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Computational Geodynamics

FEM for the 1D advection-diffusion eq

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June 23, 2017



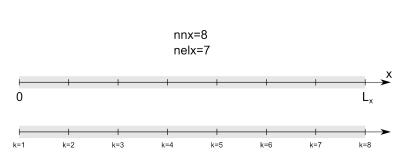


Introduction

From the strong form to the weak form

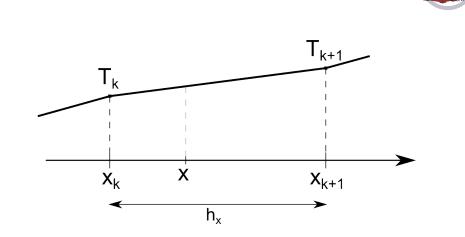
Discretisation

C. Thieulot | FEM for the 1D advection-diffusion equation



- domain Ω of length L_x
- ▶ 1D grid, nnx nodes, nelx elements







We start with the 1D advection-diffusion equation

$$\rho c_{p} \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + H$$

- This is the strong form of the ODE to solve.
- I multiply this equation by a function f(x) and integrate it over Ω :

$$\int_{\Omega} f(x)\rho c_{\rho} \frac{\partial T}{\partial t} dx + \int_{\Omega} f(x)\rho c_{\rho} u \frac{\partial T}{\partial x} dx = \int_{\Omega} f(x) \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x}\right) dx + \int_{\Omega} f(x) H dx$$



I integrate the r.h.s. by parts:

$$\int_{\Omega} f(x) \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) dx = \left[f(x) k \frac{\partial T}{\partial x} \right]_{\partial \Omega} - \int_{\Omega} \frac{\partial f}{\partial x} k \frac{\partial T}{\partial x} dx$$

► Assuming there is no heat flux prescribed on the boundary (i.e. $q_x = -k\partial T/\partial x = 0$), then:

$$\int_{\Omega} f(x) \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) dx = - \int_{\Omega} \frac{\partial f}{\partial x} k \frac{\partial T}{\partial x} dx$$

We then obtain the weak form of the diffusion equation in 1D:

$$\int_{\Omega} f(x)\rho c_{\rho} \frac{\partial T}{\partial t} dx + \int_{\Omega} f(x)\rho c_{\rho} u \frac{\partial T}{\partial x} dx + \int_{\Omega} \frac{\partial f}{\partial x} k \frac{\partial T}{\partial x} dx = \int_{\Omega} f(x) H dx$$

We then use the additive property of the integral:

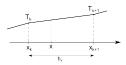
$$\int_{\Omega} \cdots = \sum_{\textit{elts}} \int_{\Omega_{\textit{e}}} \ldots$$

so that

$$\sum_{ells} \left(\underbrace{\int_{\Omega_e} f\rho c_p \frac{\partial T}{\partial t} dx}_{\Lambda_f^e} + \underbrace{\int_{\Omega_e} f\rho c_p u \frac{\partial T}{\partial x} dx}_{\Sigma_f^e} + \underbrace{\int_{\Omega_e} \frac{\partial f}{\partial x} k \frac{\partial T}{\partial x} dx}_{\Upsilon_f^e} - \underbrace{\int_{\Omega_e} fHdx}_{\Omega_f^e} \right) = 0$$





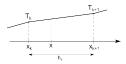


In the element, we have seen that the temperature can be written:

$$\boldsymbol{T}(\boldsymbol{x}) = \boldsymbol{N}_k(\boldsymbol{x}) T_k + \boldsymbol{N}_{k+1}(\boldsymbol{x}) T_{k+1}$$







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In the previous presentation we have computed Λ_f^e and Υ_f^e . Let us now turn to Σ_f^e and Ω_f^e .



$$\Sigma_{f}^{e} = \int_{x_{k}}^{x_{k+1}} f(x) \rho c_{p} u \frac{\partial T}{\partial x} dx$$



$$\Sigma_{f}^{e} = \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{p}u \frac{\partial T}{\partial x} dx$$

$$= \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{p}u \frac{\partial [N_{k}(x)T_{k} + N_{k+1}(x)T_{k+1}]}{\partial x} dx$$



