \\ & & & \cdot & \cdot & \cdot & \\ & 0 & & & \cdot & \cdot & -a_E^{N-1} \\ & & & & & -a_W^N & a_P^N \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} \phi_P^1 \\ \cdot \\ \phi_P^{i-1} \\ \phi_P^i \\ \phi_P^{i+1} \\ \cdot \\ \phi_P^N \end{bmatrix}}_{\boldsymbol{\phi}} = \underbrace{\begin{bmatrix} b_P^1 \\ b_P^2 \\ \cdot \\ b_P^i \\ \cdot \\ \cdot \\ b_P^N \end{bmatrix}}_{\mathbf{b}} .$$

When using a QUICK discretization or a central differencing scheme of 4th order, there are also coefficients for the farther points EE and WW (see Fig. 4.18):

$$a_{\mathrm{P}}\phi_{\mathrm{P}} - a_{\mathrm{EE}}\phi_{\mathrm{EE}} - a_{\mathrm{E}}\phi_{\mathrm{E}} - a_{\mathrm{W}}\phi_{\mathrm{W}} - a_{\mathrm{WW}}\phi_{\mathrm{WW}} = b_{\mathrm{P}}\,, \tag{4.23}$$

i.e., in the corresponding coefficient matrix **A** two additional non-zero diagonals appear:

$$\mathbf{A} = \begin{bmatrix} a_{\mathrm{P}}^{1} & -a_{\mathrm{E}}^{1} & -a_{\mathrm{EE}}^{1} & & & & & & \\ -a_{\mathrm{W}}^{2} & a_{\mathrm{P}}^{2} & -a_{\mathrm{E}}^{2} & -a_{\mathrm{EE}}^{2} & & & 0 & & \\ -a_{\mathrm{WW}}^{3} & -a_{\mathrm{W}}^{3} & a_{\mathrm{P}}^{3} & -a_{\mathrm{E}}^{3} & -a_{\mathrm{EE}}^{3} & & & & \\ & \cdot & \cdot & \cdot & \cdot & \cdot & & & \\ & & -a_{\mathrm{WW}}^{i} & -a_{\mathrm{W}}^{i} & a_{\mathrm{P}}^{i} & -a_{\mathrm{E}}^{i} & -a_{\mathrm{EE}}^{i} & & \\ & & & \cdot & \cdot & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot & \cdot & -a_{\mathrm{EE}}^{N-2} \\ & & 0 & & & \cdot & \cdot & \cdot & -a_{\mathrm{E}}^{N-1} \\ & & & & & & -a_{\mathrm{WW}}^{N} & -a_{\mathrm{W}}^{N} & a_{\mathrm{P}}^{N} \end{bmatrix}.$$

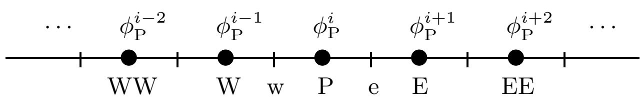


Fig. 4.18. CV dependencies with higher order scheme for 1-D transport problem

For the two- and three-dimensional cases fully analogous considerations can be made for the assembly of the discrete equation systems. For a two-dimensional rectangular domain with $N \times M$ CVs (see Fig. 4.19), we have, for instance, in the case of the discretization given in Sect. 4.6 equations of the form

$$a_{\mathrm{P}}^{i,j}\phi_{\mathrm{P}}^{i,j} - a_{\mathrm{E}}^{i,j}\phi_{\mathrm{E}}^{i,j} - a_{\mathrm{W}}^{i,j}\phi_{\mathrm{W}}^{i,j} - a_{\mathrm{S}}^{i,j}\phi_{\mathrm{S}}^{i,j} - a_{\mathrm{N}}^{i,j}\phi_{\mathrm{N}}^{i,j} = b_{\mathrm{P}}^{i,j}$$

for $i = 1,\ldots,N$ and $j = 1,\ldots,M$. In the case of a lexicographical columnwise numbering of the nodal values (index j is counted up first) and a corresponding arrangement of the unknown variables $\phi_{\mathrm{P}}^{i,j}$ (see Fig. 4.19), the system matrix **A** takes the following form:

$$
\mathbf{A} = \begin{bmatrix}
a_{\mathrm{P}}^{1,1} & -a_{N}^{1,1} & \cdot & 0 & \cdot & -a_{\mathrm{E}}^{1,1} & & & & \\
-a_{\mathrm{S}}^{1,2} & \cdot & \cdot & & & & \cdot & & 0 & \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & & \\
0 & & \cdot & \cdot & \cdot & & & & \cdot & \\
\cdot & & & \cdot & \cdot & \cdot & & & & -a_{\mathrm{E}}^{N-1,M} \\
-a_{\mathrm{W}}^{2,1} & & & & \cdot & \cdot & \cdot & & & \cdot \\
 & \cdot & & & & \cdot & \cdot & \cdot & & 0 \\
 & & \cdot & & & & \cdot & \cdot & \cdot & \cdot \\
 & 0 & & \cdot & & & & \cdot & \cdot & -a_{\mathrm{N}}^{N,M-1} \\
 & & & & -a_{\mathrm{W}}^{N,M} & \cdot & 0 & \cdot & -a_{\mathrm{S}}^{N,M} & a_{\mathrm{P}}^{N,M}
\end{bmatrix} .
$$

