Advanced Heat Transfer

Part IV: Numerical Heat Transfer Methods

2. Diffusion Problems

(Application of the Finite Volume Method)

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Diffusion Problems — Outline

Bear in Mind

- Although some topics are introduced in sections dedicated to particular classes of heat transfer problems (for instance, for 1D steady-state heat conduction) they are still valid and applicable to other classes of problems. Examples of such topics:
  - Boundary conditions;
  - Linearization of source term;
  - Properties of discretization schemes;
  - Methods for solving algebraic (discretized) equations;
  - ...

  The introduction of such topics in an early stage – where simple classes of problems are being considered – is recommended to simplify its comprehension.
- In the following slides, temperature is considered as the dependent variable – ϕ in the general transport equation. However, application to other intensive properties are still valid (and straightforward) as long as they are described by the same general transport equation.

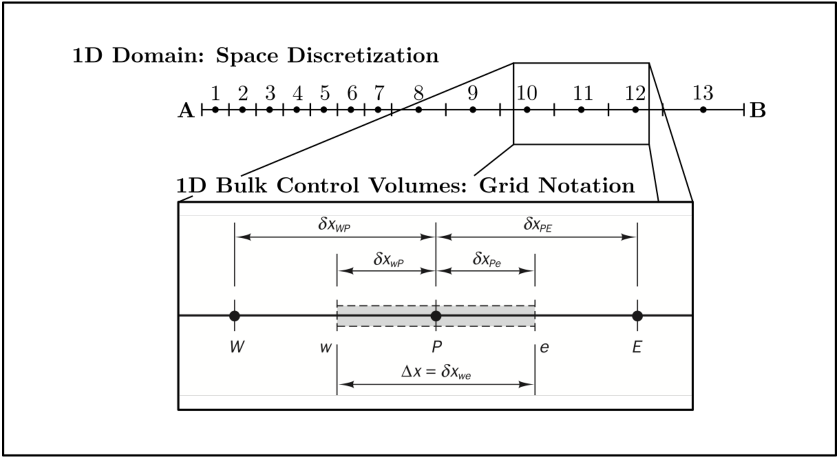
1. One-Dimensional (1D) Steady-State Heat Diffusion

Governing Equation: Differential and Integral Forms

- Pure heat conduction (diffusion) in steady-state conditions is the simplest transport process.
- The steady-state heat diffusion equation (governing equation) can be retrieved from the general transport equation neglecting the transient and convective terms and considering $\phi = T$, $\Gamma = k$, and $S_\phi = \dot{q}$.
  - Differential form:
  $$\mathrm{div}\,(k\,\mathrm{grad}\,T) + \dot{q} = 0$$
  - Integral form:
  $$\underbrace{\int_A \mathbf{n} \cdot (k\,\mathrm{grad}\;T)\,dA}_{F^d} + \underbrace{\int_{\Delta V} \dot{q}\,dV}_{Q} = 0$$
    - The physical interpretation of the last equation corresponds to the statement of the energy conservation principle applied to a control volume: the net conduction heat rate leaving the the control volume ($-F^d$) is equal to the net rate of thermal energy generation (Q).

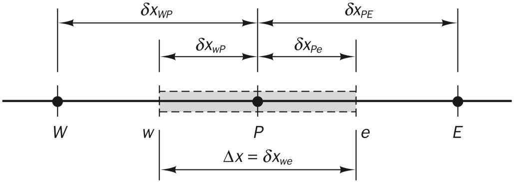
1. 1D Steady-State Heat Diffusion

1D Grid – Space Discretization and Grid Notation (Grid-Point Cluster)



1. 1D Steady-State Heat Diffusion

1D Grid Notation – Nodes, Faces, and Dimensions



W, P, and E – nodal points (nodes); w and e – CV boundaries (cell faces); Δx – CV width. W (w) – west node (face); E (e) – east node (face); and P – gen. node.

Net Rate of Thermal Energy Increase due to Diffusion Across CV Faces

$$F^d \equiv \int_A n_x \left(k \frac{dT}{dx} \right) dA = \sum_k \int_{A_k} n_x \left(k \frac{dT}{dx} \right) dA = \int_{A_\mathrm{e}} n_x \left(k \frac{dT}{dx} \right) dA +$$

$$\int_{A_\mathrm{w}} n_x \left(k \frac{dT}{dx} \right) dA = \underbrace{k_\mathrm{e} A_\mathrm{e} \left(\frac{dT}{dx} \right)_\mathrm{e}}_{F^d_\mathrm{e}} - \underbrace{k_\mathrm{w} A_\mathrm{w} \left(\frac{dT}{dx} \right)_\mathrm{w}}_{F^d_\mathrm{w}}$$

1. 1D Steady-State Heat Diffusion

Net Rate of Thermal Energy Increase due to Diffusion Across CV Faces

The same result for F^d can be obtained by volume integration – instead of applying the Gauss's divergence theorem and integrate the flux over the CV boundaries.

$$F^d \equiv \int_A \mathbf{n} \cdot (k \,\mathrm{grad}\, T)\, dA = \int_{\Delta V} \mathrm{div}\,(k \,\mathrm{grad}\, T)\, dV$$

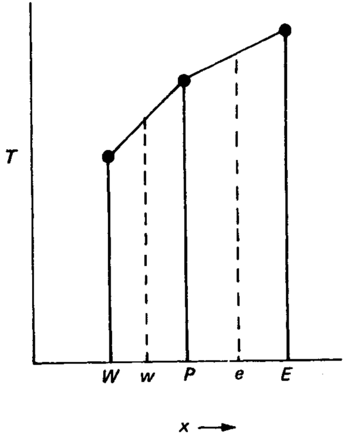
For 1D Cartesian coordinates,

$$\int_{x_\mathrm{w}}^{x_\mathrm{e}} \frac{d}{dx}\left(k \frac{dT}{dx}\right) A dx = \underbrace{k_\mathrm{e} A_\mathrm{e} \left(\frac{dT}{dx}\right)_\mathrm{e}}_{F_\mathrm{e}^d} - \underbrace{k_\mathrm{w} A_\mathrm{w} \left(\frac{dT}{dx}\right)_\mathrm{w}}_{F_\mathrm{w}^d}$$

1. 1D Steady-State Heat Diffusion

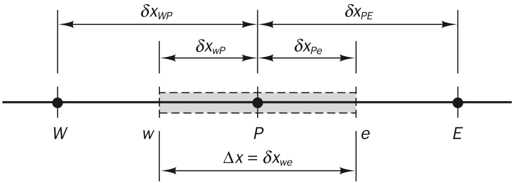
Profile Assumption

Since the dependent variable (temperature) is only known (calculated) at the nodal points W, P, and E and temperature gradients are required at the CV faces w and e, a suitable temperature profile between nodal points must be established – interpolation formula. A piecewise-linear profile – the simplest profile assumption – is herein considered.



1. 1D Steady-State Heat Diffusion

1D Grid Notation – Nodes, Faces, and Dimensions



Diffusive Fluxes Discretization

Assuming linear approximations to compute gradients at the control volume faces – central differencing scheme (second-order accurate scheme).

$$F_{\mathrm{e}}^{d} \equiv k_{\mathrm{e}} A_{\mathrm{e}} \left(\frac{dT}{dx}\right)_{\mathrm{e}} = k_e A_e \left(\frac{T_{\mathrm{E}} - T_{\mathrm{P}}}{\delta_{x_{\mathrm{PE}}}}\right)$$

$$F_{\mathrm{w}}^{d} \equiv k_{\mathrm{w}} A_{\mathrm{w}} \left(\frac{dT}{dx}\right)_{\mathrm{w}} = k_{\mathrm{w}} A_{\mathrm{w}} \left(\frac{T_{\mathrm{P}} - T_{\mathrm{W}}}{\delta_{x_{\mathrm{WP}}}}\right)$$

1. 1D Steady-State Heat Diffusion

Nonuniform Thermal Conductivity – Interface Values

The value of the heat diffusion coefficient may vary spatially (composite materials) and/or depend on the value of the dependent variable (temperature). The heat diffusion coefficient at the CV faces can be evaluated by linear interpolation taking into account the corresponding values at the nodes and the distance between nodes.

$$k_{\mathrm{w}} = \frac{\delta_{x_{\mathrm{wP}}} k_{\mathrm{W}} + \left(\delta_{x_{\mathrm{WP}}} - \delta_{x_{\mathrm{wP}}}\right) k_{\mathrm{P}}}{\delta_{x_{\mathrm{WP}}}} \qquad k_{\mathrm{e}} = \frac{\delta_{x_{\mathrm{Pe}}} k_{\mathrm{E}} + \left(\delta_{x_{\mathrm{PE}}} - \delta_{x_{\mathrm{Pe}}}\right) k_{\mathrm{P}}}{\delta_{x_{\mathrm{PE}}}}$$

For a uniform grid (equally spaced grid) where the CV faces w and e are midway between nodes W and P and P and E, respectively, the linearly interpolated thermal conductivity values are given as follows:

$$k_{\mathrm{w}} = \frac{k_{\mathrm{W}} + k_{\mathrm{P}}}{2} \qquad k_{\mathrm{e}} = \frac{k_{\mathrm{P}} + k_{\mathrm{E}}}{2}$$

1. 1D Steady-State Heat Diffusion

Net Rate of Thermal Energy Generation in the CV

The volumetric rate of thermal energy generation, $\dot{q}$, may be a function of the dependent variable (temperature). In such cases and since the discretized equations are solved by techniques for linear algebraic equations, the volume integral should be written in a linear form as follows:

$$Q \equiv \int_{\Delta V} \dot{q} dV = \bar{\dot{q}} \Delta V = \underbrace{(s_{\mathrm{C}} + s_{\mathrm{P}} T_{\mathrm{P}})}_{s \equiv \bar{\dot{q}}} \Delta V = \overbrace{(s_{\mathrm{C}} + s_{\mathrm{P}} T_{\mathrm{P}}) \, \delta_{\mathrm{we}}}^{S = S_{\mathrm{C}} + S_{\mathrm{P}} T_{\mathrm{P}}} A_{\mathrm{P}}$$

- s_{C} – constant part of the linear function of T_{P} (function s) representing the average rate of thermal energy generation per unit volume ($\bar{\dot{q}}$).
- s_{P} – coefficient of T_{P} in the linear function $s(T_{\mathrm{P}})$.
- To calculate $\bar{\dot{q}}$ through the function $s(T_{\mathrm{P}})$, the temperature at node P (T_{P}) is assumed to prevail throughout the control volume.

