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Solution procedures for time dependent problems

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Mathematical modelling in science and engineering

Lecture 5 Time dependent problems

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Time dependent form of conservation principles

Differential form for 1D examples from Lecture 1:

- Imbalance of terms in stationary formulations leads to changes of unknown field values in time
- Heat conduction the rate of change in time of the temperature at a point is equal to the imbalance between the heat flux spatial derivative and heat source at the point

$$\frac{\partial T}{\partial t} - \frac{\partial}{dx} \left(k \frac{\partial T}{dx} \right) = s(x, t)$$

• Elastodynamics – the acceleration of a point inside a body is equal to the imbalance between the internal force intensity and the external body force intensity at the point

$$\rho \frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x} \left(E \frac{\partial u}{\partial x} \right) = f(x, t)$$

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Time dependent form of conservation principles

Differential form for time dependent 1D examples from Lecture 1:

- Unknown fields as functions of time and space: T(x, t), u(x, t)
- Partial differential equations with partial derivatives
- Initial condition(s) in addition to boundary conditions
 - for all points inside the computational domain
 - $T(x,0) = T_0(x)$ for non-stationary heat conduction
 - $u(x,0) = u_0(x)$, $\frac{\partial u}{\partial t}(x,0) = v_0(x)$ for elastodynamics
 - initial conditions must agree with boundary conditions
- Initial-boundary value problems
 - $\bullet~$ well posed \rightarrow existence and uniqueness of solutions
- Stationary problems can be considered as limits of non-stationary processes, after reaching steady-state
 - stationary problems can be solved using methods for time dependent problems, with solutions converging to steady-state

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Classification of partial differential equations (PDEs)

- The most common PDEs in scientific and technical applications are second order PDEs (PDEs that involve up to the second order derivatives)
 - all second order linear PDEs can be classified as elliptic, parabolic or hyperbolic
- Stationary problems correspond usually to elliptic PDEs, with the standard form: $\partial \left(\begin{array}{c} \partial u \\ \partial u \end{array} \right)$

$$-\frac{\partial}{\partial x_i} \left(a_{ij} \frac{\partial u}{\partial x_j} \right) = f(\mathbf{x}) \qquad -(a_{ij} u_{,j})_{,i} = f$$

• Non-stationary problems, similar to heat equation, correspond to parabolic PDEs, with the standard form

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x_i} \left(a_{ij} \frac{\partial u}{\partial x_j} \right) = f(\mathbf{x}) \qquad u_{,t} - (a_{ij} u_{,j})_{,i} = f$$

• Non-stationary problems, of the type similar to elastodynamics equations, correspond to hyperbolic PDEs, with the typical form for scalar unknowns:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x_i} \left(a_{ij} \frac{\partial u}{\partial x_j} \right) = f(\mathbf{x}) \qquad u_{,tt} - (a_{ij} u_{,j})_{,i} = f$$

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Classification of partial differential equations (PDEs)

Elliptic partial differential equations:

• prototypical example – Poisson problem (Laplace problem for f=0):

$$\Delta u = f$$
 ($\Delta u = u_{,ii}$ – Laplacian operator)

- elliptic PDEs with the appropriate boundary conditions are prototypical boundary value problems (BVPs)
- the solutions to elliptic problems (BVPs) are smooth in typical situations
- the solutions to elliptic BVPs satisfy the maximum principle
 - when certain conditions are fulfilled the maximum is obtained on the boundary of the domain
- standard formulations of the finite difference and the finite element methods work well for elliptic problems
 - there are usually no problems with stability of solutions (they do not tend to infinity)
 - the systems of linear equations associated with elliptic problems are often (for symmetric coefficient arrays and some other conditions) symmetric and positive definite

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Classification of partial differential equations (PDEs)

Parabolic partial differential equations:

- parabolic equations require initial and boundary conditions for the existence and uniqueness of solutions
 - parabolic equations lead to initial-boundary value problems (IBVPs)
 - the boundary conditions and initial condition(s) must agree
- the solutions are smooth in typical situations (due to the elliptic, second order in space, terms)
 - even for non-smooth initial conditions the solution rapidly smooths out
 - with increasing time the solution further smooths out (the spatial derivatives tend to zero for problems with no sources)
- the systems of linear equations associated with parabolic problems are often (for symmetric coefficient arrays and some other conditions) symmetric and positive definite