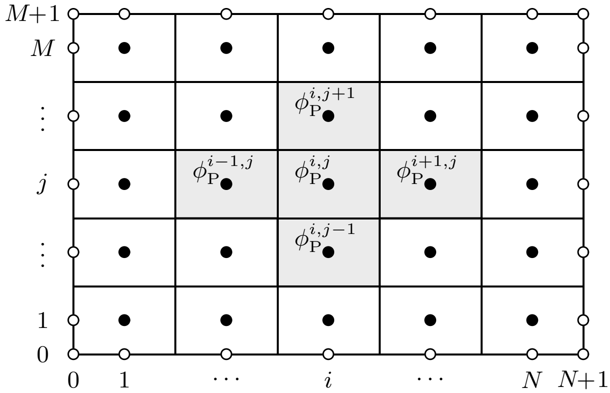


Fig. 4.19. Arrangement of CVs and nodes for 2-D transport problem

As outlined in Sect. 4.5, due to the discretization of the diffusive fluxes, in the non-Cartesian case additional coefficients can arise, whereby the number of non-zero diagonals in the system matrix increases. Using the discretization exemplarily given in Sect. 4.5, for instance, one would have additional dependencies with the points NE, NW, SE, and SW, which are required to linearly interpolate the values of ϕ in the vertices of the CV (see Fig. 4.20). Thus, in the case of a structured grid a matrix with 9 non-zero diagonals would result.

4.9 Numerical Example

As a concrete, simple (two-dimensional) example for the application of the FVM, we consider the computation of the heat transfer in a trapezoidal plate (density ρ, heat conductivity κ) with a constant heat source q all over the

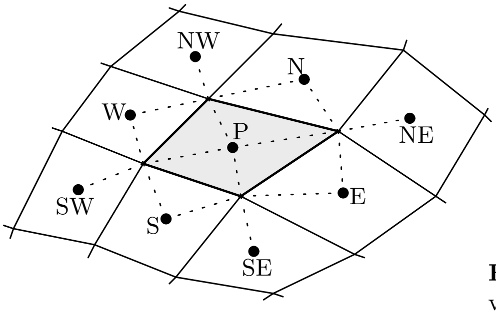


Fig. 4.20. Interpolation of vertice values for non-Cartesian CV

plate. At three sides the temperature T is prescribed and at the fourth side the heat flux is given (equal to zero). The problem data are summarized in Fig. 4.21. The problem is described by the heat conduction equation

$$-\kappa\frac{\partial^2 T}{\partial x^2} - \kappa\frac{\partial^2 T}{\partial y^2} = \rho q \tag{4.24}$$

with the boundary conditions as indicated in Fig. 4.21 (cp. Sect. 2.3.2). For the discretization we employ a grid with only two CVs as illustrated in Fig. 4.22. The required coordinates for the distinguished points for both CVs are indicated in Table 4.2.

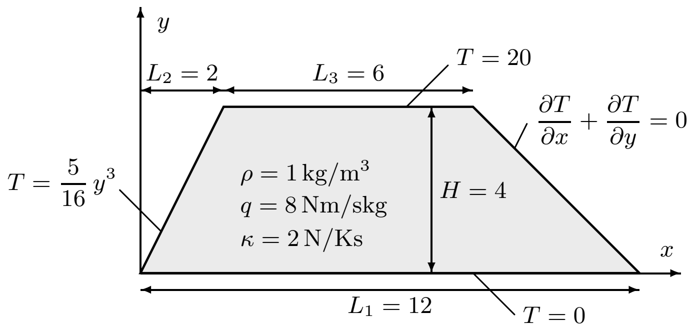


Fig. 4.21. Configuration of trapezoidal plate heat conduction example (temperature in K, length in m)

The integration of (4.24) over a control volume V and the application of the Gauß integral theorem gives:

$$\sum_c F_c = -\kappa \sum_c \int_{S_c} \left(\frac{\partial T}{\partial x} n_1 + \frac{\partial T}{\partial y} n_2\right) \mathrm{d}S_c = \int_V q\,\mathrm{d}V\,,$$

