# Solution of partial differential equations (PDEs)

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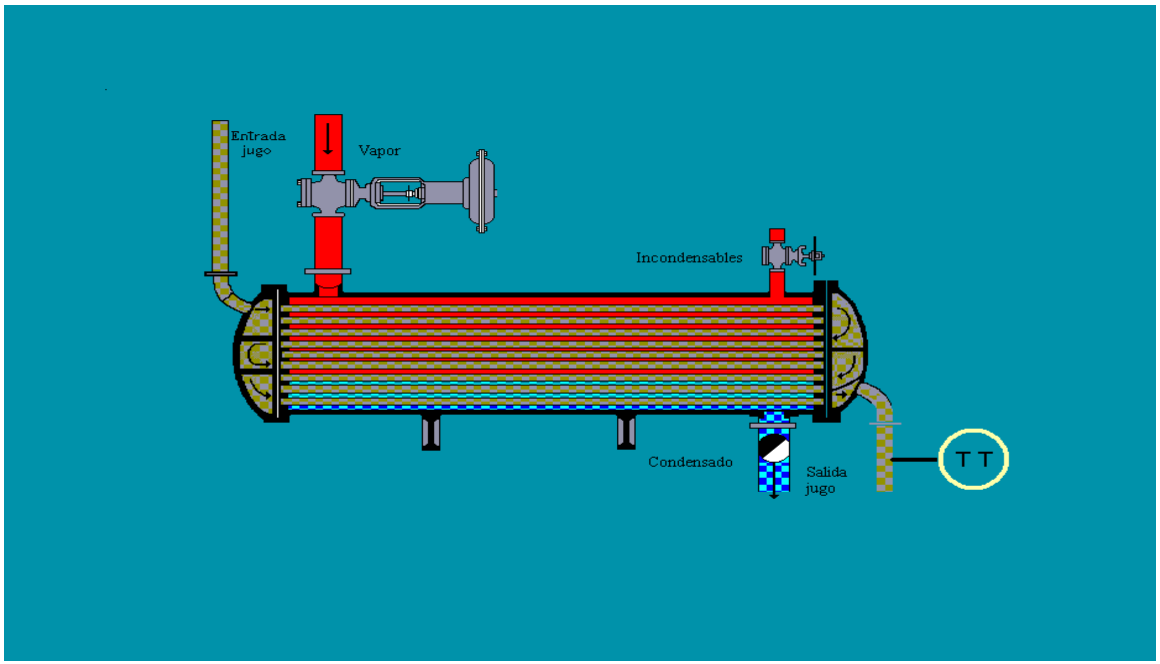
# Outline

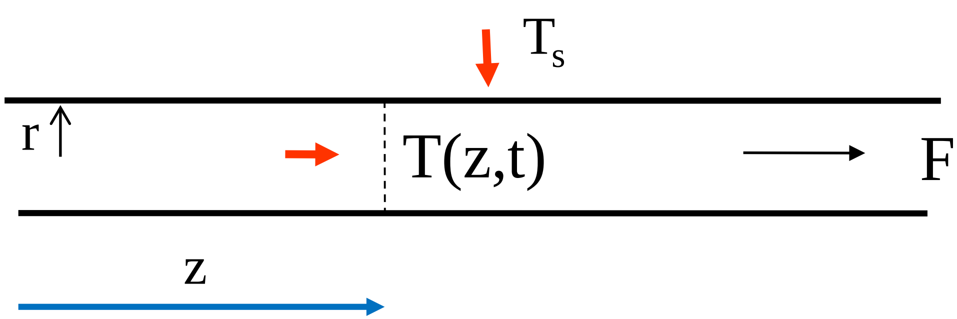
- ✓ Models with Partial Differential Equations PDEs
- ✓ Solving PDEs: converting PDEs into a set of DAEs
- ✓ Finite differences
- ✓ Weighted residuals
  - – Orthogonal collocation
  - – FEM
  - – ….

# Distributed Parameter Systems

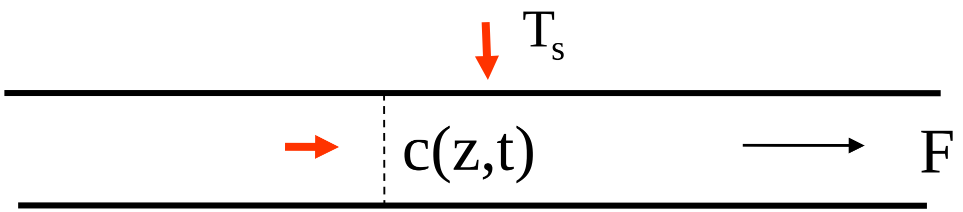


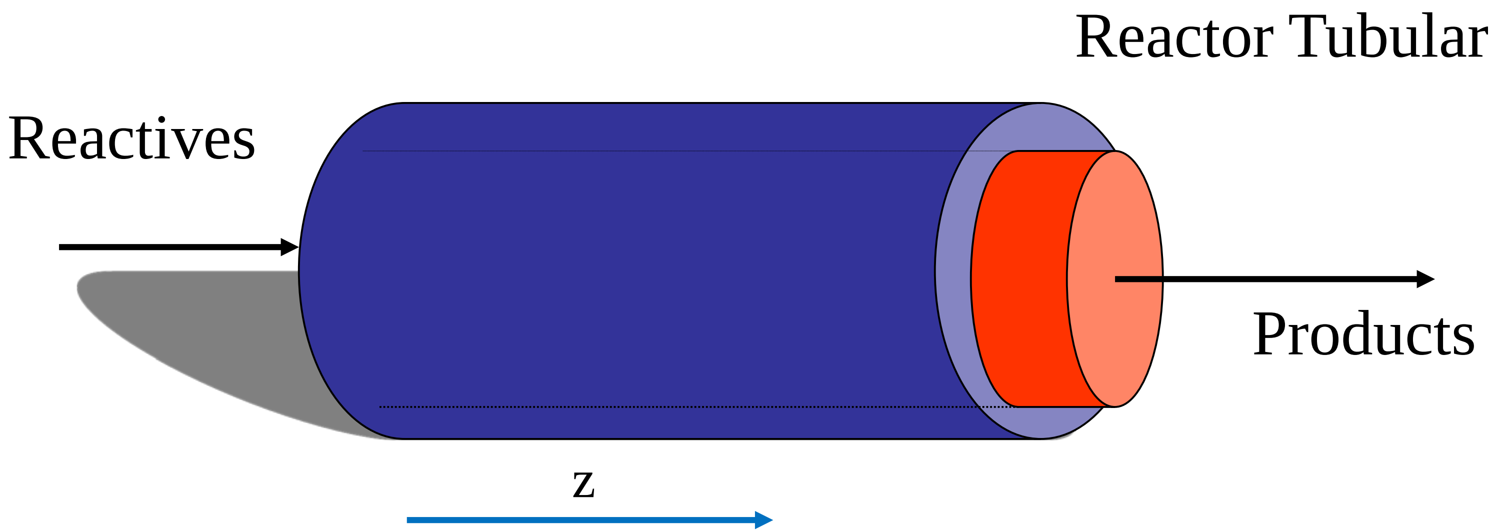

Values of variables depend on time AND spatial location

T(z,t)



# Distributed parameter systems

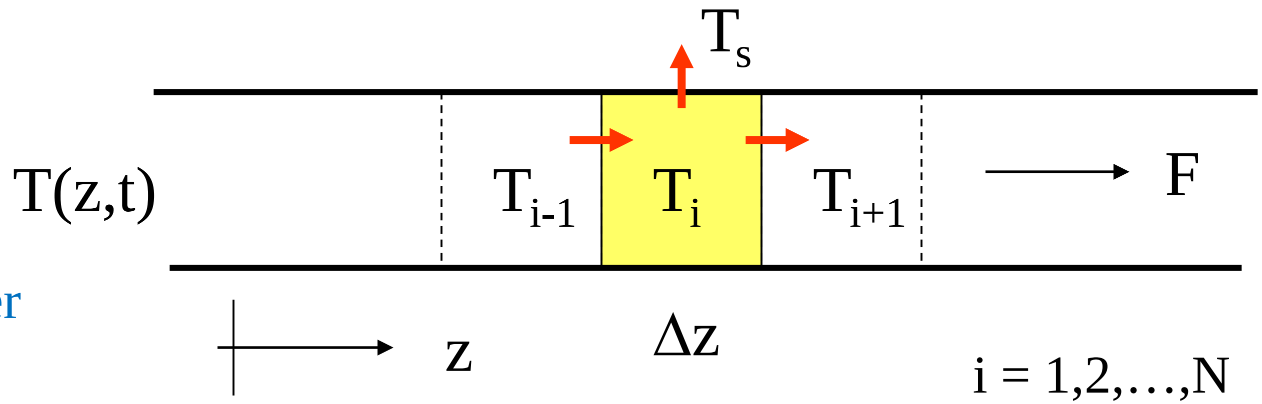



c(z,t) composition changes over time and along the reactor

# Modelling with finite volumes

Heat exchanger example

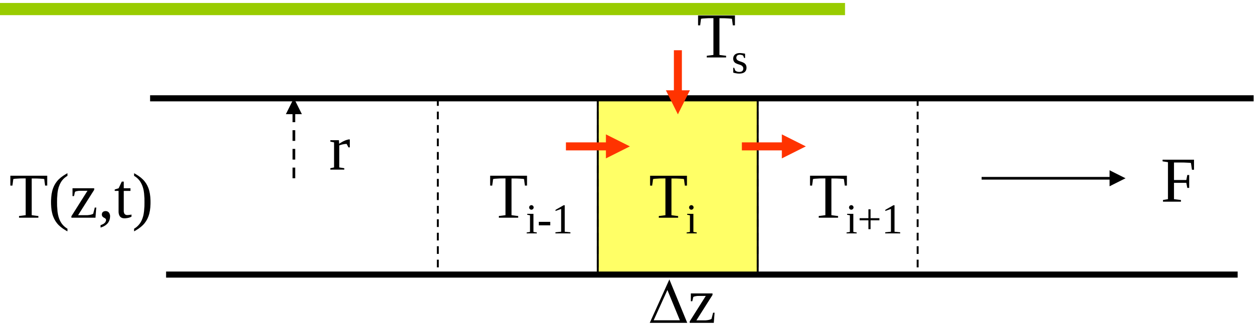



The pipe is divided into small elements of width $\Delta z$ in which T can be assumed to be constant

Energy balance on every volume

Limit when $\Delta z \to 0$

# Modelling with finite volumes




Energy balance

Transport, convection — Conduction

$$\frac{d\,\pi r^2 \Delta z \rho c_e T_i}{dt} = F\rho c_e T_{i-1} - F\rho c_e T_i + 2\pi r \Delta z U (T_s - T_i)$$

No diffusion

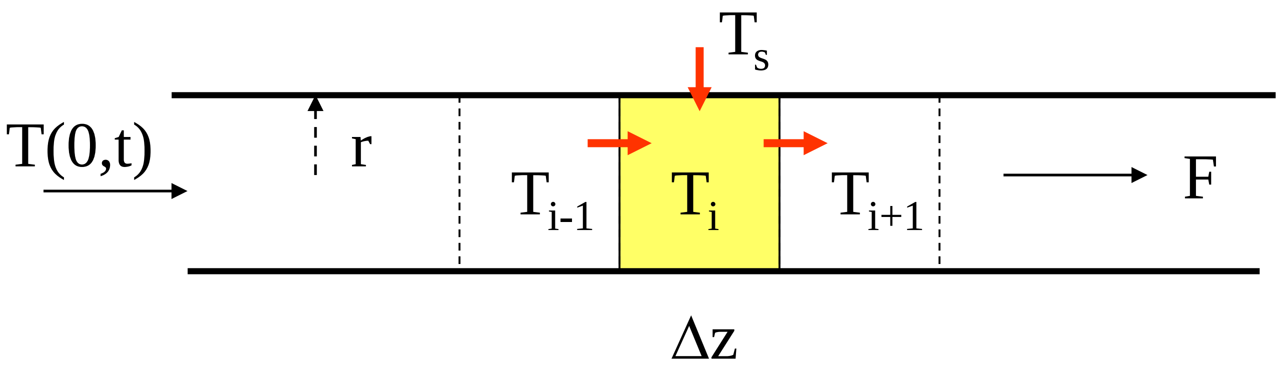
$$\frac{dT_i}{dt} = \frac{F}{\pi r^2}\frac{(T_{i-1} - T_i)}{\Delta z} + \frac{2U(T_s - T_i)}{r\rho c_e}$$

$$\lim_{\Delta z \to 0}\frac{dT_i}{dt} = \frac{F}{\pi r^2}\lim_{\Delta z \to 0}\frac{(T_{i-1} - T_i)}{\Delta z} + \lim_{\Delta z \to 0}\frac{2U(T_s - T_i)}{r\rho c_e}$$