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Classification of partial differential equations (PDEs)

Hyperbolic partial differential equations:

- hyperbolic equations require initial and boundary conditions for the existence and uniqueness of solutions
 - hyperbolic equations lead to initial-boundary value problems (IBVPs)
 - the boundary conditions and initial condition(s) must agree
- there exist curves, called characteristics, along which the solution becomes the solution of an ODE
 - for specific cases the solution along characteristics does not change
 - e.g. for discontinuous initial condition(s) the solution remain discontinuous
 - for advection problems in steady velocity fields the characteristics coincide with the streamlines of the velocity field
- hyperbolic problems correspond to wave and transport (convection, advection) phenomena
 - because of that, boundaries are often classified as inflow or outflow boundaries

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Convection equation

• The simplest time dependent problems are first order convection PDEs:

$$\frac{\partial u}{\partial t} + v_i \frac{\partial u}{\partial x_i} = f$$

where v is the convection velocity

- for *v* being the function of *x* only, the equation is linear
- when v is the function of u (or its derivatives), the equation is non-linear
- Boundary conditions:
 - the part of the boundary where the velocity vector points inside is the inflow boundary
 - on the inflow boundary the solution must be specified to indicate what is convected into the computational domain
 - the part of the boundary where the velocity vector points outside is the outflow boundary
 - on the outflow boundary the solution must not be specified to allow for free departure from the computational domain

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Convection equation

• The convection PDE can be written as

$$\left[\frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \ldots\right] \cdot [1, v_1, v_2, \ldots] = f$$

and, hence, becomes the relation for the derivative of u along the spacetime direction $[1, v_1, v_2, ...]$

- The spacetime direction $[1, v_1, v_2, ...]$ (i.e. the velocity field) determines the characteristic curves of the equation, the curves along which the PDE changes to the ODE
 - assuming the curves are parametrized by *s*,

$$(t, x_1, x_2, ...) = (t(s), x_1(s), x_2(s), ...)$$

each curve is the solution of the system of equations:

$$dt/ds = 1 \qquad dx_i/ds = v_i$$

(with the starting point e.g. at time instant t_0 and spatial point x_0)

• along such curves we have:

$$\frac{du}{ds} = f \quad \left(\text{ since } \frac{du}{ds} = \frac{\partial u}{\partial t}\frac{dt}{ds} + \frac{\partial u}{\partial x_i}\frac{dx_i}{ds} = \frac{\partial u}{\partial t} + v_i\frac{\partial u}{\partial x_i} \right)$$

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Convection equation

- The convection PDE requires an initial condition:
 - $u(x, 0) = u_0(x)$
- In case of no source term f
 - the initial "shape" $u_0(\mathbf{x})$ is convected along the direction of velocity \mathbf{v}
- For the 1D case with no source term and constant v the solution is
 - $u(x,t) = u_0(x-vt)$
 - at time instant t_n : $u(x, t_n) = u_0(x vt_n)$
 - the solution is just constant along characteristics $x = x_0 + vt$





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The finite difference method for ODEs and PDEs (recall)

The finite difference method for ODEs and PDEs – approximation of derivatives that appear in equations with formulae that use the values at discrete points:

• based on Taylor's theorem

$$f(x_0+h) = f(x_0) + \frac{f'(x_0)}{1!}h + \frac{f^{(2)}(x_0)}{2!}h^2 + \dots + \frac{f^{(n)}(x_0)}{n!}h^n + R_n(x_0+h)$$

where R_n is the remainder:

$$R_n(x_0+h) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(h)^{n+1} = O(h^{n+1}) \quad \text{for} \quad x_0 < \xi < x_0 + h$$

• for first order derivatives it gives:

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} + O(h)$$

• the formula is first order accurate, i.e. the discretization error is proportional to the first power of the distance (grid size) *h*

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The finite difference method for PDEs (recall)

Approximation of partial derivatives appearing in equations using formulae with the values at discrete points:

- for example, given points $u_{x_{i-1}}^{t_n}, u_{x_i}^{t_n}, u_{x_{i+1}}^{t_n}, u_{x_i}^{t_{n+1}}$ $(u_{x_i}^{t_n} = u(t_n, x_i))$
- and $\Delta t = t_{n+1} t_n$, $\Delta x = x_{i+1} x_i = x_i x_{i-1}$:



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The finite difference method and convection equations

- For the convection equation one of possible simple finite difference formulations is:
 - given the solution at time t_n (for t_0 taken from the initial condition) and each point x_i within the computational domain ...
 - calculate the solution at time t_{n+1} for each point x_i according to the formula: t_{n+1} t_n d_n d_n

$$\frac{u_{x_i}^{t_{n+1}} - u_{x_i}^{t_n}}{\Delta t} + v \cdot \frac{u_{x_{i+1}}^{t_n} - u_{x_i}^{t_n}}{\Delta x} = f(t_n, x_i)$$

• The formulated method is explicit, we do not have to solve a system of equations, but just calculate:

$$u_{x_{i}}^{t_{n+1}} = u_{x_{i}}^{t_{n}} - \Delta t \left(v \cdot \frac{u_{x_{i+1}}^{t_{n}} - u_{x_{i}}^{t_{n}}}{\Delta x} - f(t_{n}, x_{i}) \right)$$

• Usually explicit methods are stable (their solutions do not grow to infinity) only when suitable limits for time steps Δt are satisfied, e.g.:

 $\frac{\Delta t \cdot v}{\Delta x} < CFL_{\text{limit}} \quad (CFL \text{ is the, so called, Courant-Friedrichs-Lewy number})$

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The finite difference method and convection equations

- Hyperbolic problems pose important difficulties for numerical approximation
 - the methods that use characteristics (e.g. find characteristics and then solve the equations along characteristics) are difficult for systems of PDEs (PDEs for vector problems) and do not work well when, as is often found in practice, additional terms (e.g. with second order derivatives) appear in the equations
 - classical finite difference and finite element methods have problems with stability and accuracy (even for small time steps)
 - when exact solutions are not smooth the approximations exhibit spurious oscillations
 - for the finite difference methods, one of possible solutions is to use, so called, upwind differencing, where the choice of the difference formulae used for spatial derivatives depends upon the actual direction of velocity:

$$\frac{u_{x_i}^{t_{n+1}} - u_{x_i}^{t_n}}{\Delta t} + v \cdot \frac{u_{x_i}^{t_n} - u_{x_{i-1}}^{t_n}}{\Delta x} = f(t_n, x_i) \quad \text{for } v > 0$$

$$\frac{u_{x_i}^{t_{n+1}} - u_{x_i}^{t_n}}{\Delta t} + v \cdot \frac{u_{x_{i+1}}^{t_n} - u_{x_i}^{t_n}}{\Delta x} = f(t_n, x_i) \qquad \text{for } v < 0$$

• the above upwind scheme is stable for CFL < 1 and is first order accurate in time and in space

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Accuracy, stability, consistency, convergence

Numerical approximation methods have several properties related to the behaviour of the discretization error $e_h = u - u_h$:

- The step size or grid size parameter *h* is assumed to be the most important parameter in studying the behaviour of *e*_h
 - it can be taken as the largest step size or grid cell (element) size (in the latter case some definition for 2D and 3D grids has to be adopted, e.g. the radius of the smallest ball (circle) that contains each grid cell or the longest element edge for the whole mesh)
- The most important property is the convergence of a numerical method
 - A numerical method converges if some suitable norm of discretization error tends to zero with the discretization parameter *h* going to zero

 $||e_h|| \to 0$ for $h \to 0$

- The order of accuracy of a discretization error specifies how fast the method converges to the exact solution with the step size or grid size tending to zero
 - it does not say how large is the error for a given value of *h*

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Accuracy, stability, consistency, convergence