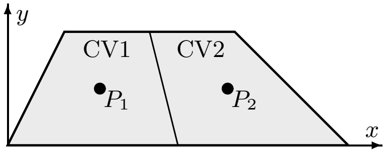


Fig. 4.22. CV definition for trapezoidal plate

Table 4.2. Coordinates of distinguished points for discretized trapezoidal plate

	CV1		CV2	
Point	x	y	x	y
P	13/4	2	31/4	2
e	11/2	2	10	2
w	1	2	11/2	2
n	7/2	4	13/2	4
s	3	0	9	0
nw	2	4	5	4
ne	5	4	8	4
se	6	0	12	0
sw	0	0	6	0
Volume	18		18	

where the summation has to be carried out over $c = \mathrm{s}, \mathrm{n}, \mathrm{w}, \mathrm{e}$. For the approximation of the integrals we employ the midpoint rule and the derivatives at CV faces are approximated by second-order central differences. Thus, the approximations of the fluxes for CV1 is:

$$F_\mathrm{e} = -\kappa \int_{S_\mathrm{e}} \left(\frac{4}{\sqrt{17}} \frac{\partial T}{\partial x} + \frac{1}{\sqrt{17}} \frac{\partial T}{\partial y} \right) \mathrm{d}S_\mathrm{e} \approx$$

$$\approx D_\mathrm{e} (T_\mathrm{E} - T_\mathrm{P}) + N_\mathrm{e}(T_\mathrm{ne} - T_\mathrm{se}) = -\frac{17}{9} (T_\mathrm{E} - T_\mathrm{P}) - 10 \, ,$$

$$F_\mathrm{w} = -\kappa \int_{S_\mathrm{w}} \left(-\frac{2}{\sqrt{5}} \frac{\partial T}{\partial x} + \frac{1}{\sqrt{5}} \frac{\partial T}{\partial y} \right) \mathrm{d}S_\mathrm{w} =$$

$$= -\kappa \int_{S_\mathrm{w}} \left(-\frac{2}{\sqrt{5}} \frac{120}{16} x^2 + \frac{1}{\sqrt{5}} \frac{15}{16} y^2 \right) \mathrm{d}S_\mathrm{w} = 60 \, ,$$

$$F_\mathrm{s} = -\kappa \int_{S_\mathrm{s}} \left(-\frac{\partial T}{\partial y} \right) \mathrm{d}S_\mathrm{s} \approx -\kappa \left(\frac{\partial T}{\partial y} \right)_\mathrm{s} (x_\mathrm{se} - x_\mathrm{sw}) \approx$$

$$\approx -\kappa \left(\frac{T_\mathrm{P} - T_\mathrm{S}}{y_\mathrm{P} - y_\mathrm{S}} \right) (x_\mathrm{se} - x_\mathrm{sw}) = 6 T_\mathrm{P} \, ,$$

$$F_\mathrm{n} = -\kappa \int\limits_{S_\mathrm{n}} \frac{\partial T}{\partial y}\, \mathrm{d}S_\mathrm{n} \approx -\kappa \left(\frac{\partial T}{\partial y}\right)_\mathrm{n} (x_\mathrm{ne} - x_\mathrm{nw}) \approx$$
$$\approx -\kappa \left(\frac{T_\mathrm{N} - T_\mathrm{P}}{y_\mathrm{N} - y_\mathrm{P}}\right) (x_\mathrm{ne} - x_\mathrm{nw}) = 3T_\mathrm{P} - 60\,.$$

The flux F_w has been computed exactly from the given boundary value function. Similarly, one obtains for CV2:

$$F_\mathrm{e} = 0\,, \quad F_\mathrm{w} \approx \frac{17}{9}(T_\mathrm{P} - T_\mathrm{W}) + 10\,, \quad F_\mathrm{s} \approx 6T_\mathrm{P}\,, \quad F_\mathrm{n} \approx 3T_\mathrm{P} - 60\,.$$

For both CVs we have $\delta V = 18$, such that the following discrete balance equations result:

$$\frac{98}{9}T_\mathrm{P} - \frac{17}{9}T_\mathrm{E} = 154 \quad \text{and} \quad \frac{98}{9}T_\mathrm{P} - \frac{17}{9}T_\mathrm{W} = 194\,.$$

We have $T_\mathrm{P} = T_1$ and $T_\mathrm{E} = T_2$ for CV1, and $T_\mathrm{P} = T_2$ and $T_\mathrm{W} = T_1$ for CV2. This gives the linear system of equations

$$98T_1 - 17T_2 = 1386 \quad \text{and} \quad 98T_2 - 17T_1 = 1746$$

for the two unknown temperatures T_1 and T_2. Its solution gives $T_1 \approx 17,77$ and $T_2 \approx 20,90$.