1. 1D Steady-State Heat Diffusion

Bulk Control Volumes – Discretized Governing Equation

$$F_{\mathrm{e}}^{d} - F_{\mathrm{w}}^{d} + Q = 0 \Leftrightarrow A_{\mathrm{e}} f_{\mathrm{e}}^{d} - A_{\mathrm{w}} f_{\mathrm{w}}^{d} + A_{\mathrm{P}} S = 0 \Leftrightarrow$$

$$\Leftrightarrow k_{\mathrm{e}} A_{\mathrm{e}} \left(\frac{T_{\mathrm{E}} - T_{\mathrm{P}}}{\delta_{x_{\mathrm{PE}}}} \right) - k_{\mathrm{w}} A_{\mathrm{w}} \left(\frac{T_{\mathrm{P}} - T_{\mathrm{W}}}{\delta_{x_{\mathrm{WP}}}} \right) + \left(s_{\mathrm{C}} + s_{\mathrm{P}} T_{\mathrm{P}} \right) \delta_{\mathrm{we}} A_{\mathrm{P}} = 0$$

Considering $A_{\mathrm{w}} = A_{\mathrm{P}} = A_{\mathrm{e}} = A$ (1D heat conduction) and rearranging,

$$\underbrace{\left(\frac{k_{\mathrm{w}}}{\delta_{x_{\mathrm{WP}}}} + \frac{k_{\mathrm{e}}}{\delta_{x_{\mathrm{PE}}}} - s_{\mathrm{P}} \delta_{\mathrm{we}} \right)}_{a_{\mathrm{P}}} T_{\mathrm{P}} = \underbrace{\frac{k_{\mathrm{w}}}{\delta_{x_{\mathrm{WP}}}}}_{a_{\mathrm{W}}} T_{\mathrm{W}} + \underbrace{\frac{k_{\mathrm{e}}}{\delta_{x_{\mathrm{PE}}}}}_{a_{\mathrm{E}}} T_{\mathrm{E}} + s_{\mathrm{C}} \delta_{\mathrm{we}} \Leftrightarrow$$

$$\Leftrightarrow \underbrace{\left(a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}} \right)}_{a_{\mathrm{P}}} T_{\mathrm{P}} = a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + \underbrace{S_{\mathrm{C}}}_{b} \Leftrightarrow$$

$$\Leftrightarrow \boxed{a_{\mathrm{P}} T_{\mathrm{P}} = a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + b}$$

The discretized equation contains the value of T at the central node (node P) and at the neighboring nodes W and E.

1. 1D Steady-State Heat Diffusion

Properties of Discretization Schemes

Physically realistic numerical results are only obtained when the discretization schemes fulfill certain fundamental rules, in particular:

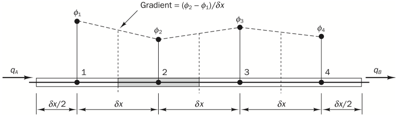
- Conservativeness (basic rule)
- Boundedness (basic rule)
- Accuracy
- Transportiveness (relevant for convection-diffusion problems – introduced later)

Basic rule – rule that must be respected for every discretization scheme. Otherwise, physically unrealistic values can be obtained or solution convergence can be compromised (*i.e.*, no converged solution is obtained).

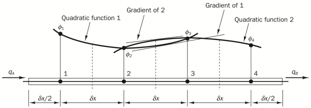
Properties of Discretization Schemes – Conservativeness

- The conservativeness property states that the flux of a property ϕ leaving a control volume across a certain face must be equal to the flux of ϕ entering the adjacent control volume through the same face.
- To ensure conservativeness, the flux through a common face must be represented in a consistent manner (using the same expression) in adjacent control volumes – see figures below.

Consistent definition of diffusive fluxes



Inconsistent definition of diffusive fluxes



- If discretization scheme conservativeness is ensured, the conservation law is satisfied either locally and globally.

1. 1D Steady-State Heat Diffusion

Properties of Discretization Schemes – Boundedness (1/2)

- In the absence of sources, the boundedness property states that the internal nodal values of property ϕ should be bounded by its boundary values. (For instance, the source-free, constant-property, and steady-state heat conduction problem (described by Laplace equation) has maximum and minimum values of temperature at the medium boundaries (if the medium is not in thermal equilibrium) and, consequently, the temperature of all internal points are bounded by such limits.)
- To ensure boundedness, all coefficients of the discretized equations (a_{P} and a_{nb} – neighboring node coefficients (a_{W}, a_{E}, ...)) should have the same sign (usually all positive). (Physically, this implies that an increase in the variable ϕ at one node should result in an increase in ϕ at neighboring nodes, considering other conditions unchanged.)
- In the existence of a source term ($S = S_{\mathrm{C}} + S_{\mathrm{P}} T_{\mathrm{P}} \neq 0$), in order to avoid a negative center-point coefficient (a_{P}) – which would violate the boundedness property –, the coefficient S_{P} must be less than or equal to zero.

1. 1D Steady-State Heat Diffusion

Properties of Discretization Schemes – Boundedness (2/2)

- For satisfying boundedness, the differencing scheme should provide coefficients in compliance with the Scarborough criterion. Scarborough criterion states that a sufficient condition for a convergent iterative method can be expressed in terms of the values of the coefficients of the discretized equations as follows:

$$\begin{cases} \sum_{\mathrm{nb}} |a_{\mathrm{nb}}| \leq |a_{\mathrm{P}}|\,, & \text{at all nodes.} \\ \sum_{\mathrm{nb}} |a_{\mathrm{nb}}| < |a_{\mathrm{P}}|\,, & \text{at one node at least.} \end{cases}$$

- The Scarborough criterion is observed if, for all nodes (and at least for one node), the absolute value of the coefficient a_{P} is greater or equal (greater) to the sum of the absolute values of the neighboring coefficients (a_{nb}).
- A matrix of coefficients which verifies the Scarborough criterion is known as diagonally dominant.

1. 1D Steady-State Heat Diffusion

Properties of Discretization Schemes – Accuracy (1/3)

For an equally spaced (uniform) 1D grid, consider the following two Taylor series expansions:

$$\phi(x+\Delta x) = \phi(x) + \left(\frac{\partial \phi}{\partial x}\right)_x \Delta x + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_x \frac{\Delta x^2}{2} + \left(\frac{\partial^3 \phi}{\partial x^3}\right)_x \frac{\Delta x^3}{6} + \ldots$$

$$\phi(x-\Delta x) = \phi(x) - \left(\frac{\partial \phi}{\partial x}\right)_x \Delta x + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_x \frac{\Delta x^2}{2} - \left(\frac{\partial^3 \phi}{\partial x^3}\right)_x \frac{\Delta x^3}{6} + \ldots$$

Subtracting the last equation from the first equation, the following equation is obtained for the first derivative (equation known as the central difference formula for the first derivative):

$$\left(\frac{\partial \phi}{\partial x}\right)_x = \frac{\phi(x+\Delta x) - \phi(x-\Delta x)}{2\Delta x} - \left(\frac{\partial^3 \phi}{\partial x^3}\right)_x \frac{\Delta x^2}{6} - \left(\frac{\partial^5 \phi}{\partial x^5}\right)_x \frac{\Delta x^4}{60} \ldots$$

1. 1D Steady-State Heat Diffusion

Properties of Discretization Schemes – Accuracy (2/3)

The previous equation, if applied to evaluate the temperature gradient at the control volume face w – for instance, for the 1D heat diffusion equation discretization – reads as follows:

$$\left(\frac{dT}{dx}\right)_{\mathrm{w}} = \frac{T_{\mathrm{P}} - T_{\mathrm{W}}}{2\,(\Delta x/2)} \underbrace{- \left(\frac{d^3T}{dx^3}\right)_{\mathrm{w}} \frac{\Delta x^2}{6} + \ldots}_{\text{Truncated Terms}} \Rightarrow \left(\frac{dT}{dx}\right)_{\mathrm{w}} = \frac{T_{\mathrm{P}} - T_{\mathrm{W}}}{\Delta x} + \mathcal{O}(\Delta x^2)$$

The last equation requires besides nodal values of T (at points W and P), higher-order derivatives. Since the higher-order derivatives are unknown the corresponding terms are neglected and, consequently, the difference approximation becomes

$$\left(\frac{dT}{dx}\right)_{\mathrm{w}} \approx \frac{T_{\mathrm{P}} - T_{\mathrm{W}}}{\Delta x}$$

The linear temperature profile between nodal points assumed previously to compute diffusive heat fluxes at the cell faces (see Slide 8) is equivalent to neglect the stated truncated terms of the series expansion.

1. 1D Steady-State Heat Diffusion

Properties of Discretization Schemes – Accuracy (3/3)

The error derived from truncating the series – commonly referred to as the Taylor series truncation error (TSTE), or shortly, truncation (or discretization) error – at the cell face w is written as

$$\epsilon_{\mathrm{w}} = -\frac{(\Delta x)^2}{6}\left(\frac{d^3 T}{dx^3}\right)_{\mathrm{w}} - \frac{(\Delta x)^4}{60}\left(\frac{d^5 T}{dx^5}\right)_{\mathrm{w}} + \dots$$

Since the leading term of the truncation error (term with the smallest grid spacing exponent) is proportional to the grid spacing squared ($\epsilon \propto (\Delta x)^2$), the current finite-difference approximation for the first derivative (central differencing scheme) is second-order accurate – truncation error of the order of the magnitude of $(\Delta x)^2$. The order of the difference approximation provides a measure of the accuracy of the discretization scheme. The order of the approximation provides the rate at which the error decreases as the grid spacing is reduced.

Truncation errors are inevitable unless the higher-order derivatives are zero, which rarely occurs in practical problems. The truncation error can be reduced by selecting finer grids, *i.e.*, decreasing the grid spacing.

Suggested Problem:

Problem 1

1. 1D Steady-State Heat Diffusion

Nonlinearities

- The discretized equation for a bulk (interior) CV with a central node P (last equation of Slide 12) is a linear algebraic equation – assuming that coefficients a_{W}, a_{P}, a_{E}, and b do not depend on temperature.
- However, nonlinearites in the mathematical model formulation can arise if: (i) the thermal conductivity (k) depends on temperature; (ii) the volumetric rate of thermal energy generation ($\dot{q}$) is a nonlinear function of temperature; or (iii) boundary conditions are nonlinear functions of temperature. In such cases, the solution for the set of algebraic equations requires successive iterations in accordance to the following procedure:
  1. Provide an initial guess for the temperature of all nodes, T;
  2. Calculate/update coefficients a_{W}, a_{P}, a_{E}, and b taking into account the previous estimate for the temperature, T^*;
  3. Solve the system of linear algebraic equations to obtain new temperature values, T;
  4. Repeat Steps 2–3 until a converged solution for all nodes is obtained.