- Consistency is a measure to which extent the exact solution *u* satisfies the discrete problem
 - A numerical method is consistent if the exact solution satisfies the discrete problem in the limit $h \to 0$
- Stability determines whether the numerical (discrete) solution does not amplifies too much disturbances in problem parameters
 - the stability of numerical schemes correspond to the well-posedness of differential problems (continuous dependence on data)
 - in practical applications stability says whether the numerical solution can grow significantly (e.g. tend to infinity) in some circumstances
 - conditionally stable numerical schemes are stable for specific values of h
 - unconditionally stable schemes are stable for all values of h
- The fundamental theorem of numerical analysis states that the solutions of a scheme that is stable and consistent converge to the exact solution of the discretized problem

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The finite difference method for ODEs (recall)

• There are several fundamental simple finite difference approximations for ODEs of the form du

$$\frac{du}{dt} = f(t, u)$$

• The first order accurate explicit (forward) Euler method:

$$\frac{u^{t_{n+1}}-u^{t_n}}{\Delta t}=f(t_n,u^{t_n}) \qquad \rightarrow \qquad u^{t_{n+1}}=u^{t_n}+\Delta tf(t_n,u^{t_n})$$

• The first order accurate implicit (backward) Euler method:

$$\frac{u^{t_{n+1}} - u^{t_n}}{\Delta t} = f(t_{n+1}, u^{t_{n+1}}) \qquad \to \qquad u^{t_{n+1}} - \Delta t f(t_{n+1}, u^{t_{n+1}}) = u^{t_n}$$

• The second order accurate implicit Crank-Nicolson method:

$$\frac{u^{t_{n+1}}-u^{t_n}}{\Delta t} = \frac{1}{2} \left(f(t_{n+1}, u^{t_{n+1}}) + f(t_n, u^{t_n}) \right) \rightarrow u^{t_{n+1}} - \frac{\Delta t}{2} f(t_{n+1}, u^{t_{n+1}}) = u^{t_n} + \frac{\Delta t}{2} f(t_n, u^{t_n})$$

• Implicit methods are more stable than explicit methods, but require the solution of an algebraic equation, that may be non-linear, at each step

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The finite difference method for ODEs (recall)

Explicit Euler time integration



Stability of time integration - dependence on the size of time step (blue - large, red - small) ... and the type of approximation





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The finite difference method for the heat conduction equation

1D heat conduction equation (no convection - parabolic problem):

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) = s(x, t)$$

- Finite difference approximations:
 - second order derivative in space the most popular approach: central difference

$$\frac{\partial}{dx} \left(k \frac{\partial T}{dx} \right) |_{(t,x_i)} \approx \frac{\partial}{dx} \left(k \frac{T_{x_{i+1}}^t - T_{x_i}^t}{\Delta x} \right) |_{(t,x_i)} \approx k \frac{\frac{T_{x_{i+1}}^t - T_{x_i}^t}{\Delta x} - \frac{T_{x_i}^t - T_{x_{i-1}}^t}{\Delta x}}{\Delta x}$$
$$\approx \frac{k}{\Delta x^2} \left(T_{x_{i+1}}^t - 2T_{x_i}^t + T_{x_{i-1}}^t \right)$$

• the PDE becomes an ODE

$$\frac{dT}{dt}|_{(t,x_i)} = \frac{k}{\Delta x^2} \left(T_{x_{i+1}}^t - 2T_{x_i}^t + T_{x_{i-1}}^t \right) + s(x_i, t) = f(t)$$

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The finite difference method for the heat conduction equation

1D heat conduction equation (no convection - parabolic problem):

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) = s(x, t)$$

- Finite difference approximations:
 - the obtained ODE is solved by one of basic methods, giving:
 - for the explicit Euler method

$$T_{x_i}^{t_n+1} = T_{x_i}^{t_n} + k rac{\Delta t}{\Delta x^2} \left(T_{x_{i+1}}^{t_n} - 2T_{x_i}^{t_n} + T_{x_{i-1}}^{t_n}
ight) + s(x_i, t_n)$$

• for the implict Euler method

$$T_{x_i}^{t_{n+1}} - k \frac{\Delta t}{\Delta x^2} \left(T_{x_{i+1}}^{t_{n+1}} - 2T_{x_i}^{t_{n+1}} + T_{x_{i-1}}^{t_{n+1}} \right) - s(x_i, t_{n+1}) = T_{x_i}^{t_n}$$