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$$= \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{p}u \frac{\partial N_{k}}{\partial x} T_{k} dx + \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{p}u \frac{\partial N_{k+1}}{\partial x} T_{k+1} dx$$



$$\begin{split} \Sigma_{f}^{\varrho} &= \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{\rho} u \frac{\partial T}{\partial x} dx \\ &= \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{\rho} u \frac{\partial [N_{k}(x)T_{k}+N_{k+1}(x)T_{k+1}]}{\partial x} dx \\ &= \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{\rho} u \frac{\partial N_{k}}{\partial x} T_{k} dx + \int_{x_{k}}^{x_{k+1}} f(x)\rho c_{\rho} u \frac{\partial N_{k+1}}{\partial x} T_{k+1} dx \\ &= \left(\int_{x_{k}}^{x_{k+1}} f(x)\rho c_{\rho} u \frac{\partial N_{k}}{\partial x} dx\right) T_{k} + \left(\int_{x_{k}}^{x_{k+1}} f(x)\rho c_{\rho} u \frac{\partial N_{k+1}}{\partial x} dx\right) T_{k+1} \end{split}$$



• Taking $f(x) = N_k(x)$ and omitting '(x)' in the rhs:

$$\Sigma_{N_{k}} = \left(\int_{x_{k}}^{x_{k+1}} \rho c_{p} u N_{k} \frac{\partial N_{k}}{\partial x} dx\right) T_{k} + \left(\int_{x_{k}}^{x_{k+1}} \rho c_{p} u N_{k} \frac{\partial N_{k+1}}{\partial x} dx\right) T_{k+1}$$



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• Taking $f(x) = N_{k+1}(x)$ and omitting '(x)' in the rhs:

$$\Sigma_{N_{k+1}} = \left(\int_{x_k}^{x_{k+1}} \rho c_p u N_{k+1} \frac{\partial N_k}{\partial x} dx\right) T_k + \left(\int_{x_k}^{x_{k+1}} \rho c_p u N_{k+1} \frac{\partial N_{k+1}}{\partial x} dx\right) T_{k+1}$$



$$\begin{pmatrix} \Sigma_{N_k} \\ \Sigma_{N_{k+1}} \end{pmatrix} = \begin{pmatrix} \int_{x_k}^{x_{k+1}} \rho c_p u N_k \frac{\partial N_k}{\partial x} dx & \int_{x_k}^{x_{k+1}} \rho c_p u N_k \frac{\partial N_{k+1}}{\partial x} dx \\ \int_{x_k}^{x_{k+1}} \rho c_p u N_{k+1} \frac{\partial N_k}{\partial x} dx & \int_{x_k}^{x_{k+1}} \rho c_p u N_{k+1} \frac{\partial N_{k+1}}{\partial x} dx \end{pmatrix} \cdot \begin{pmatrix} T_k \\ T_{k+1} \end{pmatrix}$$

or,



$$\begin{pmatrix} \Sigma_{N_{k}} \\ \Sigma_{N_{k+1}} \end{pmatrix} = \begin{pmatrix} \int_{x_{k}}^{x_{k+1}} \rho c_{p} u N_{k} \frac{\partial N_{k}}{\partial x} dx & \int_{x_{k}}^{x_{k+1}} \rho c_{p} u N_{k} \frac{\partial N_{k+1}}{\partial x} dx \\ \int_{x_{k}}^{x_{k+1}} \rho c_{p} u N_{k+1} \frac{\partial N_{k}}{\partial x} dx & \int_{x_{k}}^{x_{k+1}} \rho c_{p} u N_{k+1} \frac{\partial N_{k+1}}{\partial x} dx \end{pmatrix} \cdot \begin{pmatrix} T_{k} \\ T_{k+1} \end{pmatrix}$$

or,

$$\begin{pmatrix} \Sigma_{N_k} \\ \Sigma_{N_{k+1}} \end{pmatrix} = \begin{bmatrix} \int_{x_k}^{x_{k+1}} \rho C_{\rho} U \begin{pmatrix} N_k \frac{\partial N_k}{\partial x} & N_k \frac{\partial N_{k+1}}{\partial x} \\ N_{k+1} \frac{\partial N_k}{\partial x} & N_{k+1} \frac{\partial N_{k+1}}{\partial x} \end{pmatrix} dx \end{bmatrix} \cdot \begin{pmatrix} T_k \\ T_{k+1} \end{pmatrix}$$



Finally, we have already defined the vectors

$$\mathbf{N}^{T} = \begin{pmatrix} \mathbf{N}_{k}(x) \\ \mathbf{N}_{k+1}(x) \end{pmatrix} \qquad \mathbf{B}^{T} = \begin{pmatrix} \frac{\partial \mathbf{N}_{k}}{\partial x} \\ \frac{\partial \mathbf{N}_{k+1}}{\partial x} \end{pmatrix} \qquad \mathbf{T}^{e} = \begin{pmatrix} T_{k} \\ T_{k+1} \end{pmatrix}$$

so that

$$\begin{pmatrix} \Sigma_{N_k} \\ \\ \Sigma_{N_{k+1}} \end{pmatrix} = \left(\int_{x_k}^{x_{k+1}} \mathbf{N}^T \rho \mathbf{c}_{\mathbf{p}} u \mathbf{B} dx \right) \cdot \mathbf{T}^e$$