Source-Term Linearization – Suggested Approaches (1/2)

The source term dependency on temperature (if any) should comply with the following linear form:

$$\boxed{s\left(T_{\mathrm{P}}\right) = s_{\mathrm{C}} + s_{\mathrm{P}}\, T_{\mathrm{P}}}$$

1. Considering the source term defined by $s\left(T_{\mathrm{P}}\right) = c_0 + c_1\, T_{\mathrm{P}}$, with $|c_1| > 0$, the recommended values for s_{C} and s_{P} can be calculated as follows:

$$s_{\mathrm{C}} = c_0 + c_1'\, T_{\mathrm{P}}^* \qquad\qquad s_{\mathrm{P}} = \left(c_1 - c_1'\right)$$

$$c_1' = \begin{cases} 0, & \text{if problem solvable without iterations.} \\ \geq c_1, & \text{if } c_1 > 0 \text{ and iterative solution procedure required.} \\ > 0, & \text{if } c_1 < 0 \text{ and iter. convergence slowdown pursued.} \end{cases}$$

A progressive increase of c_1' above c_1 (0) when $c_1 > 0$ or ($c_1 < 0$) promotes a slowdown in the iterative convergence procedure which can be beneficial to successfully achieve a converged solution.

1. 1D Steady-State Heat Diffusion

Source-Term Linearization – Suggested Approaches (2/2)

2. Considering the source term defined by a polynomial function $s\left(T_{\mathrm{P}}\right)=\sum_{i=0}^{n} c_i T_{\mathrm{P}}^{i}$, with $n \geq 2$, the recommended values for s_{C} and s_{P} can be calculated as follows:

$$s_{\mathrm{C}} = c_0 - \sum_{i=0}^{n-1}\left(i c_{i+1} - c'_{i+1}\right)\left(T_{\mathrm{P}}^{*}\right)^{i+1} \quad s_{\mathrm{P}} = \sum_{i=1}^{n}\left(i c_i - c'_i\right)\left(T_{\mathrm{P}}^{*}\right)^{i-1}$$

$$c'_1 = c'_i = c'_n = \begin{cases} 0, & \text{if } \sum_{i=1}^{n} i c_i \leq 0. \\ > 0, & \text{if } \sum_{i=1}^{n} i c_i \leq 0 \text{ and conv. slowd. pursued.} \\ \geq i c_i, & \text{if } \sum_{i=1}^{n} i c_i > 0. \end{cases}$$

3. More generally, the recommended linearization practice (expressions for s_{C} and s_{P}) is derived from the application of the following truncated Taylor series expansion:

$$s\left(T_{\mathrm{P}}\right) \equiv s_{\mathrm{C}} + s_{\mathrm{P}} T_{\mathrm{P}} = s\left(T_{\mathrm{P}}^{*}\right) + \left(T_{\mathrm{P}} - T_{\mathrm{P}}^{*}\right)\left(\frac{ds}{dT_{\mathrm{P}}}\right)_{T_{\mathrm{P}}=T_{\mathrm{P}}^{*}}$$

1. 1D Steady-State Heat Diffusion

Source-Term Linearization – Examples (1/3)

Function	$s\,(T_\mathrm{P})$	s_C	s_P	Option (Opt.)
1	$2 - 7\,T_\mathrm{P}$	2	-7	1
		$2 + 5\,T_\mathrm{P}^*$	-12	2
		$2 - 4\,T_\mathrm{P}^*$	-3	3
2	$9 + 2\,T_\mathrm{P}$	9	2	1
		$9 + 2\,T_\mathrm{P}^*$	0	2
		$9 + 4\,T_\mathrm{P}^*$	-2	3
3	$3 - 6\,T_\mathrm{P}^2$	$3 + 6\,(T_\mathrm{P}^*)^2$	$-12\,T_\mathrm{P}^*$	1
		$3 + 10\,(T_\mathrm{P}^*)^2$	$-16\,T_\mathrm{P}^*$	2

- Function 1: Opt. 1 is the recommended linearization procedure. Opt. 2 may be advantageous for convergence because it promotes a slowdown in the iterative solution procedure. Convergence with Opt. 3 is possible but this option fails to take advantage of the dependence of s on T.
- Function 2: Opt. 1 is only applicable when no iterations are required to solve the problem. Otherwise apply Opts. 2 or 3. Opt. 3 is slower (requires more iterations) than Opt. 2 but it can be more robust (avoid solution divergence).

Source-Term Linearization – Examples (2/3)

Function	$s\,(T_\mathrm{P})$	s_C	s_P	Option (Opt.)
2	$9 + 2\,T_\mathrm{P}$	9	2	1
		$9 + 2\,T_\mathrm{P}^*$	0	2
		$9 + 4\,T_\mathrm{P}^*$	-2	3
3	$3 - 6\,T_\mathrm{P}^2$	$3 + 6\,(T_\mathrm{P}^*)^2$	$-12\,T_\mathrm{P}^*$	1
		$3 + 10\,(T_\mathrm{P}^*)^2$	$-16\,T_\mathrm{P}^*$	2
		$3 + 12\,(T_\mathrm{P}^*)^2$	$-18\,T_\mathrm{P}^*$	3
4	$2 + 3\,T_\mathrm{P}^3$	$2 - 6\,(T_\mathrm{P}^*)^3$	$9\,(T_\mathrm{P}^*)^2$	1
		$2 - 6\,(T_\mathrm{P}^*)^3$	$-9\,(T_\mathrm{P}^*)^2$	2
		$2 + 3\,(T_\mathrm{P}^*)^3$	0	3

- Function 3: all options are suitable but as decreasing the slope value (from $-12\,T_\mathrm{P}^*$ to $-18\,T_\mathrm{P}^*$), the convergence rate of the iterative procedure is slowed down – it may be useful to successfully obtain a converged solution. (Opt. 1 is derived from the direct application of the last equation of Slide 23 – note that Opt. 1 provides the line tangent to the curve $s\,(T_\mathrm{P})$ at $T_\mathrm{P} = T_\mathrm{P}^*$.)

1. 1D Steady-State Heat Diffusion

Source-Term Linearization – Examples (3/3)

Function	$s\,(T_\mathrm{P})$	s_C	s_P	Option (Opt.)
4	$2 + 3T_\mathrm{P}^3$	$2 - 6\,(T_\mathrm{P}^*)^3$	$9\,(T_\mathrm{P}^*)^2$	1
		$2 - 6\,(T_\mathrm{P}^*)^3$	$-9\,(T_\mathrm{P}^*)^2$	2
		$2 + 3\,(T_\mathrm{P}^*)^3$	0	3

- Function 4: Opt. 1 is obtained applying the last equation of Slide 23. However, Opt. 1 has a positive s_P value, and consequently, it is not recommended since the source term is nonlinear and the problem solution would require an iterative procedure. (For avoiding divergence, s_P should not be positive because it may result in a negative center-point coefficient, a_P.) Opt. 2 is incorrect because it does not agree with the prescribed $s\,(T_\mathrm{P})$ function – note that when a converged solution is obtained T_P is equal to T_P^* and, in such case, the source term of Opt. 2 is described by a different function ($2 - 15\,T_\mathrm{P}^3$) than the prescribed one ($2 + 3\,T_\mathrm{P}^3$). Opt. 3 is the appropriate linearization procedure. (If a convergence slowdown is pursued – for instance, to improving the robustness against solution divergence due to other nonlinearity sources – a negative value for s_P can be recommended.)

1. 1D Steady-State Heat Diffusion

Under-relaxation Strategies for the Iterative Sol. of Nonlinear Probs.

- During the iterative solution procedure adopted for handling nonlinearities (see Slide 21) the coefficient values – calculated based on the solution of the previous iteration (T^*) – may change very abruptly which may lead to divergence issues, and consequently, no reliable solution can be obtained.
- To avoid very steep changes in the discretized equation coefficients it is recommended to slowdown solution changes between successive iterations – process known as under-relaxation. Therefore, the temperature solution at node P (T_P) is calculated as shown below, where α corresponds to the under-relaxation factor ($0 < \alpha < 1$), and T^*_P and $\tilde{T}_\mathrm{P}$ are the solution from the previous iteration and the solution computed with the boxed equation of Slide 12, respectively.

$$T_\mathrm{P} = \alpha\,\tilde{T}_\mathrm{P} + (1-\alpha)\,T^*_\mathrm{P}$$

- Under-relaxation can also be applied to other quantities (*viz.* thermal conductivities, boundary conditions, and source terms) – besides to the dependent variable (T).

Suggested Problem:
Problem 3

1. 1D Steady-State Heat Diffusion

Boundary Control Volumes – Discretized Boundary Conditions

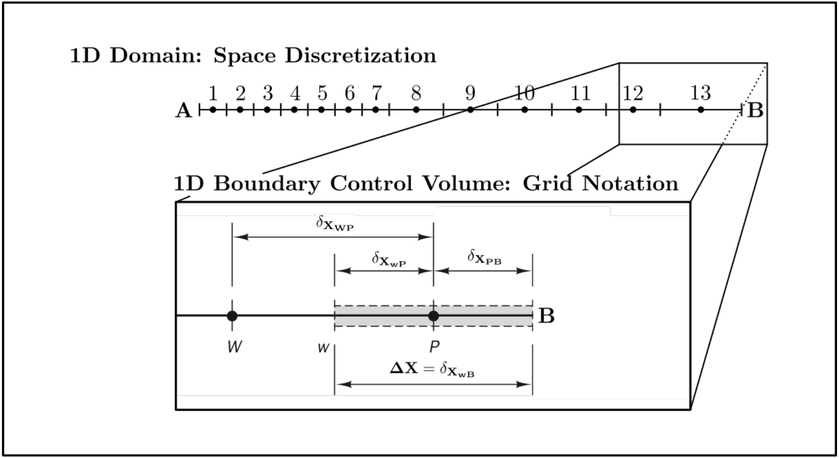
Three types of boundary conditions are herein considered:

- prescribed temperature (boundary condition of first kind or Dirichlet boundary condition);
- specified heat flux (boundary condition of second kind or Neumann boundary condition); and
- convection boundary condition (boundary condition of third kind or Robin boundary condition).

The application of such conditions into the discretized equations of boundary control volumes is illustrated in the slides that follow, in particular, for the right (last) control volume.
(Note that the physical domain boundaries $x = x_{\mathrm{A}}$ and $x = x_{\mathrm{B}}$ are coincident with the west and east faces of the first and last control volumes, respectively.)