• for the Crank-Nicolson method

 $2T_{x_{i}}^{t_{n+1}} - k\frac{\Delta t}{\Delta x^{2}} \left(T_{x_{i+1}}^{t_{n+1}} - 2T_{x_{i}}^{t_{n+1}} + T_{x_{i-1}}^{t_{n+1}} \right) - s(x_{i}, t_{n+1}) = 2T_{x_{i}}^{t_{n}} + k\frac{\Delta t}{\Delta x^{2}} \left(T_{x_{i+1}}^{t_{n}} - 2T_{x_{i}}^{t_{n}} + T_{x_{i-1}}^{t_{n}} \right) + s(x_{i}, t_{n})$

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The finite difference method for the heat conduction equation

1D heat conduction equation (no convection - parabolic problem):

$$\frac{\partial T}{\partial t} - \frac{\partial}{dx} \left(k \frac{\partial T}{dx} \right) = s(x, t)$$

- Finite difference approximations:
 - the finite difference formulae link several values at particular points and time instants, creating, so called, finite difference stencils:



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The combined FEM+FDM approach to the heat conduction equation

1D heat conduction equation (no convection - parabolic problem):

$$\frac{\partial T}{\partial t} - \frac{\partial}{dx} \left(k \frac{\partial T}{dx} \right) = s(x, t)$$

- The combined FEM+FDM approach the method of lines
 - the finite element discretization in space (homogeneous Dirichlet boundary conditions assumed for simplicity)

$$\int_0^1 \frac{\partial T}{\partial t}(x,t)w(x)dx + \int_0^1 k \frac{\partial T}{\partial x} \frac{dw}{dx}dx = \int_0^1 s(x,t) \cdot w(x)dx \quad \forall w \in V_0$$

- since all the functions depending on *x* are integrated, the terms in the equation are functions of time only, ...
- ... and the equation becomes an ODE, that can written in a concise form:

$$(T_{t}, w) + k(T_{x}, w_{x}) = (s, w) \quad \forall w \in V_0$$

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The combined FEM+FDM approach to the heat conduction equation

1D heat conduction equation (no convection - parabolic problem):

$$\frac{\partial T}{\partial t} - \frac{\partial}{dx} \left(k \frac{\partial T}{dx} \right) = s(x, t)$$

- The combined FEM+FDM approach the method of lines
 - the finite difference discretization in time:
 - backward Euler implicit, unconditionally stable, first order accurate

$$\left(\frac{T^{n+1}-T^n}{\Delta t},w\right)+k(T^{n+1}_{,x},w_{,x})=(s(t_n,x),w)\qquad\forall w\in V_0$$

• Crank-Nicolson - implicit, unconditionally stable, second order accurate

$$\left(\frac{T^{n+1}-T^n}{\Delta t},w\right) + \frac{1}{2}k\left(\left(T^{n+1}_{,x},w_{,x}\right) + \left(T^n_{,x},w_{,x}\right)\right) = \frac{1}{2}\left(\left(s(t_{n+1},x),w\right) + \left(s(t_n,x),w\right)\right) \quad \forall w \in V_0$$

- initial condition $T_0(x)$ at t_0 is specified
- boundary condition types are the same as for the stationary problems
- at each time step a system of linear equations is solved

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The combined FEM+FDM approach for non-stationary problems

Non-stationary heat conduction in several space variables - notation

- $T(\mathbf{x}, t)$ temperature as function of time and space
 - $T^n(\mathbf{x}) = T(\mathbf{x}, t^n)$
- assumption for finite element discretization:

$$T(\boldsymbol{x},t) = \sum_{L=1}^{N} \mathrm{T}_{L}(t)\psi_{L}(\boldsymbol{x})$$

 $\mathbf{T}(t) = {\mathbf{T}_L(t)}$ - the set of degrees of freedom for the approximation of *T* • hence

$$\frac{\partial T(\boldsymbol{x},t)}{\partial t} = \sum_{L=1}^{N} \frac{d\mathbf{T}_{L}}{dt} \psi_{L}(\boldsymbol{x}) = \sum_{L=1}^{N} \dot{\mathbf{T}}_{L} \psi_{L}(\boldsymbol{x}) \qquad T^{n}(\boldsymbol{x}) = \sum_{L=1}^{N} \mathbf{T}_{L}^{n} \psi_{L}(\boldsymbol{x})$$