Partial Differential Equation (PDE)

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

# Modelling with finite volumes




First order PDE

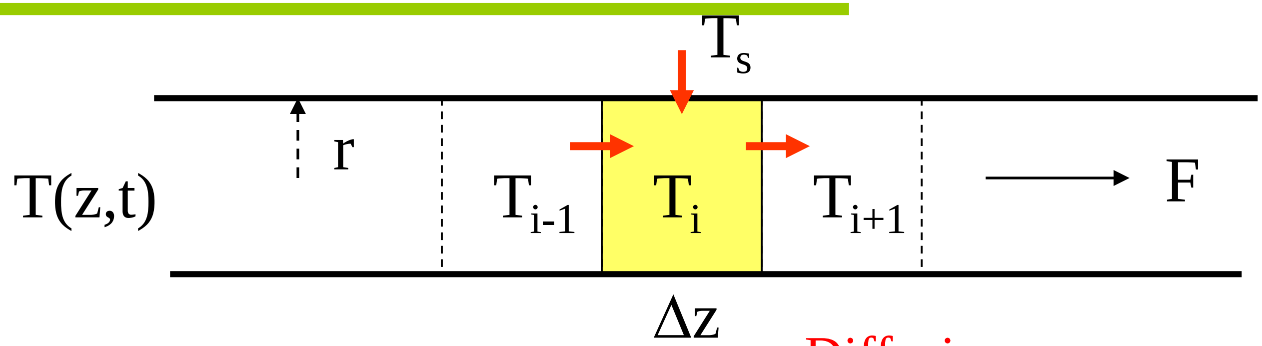
$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

Initial conditions $T(z,0)$

Boundary condition at z = 0 $T(0,t) = T_{input}$

In addition to the values of $T_s(t)$ and F(t), initial values at t = 0 for T and values over time of the temperature of the inflow have to be given (boundary conditions)

# Adding diffusion




Diffusion

$$\frac{d\,\pi r^2 \Delta z \rho c_e T_i}{dt} = F\rho c_e T_{i-1} - F\rho c_e T_i - k\pi r^2 \left.\frac{\partial T}{\partial z}\right|_{i-1} + k\pi r^2 \left.\frac{\partial T}{\partial z}\right|_{i+1} + 2\pi r \Delta z U (T_s - T_i)$$

$$\frac{dT_i}{dt} = \frac{F}{\pi r^2}\frac{(T_{i-1} - T_i)}{\Delta z} + \frac{k}{\rho c_e}\frac{-\left.\frac{\partial T}{\partial z}\right|_{i-1} + \left.\frac{\partial T}{\partial z}\right|_{i+1}}{\Delta z} + \frac{2U(T_s - T_i)}{r\rho c_e}$$

k thermal conductivity

$$\Delta z \rightarrow 0$$

D thermal difusivity

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + D\frac{\partial^2 T(z,t)}{\partial z^2} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

Second order PDE

# Differential equations

$$\frac{dx}{dt} = f(x,u) \qquad x(0) = x_0$$

**ODE, DAE with initial values** Can be solved with well known integration methods: Runge-Kutta, DASSL, etc

$$\frac{dx}{dt} = f(x,u) \qquad x(0) = x_0$$

$$x(t_f) = x_f$$

**ODE , DAE with two points boundary conditions** require several iterations to fulfil the terminal conditions

$$\frac{\partial x(z,t)}{\partial t} = -v\frac{\partial x(z,t)}{\partial z} + D\frac{\partial^2 x(z,t)}{\partial z^2} + F(x,t)$$

**PDE partial differential equations ,** must be discretized

$$B_0 \frac{\partial x(0,t)}{\partial z} = f(x(0,t),t) \qquad B_L \frac{\partial x(L,t)}{\partial z} = f(x(L,t),t)$$

Boundary conditions

$$x(z,0) = x_0$$

Initial conditions

# Boundary conditions

$$\frac{\partial x(z,t)}{\partial t} = -v\frac{\partial x(z,t)}{\partial z} + D\frac{\partial^2 x(z,t)}{\partial z^2} + F(x,t)$$

$$x(0,t) = \varphi(t)$$
$$x(L,t) = \phi(t)$$

Dirichlet type boundary conditions

$$\frac{\partial x(0,t)}{\partial z} = f_0(x(0,t),t)$$
$$\frac{\partial x(L,t)}{\partial z} = f_L(x(L,t),t)$$

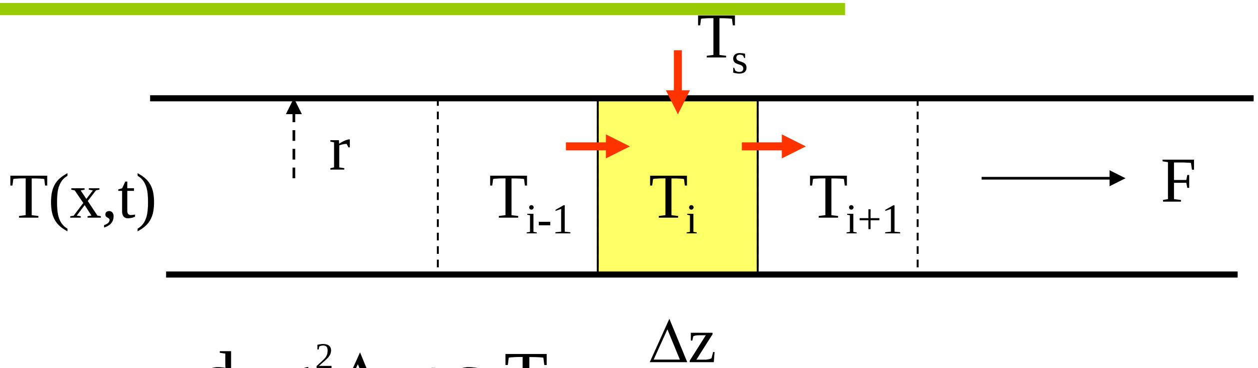
Neumann type boundary conditions

Cauchy type boundary conditions mixes Dirichlet and Neumann

$$A_0 x(0,t) + B_0\frac{\partial x(0,t)}{\partial z} = f_0(x(0,t),t)$$
$$A_L x(L,t) + B_L\frac{\partial x(L,t)}{\partial z} = f_L(x(L,t),t)$$

Robin type boundary conditions

# Solution with Finite Volumes




Energy balance

$$\frac{d\,\pi r^2 \Delta z \rho c_e T_i}{dt} = F\rho c_e T_{i-1} - F\rho c_e T_i + 2\pi r \Delta z U (T_s - T_i)$$

No diffusion

Set of ODEs

$$\frac{dT_i}{dt} = \frac{F}{\pi r^2}\frac{(T_{i-1} - T_i)}{\Delta z} + \frac{2U(T_s - T_i)}{r\rho c_e}$$

$$i = 1,2,\ldots,N \qquad T_0 = T_{input}(t)$$

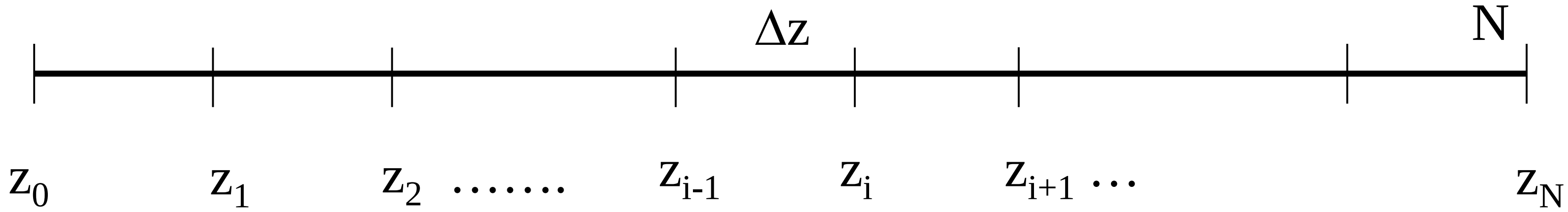
Boundary condition

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

# Solution with Finite Differences

- ✓ The space z is discretized according to a regular mesh, and the derivatives with respect to space at the mesh nodes are approximated by interpolation using the values of the function in the surrounding nodes.

$$\Delta z = \frac{L}{N}$$




Taylor expansions

$$x(z_{i+1},t) = x(z_i,t) + \frac{\partial x(z_i,t)}{\partial z}\Delta z + \frac{1}{2!}\frac{\partial^2 x(z_i,t)}{\partial z^2}\Delta z^2 + \ldots$$

$$x(z_{i-1},t) = x(z_i,t) - \frac{\partial x(z_i,t)}{\partial z}\Delta z + \frac{1}{2!}\frac{\partial^2 x(z_i,t)}{\partial z^2}\Delta z^2 + \ldots$$

# Approximating derivatives

$$x(z_{i+1},t) = x(z_i,t) + \frac{\partial x(z_i,t)}{\partial z}\Delta z + \frac{1}{2!}\frac{\partial^2 x(z_i,t)}{\partial z^2}\Delta z^2 + \ldots$$

$$x(z_{i-1},t) = x(z_i,t) - \frac{\partial x(z_i,t)}{\partial z}\Delta z + \frac{1}{2!}\frac{\partial^2 x(z_i,t)}{\partial z^2}\Delta z^2 + \ldots$$

From the Taylor series development, several approximations of different orders of the derivatives can be computed:

$$\frac{\partial x(z_j,t)}{\partial z} \cong \begin{cases} \dfrac{x(z_{j+1},t) - x(z_j,t)}{\Delta z} \\ \dfrac{x(z_j,t) - x(z_{j-1},t)}{\Delta z} \\ \dfrac{x(z_{j+1},t) - x(z_{j-1},t)}{2\Delta z} \end{cases}$$

First order

second order

$$\frac{\partial^2 x(z_j,t)}{\partial z^2} \cong \frac{x(z_{j+1},t) - 2x(z_j,t) + x(z_{j-1},t)}{\Delta z^2}$$

# Finite differences

$$\frac{\partial x(z_j,t)}{\partial z} \cong \frac{x(z_{j+1},t)-x(z_{j-1},t)}{2\Delta z}$$

$$\frac{\partial x(z,t)}{\partial t} = -v\frac{\partial x(z,t)}{\partial z} + D\frac{\partial^2 x(z,t)}{\partial z^2}$$

PDE

$$\frac{\partial^2 x(z_j,t)}{\partial z^2} \cong \frac{x(z_{j+1},t)-2x(z_j,t)+x(z_{j-1},t)}{\Delta z^2}$$

Set of ODE

$$\frac{dx(z_j,t)}{dt} = -v\frac{x(z_{j+1},t)-x(z_{j-1},t)}{2\Delta z} + D\frac{x(z_{j+1},t)-2x(z_j,t)+x(z_{j-1},t)}{\Delta z^2}$$

$j = 1, 2, 3\ldots, N-1$

At $z_0$ and $z_N$ other expressions or boundary conditions are required

$$x(z_0,t) = T_{input}(t)$$

$$\frac{\partial x(z_N,t)}{\partial z} \approx \frac{x(z_N,t)-x(z_{N-1},t)}{\Delta z} = 0$$

# Finite differences

PDEs are approximated by a set of ODEs / DAEs that can be integrated in standard simulation environments

$$\frac{dx(z_j,t)}{dt} = -v\frac{x(z_{j+1},t) - x(z_{j-1},t)}{2\Delta z} + D\frac{x(z_{j+1},t) - 2x(z_j,t) + x(z_{j-1},t)}{\Delta z^2}$$

j = 1, 2, 3…,N-1

$$B_0 \frac{x(z_1,t) - x(0,t)}{\Delta z} = f(x(0,t),t) \qquad x(z_j,0) = x_0$$

$$B_L \frac{x(z_N,t) - x(z_{N-1},t)}{\Delta z} = f(x(z_N,t),t)_0$$

Stability and convergence to the true solution depends on the mesh and the type of approximation of the derivatives.