Prove that

$$\mathbf{K}_{a}^{e} =
ho c_{p} u \left(egin{array}{cc} -1/2 & 1/2 \ -1/2 & 1/2 \end{array}
ight)$$



Let us now look at the source term:

$$\Omega_f^e = \int_{x_k}^{x^{k+1}} f(x) H(x) dx$$

• Taking $f(x) = N_k(x)$

$$\Omega_{N_k} = \int_{x_k}^{x^{k+1}} N_k(x) H(x) dx$$



Let us now look at the source term:

$$\Omega_f^{\boldsymbol{\varrho}} = \int_{x_k}^{x^{k+1}} f(x) \boldsymbol{H}(x) dx$$

• Taking $f(x) = N_k(x)$

$$\Omega_{N_k} = \int_{x_k}^{x^{k+1}} N_k(x) H(x) dx$$

• Taking $f(x) = N_{k+1}(x)$

$$\Omega_{N_{k+1}} = \int_{x_k}^{x^{k+1}} N_{k+1}(x) H(x) dx$$



$$\begin{pmatrix} \Omega_{N_k} \\ \Omega_{N_{k+1}} \end{pmatrix} = \begin{pmatrix} \int_{x_k}^{x^{k+1}} N_k(x) H(x) dx \\ \int_{x_k}^{x^{k+1}} N_{k+1}(x) H(x) dx \end{pmatrix}$$



$$\begin{pmatrix} \Omega_{N_k} \\ \Omega_{N_{k+1}} \end{pmatrix} = \begin{pmatrix} \int_{x_k}^{x^{k+1}} N_k(x) H(x) dx \\ \int_{x_k}^{x^{k+1}} N_{k+1}(x) H(x) dx \end{pmatrix}$$
$$\begin{pmatrix} \Omega_{N_k} \\ \Omega_{N_{k+1}} \end{pmatrix} = \begin{bmatrix} \int_{x_k}^{x^{k+1}} \begin{pmatrix} N_k(x) H(x) \\ N_{k+1}(x) H(x) \end{pmatrix} dx \end{bmatrix}$$

so that

or,

$$\begin{pmatrix} \Omega_{N_k} \\ \Omega_{N_{k+1}} \end{pmatrix} = \left(\int_{x_k}^{x^{k+1}} \mathbf{N}^T \mathbf{H}(x) dx \right)$$





The weak form discretised over 1 element becomes

$$\underbrace{\left(\int_{x_{k}}^{x_{k+1}} \mathbf{N}^{T} \rho c_{p} \mathbf{N} dx\right)}_{\mathbf{M}^{e}} \cdot \dot{\mathbf{T}}^{e} + \underbrace{\left(\int_{x_{k}}^{x_{k+1}} \mathbf{N}^{T} \rho c_{p} u \mathbf{B} dx\right)}_{\mathbf{K}^{e}_{a}} \cdot \mathbf{T}^{e}$$
$$+ \underbrace{\left(\int_{x_{k}}^{x_{k+1}} \mathbf{B}^{T} k \mathbf{B} dx\right)}_{\mathbf{K}^{e}_{d}} \cdot \mathbf{T}^{e} = \underbrace{\left(\int_{x_{k}}^{x_{k+1}} \mathbf{N}^{T} H(x) dx\right)}_{\mathbf{F}^{e}}$$

or,

$$M^e \cdot \dot{T}^e + (K^e_d + K^e_a) \cdot T^e = F^e$$

or,

$$\boldsymbol{M}^{e} \cdot \frac{\partial \boldsymbol{T}^{e}}{\partial t} + (\boldsymbol{K}^{e}_{a} + \boldsymbol{K}^{e}_{d}) \cdot \boldsymbol{T}^{e} = \boldsymbol{F}^{e}$$

The author wishes to thank 85. Huismans and P. Steer for stimuularing discussions and any reviews of the manuscript. Technical support by Anshui Gupta throughout the code development is apprexiated. This work was funded through howregian Research Connell Corant 1774/80/Y83 and EU. International Reintegration presented in how zero conducted at the Research Cora research of the serve conducted at the Research Cora tainonal Science.¹³ Prof. Tarsa Gerya is thanked for his rapid and constructive review of the manuscript.