• and $\dot{\mathbf{T}} = \{\dot{\mathbf{T}}_L\}$ $\mathbf{T}^n = \{\mathbf{T}_L^n\}$

• test functions in the standard way:

$$w = \sum_{K=1}^{N} W_{K} \psi_{K}(\boldsymbol{x})$$

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The combined FEM+FDM approach for non-stationary problems

Non-stationary heat equations in several space variables

$$\frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial x_i^2} = s(x, t) \qquad \qquad T_{,t} - k T_{,ii} = s(x, t)$$

• weak formulation (Dirichlet boundary conditions for simplicity)

$$(T_{t}, w) + k(T_{t}, w, i) = (s, w) \quad \forall w \in V_0$$

• finite element space discretization leads to

$$\sum_{L=1}^{N} (\psi_{K}, \psi_{L}) \dot{\mathbf{T}}_{L} + \sum_{L=1}^{N} k \left(\frac{d\psi_{K}}{dx}, \frac{d\psi_{L}}{dx} \right) \mathbf{T}_{L} = (s, \psi_{K}) \text{ for } K = 1, 2, ..., N$$

• that can be written as

 $\mathbf{M}\dot{\mathbf{T}} + \mathbf{K}\mathbf{T} = \mathbf{b}$

with

$$\mathbf{M}_{K,L} = (\psi_K, \psi_L) \quad \mathbf{K}_{K,L} = k \left(\frac{d\psi_K}{dx_i}, \frac{d\psi_L}{dx_i} \right) \quad \mathbf{b}_K^n = (\psi_K, \psi_L) \mathbf{T}_L^n + \Delta t(s(t_n, x), \psi_K)$$

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The combined FEM+FDM approach for non-stationary problems

• FDM for linear ODEs of the form

 $M\dot{T} + KT = b$

• explicit Euler time integration:

$$\mathbf{MT}^{n+1} = \mathbf{MT}^n - \Delta t \mathbf{KT}^n + \Delta t \mathbf{b}^n$$

• implicit Euler time integration:

$$\mathbf{MT}^{n+1} + \Delta t \mathbf{KT}^{n+1} = \mathbf{MT}^n + \Delta t \mathbf{b}^{n+1}$$

• Crank-Nicolson time integration:

$$\mathbf{MT}^{n+1} + \frac{1}{2}\Delta t\mathbf{KT}^{n+1} = \mathbf{MT}^n - \frac{1}{2}\Delta t\mathbf{KT}^n + \frac{1}{2}\Delta t\left(\mathbf{b}^n + \mathbf{b}^{n+1}\right)$$

• the above time integration schemes can be generalized into the so called α -method

$$\mathbf{MT}^{n+1} + \alpha \Delta t \mathbf{KT}^{n+1} = \mathbf{MT}^n - (1 - \alpha) \Delta t \mathbf{KT}^n + \Delta t \left((1 - \alpha) \mathbf{b}^n + \alpha \mathbf{b}^{n+1} \right)$$

with: $\alpha = 0$ - for explicit Euler, $\alpha = 1$ - for implicit Euler, $\alpha = 0.5$ - for
Crank-Nicolson,

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The combined FEM+FDM approach for non-stationary problems

- The method of lines
 - the same discretization steps as for the non-stationary heat equation can be done for other time-dependent problems
 - for first order equations the resulting systems of ordinary differential equations may be written as:

$M\dot{T} + KT = b$

• for second order hyperbolic problems the ODEs have the form:

$\mathbf{M}\ddot{\mathbf{U}} + \mathbf{C}\dot{\mathbf{U}} + \mathbf{K}\mathbf{U} = \mathbf{b}$

- due to interpretations in mechanics the matrix M is usually caled "the mass matrix", while the matrix K is "the stiffness matrix"
- any method, explicit or implicit, can be used to solve the above ODEs
 - typical choices include: the introduced variations of the α -method, Runge-Kutta methods, a family of Newmark methods for second order equations, discontinuous Galerkin time discretization, etc.
 - in order not to solve a system of linear equations at each time step, so called "mass lumping" (diagonalization of **M**) is performed for explicit methods