Further discretization of the time domain leads to a set of algebraic equations

# Using macros with EcosimPro

They allow for a compact writing of PDEs

The .el file should incorporate the  include declaration of the file where the macros are stored

#include c:\ecosimpro\macros\macroscgm.h“

Different formats according to the order of the approximation and boundaries included:

PDE_1D_2der(0,1,N,T,Tx,Txx)
PDE_1D_EXTR_2der(0,1,N,T,Tx,Txx,TRUE,Tx1,TRUE,TxN)
….

# Example

```
#include "C:\programas\EcosimPro\MACROS\macros.h"

COMPONENT FourierCartes2(INTEGER N=50)
DATA
    REAL L= 1..0 "length (m)"
DECLS
    REAL T[N]
    REAL Tx[N
          REAL Txx[N]
          REAL Tx1    "valor frontera inicial"
    REAL TxN    "valor frontera final"
INIT
    FOR(i IN 2,N)
           T[i]= 0.0
    END FOR
CONTINUOUS
    -- valores frontera
    Tx1= 0.0
    TxN= 1 - T[N]**4
    -- calcula derivadas con respecto a x, la
    primera con
    -- condiciones extremo impuestas, la segunda no
    PDE_1D_EXTR_2der(0,1,N,T,Tx,Txx,TRUE,Tx1,TRUE,Tx
    N)

    EXPAND (i IN 1,N)
           T[i]' = Txx[i]
END COMPONENT
```

Tx and Txx are substituted by the corresponding expressions of the FD discretization

# Weighted residuals

The weighted residuals approach assumes that, according to the Fourier series theorem, the solution of the PDE can be approximated by:

$$\hat{x}(z,t) = \sum_{i=0}^{N} a_i(t)\phi_i(z)$$

Time varying linear combination of known spatial functions $\phi_i$

Where the $\phi_i(z)$ are known (basis) functions normally chosen orthogonal among them and verifying the boundary conditions. Substitution of the approximated solution in the PDE leads to the residual:

$$R(z,t) = \frac{\partial \hat{x}(z,t)}{\partial t} + v\frac{\partial \hat{x}(z,t)}{\partial z} - D\frac{\partial^2 \hat{x}(z,t)}{\partial z^2} - F(\hat{x},t)$$

and the best choice of $a_i(t)$ is the one that minimizes the residuals

# Weighted residuals

Given the spatial basis functions $\phi_i(z)$, the weighted residual family of methods, looks for the functions $a_i(t)$ that cancels a weighted integral of the residuals R over the considered spatial domain $\Omega$. The weights are denoted as the functions $W_i(z)$:

$$\int_{\Omega} W_i(z) R(z,t) dz = 0 \quad i = 1,2,\ldots N$$

This (plus the boundaries) provides a set of ODEs that allows computing the $a_i$ functions

Depending on the choice of the $W_i(z)$, different methods arise:

- Least squares
- Collocation
- Galerkin….

# Weighted residuals

$$W_i = R(z,t) \qquad \Rightarrow \int_\Omega R(z,t)^2 dz = 0$$

**Least squares**

$$W_i = \phi_i(z) \qquad \Rightarrow \int_\Omega \phi_i(z) R(z,t) dz = 0$$

**Galerkin**

$$W_i = \delta(z - z_i) \qquad \Rightarrow R(z_i, t) = 0$$

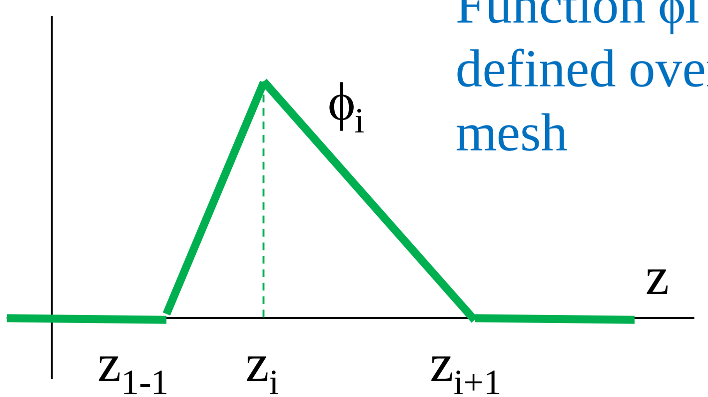
**Collocation**

The choice of the functions $\phi_i(z)$ is very important and can be defined locally (FEM) or globally (spectral methods). Normally the spatial domain is discretized in a set of elements where the $\phi_i(z)$ are defined using simple functions to facilitate the computation.

# Finite Element Method FEM

$$\int_{\Omega} \phi_i(z) R(z,t) dz = 0$$

The spatial domain considered in the problem is discretized using a set of elements forming a mesh, and the spatial functions $\phi_i$ are defined locally on them. The spatial profile of x can be obtained as a linear combination of the $\phi_i$

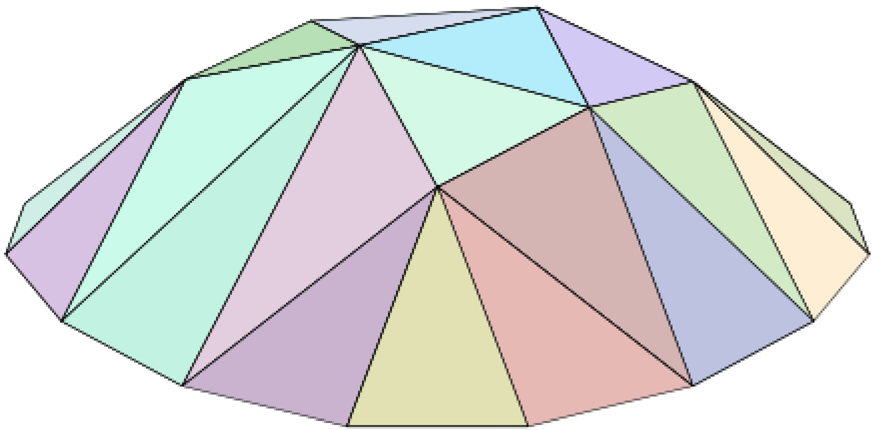



Function $\phi i$ defined over the mesh

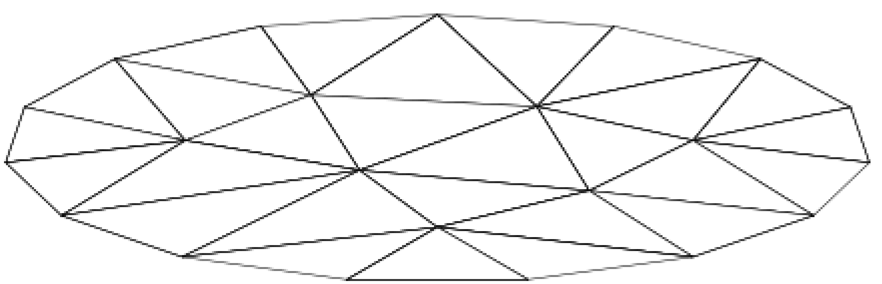
$$\phi_i = \begin{cases} \dfrac{z - z_{i-1}}{z_i - z_{i-1}} & \text{if} \quad z \in [z_{i-1}, z_i] \\ \dfrac{z_{i+1} - z}{z_{i+1} - z_i} & \text{if} \quad z \in [z_i, z_{i+1}] \\ 0 & \text{otherwise} \end{cases}$$

Mesh corresponding to 1-dimensional discretization of the space z

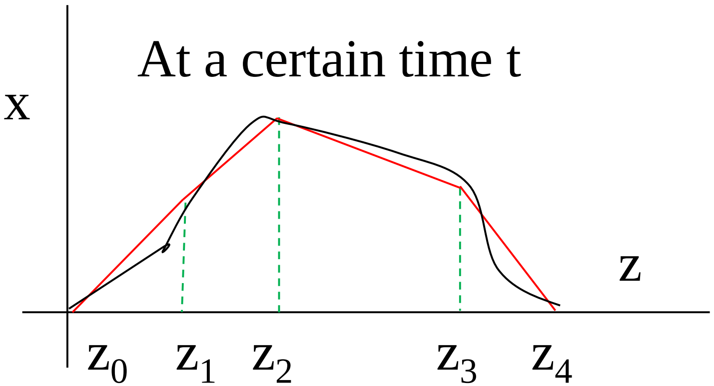
# FEM



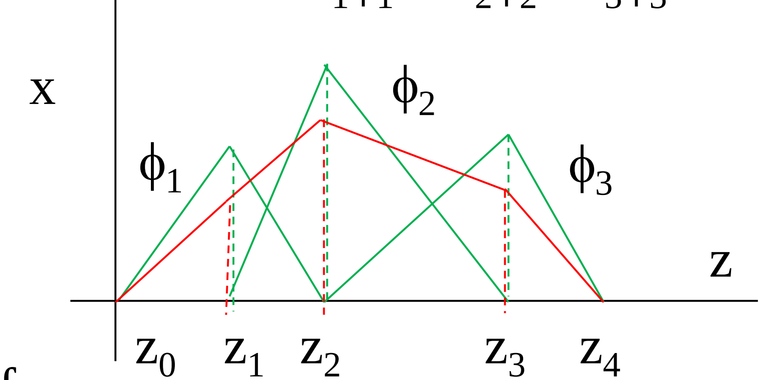
Approximation of a variable over the mesh



2-dimensional mesh showing the elements



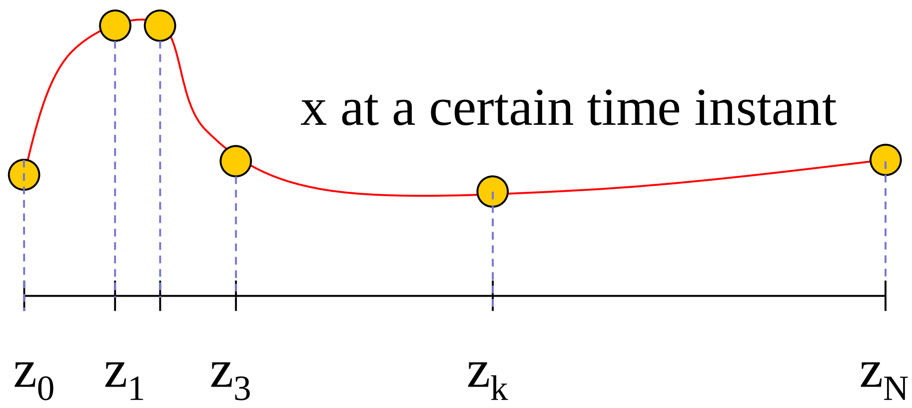

$x \approx a_1\phi_1 + a_2\phi_2 + a_3\phi_3$




The spatial profile of x can be obtained as a linear combination of the $\phi_i$

1-dimensional problems

# Collocation methods




A set of collocation points $z_i$ are placed on the spatial domain and the approximate solution is forced to coincide with the exact one at these points:

$$\frac{\partial \hat{x}(z_i, t)}{\partial t} + v\frac{\partial \hat{x}(z_i, t)}{\partial z} - D\frac{\partial^2 \hat{x}(z_i, t)}{\partial z^2} - F(\hat{x}(z_i, t), t) = 0 \qquad R(z_i, t) = 0$$

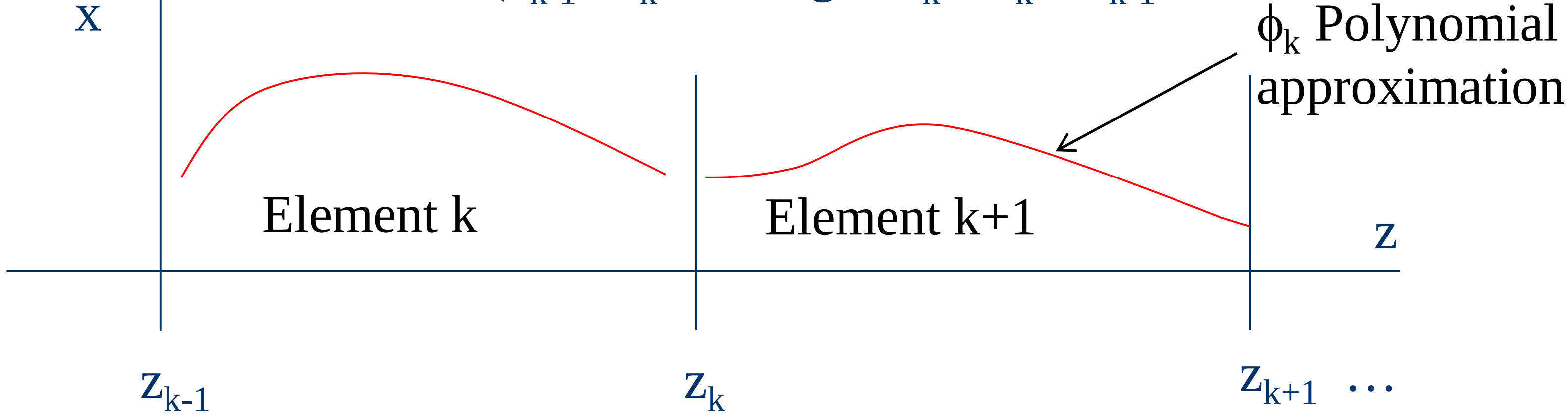
$i = 1.2.,\ldots$

This provides a set of differential equations that allows computing the $a_i(t)$ by integration

$$\hat{x}(z_i, t) = \sum_{i=0}^{N} a_i(t)\phi_i(z_i)$$

# Collocation on finite elements

The spatial domain is divided in a mesh of K intervals or elements $(z_{k-1}, z_k]$ of length $\Delta_k = z_k - z_{k-1}$