Appendix A. FEM formulation of equations

The Galerkin finite element equation corresponding to Eq. (12) is

$$(\boldsymbol{K}_{\mu} + \boldsymbol{K}_{\lambda}) \cdot \boldsymbol{v} = \boldsymbol{E}$$

with

$$\begin{split} & \boldsymbol{K}_{\mu} = \int_{\Omega} \boldsymbol{B}^{T} \cdot \boldsymbol{D}_{\mu} \cdot \boldsymbol{B} d\Omega \\ & \boldsymbol{K}_{\pm} = \int_{\Omega}^{T} \boldsymbol{B}^{T} \cdot \boldsymbol{D}_{\pm} \cdot \boldsymbol{B} d\Omega \\ & \boldsymbol{B} = \int_{\Omega} \boldsymbol{N}^{T} \boldsymbol{p} \boldsymbol{g} d\Omega \\ & \boldsymbol{D}_{\mu}^{D} = \mu \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \boldsymbol{D}_{\pm}^{2D} = \lambda \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{split}$$

and where N is the vector of shape functions, and B is the matrix of spatial derivatives of the shape functions.

The finite element equation corresponding to the heat transfer equation is

$$\begin{split} \mathbf{M}_{c} \cdot \frac{\partial \mathbf{T}}{\partial t} + (\mathbf{K}_{a} + \mathbf{K}_{d}) \cdot \mathbf{T} &= \mathbf{F} \\ \text{where} \\ \mathbf{M}_{c} &= \int_{\Omega} \mathbf{N}^{T} \rho c_{P} \mathbf{N} \, d\Omega \\ \mathbf{K}_{a} &= \int_{\Omega} (\mathbf{N}^{*})^{T} \rho c_{P} \mathbf{\nu} \cdot \mathbf{B} \, d\Omega \end{split}$$

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Thieulot, PEPI 188, 2011



where T is the vector of the nodal temperatures.

In the case where advection dominates over diffusion, the standard Galerkin approach of the advection term leads to problematic oscillations, and a stabilisation scheme is needed. A streamline-upwind Petrov-Galerkin (SUPG) method is therefore implemented, which translates in the modified N^{*} term in Eq. (A1):

 $(N^*)^T = N^T + \tau \boldsymbol{v} \cdot \boldsymbol{B}$

where τ a dimensionless parameter. The case $\tau = 0$ is equivalent to the Bubnov-Galerkin method. The choice of the parameter τ in the context of FEM stabilisation schemes is discussed in Tezduyar and Osawa (2000) and is calculated as follows:

$$\tau = \left(\frac{1}{(\tau_1)^r} + \frac{1}{(\tau_2)^r} + \frac{1}{(\tau_3)^r}\right)^{-1}$$

with often r = 1 or r = 1/2 and

$$\tau_1 = \frac{h}{2|v|}, \quad \tau_2 = \theta dt, \quad \tau_3 = \frac{h^2 \rho c_P}{k}$$
(A.2)

where h is a measure of the element size and θ is related to the time discretistion scheme $|\theta = 1/2$ in this case as it corresponds to the implemented mid-point implicit scheme, see for instance fraun (2023). In order to illustrate the benchfold aspect of the SURG schemetrino rd is scalar field containing a steep from (diffusion and source terms are multi). In Fig. 19 is shown the analytical initial scalar field. It is a challenging benchmark as the numerical treatment oracte terms are multi and the schemetric diffusion and the advection of such a discontinuity often leads to non-negligible oscillations. The unit segment is discretised by means of 30 elenets, over which and unit velocity field is prescribed. The time step placed at n < 1/4 and after 220 time steps, it is expected to have reached the position n < 3/4.

In Fig. 19 are shown the advected field for various values of the dimensionless coefficient y ~t/µ/h. The clarkin scheme (y = 0) leads to strong oscillations, as already described by Donea and Huerta (2003). Using Eq. (A2.) one arrives to y = 0.045, which leads to a desired removal of the oscillations through a small amount of numerical diffusion. Braun (2003) argues for a constant





We start from

$$M \cdot \dot{T} + K \cdot T = F$$

Let us then write this equation at times *t* and $t + \delta t$:

$$\mathbf{M}(t) \cdot \dot{\mathbf{T}}(t) + \mathbf{K}(t) \cdot \mathbf{T}(t) = \mathbf{F}(t)$$

$$\mathbf{M}(t + \delta t) \cdot \dot{\mathbf{T}}(t + \delta t) + \mathbf{K}(t + \delta t) \cdot \mathbf{T}(t + \delta t) = \mathbf{F}(t + \delta t)$$