1. 1D Steady-State Heat Diffusion

1D Grid – Space Discretization and Grid Notation (Grid-Point Cluster)



1. 1D Steady-State Heat Diffusion

Discretized Boundary Conditions: Prescribed Temperature (1/2)

Prescribed temp. at the right boundary of the domain: $T\left(x = x_\mathrm{B}\right) = T_\mathrm{B}$

$$f_\mathrm{e}^d - f_\mathrm{w}^d + S = 0 \Leftrightarrow k_\mathrm{B} \frac{(T_B - T_P)}{\delta_{x_\mathrm{PB}}} - k_\mathrm{w} \frac{(T_P - T_W)}{\delta_{x_\mathrm{WP}}} + (S_\mathrm{C} + S_\mathrm{P} T_\mathrm{P}) = 0$$

Rearranging,

$$\underbrace{\left(\frac{k_\mathrm{w}}{\delta_{x_\mathrm{WP}}} \overbrace{- S_\mathrm{P} + \frac{k_\mathrm{B}}{\delta_{x_\mathrm{PB}}}}^{-S_\mathrm{P}^\mathrm{T}} \right)}_{a_\mathrm{P}} T_\mathrm{P} = \underbrace{\frac{k_\mathrm{w}}{\delta_{x_\mathrm{WP}}}}_{a_\mathrm{W}} T_\mathrm{W} + \underbrace{0}_{a_\mathrm{E}} T_\mathrm{E} + \overbrace{S_\mathrm{C} + \frac{k_\mathrm{B}}{\delta_{x_\mathrm{PB}}} T_\mathrm{B}}^{b \equiv S_\mathrm{C}^\mathrm{T}} \Leftrightarrow$$

$$\Leftrightarrow a_\mathrm{P} T_\mathrm{P} = a_\mathrm{W} T_\mathrm{W} + a_\mathrm{E} T_\mathrm{E} + b$$

Discretized Boundary Conditions: Prescribed Temperature (2/2)

Prescribed temp. at the right boundary of the domain: $T\left(x = x_{\mathrm{B}}\right) = T_{\mathrm{B}}$

$$\boxed{a_{\mathrm{P}} T_{\mathrm{P}} = a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + b}$$

$$a_{\mathrm{P}} = a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}^{\mathrm{T}}$$

$$a_{\mathrm{W}} = \frac{k_{\mathrm{w}}}{\delta_{x_{\mathrm{WP}}}}$$

$$a_{\mathrm{E}} = 0$$

$$S^{\mathrm{T}} = S_{\mathrm{C}}^{\mathrm{T}} + S_{\mathrm{P}}^{\mathrm{T}} T_{\mathrm{P}}$$

$$b \equiv S_{\mathrm{C}}^{\mathrm{T}} = S_{\mathrm{C}} + \frac{k_{\mathrm{B}}}{\delta_{\mathrm{x_{PB}}}} T_{\mathrm{B}}$$

$$S_{\mathrm{P}}^{\mathrm{T}} = S_{\mathrm{P}} - \frac{k_{\mathrm{B}}}{\delta_{\mathrm{x_{PB}}}}$$

Note that: (i) for a uniform grid $\delta_{\mathrm{x_{PB}}} = 1/2\delta_{\mathrm{x_{WP}}}$; and (ii) in the absence of thermal energy generation (energy source) $S = 0$ ($S_{\mathrm{C}} = 0$ and $S_{\mathrm{P}} = 0$).

Discretized Boundary Conditions: Specified Heat Flux (1/2)

Specified heat flux at the right boundary of the domain: $\left(k\frac{dT}{dx}\right)\Big|_{x=x_\mathrm{B}} = q''_\mathrm{B}$

$$f_\mathrm{e}^d - f_\mathrm{w}^d + S = 0 \Leftrightarrow q''_\mathrm{B} - k_\mathrm{w}\frac{(T_P - T_W)}{\delta_{x_\mathrm{WP}}} + (S_\mathrm{C} + S_\mathrm{P}\,T_\mathrm{P}) = 0$$

Rearranging,

$$\underbrace{\left(\frac{k_\mathrm{w}}{\delta_{x_\mathrm{WP}}}\overbrace{-S_\mathrm{P}}^{-S_\mathrm{P}^\mathrm{T}}\right)}_{a_\mathrm{P}} T_\mathrm{P} = \underbrace{\frac{k_\mathrm{w}}{\delta_{x_\mathrm{WP}}}}_{a_\mathrm{W}} T_\mathrm{W} + \underbrace{0}_{a_\mathrm{E}} T_\mathrm{E} + \overbrace{S_\mathrm{C} + q''_\mathrm{B}}^{b\equiv S_\mathrm{C}^\mathrm{T}} \Leftrightarrow$$

$$\Leftrightarrow a_\mathrm{P}\,T_\mathrm{P} = a_\mathrm{W}\,T_\mathrm{W} + a_\mathrm{E}\,T_\mathrm{E} + S_\mathrm{C}^\mathrm{T}$$

1. 1D Steady-State Heat Diffusion

Discretized Boundary Conditions: Specified Heat Flux (2/2)

Specified heat flux at the right boundary of the domain: $\left(k\frac{dT}{dx}\right)\Big|_{x=x_{\mathrm{B}}} = q''_{\mathrm{B}}$

$$\boxed{a_{\mathrm{P}}\,T_{\mathrm{P}} = a_{\mathrm{W}}\,T_{\mathrm{W}} + a_{\mathrm{E}}\,T_{\mathrm{E}} + b}$$

$$a_{\mathrm{P}} = a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}^{\mathrm{T}}$$

$$a_{\mathrm{W}} = \frac{k_{\mathrm{w}}}{\delta_{x_{\mathrm{WP}}}}$$

$$a_{\mathrm{E}} = 0$$

$$S^{\mathrm{T}} = S_{\mathrm{C}}^{\mathrm{T}} + S_{\mathrm{P}}^{\mathrm{T}}\,T_{\mathrm{P}}$$

$$b \equiv S_{\mathrm{C}}^{\mathrm{T}} = S_{\mathrm{C}} + q''_{\mathrm{B}}$$

$$S_{\mathrm{P}}^{\mathrm{T}} = S_{\mathrm{P}}$$

Note that: (i) for a uniform grid $\delta_{\mathrm{x_{PB}}} = 1/2\delta_{\mathrm{x_{WP}}}$; and (ii) in the absence of thermal energy generation (energy source) $S = 0$ ($S_{\mathrm{C}} = 0$ and $S_{\mathrm{P}} = 0$).

1. 1D Steady-State Heat Diffusion

Discretized Bound. Conditions: Convection Boundary Condition (1/2)

Imposed convective heat flux at the right boundary of the domain: $\left(k\frac{dT}{dx}\right)\Big|_{x=x_\mathrm{B}} = h\left[T_\infty - T\left(x = x_\mathrm{B}\right)\right]$

$$f_\mathrm{e}^d - f_\mathrm{w}^d + S = 0 \Leftrightarrow \overbrace{\left(\frac{\delta_{x_\mathrm{PB}}}{k_\mathrm{B}} + \frac{1}{h}\right)^{-1}}^{U_\mathrm{B}} \left(T_\infty - T_\mathrm{P}\right) - k_\mathrm{w}\frac{\left(T_P - T_W\right)}{\delta_{x_\mathrm{WP}}} + \left(S_\mathrm{C} + S_\mathrm{P}\,T_\mathrm{P}\right) = 0$$

Rearranging,

$$\underbrace{\left(\frac{k_\mathrm{w}}{\delta_{x_\mathrm{WP}}} \overbrace{-S_\mathrm{P} + U_\mathrm{B}}^{-S_\mathrm{P}^\mathrm{T}}\right)}_{a_\mathrm{P}} T_\mathrm{P} = \underbrace{\frac{k_\mathrm{w}}{\delta_{x_\mathrm{WP}}}}_{a_\mathrm{W}} T_\mathrm{W} + \underbrace{0}_{a_\mathrm{E}} T_\mathrm{E} + \overbrace{S_\mathrm{C} + U_\mathrm{B}\,T_\infty}^{b \equiv S_\mathrm{C}^\mathrm{T}} \Leftrightarrow$$

$$\Leftrightarrow a_\mathrm{P}\,T_\mathrm{P} = a_\mathrm{W}\,T_\mathrm{W} + a_\mathrm{E}\,T_\mathrm{E} + b$$

1. 1D Steady-State Heat Diffusion

Discretized Bound. Conditions: Convection Boundary Condition (2/2)

Imposed convective heat flux at the right boundary of the domain: $\left(k\frac{dT}{dx}\right)\Big|_{x=x_{\mathrm{B}}} = h\left[T_\infty - T\left(x = x_{\mathrm{B}}\right)\right]$

$$\boxed{a_{\mathrm{P}}\,T_{\mathrm{P}} = a_{\mathrm{W}}\,T_{\mathrm{W}} + a_{\mathrm{E}}\,T_{\mathrm{E}} + b}$$

$$a_{\mathrm{P}} = a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}^{\mathrm{T}}$$

$$a_{\mathrm{W}} = \frac{k_{\mathrm{w}}}{\delta_{x_{\mathrm{WP}}}}$$

$$a_{\mathrm{E}} = 0$$

$$S^{\mathrm{T}} = S_{\mathrm{C}}^{\mathrm{T}} + S_{\mathrm{P}}^{\mathrm{T}}\,T_{\mathrm{P}}$$

$$b \equiv S_{\mathrm{C}}^{\mathrm{T}} = S_{\mathrm{C}} + U_{\mathrm{B}}\,T_\infty$$

$$S_{\mathrm{P}}^{\mathrm{T}} = S_{\mathrm{P}} - U_{\mathrm{B}}$$

$$U_{\mathrm{B}} = \left(\frac{\delta_{x_{\mathrm{PB}}}}{k_{\mathrm{B}}} + \frac{1}{h}\right)^{-1}$$

Note that: (i) for a uniform grid $\delta_{\mathrm{x_{PB}}} = 1/2\delta_{\mathrm{x_{WP}}}$; and (ii) in the absence of thermal energy generation (energy source) $S = 0$ ($S_{\mathrm{C}} = 0$ and $S_{\mathrm{P}} = 0$).

1. 1D Steady-State Heat Diffusion

Discretized Boundary Conditions: Summary

BC	Boundary	a_W	a_E	b	S_P^T	a_P
1^{st}	L	0	$\frac{k_e}{\delta_{x_{PE}}}$	$S_C + \frac{k_A}{\delta_{x_{AP}}} T_A$	$S_P - \frac{k_A}{\delta_{x_{AP}}}$	$a_W + a_E - S_P^T$
	R	$\frac{k_w}{\delta_{x_{WP}}}$	0	$S_C + \frac{k_B}{\delta_{x_{PB}}} T_B$	$S_P - \frac{k_B}{\delta_{x_{PB}}}$	
2^{nd}	L	0	$\frac{k_e}{\delta_{x_{PE}}}$	$S_C + q''_A$	S_P	
	R	$\frac{k_w}{\delta_{x_{WP}}}$	0	$S_C + q''_B$	S_P	
3^{rd}	L	0	$\frac{k_e}{\delta_{x_{PE}}}$	$S_C + U_A T_\infty$	$S_P - U_A$	
	R	$\frac{k_w}{\delta_{x_{WP}}}$	0	$S_C + U_B T_\infty$	$S_P - U_B$	

First Column – boundary condition kind; and Second Column – L (left boundary) and R (right boundary).