Exercises for Chap. 4

Exercise 4.1. Determine the leading error terms for the one-dimensional midpoint and trapezoidal rules by Taylor series expansion and compare the results.

Exercise 4.2. Let the concentration of a pollutant $\phi = \phi(x)$ in a chimney be described by the differential equation

$$-3\phi' - 2\phi'' = x\cos(\pi x) \quad \text{for} \quad 0 < x < 6$$

with the boundary conditions $\phi'(0) = 1$ and $\phi(6) = 2$. Compute the values ϕ_1 and ϕ_2 in the centers of the two control volumes CV1 $= [0, 4]$ and CV2 $= [4, 6]$ with a finite-volume discretization using the UDS method for the convective term.

Exercise 4.3. Consider the heat conduction in a square plate with the problem data given in Fig. 4.23. Compute the solution with a finite-volume method for the two grids illustarted in Fig. 4.24. Compare the results with the analytic solution $T_\mathrm{a}(x, y) = 20 - 2y^2 + x^3y - xy^3$.

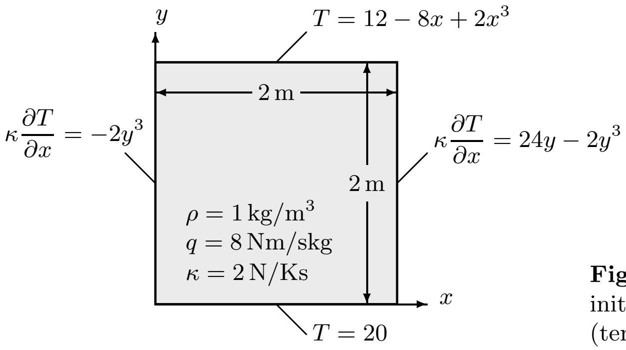


Fig. 4.23. Problem definition for Exercise 4.3 (temperatures in K)

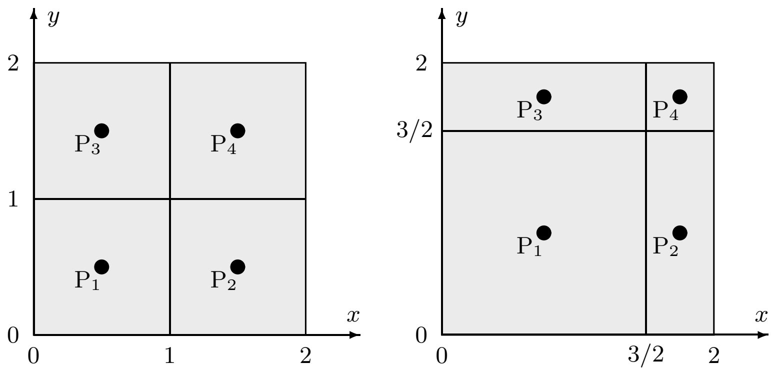


Fig. 4.24. Numerical grids for Exercise 4.3

Exercise 4.4. Formulate a finite-volume method of 2nd order for equidistant grids for the bar equation (2.38). Use this for computing the displacement of a bar of length $L = 60\,\mathrm{m}$ with the boundary conditions (2.39) with $A(x) = 1 + x/60$, $u_0 = 0$, and $k_L = 4\,\mathrm{N}$ employing a discretization with three equidistant CVs.

Exercise 4.5. Formulate a finite-volume method of 4th order for the membrane equation (2.17) for an equidistant Cartesian grid.

Exercise 4.6. Consider the integral

$$I = \int_{S_e} \phi \, \mathrm{d}S$$

for the function $\phi = \phi(x, y)$ over the face S_e of the CV $[1, 3]^2$. (i) Determine the leading error term and the order (with respect to the length Δy of S_e) for the approximation

$$I \approx \phi(3, \alpha)\Delta y$$

depending on the parameter $\alpha \in [1, 3]$. (ii) Compute I for the function $\phi(x, y) = x^3 y^4$ directly (analytically) and with the approximation defined in (i) with $\alpha = 2$. Compare the two solutions.

Exercise 4.7. The velocity vector of a two-dimensional flow is given by

$$\mathbf{v} = (v_1(x, y), v_2(x, y)) = (x \cos \pi y, x^4 y)\,.$$

Let the flux through the surface S of the control volume $V = [1, 2]^2$ be defined by

$$I = \int_S v_i n_i \, \mathrm{d}S\,.$$

(i) Approximate the integral with the Simpson rule. (ii) Transform the integral with the Gauß integral theorem into a volume integral (over V) and approximate this with the midpoint rule.