To insure numerical stability, a second order accurate, mid-point implicit scheme ($\alpha = 0.5$) is used to represent the time derivative of temperature :

$$\frac{T(t+\delta t)-T(t)}{\delta t} = \alpha \dot{T}(t+\delta t) + (1-\alpha) \dot{T}(t)$$

- $\alpha = 0$: fully explicit scheme
- $\alpha = 1$: fully implicit scheme



One can multiply Eq.(1) by 1 – α and Eq. (1) by α and sum them :

$$(1 - \alpha)\mathbf{M}(t) \cdot \dot{\mathbf{T}}(t) + (1 - \alpha)\mathbf{K}(t) \cdot \mathbf{T}(t) = (1 - \alpha)\mathbf{F}(t) +\alpha\mathbf{M}(t + \delta t) \cdot \dot{\mathbf{T}}(t + \delta t) + \alpha\mathbf{K}(t + \delta t) \cdot \mathbf{T}(t + \delta t) + \alpha\mathbf{F}(t + \delta t)$$

Assuming $\boldsymbol{M}(t) \approx \boldsymbol{M}(t + \delta t)$, and $\boldsymbol{F}(t) \approx \boldsymbol{F}(t + \delta t)$, then

$$\boldsymbol{M}(t) \cdot \frac{T(t+\delta t) - T(t)}{\delta t} + (1-\alpha)\boldsymbol{K}(t) \cdot \boldsymbol{T}(t) = \boldsymbol{F}(t) + \alpha \boldsymbol{K}(t+\delta t) \cdot \boldsymbol{T}(t+\delta t)$$

and finally

$$[\boldsymbol{M}(t) + \alpha \boldsymbol{K}(t) \,\delta t] \cdot \boldsymbol{T}(t + \delta t) = [\boldsymbol{M}(t) - (1 - \alpha)\boldsymbol{K}(t) \,\delta t] \cdot \boldsymbol{T}(t) + \boldsymbol{F}(t) \,\delta t$$



Another approach (to arrive at the same result):

$$\boldsymbol{M}\cdot\dot{\boldsymbol{T}}+\boldsymbol{K}\cdot\boldsymbol{T}=\boldsymbol{F}$$

Looking at the Crank-Nicolson algorithm presented earlier, one can write:

$$\boldsymbol{M} \cdot \frac{\boldsymbol{T}(t+\delta t) - \boldsymbol{T}(t)}{\delta t} + \boldsymbol{K} \cdot (\alpha \boldsymbol{T}(t+\delta t) + (1-\alpha)\boldsymbol{T}(t)) = \boldsymbol{F}$$

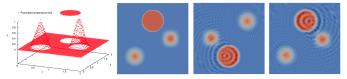
which yields

 $[\boldsymbol{M}(t) + \alpha \boldsymbol{K}(t) \,\delta t] \cdot \boldsymbol{T}(t + \delta t) = [\boldsymbol{M}(t) - (1 - \alpha) \boldsymbol{K}(t) \,\delta t] \cdot \boldsymbol{T}(t) + \boldsymbol{F}(t) \,\delta t$





Advection is notoriously difficult to get right:



- It often needs to be stabilised
- A standard approach is the Streamline Upwind Petrov Galerkin (SUPG) method.
- ► The advection matrix is computed as follows:

$$\mathbf{K}_{a}^{e} = \int_{x_{k}}^{x_{k+1}} (\mathbf{N}^{\star})^{T} \rho c_{\rho} u \mathbf{B} dx \quad \text{with} \quad \mathbf{N}^{\star} = \mathbf{N} + \tau u \mathbf{B}$$

FEM in 1D Advection stabilisation

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where τ a dimensionless parameter. The case $\tau = 0$ is equivalent to the Bubnov-Galerkin method. The choice of the parameter τ in the context of FEM stabilisation schemes is discussed in Tezduyar and Osawa (2000) and is calculated as follows:

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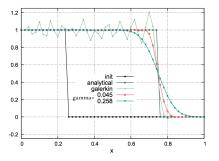


Prove that in the SUPG case

$$(\mathbf{K}_{a}^{e})_{SUPG} = \mathbf{K}_{a}^{e} + \rho c_{p} \frac{\tau u^{2}}{h_{x}} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$



Reproduce the advection example presented in Appendix A of *Thieulot, PEPI 188, 2011* ($\rho = 1, c_p = 1$). Implement the SUPG stabilisation and vary the value of the τ parameter. Implement the implicit, explicit and mid-point algorithms look at their influence on the results.



where
$$\tau = \gamma h / v$$
.