Boundary conditions are considered in the discretized equations of boundary control volumes by suppressing the link to the boundary side ($a_W = 0$ or $a_E = 0$) and introducing the boundary side heat flux through additional terms on S_C^T ($\equiv b$) and/or S_P^T.

Suggested Problem:
Problem 5

1. 1D Steady-State Heat Diffusion

Solution of Discretized Equations (1/2)

For each nodal point, the discretization process yields the following equation

$$a_{\mathrm{P}} T_{\mathrm{P}} = a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + b$$

which can be re-written as

$$a_i T_i = b_i T_{i+1} + c_i T_{i-1} + d_i$$

and the system of linear algebraic equations can be presented in a matrix form as follows

$$\underbrace{\begin{bmatrix} a_1 & -b_1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ -c_2 & a_2 & -b_2 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & -c_3 & a_3 & -b_3 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -c_{N-2} & a_{N-2} & -b_{N-2} & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & -c_{N-1} & a_{N-1} & -b_{N-1} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & -c_N & a_N \end{bmatrix}}_{[a]} \underbrace{\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{N-2} \\ T_{N-1} \\ T_N \end{bmatrix}}_{[T]} = \underbrace{\begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_{N-2} \\ d_{N-1} \\ d_N \end{bmatrix}}_{[b]}$$

1. 1D Steady-State Heat Diffusion

Solution of Discretized Equations (2/2)

- The solution for the temperature distribution can be calculated through direct matrix inversion methods – such as, Cramer's rule and Gauss elimination – as follows:

$$\left[a\right]\left[T\right] = \left[b\right] \Leftrightarrow \left[T\right] = \left[a\right]^{-1}\left[b\right]$$

- In alternative, other more efficient (economical) methods that take advantage of matrix sparsity (matrix $[a]$ is a tridiagonal matrix) can be considered such as, the Thomas algorithm (or tridiagonal matrix algorithm – TDMA).
- The solution techniques for linear algebraic equations suggested before belong to the class of direct methods – methods requiring no iterations. An alternative class of methods are the indirect or iterative methods.
- The number of operations required by direct methods to solve a system of N equations with N unknowns can be determined in advance – on the order of N^3 – but not for iterative methods.

Solution of Discretized Equations – Application to Problem 5(c) (1/3)

Taking into account the discretized equations developed for Problem 5(c), determine the corresponding solution considering $L = 1$ (domain length) and 10 (equally-sized) control volumes.

The expressions developed for the coefficients a_{W}, a_{P}, a_{E}, and b should be evaluated taking into account the conditions considered – see the values for these coefficients in the next table.

Node	a_{W}	a_{E}	$b\left(= S_{\mathrm{C}}, S_{\mathrm{C}}^{\mathrm{T}}\right)$	S_{P}, $S_{\mathrm{P}}^{\mathrm{T}}$	a_{P}
1	0.000	30.000	1057.143	-8.571	38.571
$2, \ldots, 9$	30.000	30.000	200.000	0.000	60.000
10	30.000	0.000	3200.000	-60.000	90.000

1. 1D Steady-State Heat Diffusion

Solution of Discretized Equations – Application to Problem 5(c) (2/3)

The equation for the first node ($i = 1$) reads as follows:

$$a_{\mathrm{P}}\, T_{\mathrm{P}} = a_{\mathrm{W}}\, T_{\mathrm{W}} + a_{\mathrm{E}}\, T_{\mathrm{E}} + b \Leftrightarrow$$
$$\Leftrightarrow 38.571\, T_1 = 0\, T_{\mathrm{W}} + 30\, T_2 + 1057.143 \Leftrightarrow 38.571\, T_1 - 30\, T_2 = 1057.143$$

The equation for any interior node i ($2 \leq i \leq 9$) reads as follows:

$$a_{\mathrm{P}}\, T_{\mathrm{P}} = a_{\mathrm{W}}\, T_{\mathrm{W}} + a_{\mathrm{E}}\, T_{\mathrm{E}} + b \Leftrightarrow$$
$$\Leftrightarrow 60\, T_i = 30\, T_{i-1} + 30\, T_{i+1} + 200 \Leftrightarrow -30\, T_{i-1} + 60\, T_i - 30\, T_{i+1} = 200$$

The equation for the last node ($i = 10$) reads as follows:

$$a_{\mathrm{P}}\, T_{\mathrm{P}} = a_{\mathrm{W}}\, T_{\mathrm{W}} + a_{\mathrm{E}}\, T_{\mathrm{E}} + b \Leftrightarrow$$
$$\Leftrightarrow 90\, T_{10} = 30\, T_9 + 0\, T_{\mathrm{E}} + 3200 \Leftrightarrow -30\, T_9 + 90\, T_{10} = 3200$$

1. 1D Steady-State Heat Diffusion

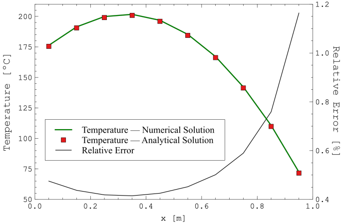
Solution of Discretized Equations – Application to Problem 5(c) (3/3)

The previous equations can be presented in a matrix form as follows

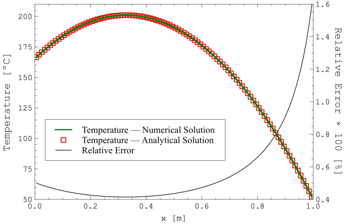
$$\begin{bmatrix} 38.571 & -30 & 0 & \cdots & 0 & 0 & 0 \\ -30 & 60 & -30 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -30 & 60 & -30 \\ 0 & 0 & 0 & \cdots & 0 & -30 & 90 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_9 \\ T_{10} \end{bmatrix} = \begin{bmatrix} 1057.143 \\ 200 \\ \vdots \\ 200 \\ 3200 \end{bmatrix} \Leftrightarrow [T] = [a]^{-1}[b]$$

The results for uniform grids with 10 and 100 CVs are presented in the following figure. Analytical results are also provided for comparison purposes.

10 Control Volumes



100 Control Volumes



1. 1D Steady-State Heat Diffusion

Methods for Solving Algebraic Equations – TDMA

- Tridiagonal matrix algorithm is an efficient method ($\mathcal{O}(N)$ – requires computational storage and computational time proportional to N) for solving a system of N linear algebraic equations represented by

$$a_i T_i = b_i T_{i+1} + c_i T_{i-1} + d_i$$

  where $i = 1, \ldots, N$. Note that for $i = 1$ and $i = N$ (first and last nodal points of the domain), $c_1 = 0$ and $b_N = 0$, respectively.

- Tridiagonal matrix algorithm is comprised by two main steps: (i) forward elimination; and (ii) backward substitution. In the forward elimination stage, the dependency of T_{i-1} on T_i is eliminated for nodes $i = 2$ to $i = N$. Consequently, the equation for T_i only depends on T_{i+1} for $i = 1$ to $i = N - 1$ and T_N is directly computed based on the values of a_i, b_i, c_i, and d_i. Once T_N is known the remaining temperatures are calculated (backward substitution step).

1. 1D Steady-State Heat Diffusion

TDMA: Forward Elimination Step (1/2)

- In the forward elimination stage, each equation for T_i $(i = 1, \ldots, N-1)$ is rewritten in such a way that it only depends on T_{i+1} as follows.
  - Starting with $i = 1$,

$$a_i T_i = b_i T_{i+1} + c_i T_{i-1} + d_i \Rightarrow$$

$$\Rightarrow a_1 T_1 = b_1 T_2 + d_1 \Leftrightarrow T_1 = \underbrace{\frac{b_1}{a_1}}_{P_1} T_2 + \underbrace{\frac{d_1}{a_1}}_{Q_1} \Leftrightarrow T_1 = P_1 T_2 + Q_1$$

  - For $i = 2$,

$$a_2 T_2 = b_2 T_3 + c_2 T_1 + d_2 \Leftrightarrow a_2 T_2 =$$

$$c_2 b_2 T_3 + \underbrace{(P_1 T_2 + Q_1)}_{T_1} + d_2 \Leftrightarrow T_2 = \underbrace{\frac{b_2}{a_2 - c_2 P_1}}_{P_2} T_3 + \underbrace{\frac{d_2 + c_2 Q_1}{a_2 - c_2 P_1}}_{Q_2} \Leftrightarrow$$

$$T_2 = P_2 T_3 + Q_2$$

TDMA: Forward Elimination Step (2/2)

- For $2 \leq i \leq N-1$,

$$T_i = P_i T_{i+1} + Q_i$$

where

$$P_i = \frac{b_i}{a_i - c_i P_{i-1}} \qquad Q_i = \frac{d_i + c_i Q_{i-1}}{a_i - c_i P_{i-1}}$$

- Finally, T_N can be written as follows,

$$a_i T_i = b_i T_{i+1} + c_i T_{i-1} + d_i \Rightarrow a_N T_N = c_N T_{N-1} + d_N \Leftrightarrow$$

$$T_N = \frac{c_N}{a_N} T_{N-1} + d_N \Leftrightarrow T_N = \frac{c_N}{a_N} \underbrace{(P_{N-1} T_N + Q_{N-1})}_{T_{N-1}} + \frac{d_N}{a_N} \Leftrightarrow$$

$$T_N = \underbrace{\frac{d_N + c_N Q_{N-1}}{a_N - c_N P_{N-1}}}_{Q_N} \Leftrightarrow T_N = Q_N$$

Note that Q_N is calculated taking into account only the known values of a_i, b_i, c_i, and d_i for $1 \leq i \leq N$.

1. 1D Steady-State Heat Diffusion

TDMA: Forward and Backward Steps (Summary)

1. **Forward elimination step**
   - Determine $P_1, P_2, \ldots, P_{N-1}$ and $Q_1, Q_2, \ldots, Q_N$ (according to this order – forward) and using the expressions listed in the following table.

i	1	$2, \ldots, N-1$	N
P_i	b_1/a_1	$b_i/\left(a_i - c_i P_{i-1}\right)$	–
Q_i	d_1/a_1	$\left(d_i + c_i Q_{i-1}\right)/\left(a_i - c_i P_{i-1}\right)$	$\left(d_N + c_N Q_{N-1}\right)/\left(a_N - c_N P_{N-1}\right)$

   - Set $T_N = Q_N$.