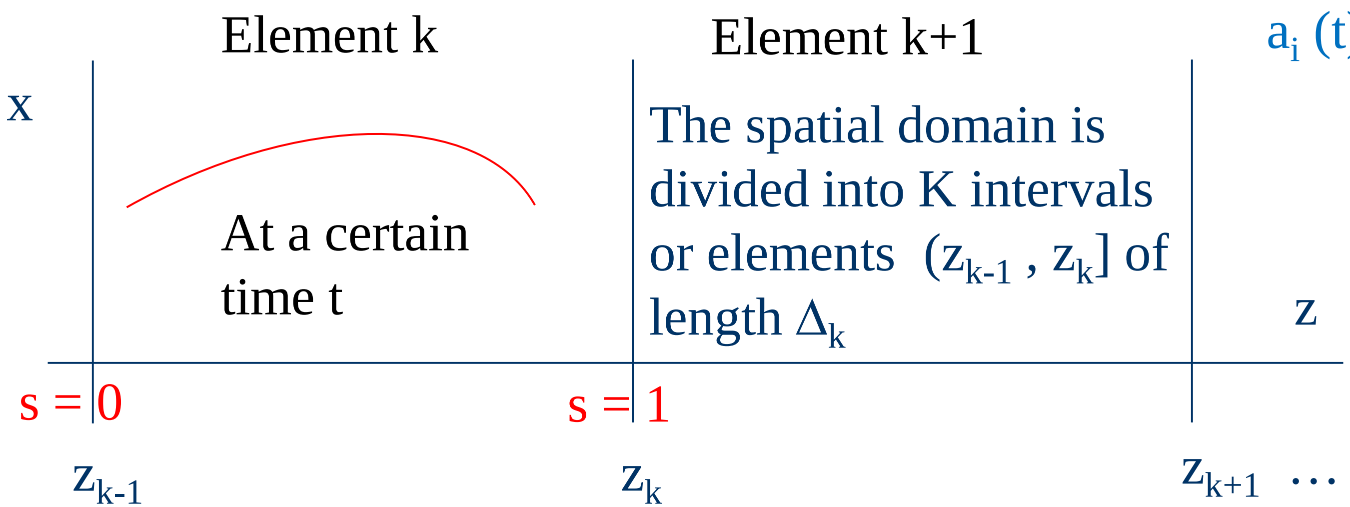

On every element or interval $(z_{k-1}, z_k]$ the spatial functions $\phi_k$ are chosen as a polynomial formula. This provides a smooth approximation within the finite element.

There are many types of polynomials approximations that can be used

The number K of elements does not need to be large

# Collocation on finite elements

$\phi_i(z) = P_j(z(s))$
$a_i\,(t) = x_{kj}(t)$




$x_{kj}(t)$ parameters to be determined

The solution x in the element k at time t is approximated by a linear combination of known polynomials $P_j(s)$ of order P. Lagrange interpolation polynomials are often preferred

s normalized spatial z variable

$$\mathbf{x}(z,t) \approx \sum_{j=0}^{P} P_j(s)\,\mathbf{x}_{kj}(t)$$

$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1] \qquad k = 1,\ldots,K$$

$$\frac{\partial \mathbf{x}(z,t)}{\partial z} \approx \sum_{j=0}^{P} \frac{\partial P_j(s)}{\partial s}\frac{\mathbf{x}_{kj}(t)}{\Delta_k}$$

s normalized distance

# Example Lagrange polynomial

P =2 :

$$s_0 = 0 \quad s_1 = 0.33333 \quad s_2 = 1$$

$$P_j(s) = \prod_{i=0, i\neq j}^{P} \frac{s - s_i}{s_j - s_i}$$

$$P_0 = \frac{s - s_1}{s_0 - s_1}\frac{s - s_2}{s_0 - s_2} = \frac{s - 0.333}{(0 - 0.333)}\frac{s - 1}{(0 - 1)} = 3s^2 - 4s + 1 \qquad \frac{\partial P_0}{\partial s} = 6s - 4$$

$$P_1 = \frac{s - s_0}{s_1 - s_0}\frac{s - s_2}{s_1 - s_2} = -1.5s^2 + 1.5s \qquad \frac{\partial P_1}{\partial s} = -3s + 1.5$$

$$P_2 = \frac{s - s_0}{s_2 - s_0}\frac{s - s_1}{s_2 - s_1} = 1.5s^2 - 0.5s \qquad \frac{\partial P_2}{\partial s} = 3s - 0.5$$

$$x(z_{k-1} + s_j\Delta_k, t) = x_{kj}(t)$$

$$x(z,t) \approx \sum_{j=0}^{P} P_j(s)\mathbf{x}_{kj}(t)$$

$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1]$$

# Example Lagrange polynomial

$$P_j(s) = \prod_{i=0, i\neq j}^{P} \frac{s - s_i}{s_j - s_i}$$

$P = 3:$

$s_0 = 0 \quad s_1 = 0.155051 \quad s_2 = 0.644949 \quad s_3 = 1$

$$P_0 = \frac{s-s_1}{s_0-s_1}\frac{s-s_2}{s_0-s_2}\frac{s-s_3}{s_0-s_3} = -10s^3 + 18s^2 - 9s + 1$$

$$P_1 = \frac{s-s_0}{s_1-s_0}\frac{s-s_2}{s_1-s_2}\frac{s-s_3}{s_1-s_3} = 15.5808\, s^3 - 25.6296 s^2 + 10.0488 s$$

$$P_2 = \frac{s-s_0}{s_2-s_0}\frac{s-s_1}{s_2-s_1}\frac{s-s_3}{s_2-s_3} = -8.9141 s^3 + 10.2963 s^2 - 1.3821 s$$

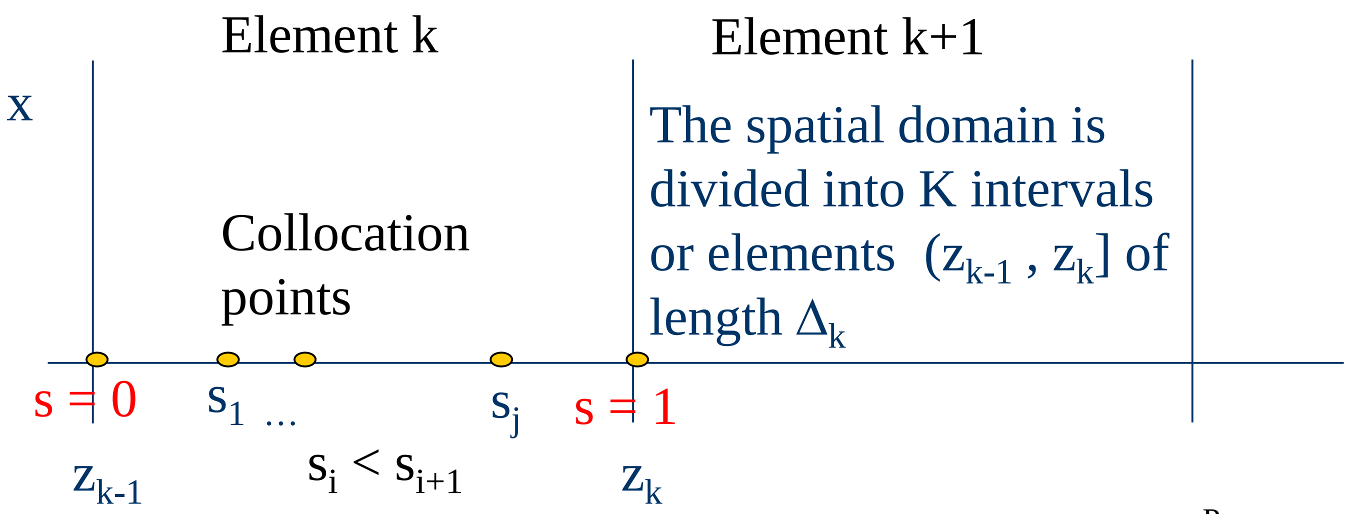
$$P_3 = \frac{s-s_0}{s_3-s_0}\frac{s-s_1}{s_3-s_1}\frac{s-s_2}{s_3-s_2} = 3.3333 s^3 - 2.6667 s^2 + 0.3333 s$$

$$x(z_{k-1} + s_j \Delta_k, t) = x_{kj}(t)$$

$$x(z,t) \approx \sum_{j=0}^{P} P_j(s)\mathbf{x}_{kj}(t)$$

$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1]$$

# Collocation points



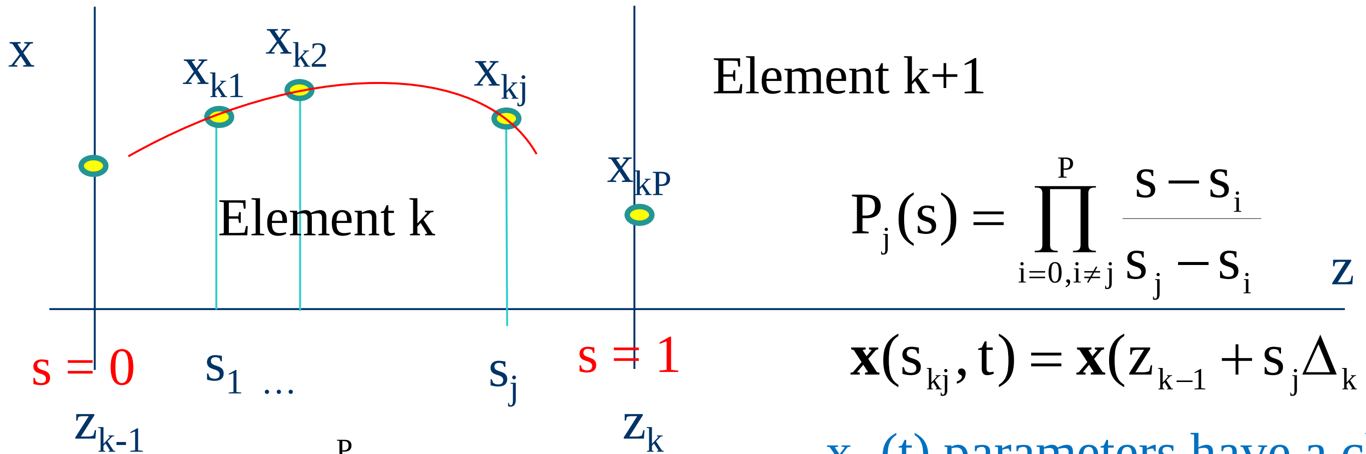

The spatial domain is divided into K intervals or elements $(z_{k-1}, z_k]$ of length $\Delta_k$

The same P+1 s-points used in the definition of the P(s) Lagrange polynomials are used as collocation points $s_i$ within every element k

$$P_j(s) = \prod_{i=0, i \neq j}^{P} \frac{s - s_i}{s_j - s_i}$$

Important property: $P_j(s_i) = 1$ for $i = j$
$P_j(s_i) = 0$ for $i \neq j$

# Lagrange interpolation polynomials




$$P_j(s) = \prod_{i=0, i \neq j}^{P} \frac{s - s_i}{s_j - s_i}$$

$$\mathbf{x}(s_{kj}, t) = \mathbf{x}(z_{k-1} + s_j \Delta_k, t) = \mathbf{x}_{kj}(t)$$

$$\mathbf{x}(z,t) \approx \sum_{j=0}^{P} P_j(s) \mathbf{x}_{kj}(t)$$

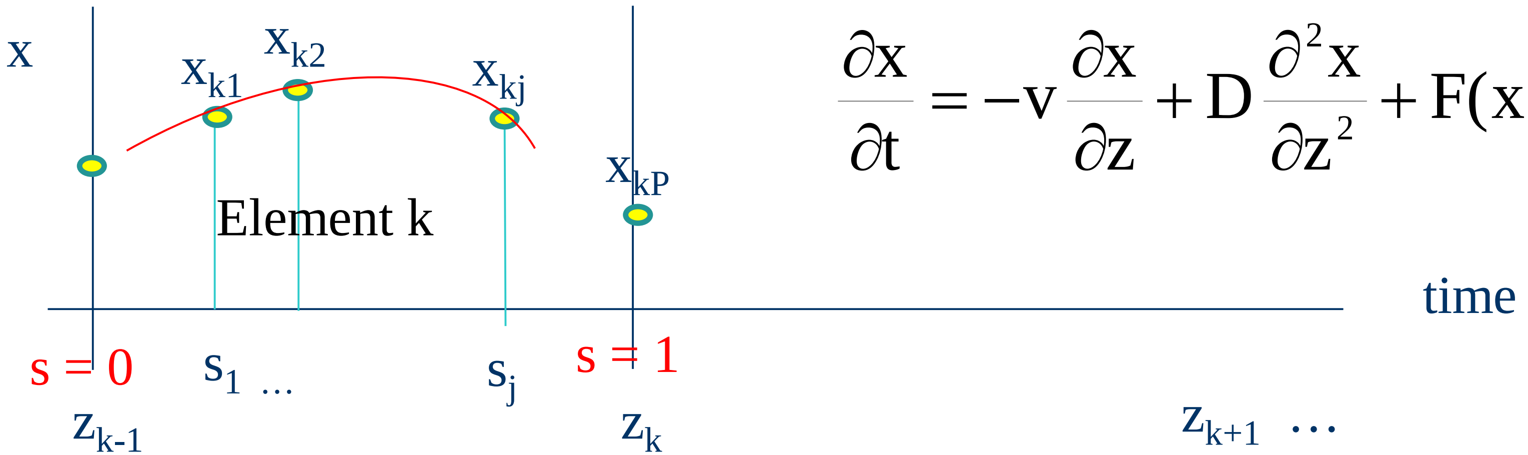
$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1]$$

$x_{kj}(t)$ parameters have a clear meaning using Lagrange polynomials: they coincide with the value of the x variable at location $s_{kj}$

This provides an easy rule for substitution in the PDE of the proposed solution at the $s_i$ collocation points of every k finite element

$$\mathbf{x}(z,t) \approx \mathbf{x}_{kj}(t) \qquad \frac{\partial \mathbf{x}(z,t)}{\partial z} \approx \sum_{j=0}^{P} \frac{\partial P_j(s_i)}{\partial s} \frac{\mathbf{x}_{kj}(t)}{\Delta_k} \qquad \frac{\partial^2 \mathbf{x}(z,t)}{\partial z^2} \approx \sum_{j=0}^{P} \frac{\partial^2 P_j(s_i)}{\partial s^2} \frac{\mathbf{x}_{kj}(t)}{\Delta_k^2}$$

# Collocation on finite elements




$$\frac{\partial x}{\partial t} = -v\frac{\partial x}{\partial z} + D\frac{\partial^2 x}{\partial z^2} + F(x,t)$$

The PDE equations are required to be satisfied at the collocation points $s_i$:

$$\frac{d\mathbf{x}_{ki}(t)}{dt} = -v\sum_{j=0}^{P}\frac{\partial P_j(s_{ki})}{\partial s}\frac{\mathbf{x}_{kj}(t)}{\Delta_k} +$$

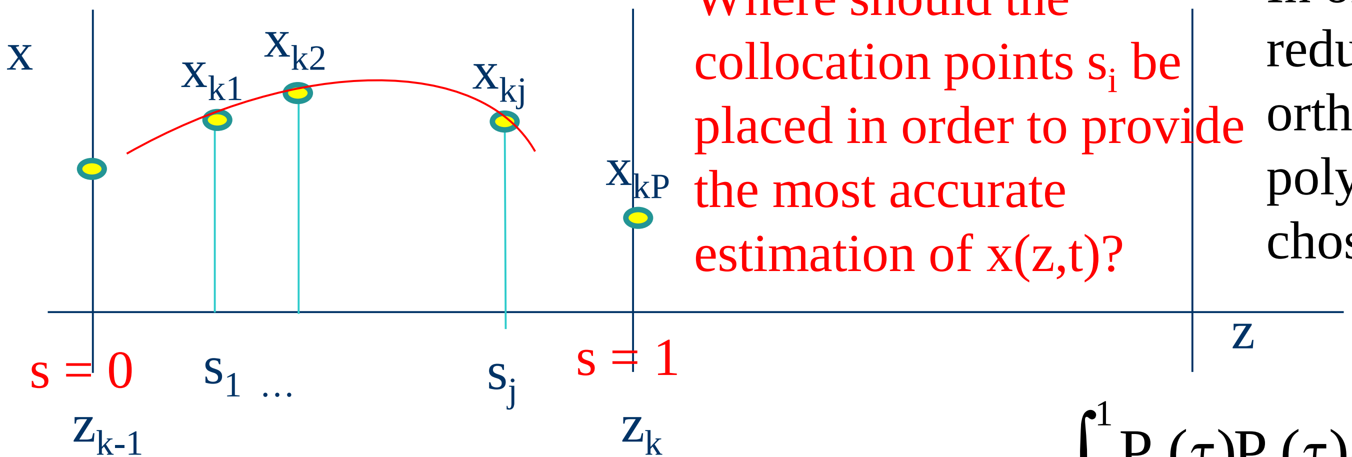
$$+ D\sum_{j=0}^{P}\frac{\partial^2 P_j(s_{ki})}{\partial s^2}\frac{\mathbf{x}_{kj}(t)}{\Delta_k^2} + F(\mathbf{x}_{ki}(t), t)$$

the P+1 collocation points are located at fixed positions $s_j$ in every element k. Different methods exist to choose them

k = 1,..K
i = 1,…P

This provides a set of equations that allows computing the values of the unknown $x_{ki}(t)$

# Orthogonal collocation




Where should the collocation points $s_i$ be placed in order to provide the most accurate estimation of x(z,t)?

In order to reduce P, orthogonal polynomials are chosen

$$\int_0^1 P_j(\tau) P_i(\tau) d\tau = 0 \quad i \neq j$$

$$\frac{d\mathbf{x}_{ki}(t)}{dt} = -v \sum_{j=0}^{P} \frac{\partial P_j(s_{ki})}{\partial s} \frac{\mathbf{x}_{kj}(t)}{\Delta_k} + D \sum_{j=0}^{P} \frac{\partial^2 P_j(s_{ki})}{\partial s^2} \frac{\mathbf{x}_{kj}(t)}{\Delta_k^2} + F(\mathbf{x}_{ki}(t), t) \qquad \begin{array}{l} k = 1,..K \\ i = 1, \ldots P \end{array}$$

Equations are not enforced at $s_0 = 0$. Instead, the continuity of the states through the elements and boundary conditions at s = 0 are used to generate the additional equations that allows computing all $x_{ki}$

# Orthogonal collocation

*Shifted Gauss–Legendre and Radau roots as collocation points.*

| Degree *P* | Legendre Roots | Radau Roots |
|---|---|---|
| 1 | 0.500000 | 1.000000 |
| 2 | 0.211325 | 0.333333 |
| | 0.788675 | 1.000000 |
| 3 | 0.112702 | 0.155051 |
| | 0.500000 | 0.644949 |
| | 0.887298 | 1.000000 |
| 4 | 0.069432 | 0.088588 |
| | 0.330009 | 0.409467 |
| | 0.669991 | 0.787659 |
| | 0.930568 | 1.000000 |
| 5 | 0.046910 | 0.057104 |
| | 0.230765 | 0.276843 |
| | 0.500000 | 0.583590 |
| | 0.769235 | 0.860240 |
| | 0.953090 | 1.000000 |

$s_0$ is always = 0

Legendre: better accuracy
Radau: better robustness

Collocation points $s_i$, i = 1,…,P are selected as the roots of Gauss-Jacobi type polynomials, typically:

$$P_P^{Legendre}(s) = \sum_{j=0}^{P} (-1)^{P-j} s^j \gamma_j$$

$$\gamma_0 = 1$$

$$\gamma_j = \frac{(P-j+1)(P+j)}{j^2}$$

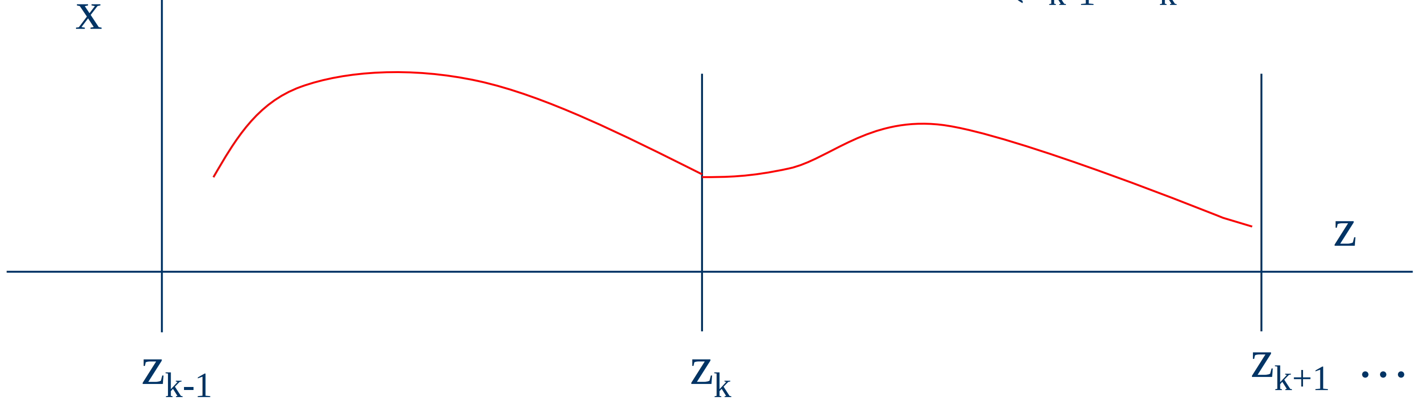
$$P_P^{Radau}(s) = \sum_{j=0}^{P} (-1)^{P-j} s^j \gamma_j$$

$$\gamma_0 = 1$$

$$\gamma_j = \frac{(P-j+1)(P+j+1)}{j^2}$$

# Orthogonal collocation

The continuity of the state profiles is enforced over the finite elements $(z_{k-1}, z_k]$




$$\mathbf{x}(z_k, t) = \mathbf{x}_{k+1,0}(t) = \mathbf{x}_{k,P}(t)$$

$$\mathbf{x}(z_0, t) = \mathbf{x}_{10} = \text{boundary}$$

Simultaneous methods are adequate for unstable systems

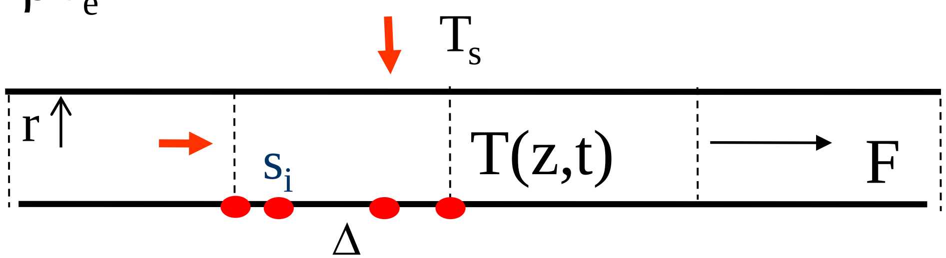
Note that dealing with control profiles, discontinuities can be allowed at the element boundaries if these conditions are not enforced on them