2. **Backward substitution step**
   - Once T_N, $P_{N-1}, \ldots, P_1$, and $Q_{N-1}, \ldots, Q_1$ are known (from the forward elimination step), the direct calculation of $T_{N-1}, \ldots, T_1$ is performed from $i = N-1$ to $i = 1$ (backward) with the equation:

$$\boxed{T_i = P_i T_{i+1} + Q_i}$$

2. One-Dimensional (1D) Transient Heat Diffusion

Governing Equation: Differential and Integral Forms

- The unsteady heat diffusion equation (governing equation) can be retrieved from the general transport equation neglecting the convective term and considering $\phi = T$, $\Gamma = k/c_p$, and $S_\phi = \dot{q}/c_p$.
  - Differential form:

$$\rho c_p \frac{\partial T}{\partial t} = \mathrm{div}\,(k\,\mathrm{grad}\,T) + \dot{q}$$

  - Integral form:

$$\int_t^{t+\Delta_t} \left(\int_{\Delta V} \rho c_p \frac{\partial T}{\partial t} dV \right) dt =$$

$$\int_t^{t+\Delta_t} \left[\int_A \mathbf{n} \cdot (k\,\mathrm{grad}\,T)\, dA + \int_{\Delta V} \dot{q} dV \right] dt$$

2. 1D Transient Heat Diffusion

Governing Equation: Differential and Integral Forms

- The unsteady 1D (Cartesian) heat diffusion equation (governing equation) reads as follows.
  - Differential form:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \dot{q}$$

  - Integral form:

$$\int_{\Delta V}\left(\int_{t}^{t+\Delta_t} \rho c_p \frac{\partial T}{\partial t} dt\right) dV =$$

$$\int_{t}^{t+\Delta_t}\left[\int_{\Delta V} \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) dV + \int_{\Delta V} \dot{q} dV\right] dt$$

2. 1D Transient Heat Diffusion

Transient Term – Discretization

$$\int_{\Delta V}\left(\int_t^{t+\Delta_t}\rho c_p \frac{\partial T}{\partial t}dt\right)dV = \rho \Delta V c_p \left[T_\mathrm{P}\left(t+\Delta t\right) - T_\mathrm{P}\left(t\right)\right] =$$

$$\rho A_\mathrm{P} \delta_{x_\mathrm{we}} c_p \left(T_\mathrm{P}^1 - T_\mathrm{P}^0\right)$$

(The temperature at the node (T_P) is assumed to prevail over the whole CV.)

Diffusive and Source Term – Spatial Discretization

$$\int_t^{t+\Delta_t}\left(\underbrace{\int_A \mathbf{n}\cdot\left(k\,\mathrm{grad}\,T\right)dA}_{F^d} + \underbrace{\int_{\Delta V}\dot{q}dV}_{Q}\right)dt =$$

$$\int_t^{t+\Delta_t}\underbrace{\left[k_\mathrm{e}A_\mathrm{e}\left(\frac{T_\mathrm{E}-T_\mathrm{P}}{\delta_{x_\mathrm{PE}}}\right) - k_\mathrm{w}A_\mathrm{w}\left(\frac{T_\mathrm{P}-T_\mathrm{W}}{\delta_{x_\mathrm{WP}}}\right) + \left(s_\mathrm{C}+s_\mathrm{P}T_\mathrm{P}\right)\delta_\mathrm{we}A_\mathrm{P}\right]}_{F^d+Q=F^d_\mathrm{e}-F^d_\mathrm{w}+Q \text{ – see Slide 12}}dt$$

2. 1D Transient Heat Diffusion

Temporal Temperature Profile Assumption

To compute the integral $\int_t^{t+\Delta t} \left(F^d + Q\right) dt$, the following assumption on how local temperatures (T_W, T_P, and T_E) vary with time is considered

$$T = fT^1 + (1 - f)\, T^0$$

where $0 \leq f \leq 1$ is a weighting factor. (T^0 and T^1 correspond to the temperature at time t and time $t + \Delta t$, respectively). Consequently, the time integral of temperature T_P is given as follows:

$$\int_t^{t+\Delta t} T_\mathrm{P}\, dt = \left[fT_\mathrm{P}^1 + (1 - f)\, T_\mathrm{P}^0\right] \Delta t$$

$$f = \begin{cases} 0, & \text{Temperature at time } t\ (T^0) \text{ prevails over } [t,\, t + \Delta t[. \\ 1, & \text{Temp. at the end of time step } (T^1) \text{ is considered over }]t,\, t + \Delta t]. \\ 0.5, & \text{Temperatures at } t\ (T^0) \text{ and } t + \Delta t\ (T^1) \text{ are equally weighted.} \end{cases}$$

2. 1D Transient Heat Diffusion

Bulk Control Volumes – Discretized Governing Equation

The integral form of the governing equation reads as follows:

$$\int_{\Delta V}\left(\int_t^{t+\Delta_t}\rho c_p\frac{\partial T}{\partial t}dt\right)dV=\int_t^{t+\Delta_t}\left(\int_A \mathbf{n}\cdot(k\mathrm{grad}\,T)\,dA+\int_{\Delta V}\dot{q}dV\right)dt$$

Substituting the expressions for each integral (see previous slides) and considering $A_\mathrm{w}=A_\mathrm{P}=A_\mathrm{e}$, we have

$$\begin{aligned}\rho c_p\delta_{x_\mathrm{we}}\left(T_\mathrm{P}^1-T_\mathrm{P}^0\right)&=\\ f\left[k_\mathrm{e}\left(\frac{T_\mathrm{E}^1-T_\mathrm{P}^1}{\delta_{x_\mathrm{PE}}}\right)-k_w\left(\frac{T_\mathrm{P}^1-T_\mathrm{W}^1}{\delta_{x_\mathrm{WP}}}\right)+\left(s_\mathrm{C}+s_\mathrm{P}T_\mathrm{P}^1\right)\delta_\mathrm{we}\right]\Delta t&+\\ (1-f)\left[k_\mathrm{e}\left(\frac{T_\mathrm{E}^0-T_\mathrm{P}^0}{\delta_{x_\mathrm{PE}}}\right)-k_w\left(\frac{T_\mathrm{P}^0-T_\mathrm{W}^0}{\delta_{x_\mathrm{WP}}}\right)+\left(s_\mathrm{C}+s_\mathrm{P}T_\mathrm{P}^0\right)\delta_\mathrm{we}\right]\Delta t&\end{aligned}$$

Bulk Control Volumes – Discretized Governing Equation

From the previous slide,

$$
\begin{aligned}
&\rho c_p \delta_{x_{\mathrm{we}}} \left(T_{\mathrm{P}}^1 - T_{\mathrm{P}}^0\right) = \\
&f \left[k_{\mathrm{e}} \left(\frac{T_{\mathrm{E}}^1 - T_{\mathrm{P}}^1}{\delta_{x_{\mathrm{PE}}}}\right) - k_w \left(\frac{T_{\mathrm{P}}^1 - T_{\mathrm{W}}^1}{\delta_{x_{\mathrm{WP}}}}\right) + \left(s_{\mathrm{C}} + s_{\mathrm{P}} T_{\mathrm{P}}^1\right) \delta_{\mathrm{we}}\right] \Delta t + \\
&(1-f) \left[k_{\mathrm{e}} \left(\frac{T_{\mathrm{E}}^0 - T_{\mathrm{P}}^0}{\delta_{x_{\mathrm{PE}}}}\right) - k_w \left(\frac{T_{\mathrm{P}}^0 - T_{\mathrm{W}}^0}{\delta_{x_{\mathrm{WP}}}}\right) + \left(s_{\mathrm{C}} + s_{\mathrm{P}} T_{\mathrm{P}}^0\right) \delta_{\mathrm{we}}\right] \Delta t
\end{aligned}
$$

This equation can be re-written as follows:

$$
\boxed{a_{\mathrm{P}} T_{\mathrm{P}}^1 = f \left(a_{\mathrm{W}} T_{\mathrm{W}}^1 + a_{\mathrm{E}} T_{\mathrm{E}}^1\right) + b}
$$

where,

$$
a_{\mathrm{P}} = f \left(a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}\right) + \rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} \qquad a_{\mathrm{W}} = \frac{k_{\mathrm{w}}}{\delta_{x_{\mathrm{WP}}}} \qquad a_{\mathrm{E}} = \frac{k_{\mathrm{e}}}{\delta_{x_{\mathrm{PE}}}}
$$

$$
b = (1-f) \left[a_{\mathrm{E}} \left(T_{\mathrm{E}}^0 - T_{\mathrm{P}}^0\right) - a_{\mathrm{W}} \left(T_{\mathrm{P}}^0 - T_{\mathrm{W}}^0\right) + S_{\mathrm{P}} T_{\mathrm{P}}^0\right] + S_{\mathrm{C}} + \rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} T_{\mathrm{P}}^0
$$

2. 1D Transient Heat Diffusion

Time Discretization Schemes

- Different values of f leads to different forms for the discretized equations – different temporal differencing schemes for the diffusive and source terms.
- For $f = 0$ (explicit scheme), the temperature T_{P}^1 only depends on known temperatures obtained (or estimated) in a previous (old) time step (T_{W}^0, T_{P}^0, and T_{E}^0). Therefore, an explicit expression to compute T_{P}^1 is obtained.
- For $0 < f \leq 1$ (implicit scheme), the temperatures at $t + \Delta t$ (T^1) are present on both sides of the discretized equation (see the boxed equation in the previous slide) and, consequently, the calculation of T_{P}^1 is implicit.
- Two extreme implicit schemes are considered based on the actual value for f:
  - $f = 0.5$ – Crank-Nicolson (or semi-implicit) scheme; and
  - $f = 1$ – fully implicit scheme.

2. 1D Transient Heat Diffusion

Explicit Discretization Scheme (1/2)

The explicit discretization method applied to the 1D heat diffusion equation is obtained considering $f = 0$ and the corresponding discretized equation is given as follows:

$$\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} T_{\mathrm{P}}^{1} = a_{\mathrm{W}} T_{\mathrm{W}}^{0} + a_{\mathrm{E}} T_{\mathrm{E}}^{0} + \left[\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} - (a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}) \right] T_{\mathrm{P}}^{0} + S_{\mathrm{C}}$$

- T_{P}^{1} is calculated by forward marching in time since the previous equation only includes values at the old time step – the evaluation of a single algebraic equation is required to obtain T_{P}^{1}.
- First-order accurate (Taylor series truncation error accuracy) in time.
- Easy to implement and solve.

2. 1D Transient Heat Diffusion

Explicit Discretization Scheme (2/2)

- Since all coefficients need to be positive to ensure a physically realistic solution, a constrain on the selection of the adopted time step, Δt, arises from the coefficient of T_{P}^0:

$$\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} - a_{\mathrm{W}} - a_{\mathrm{E}} > 0 \Rightarrow \overbrace{\boxed{\Delta t < \rho c_p \frac{(\Delta x)^2}{2k}}}^{\text{Stability Criterion}}$$

  (A constant thermal conductivity, $k_{\mathrm{w}} = k_{\mathrm{e}} = k$, and a uniform grid spacing $\delta_{x_{\mathrm{WP}}} = \delta_{x_{\mathrm{PE}}} = \Delta x$ are assumed.)