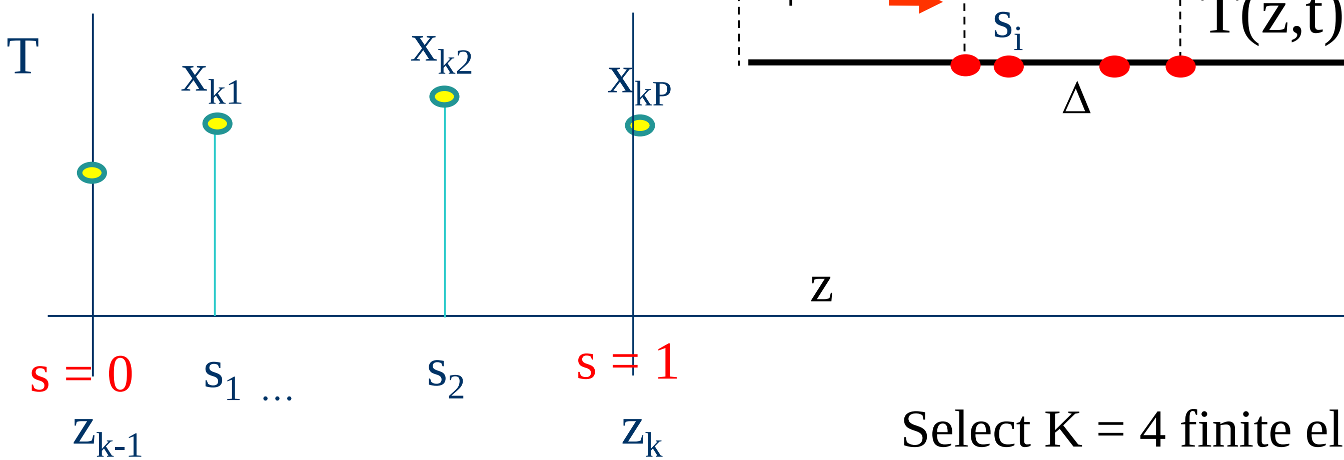
# Example: Heated pipe

Integrate over z = [0 2], from t =0 to 15

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

$$T(z,0) = 20 \qquad T(0,t) = 20$$




Select K = 4 finite elements of equal size $\Delta_k = (2 – 0)/4 = 0.5$
P = 3 , 4 collocation points

The Radau collocation points for P =3 are:
$s_0 = 0$ $s_1 = 0.155051$ $s_2 = 0.644949$ $s_3 = 1$

# Example

The Radau collocation points for P =3 are:

$s_0 = 0$ $s_1 = 0.155051$ $s_2 = 0.644949$ $s_3 = 1$

$$P_j(s) = \prod_{i=0, i\neq j}^{P} \frac{s - s_i}{s_j - s_i}$$

$$P_0 = \frac{s - s_1}{s_0 - s_1} \frac{s - s_2}{s_0 - s_2} \frac{s - s_3}{s_0 - s_3} = -10s^3 + 18s^2 - 9s + 1$$

$$P_1 = \frac{s - s_0}{s_1 - s_0} \frac{s - s_2}{s_1 - s_2} \frac{s - s_3}{s_1 - s_3} = 15.5808s^3 - 25.6296s^2 + 10.0488s$$

$$P_2 = \frac{s - s_0}{s_2 - s_0} \frac{s - s_1}{s_2 - s_1} \frac{s - s_3}{s_2 - s_3} = -8.9141s^3 + 10.2963s^2 - 1.3821s$$

$$P_3 = \frac{s - s_0}{s_3 - s_0} \frac{s - s_1}{s_3 - s_1} \frac{s - s_2}{s_3 - s_2} = 3.3333s^3 - 2.6667s^2 + 0.3333s$$

# Example

$$\frac{\partial T(z,t)}{\partial z} \approx \sum_{j=0}^{P} \frac{\partial P_j(s)}{\partial s} \frac{T_{kj}(t)}{\Delta_k} \qquad \left.\frac{\partial T(z,t)}{\partial z}\right|_{s_i} \approx \sum_{j=0}^{P} \frac{\partial P_j(s_i)}{\partial s} \frac{T_{kj}(t)}{\Delta_k}$$

$$\frac{\partial P_0(s)}{\partial s} = -30 s^2 + 36 s - 9$$

$$\frac{\partial P_1(s)}{\partial s} = 46.7423 s^2 - 51.2592 s + 10.0488$$

$$\frac{\partial P_2(s)}{\partial s} = -26.7423 s^2 + 20.5925 s - 1.3821$$

$$\frac{\partial P_3(s)}{\partial s} = 10 s^2 - 5.3333 s + 0.3333$$

$$T(z_{k-1} + s_j \Delta_k, t) = \mathbf{x}_{kj}(t) \quad = T_{kj}(t)$$

$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1]$$

# Evaluating derivatives at $s_i$

The Radau collocation points for P =3 are:
$s_0 = 0 \quad s_1 = 0.155051 \quad s_2 = 0.644949 \quad s_3 = 1$

$$\frac{\partial P_0(s_0)}{\partial s} = -9 \qquad \frac{\partial P_0(s_1)}{\partial s} = -30(0.155051)^2 + 36(0.155051) - 9 = -4.1394$$

$$\frac{\partial P_0(s_2)}{\partial s} = 1.7394 \qquad \frac{\partial P_0(s_3)}{\partial s} = -3$$

$$\frac{\partial P_1(s_0)}{\partial s} = 10.0488 \qquad \frac{\partial P_1(s_1)}{\partial s} = 3.2247 \qquad \frac{\partial P_1(s_2)}{\partial s} = -3.5679 \qquad \frac{\partial P_1(s_3)}{\partial s} = 5.5319$$

$$\frac{\partial P_2(s_0)}{\partial s} = -1.3821 \qquad \frac{\partial P_2(s_1)}{\partial s} = 1.1679 \qquad \frac{\partial P_2(s_2)}{\partial s} = 0.7753 \qquad \frac{\partial P_2(s_3)}{\partial s} = -7.5319$$

$$\frac{\partial P_3(s_0)}{\partial s} = 0.3333 \qquad \frac{\partial P_3(s_1)}{\partial s} = -0.2532 \qquad \frac{\partial P_3(s_2)}{\partial s} = 1.0532 \qquad \frac{\partial P_3(s_3)}{\partial s} = 5$$

These terms can be pre-computed and are the same for all problems with P = 3

# Example

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

$$T(z,0) = 20 \qquad T(0,t) = 20$$

Set of ODEs

$$\frac{dT_{ki}(t)}{dt} = -\frac{F}{\pi r^2}\sum_{j=0}^{P}\frac{\partial P_j(s_i)}{\partial s}\frac{T_{kj}(t)}{\Delta_k} + \frac{2U(T_s - T_{ki}(t))}{r\rho c_e}$$

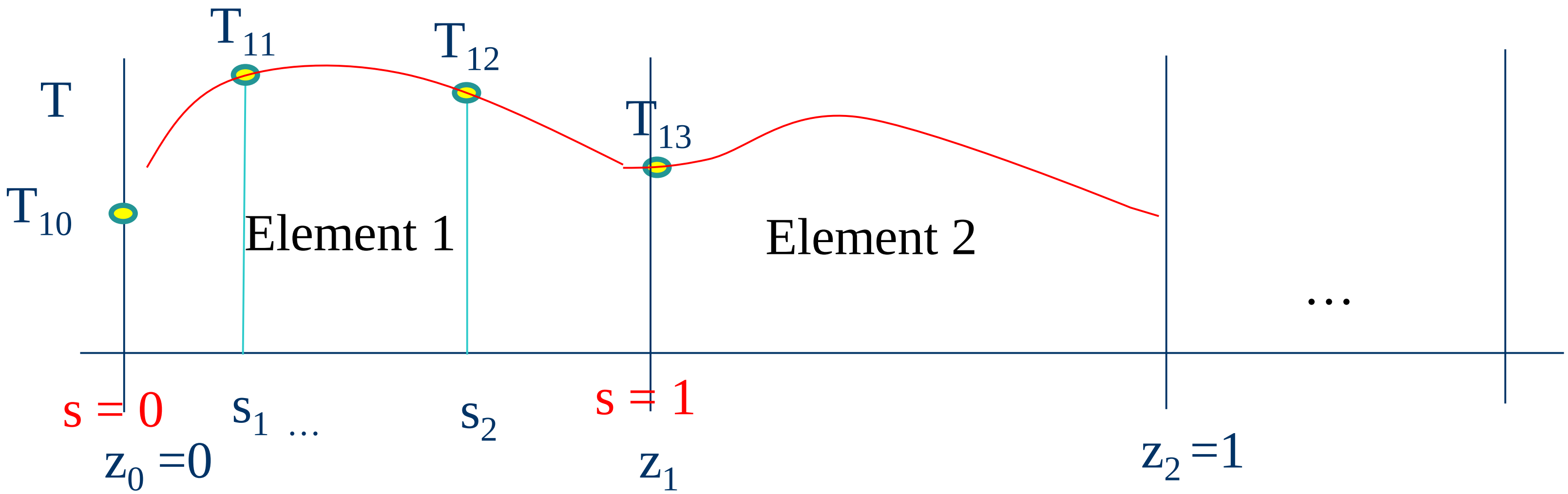
$$T_{ki}(0) = 20 \qquad T_{ki}(0,t) = 20$$

$$i = 1,2,3$$
$$k = 1,2,3,4$$

$$T(z_{k-1} + s_j\Delta_k, t) = T_{kj}(t)$$

$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1]$$

# Example




$$T(z_k, t) = T_{k+1,0}(t) = T_{k,P}(t) = \sum_{j=0}^{P} P_j(1) T_{k,j}(t)$$

$$T(0,t) = T_{10} = 20$$

$$T(0.5,t) = T_{20} = T_{13} = \sum_{j=0}^{3} P_j(1) T_{1j}(t)$$

$$T(0,t) = T_{10}(t) = 20$$

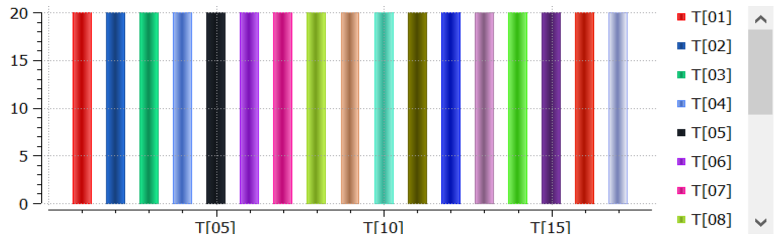
Continuity and initial conditions provide the rest of the equations for solving the temperature at points $T_{kj.}$ For other positions, one have to interpolate using:

$$T(z,t) \approx \sum_{j=0}^{P} P_j(s) T_{kj}(t) \qquad z = z_{k-1} + s\Delta_k$$