- Recommended for simple conduction problems.
- Not recommended for general transient problems due to the effect of spatial accuracy on the maximum possible time step in accordance to the stability criterion – an increase of spatial refinement leads inevitably to very small maximum (allowable) time steps.

2. 1D Transient Heat Diffusion

Crank-Nicolson Discretization Scheme (1/2)

The Crank-Nicolson discretization method applied to the 1D heat diffusion equation is obtained considering $f = 1/2$ and the corresponding discretized equation is given as follows:

$$\left[\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} + \frac{1}{2}\left(a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}\right)\right] T_{\mathrm{P}}^{1} =$$

$$a_{\mathrm{W}}\left(\frac{T_{\mathrm{W}}^{0} + T_{\mathrm{W}}^{1}}{2}\right) + a_{\mathrm{E}}\left(\frac{T_{\mathrm{E}}^{0} + T_{\mathrm{E}}^{1}}{2}\right) + \left[\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} - \frac{1}{2}\left(a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}\right)\right] T_{\mathrm{P}}^{0} + S_{\mathrm{C}}$$

- The Crank-Nicolson method – as any other implicit method – requires the simultaneous solution of the equations for all nodal points at each time step.
- Second-order accurate in time – since this method is based on central differencing.

2. 1D Transient Heat Diffusion

Crank-Nicolson Discretization Scheme (2/2)

- Although unconditionally stable[1] for all time step values, to make sure physically realistic and bounded solutions are obtained all coefficients need to be positive. For the coefficient of T_{P}^{0} the following constrain is observed:

$$\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} - \frac{1}{2}\left(a_{\mathrm{W}} + a_{\mathrm{E}}\right) > 0 \Rightarrow \overbrace{\boxed{\Delta t < \rho c_p \frac{(\Delta x)^2}{k}}}^{\text{Stability Criterion}}$$

- The Crank-Nicolson method provides greater accuracy than the explicit scheme considering sufficiently small times steps.

---

[a] A numerical method is stable if it does not magnify the errors that appear during the solution process. For temporal problems, stability guarantees that the method produces a bounded solution whenever the solution of the exact equation is bounded.

2. 1D Transient Heat Diffusion

Fully Implicit Discretization Scheme (1/2)

The fully implicit discretization method applied to the 1D heat diffusion equation is obtained considering $f = 1$ and the corresponding discretized equation is given as follows:

$$\underbrace{\left[\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t} + a_{\mathrm{W}} + a_{\mathrm{E}} - S_{\mathrm{P}}\right]}_{a_{\mathrm{P}}} T_{\mathrm{P}}^{1} = a_{\mathrm{W}}\, T_{\mathrm{W}}^{1} + a_{\mathrm{E}}\, T_{\mathrm{E}}^{1} + \underbrace{\rho c_p \frac{\delta_{x_{\mathrm{we}}}}{\Delta t}\, T_{\mathrm{P}}^{0} + S_{\mathrm{C}}}_{b}$$

- No constrains on the selection of the time step size – no stability restrictions (unconditionally stable method) – since all coefficients (a_{W}, a_{P}, a_{E}, and the coefficient of T_{P}^{0}) are positive.
- First-order accurate in time.
- Scheme recommended for general-purpose transient calculations due to its robustness and unconditional stability.

2. 1D Transient Heat Diffusion

Fully Implicit Discretization Scheme (2/2)

- Less accurate than the Crank-Nicolson scheme for small time steps.
- To obtain accurate results small time steps are required.
- The steady-state discretized equation is obtained considering $\Delta t \rightarrow \infty$.
- Since the fully implicit scheme implies that the new value for T_{P} (*i.e.*, T_{P}^{1}) prevails over the entire time step ($]t,\ t + \Delta t]$), a temperature dependent thermal conductivity ($k = f\,(T)$) should be iteratively computed taking into account T_{P}^{1} – as it is done for steady-state problems.

3. Multi-Dimensional (MD) Heat Diffusion

Governing Equation: Differential and Integral Forms

The unsteady multidimensional Cartesian (MD Carte.) heat diffusion equation (governing equation) reads as follows.

- Differential form:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) + \dot{q}$$

- Integral form:

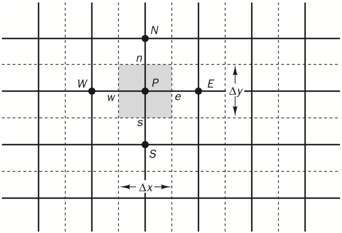
$$\int_{\Delta V}\left(\int_t^{t+\Delta_t} \rho c_p \frac{\partial T}{\partial t} dt\right) dV = \int_t^{t+\Delta_t}\left[\int_{\Delta V} \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) dV + \int_{\Delta V} \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) dV + \int_{\Delta V} \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) dV + \int_{\Delta V} \dot{q} dV\right] dt$$

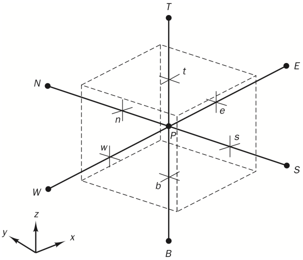
3. MD Heat Diffusion

Transient Term – Discretization

$$\int_{\Delta V}\left(\int_{t}^{t+\Delta_t}\rho c_p \frac{\partial T}{\partial t}dt\right)dV = \rho \Delta V c_p \left[T_{\mathrm{P}}\left(t+\Delta t\right) - T_{\mathrm{P}}\left(t\right)\right] = \rho \Delta V c_p \left(T_{\mathrm{P}}^1 - T_{\mathrm{P}}^0\right)$$

2D and 3D Cartesian Grid Notation – Nodes, Faces, and Dimensions





$\mathrm{S}\,(\mathrm{s})$ – south node (face); $\mathrm{N}\,(\mathrm{n})$ – north node (face); $\mathrm{B}\,(\mathrm{b})$ – bottom node (face); and $\mathrm{T}\,(\mathrm{t})$ – top node (face).

3. MD Heat Diffusion

Diffusive and Source Term – Spatial and Temporal Discretization

$$\int_t^{t+\Delta_t} \left(\int_A \mathbf{n} \cdot (k \,\mathrm{grad}\, T) + \int_{\Delta V} \dot{q} dV \right) dt =$$

$$\int_t^{t+\Delta_t} \left[\left(F_\mathrm{e}^d - F_\mathrm{w}^d \right) + \left(F_\mathrm{n}^d - F_\mathrm{s}^d \right) + \left(F_\mathrm{t}^d - F_\mathrm{b}^d \right) + Q \right] dt \Rightarrow$$

<u>Fully Implicit Scheme</u> $\Rightarrow$

$$\Bigg\{ \left[k_\mathrm{e} A_\mathrm{e} \left(\frac{T_\mathrm{E}^1 - T_\mathrm{P}^1}{\delta_{x_\mathrm{PE}}} \right) - k_\mathrm{w} A_\mathrm{w} \left(\frac{T_\mathrm{P}^1 - T_\mathrm{W}^1}{\delta_{x_\mathrm{WP}}} \right) \right] +$$

$$\left[k_\mathrm{n} A_\mathrm{n} \left(\frac{T_\mathrm{N}^1 - T_\mathrm{P}^1}{\delta_{y_\mathrm{PN}}} \right) - k_\mathrm{s} A_\mathrm{s} \left(\frac{T_\mathrm{P}^1 - T_\mathrm{S}^1}{\delta_{y_\mathrm{SP}}} \right) \right] +$$

$$\left[k_\mathrm{t} A_\mathrm{t} \left(\frac{T_\mathrm{T}^1 - T_\mathrm{P}^1}{\delta_{z_\mathrm{PT}}} \right) - k_\mathrm{b} A_\mathrm{b} \left(\frac{T_\mathrm{P}^1 - T_\mathrm{B}^1}{\delta_{z_\mathrm{BP}}} \right) \right] +$$

$$\left(s_\mathrm{C} + s_\mathrm{P} T_\mathrm{P}^1 \right) \Delta V \Bigg\} \Delta t$$

3. MD Heat Diffusion

Bulk Control Volumes – Discretized Governing Equation

Equating the discretized expression for the transient term with the sum of the discretized equations for the diffusive and source term and rearranging, we have

$$a_{\mathrm{P}}\,T_{\mathrm{P}}^{1} = a_{\mathrm{W}}\,T_{\mathrm{W}}^{1} + a_{\mathrm{E}}\,T_{\mathrm{E}}^{1} + a_{\mathrm{S}}\,T_{\mathrm{S}}^{1} + a_{\mathrm{N}}\,T_{\mathrm{N}}^{1} + a_{\mathrm{B}}\,T_{\mathrm{B}}^{1} + a_{\mathrm{T}}\,T_{\mathrm{T}}^{1} + b \Leftrightarrow$$

$$\boxed{a_{\mathrm{P}}\,T_{\mathrm{P}}^{1} = \sum_{\mathrm{nb}} a_{\mathrm{nb}}\,T_{\mathrm{nb}}^{1} + b}$$

where,

$$a_{\mathrm{P}} = a_{\mathrm{W}} + a_{\mathrm{E}} + a_{\mathrm{S}} + a_{\mathrm{N}} + a_{\mathrm{B}} + a_{\mathrm{T}} + \rho c_p \frac{\Delta V}{\Delta t} - S_{\mathrm{P}} \Leftrightarrow a_{\mathrm{P}} = \sum_{\mathrm{nb}} a_{\mathrm{nb}} + \rho c_p \frac{\Delta V}{\Delta t} - S_{\mathrm{P}} \qquad b = \rho c_p \frac{\Delta V}{\Delta t} T_{\mathrm{P}}^{0} + S_{\mathrm{C}}$$

For a uniform grid, $\delta_{x_{\mathrm{WP}}} = \delta_{x_{\mathrm{PE}}} = \Delta x$, $\delta_{y_{\mathrm{SP}}} = \delta_{y_{\mathrm{PN}}} = \Delta y$, and $\delta_{z_{\mathrm{BP}}} = \delta_{z_{\mathrm{PT}}} = \Delta z$,

Dim.	a_{W}	a_{E}	a_{S}	a_{N}	a_{B}	a_{T}	ΔV
2D	$k_{\mathrm{w}} \frac{\Delta y \cdot 1}{\Delta x}$	$k_{\mathrm{e}} \frac{\Delta y \cdot 1}{\Delta x}$	$k_{\mathrm{s}} \frac{\Delta x \cdot 1}{\Delta y}$	$k_{\mathrm{n}} \frac{\Delta x \cdot 1}{\Delta y}$	–	–	$\Delta x \Delta y \cdot 1$
3D	$k_{\mathrm{w}} \frac{\Delta y \Delta z}{\Delta x}$	$k_{\mathrm{e}} \frac{\Delta y \Delta z}{\Delta x}$	$k_{\mathrm{s}} \frac{\Delta x \Delta z}{\Delta y}$	$k_{\mathrm{n}} \frac{\Delta x \Delta z}{\Delta y}$	$k_{\mathrm{b}} \frac{\Delta x \Delta y}{\Delta z}$	$k_{\mathrm{t}} \frac{\Delta x \Delta y}{\Delta z}$	$\Delta x \Delta y \Delta z$

Suggested Problem:

Problem 9

3. MD Heat Diffusion

Solution of Discretized Equations – Methods for Solving Algebraic Equations

- Direct methods: only competitive for linear problems (not efficient for nonlinear problems).
- Iterative methods – such as, the Gauss-Seidel and line-by-line method:
  - based on a repeated application of a relatively simple algorithm;
  - more economical than direct methods, particularly for large systems of equations (extremely refined meshes);
  - recommended for nonlinear problems; and
  - total number of operations (iter. path) not predictable in advance.