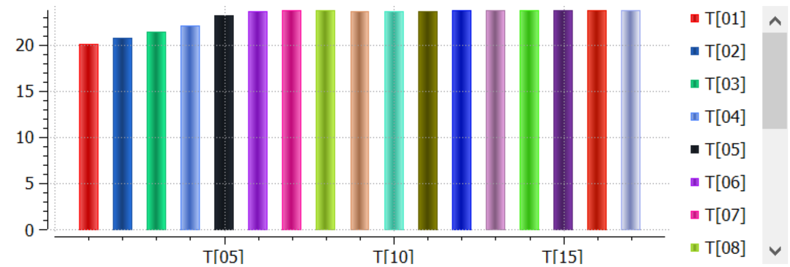
$$s \in (0,1]$$

# Heated pipe

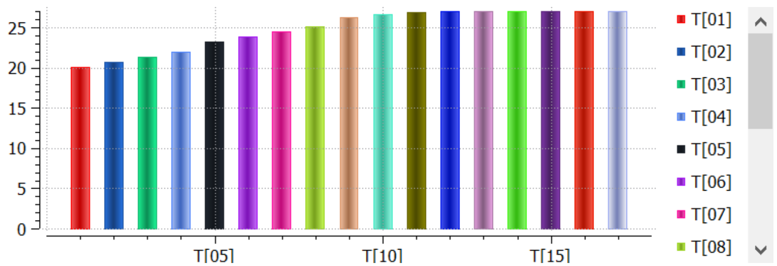
t = 0



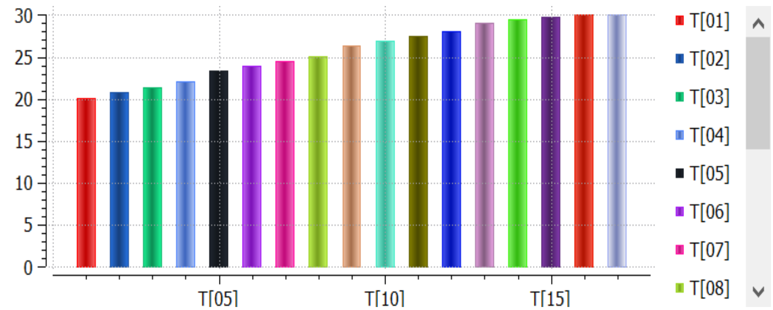

t = 2




t = 4

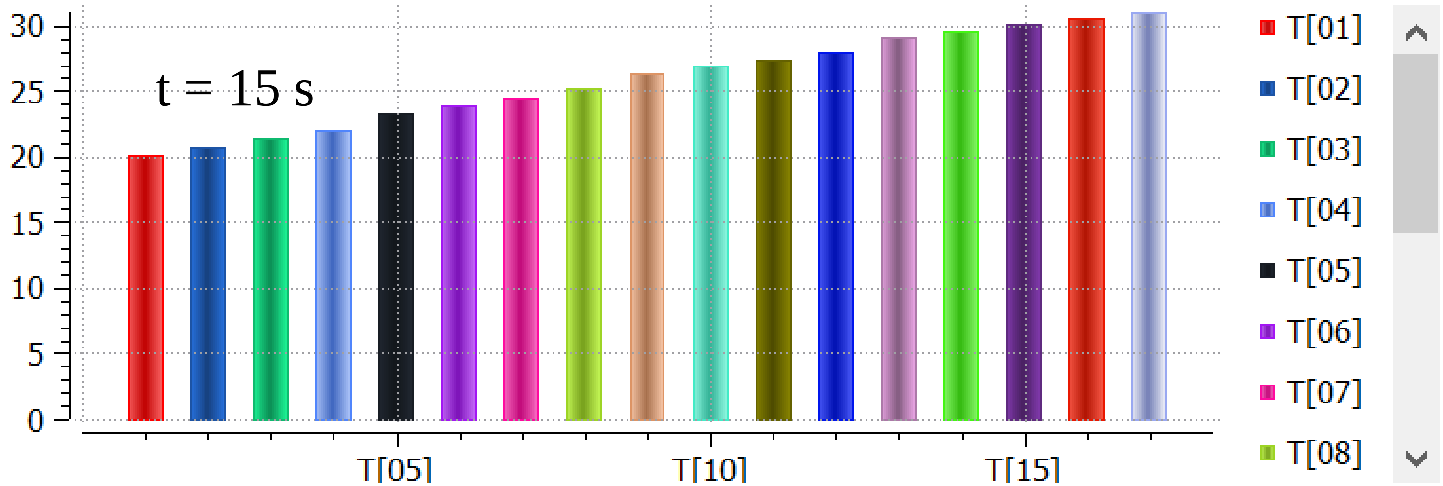


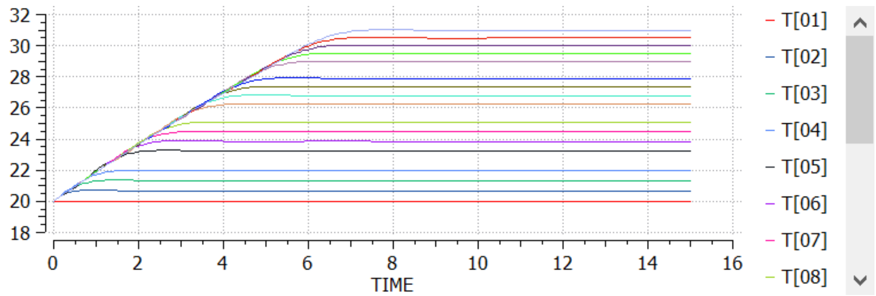

t = 6

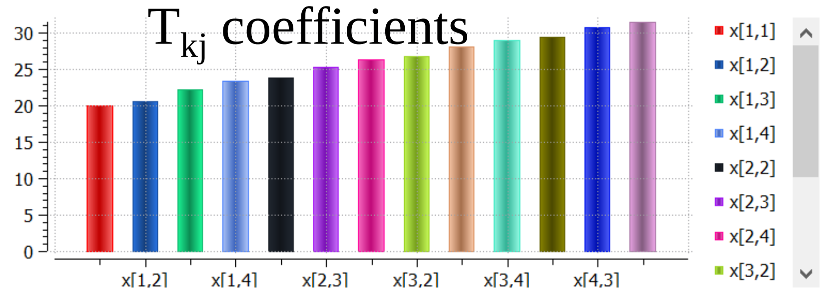



L = 2

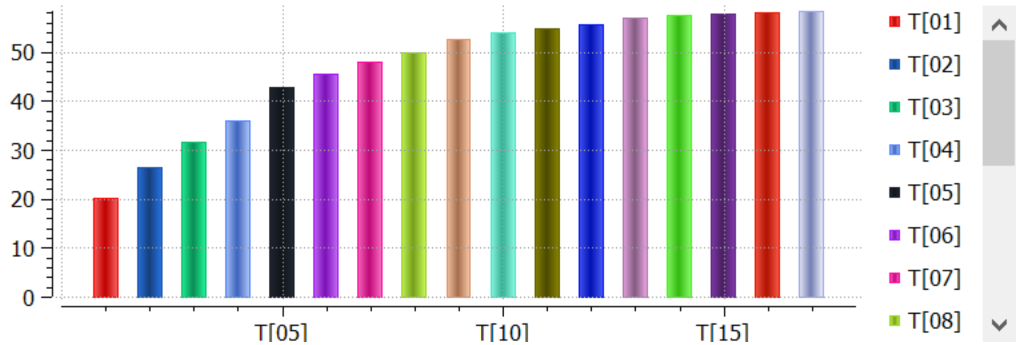
# Example: Heated pipe

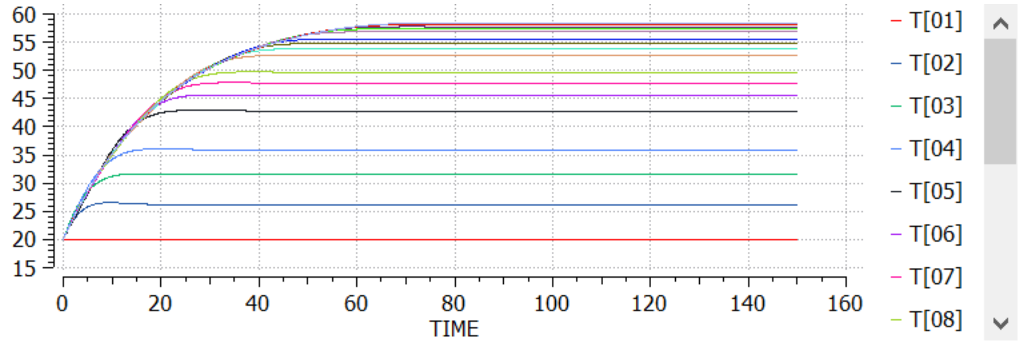


# Heated pipe




Expanding the length to L = 20

# + Diffusion

$$\frac{\partial^2 T(z,t)}{\partial z^2} \approx \sum_{j=0}^{P} \frac{\partial^2 P_j(s)}{\partial s^2} \frac{T_{kj}(t)}{\Delta_k^2}$$

$$\frac{\partial^2 P_0(s)}{\partial s^2} = -60s + 36$$

$$\frac{\partial^2 P_1(s)}{\partial s^2} = 93.4846s - 51.2592$$

$$\frac{\partial^2 P_2(s)}{\partial s^2} = -53.4846s + 20.5925$$

$$\frac{\partial^2 P_3(s)}{\partial s^2} = 20s - 5.3333$$

$$T(z_{k-1} + s_j \Delta_k, t) = T_{kj}(t)$$

$$z = z_{k-1} + s\Delta_k \qquad s \in (0,1]$$

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + D\frac{\partial^2 T(z,t)}{\partial z^2} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

$$T(z,0) = 20 \qquad T(0,t) = 20$$

$$\frac{dT_{ki}(t)}{dt} = -\frac{F}{\pi r^2}\sum_{j=0}^{P}\frac{\partial P_j(s_i)}{\partial s}\frac{T_{kj}(t)}{\Delta_k} + D\sum_{j=0}^{P}\frac{\partial^2 P_j(s_i)}{\partial s^2}\frac{T_{kj}(t)}{\Delta_k^2} + \frac{2U(T_s - T_{ki}(t))}{r\rho c_e}$$

$$T_{ki}(0) = 20 \qquad T_{ki}(0,t) = 20$$

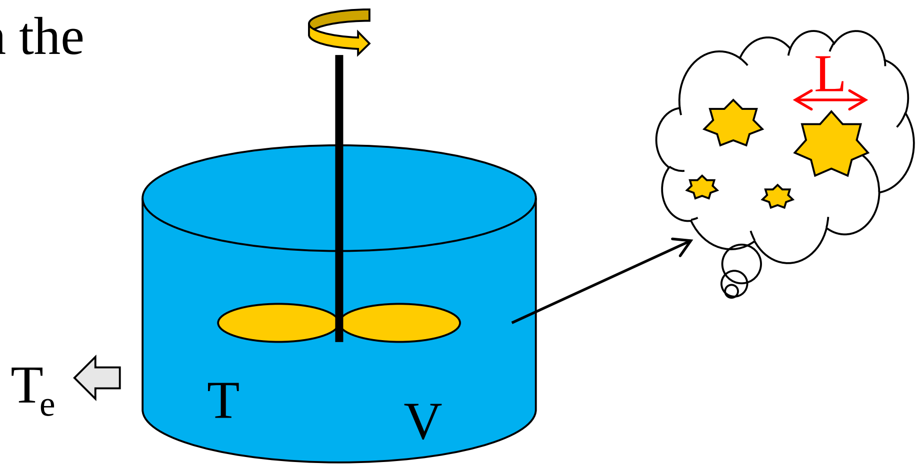
i = 1,2,3

k = 1,2,3,4

# Ice cream crystallization

Ice cream crystallization model based on population balance equations.
It allows the determination of the crystal size distribution, giving information on granulometry which characterizes product quality.

Crystals are formed spontaneously when the solution is under its saturation freezing temperature




Homogeneous mixture of crystals and syrup

Crystals growth at a rate that depends on the difference between the temperature T of the solution and its saturation freezing temperature $T_s$

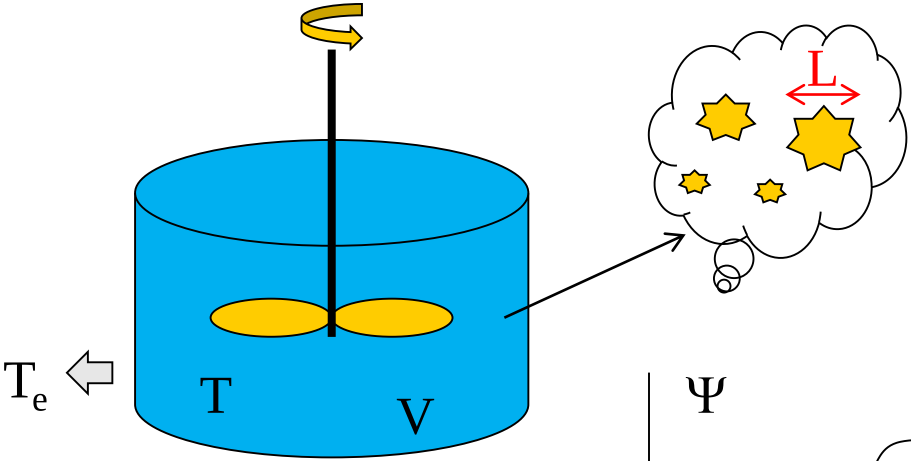
# Crystal size distribution

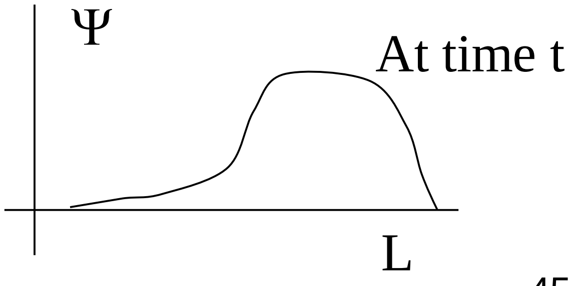
The crystal size distribution function ψ(L,t) represents the number of crystals of size L per unit volume at time t.

L crystal size

Ψ(L,t) Cristal size distribution

V Volume
T(t) temperature
$T_s$ freezing temperature
$T_e$ cooling wall temperature



# Population Balance Equation (PBE)

The model takes into account the nucleation and growth kinetics.
It allows the determination of the crystal size distribution $\Psi(L,t)$.

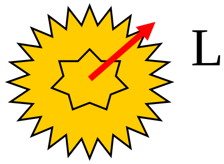
Nucleation occurs at a rate N that depends on the difference between the temperature T of the solution and its saturation freezing temperature $T_s$ creating N crystals of minimum size $L_c$ per unit time and unit volume.

$$N = \alpha (T_s - T)^{\nu} \delta(L - L_c)$$

$\delta$ Dirac Delta

Crystal growth G, defined as the change in size of a crystal per unit time, is also depending on the difference between the temperature T of the solution and its saturation freezing temperature $T_s$

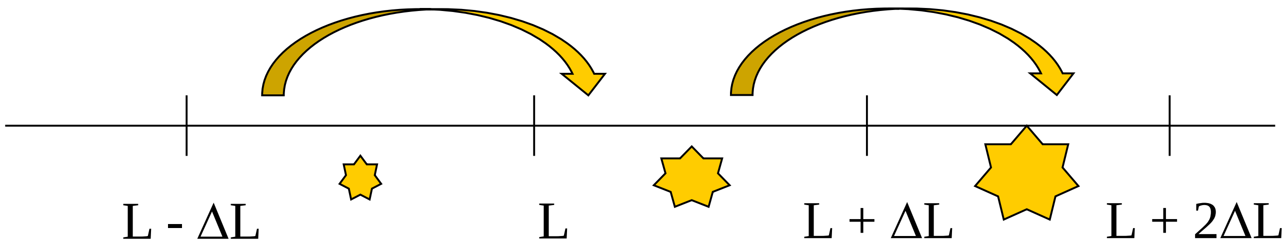
$$\frac{dL}{dt} = G = \beta (T_s - T)^{\gamma}$$




$T_s(c)$ depends on the solute concentration of the solution c

# PBE

Dynamic mass balance applied to the change in the number of crystals of sizes between L and L+ΔL. It assumes that the crystals grow size at a rate G per unit time, are formed by nucleation at a rate N per unit volume and no crystal agglomeration and breakage takes place.




At a growth rate G, crystals will grow ΔL in size in a time interval given by $\Delta L = G\,\Delta t$. So, crystals in the interval size [L - ΔL, L] will move to the interval size [L, L+ ΔL] and crystals that were in the interval [L, L+ ΔL] will move to the next interval [L+ ΔL, L+ 2ΔL] . If the number of crystals of size L per unit volume is given by ψ(L,t), then the net balance due to crystal growth in the number of crystals with sizes in [L, L+ ΔL] in the time interval $\Delta t = \Delta L/G$ is: $[\psi(L-\Delta L,t) - \psi(L,t)]V$

# PBE

Dynamic mass balance applied to the change in the number of crystals of sizes between L and L+ΔL. Considering the growth rate G and nucleation at a rate N;

$$[\psi(L, t+\Delta t) - \psi(L,t)]V = [\psi(L-\Delta L, t) - \psi(L,t)]\left[\frac{G}{\Delta L}\right]\Delta t V + N\,\delta(L - L_c)V\Delta t$$

=1

$$[\psi(L, t+\Delta t) - \psi(L,t)]V = \left[\frac{G\psi(L-\Delta L, t) - G.\psi(L,t)}{\Delta L}\right]V\Delta t + N\,\delta(L - L_c)V\Delta t$$

If $\Delta t \to 0$, $\Delta L \to 0$

$$\frac{\partial \psi(L,t)}{\partial t} + \frac{\partial (G.\psi(L,t))}{\partial L} = N\,\delta(L - L_c)$$

PBE

$G(T,c)$, $N(T)$, $\frac{dU(T)}{dt} = UA(T_e - T) + Q_{fusion}$

The PBE has to be solved together with an energy balance equation , and solute concentration c

# Moments method

It provides values of many characteristic variables of the crystal distribution

$$M_0 = \int_0^\infty \psi(L,t)dL$$ number of particles

$$M_1 = \int_0^\infty L\psi(L,t)dL$$ sum of characteristic lengths

$$M_2 = \int_0^\infty L^2\psi(L,t)dL$$ ~ total area

$$M_3 = \int_0^\infty L^3\psi(L,t)dL$$ ~ total volume

**M1/Mo** ~ mean crystal size **M3/M2** ~ mean square weighted crystal size

$$\varphi(t) = \int_{0 \text{ or } Lc}^{\infty \text{ or } Lmax} \psi(L,t)\frac{\pi L^3}{6}dL = \frac{\pi}{6}M_3$$ Volumetric ice fraction

# Moments method

$$\frac{\partial \psi(L,t)}{\partial t} + \frac{\partial (G.\psi(L,t))}{\partial L} = N\,\delta(L - L_c)$$

Assuming that G is independent of L, which is a sensible assumption, the PBE is multiplied by $L^j$ and integrated (by parts) to obtain the moments.

$$\int_0^\infty \frac{\partial L^j \psi(L,t)}{\partial t} dL + \int_0^\infty L^j \frac{\partial (G.\psi(L,t))}{\partial L} dL = \int_0^\infty L^j N\,\delta(L - L_c) dL$$

$$\frac{\partial}{\partial t}\int_0^\infty L^j \psi(L,t) dL + L^j G \psi(L,t)\Big|_0^\infty - Gj\int_0^\infty \psi(L,t) L^{j-1} dL = L_c^j N$$

$$\boxed{\frac{dM_j}{dt} = j.G.M_{j-1} + L_c{}^j N \qquad j = 0,1,2,\ldots}$$

The solution of this set of ODEs provides the moments $M_j$

# Method of characteristics

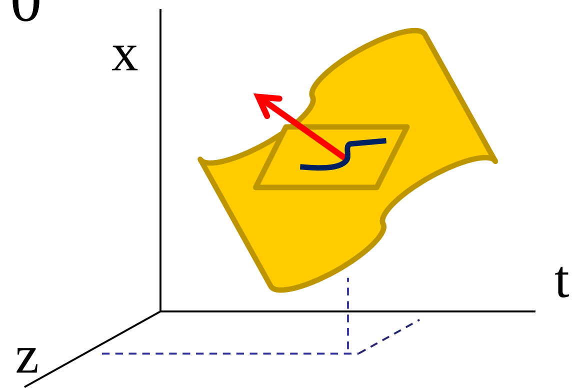
The method will be illustrated using the first order PDE:

$$a(x,z,t)\frac{\partial x(z,t)}{\partial t} + b(x,z,t)\frac{\partial x(z,t)}{\partial z} = c(x,z,t)$$

If x(z,t) is a solution of the PDE, then, at every (z,t), the vector $(x_z, x_t, -1)$ is normal to the surface x = x(z,t)

$$a(x,z,t)x_t(z,t) + b(x,z,t)x_z(z,t) - c(x,z,t) = 0$$

$$[a(x,z,t), b(x,z,t), c(x,z,t)]\begin{bmatrix} x_t(z,t) \\ x_z(z,t) \\ -1 \end{bmatrix} = 0$$




So, at every solution point, the vector [a,b,c] lies in a tangent plane to the solution surface:

$$\frac{dx}{c} = \frac{dz}{b} = \frac{dt}{a}$$

# Method of characteristics

$$\frac{dx(s)}{c(x,z,t)} = \frac{dz(s)}{b(x,z,t)} = \frac{dt(s)}{a(x,z,t)} = ds$$

With the solution parameterized by a parameter s

$$\frac{dt(s)}{ds} = a(x,z,t)$$

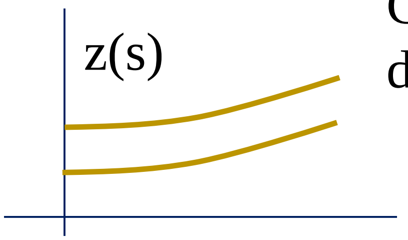
$$\frac{dz(s)}{ds} = b(x,z,t)$$

$$\frac{dx(s)}{ds} = c(x,z,t)$$

The solution of this set of ODE will be equivalent to the solution of the PDE

The solutions x(s) are obtained along the characteristic curves z(s),t(s) for different values of the parameter s

The first order PDE becomes a set of ODEs over the characteristic curves




Curves for different z(0)

# Initial and boundary conditions

$$a(x,z,t)\frac{\partial x(z,t)}{\partial t} + b(x,z,t)\frac{\partial x(z,t)}{\partial z} = c(x,z,t)$$

A family of solutions for different initial z(0)

$$x(z,0) = x_0(z)$$

$$x(0,t) = B_0(t)$$

$$\left.\frac{\partial x(z,t)}{\partial t}\right|_{z=L} = 0$$

$$\frac{dt(s)}{ds} = a(x,z,t)$$

$$\frac{dz(s)}{ds} = b(x,z,t)$$

$$\frac{dx(s)}{ds} = c(x,z,t)$$

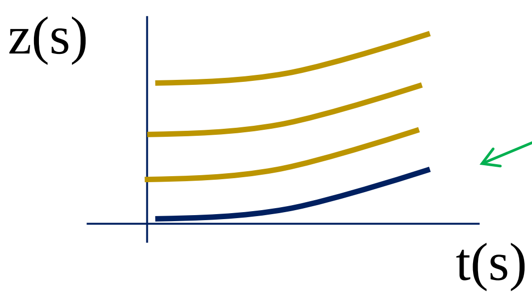
$$t(0) = 0 \qquad z(0) = z_0$$

$$x(z(0),0) = x_0(z)$$

Initial value of x depends on the chosen z

$$x(0,t(s)) = B_0(t)$$

$$\left.\frac{\partial x(z,t(s))}{\partial t}\right|_{z=L} = 0$$



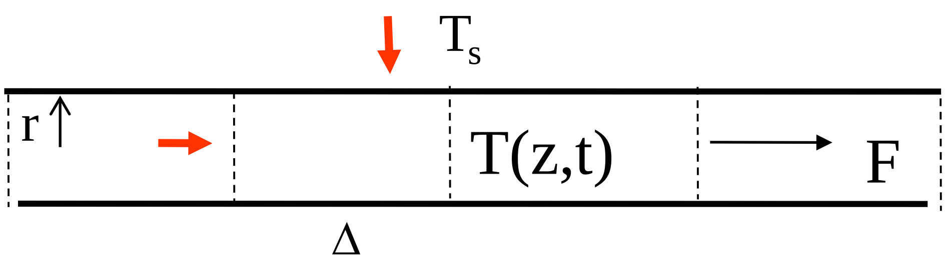

Below this characteristic curve, no solution is computed

# Example: Heated pipe

Integrate over z = [0 2], from t =0 to 15

$$\frac{\partial T(z,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(z,t)}{\partial z} + \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

$$T(z,0) = 20 \qquad T(0,t) = T_0(t)$$




$$a(T,z,t)\frac{\partial x(z,t)}{\partial t} + b(T,z,t)\frac{\partial x(z,t)}{\partial z} = c(T,z,t)$$

$$a(T,z,t) = 1$$

$$b(T,z,t) = \frac{F}{\pi r^2}$$

$$c(T,z,t) = \frac{2U(T_s - T(z,t))}{r\rho c_e}$$

$$\frac{dt}{ds} = 1$$

$$\frac{dz}{ds} = \frac{F}{\pi r^2}$$

$$\frac{dT(s)}{ds} = \frac{2U(T_s - T(s))}{r\rho c_e}$$

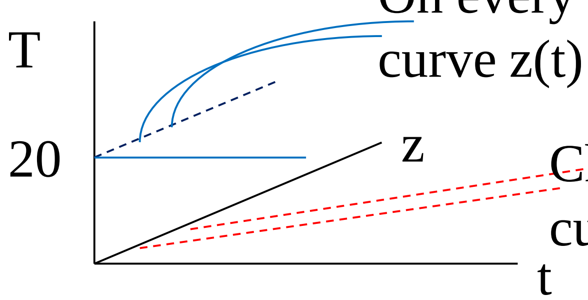
# Example: Heated pipe

$$\frac{dt}{ds} = 1$$

$$\frac{dz}{ds} = \frac{F}{\pi r^2}$$

$$\frac{dT(s)}{ds} = \frac{2U(T_s - T(s))}{r\rho c_e}$$

$$T(z,0) = 20 \qquad T(0,t) = 20$$




$$t = s$$

$$z(s) = \frac{F}{\pi r^2} s + z_0$$

$$T(s) = T_s(1 - e^{-\frac{2U}{r\rho c_e}s}) + T_0$$

$$z(t) = \frac{F}{\pi r^2} t + z_0$$

$$T(t) = T_s(1 - e^{-\frac{2U}{r\rho c_e}t}) + 20$$

On every characteristic curve z(s),t(s)