Methods for Solving Algebraic Eqs. – Gauss-Seidel Iteration Method (1/4)

- According to the Gauss-Seidel method, the values of variables are calculated by visiting each grid point in a specific order.
- Convergence is guaranteed if Scarborough criterion is satisfied.
- Slow convergence particularly for a large system of equations.

3. MD Heat Diffusion

Methods for Solving Algebraic Eqs. – Gauss-Seidel Iteration Method (2/4)

Gauss-Seidel Iteration Method – [Algorithm]. Consider a system of n equations with n unknowns $(x_1, \ldots, x_n)$ in which each equation is described by

$$\sum_{j=1}^{n} a_{ij} x_j = b_i$$

where a_{ij} corresponds to the coefficient of the x_j in the i^{th} equation. For the application of iterative methods, it is convenient to rearrange the system of equations in such a way that the contribution x_i is isolated on the LHS of the i^{th} equation as follows:

$$a_{ii} x_i = b_i - \sum_{j=1,\, j\neq i}^{n} a_{ij} x_j$$

According to the Gauss-Seidel iteration method, the solution for variable x_i obtained at the iteration k $(x_i^{(k)})$ is computed as follows:

$$x_i^{(k)} = \sum_{j=1}^{i-1} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^{(k)} + \sum_{j=i+1}^{n} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^{(k-1)} + \frac{b_i}{a_{ii}}$$

3. MD Heat Diffusion

Methods for Solving Algebraic Eqs. – Gauss-Seidel Iteration Method (3/4)

Gauss-Seidel Iteration Method – [Appli. Example]. Consider the following system of equations whose solution is to be found with the Gauss-Seidel Method.

$$\begin{cases} 2x_1 + x_2 + x_3 = 7 \\ -x_1 + 3x_2 - x_3 = 2 \\ x_1 - x_2 + 2x_3 = 5 \end{cases} \Leftrightarrow \begin{cases} x_1 = \left(7 - x_2 - x_3\right)/2 \\ x_2 = \left(2 + x_1 + x_3\right)/3 \\ x_3 = \left(5 - x_1 + x_2\right)/2 \end{cases}$$

Since the matrix of coefficients is diagonally dominant (Scarborough criterion is satisfied) the convergence of the Gauss-Seidel method is guaranteed. The initial guess (arbitrary estimate) for the three unknowns is considered equal to zero, *i.e.*, $x_1^0 = x_2^0 = x_3^0 = 0$. The first iteration of the method yields:

$$x_1^{(1)} = \left(7 - x_2^0 - x_3^0\right)/2 = \left(7 - 0 - 0\right)/2 \Leftrightarrow x_1^{(1)} = 3.50$$

$$x_2^{(1)} = \left(2 + x_1^1 + x_3^0\right)/3 = \left(2 + 3.50 + 0\right)/3 \Leftrightarrow x_2^{(1)} = 1.8(3)$$

$$x_3^{(1)} = \left(5 - x_1^1 + x_2^1\right)/2 = \left(5 - 3.50 + 1.8(3)\right)/2 \Leftrightarrow x_3^{(1)} = 1.6(6)$$

3. MD Heat Diffusion

Methods for Solving Algebraic Eqs. – Gauss-Seidel Iteration Method (4/4)

The second and subsequent iterations follow the exact same procedure.
The results of successive iterations of the Gauss-Seidel method are presented in the following table.

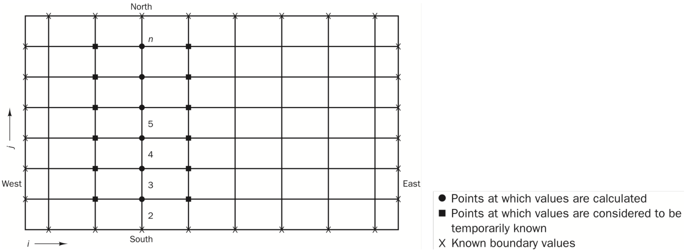
	Iteration k					
	0	1	2	3	...	13
x_1	0	3.5000	1.7500	1.3333	...	1.000
x_2	0	1.8333	1.8056	1.9537	...	2.000
x_3	0	1.6667	2.5278	2.8102	...	3.000

Methods for Solving Algebraic Equations – Line-by-line Method (1/5)

- The line-by-line method results from the combination of the TDMA (direct method for 1D problems – see Slide 44 *et seq.*) and the Gauss-Seidel method (iterative method)
- The line-by-line method consists in the iterative application of the TDMA for solving multi-dimensional (2D and 3D) problems.

Methods for Solving Algebraic Equations – Line-by-line Method (2/5)

- According to the line-by-line method, the TDMA is applied along each line of the grid (column or row) – see the figure below illustrating the TDMA application along north-south lines. Each line is assumed as a 1D domain. The influence of the nodes belonging to the neighboring lines is assumed to be known (from the initial guess or from the current or previous iteration). Once the node values of the current line have been evaluated, the TDMA is applied to the next line, taking always into account the latest (most recent) node values for every calculations.



3. MD Heat Diffusion

Methods for Solving Algebraic Equations – Line-by-line Method (3/5)

The general two-dimensional discretized transport equation reads as

$$a_{\mathrm{P}} T_{\mathrm{P}} = a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + a_{\mathrm{S}} T_{\mathrm{S}} + a_{\mathrm{N}} T_{\mathrm{N}} + b$$

Applying the method along north-south lines, the previous equation can be organized as follows:

$$a_{\mathrm{P}} T_{\mathrm{P}} = a_{\mathrm{N}} T_{\mathrm{N}} + a_{\mathrm{S}} T_{\mathrm{S}} + \underbrace{a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + b}_{\text{Temp. known value}}$$

For each central node P the neighboring contributions ($a_{\mathrm{W}} T_{\mathrm{W}}$ and $a_{\mathrm{E}} T_{\mathrm{E}}$) are considered temporarily known from the previous iteration or initial guess. The last equation is similar to the equation presented in Slide 44 to illustrate the application of the TDMA method considering $a_i T_i = a_{\mathrm{P}} T_{\mathrm{P}}$, $b_i T_{i+1} = a_{\mathrm{N}} T_{\mathrm{N}}$, $c_i T_{i-1} = a_{\mathrm{S}} T_{\mathrm{S}}$, and $d_i = a_{\mathrm{W}} T_{\mathrm{W}} + a_{\mathrm{E}} T_{\mathrm{E}} + b$.

3. MD Heat Diffusion

Methods for Solving Algebraic Equations – Line-by-line Method (4/5)

- The TDMA is applied to all lines (from the west to the east, east to west, north to south, or south to north boundaries) several times. The method terminates when specific criteria are observed (generally when the results do not change considerably between successive iteration, *i.e.*, when a converged solution is obtained).
- The sweep direction (direction of the successive application of the TDMA – from west to east, east to west, north to south, or south to north boundaries) should be selected taking into account the dominant transport direction to improve the convergence rate.
- The sweep direction has a strong effect on the convergence rate but not on the accuracy of the final converged solution.

3. MD Heat Diffusion

Methods for Solving Algebraic Equations – Line-by-line Method (5/5)

- If the dominant transport direction (defined by boundary conditions) is from the west to the east boundaries then this sweep direction should be selected since the transport of information from the boundary nodes to the interior nodes is faster – convergence rate improved. (For instance, when advection is relevant it is convenient to define the sweep direction in accordance to the fluid flow direction – from upstream to downstream).
- The line-by-line method is easily implemented in 3D.

Methods for Solving Algebraic Eqs. – Gauss-Seidel With Relaxation (1/2)

- The convergence rate of the Gauss-Seidel method can be improved (less iterations required to achieve the solution) with the application of a relaxation factor, α, as follows

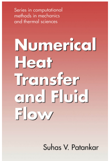
$$x_i^{(k)} = x_i^{(k-1)} + \alpha \left[\sum_{j=1}^{i-1} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^{(k)} + \sum_{j=i}^{n} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^{(k-1)} + \frac{b_i}{a_{ii}} \right]$$

3. MD Heat Diffusion

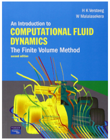
Methods for Solving Algebraic Eqs. – Gauss-Seidel With Relaxation (2/2)

- Depending on the value of the relaxation parameter, the change in the variables (successive variable adjustments towards the final solution) along the iterative procedure can be accelerated ($\alpha > 1$ – over-relaxation) or slowed down ($0 < \alpha < 1$ – under-relaxation). Note that when no relaxation is applied, *i.e.* when $\alpha = 1$, the previous equation reduces to the iteration equation for the basic Gauss-Seidel method (compared such equation with the last equation presented in Slide 67).
- A suitable relaxation parameter value influences the convergence rate (iterative convergence path) but not the final solution.
- While over-relaxation applied to Gauss-Seidel method – known as the SOR (successive over-relaxation) method – may be advantageous for speeding up the iterative procedure, in the presence of strong nonlinearites sub-relaxation may be convenient to avoid solution divergence.
- The optimum relaxation param. value is mesh- and problem-dependent.

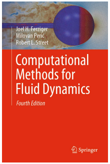
Further Reading



- Chapter 3: Discretization Methods
- Chapter 4: Heat Conduction



- Chapter 4: The FVM for Diffusion Problems
- Chapter 7: Solution of Discretised Equations
- Chapter 8: The FVM for Unsteady Flows



- Chapter 4: Finite Volume Methods
- Chapter 5: Solution of Linear Equation Systems
- Chapter 6: Methods for Unsteady Problems