Homeworks for the course on "Numerical Methods for HPC"

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0.1 Finite Element solution of transport-diffusion equation

Consider the transient convection-diffusion equation in 1-D:

$$D\frac{\partial^2 c}{\partial x^2} - v_x\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \qquad 0 \le x \le L, \;\; t \ge 0 \tag{1}$$

with boundary conditions:

$$\begin{cases} c\left(0,x\right) = \overline{c} \\ D\left.\dfrac{\partial c}{\partial x}\right|_{x=L} = \overline{q} \end{cases}$$

Since the differential operator in (1) is not self-adjoint due to the convective term, there is no classical variational principle. To solve the problem it is possible to define a restricted variational principle or slightly modify the differential operator in order to make it self-adjoint. However, the easiest and most convenient way to solve the problem is through the use of the Galerkin method, that will produce exactly the same results that would be produced by a restricted variational principle.

Let us discretize domain L in equal parts of length h by using linear finite elements. The entries of the *stiffness matrix* arising from the Laplace operator $D\nabla^2$ are identically to those arising from the classical variational principle. Hence:

$$\begin{aligned} h_{ii} &= \frac{D}{h^2}\int_{x_{i-1}}^{x_i}\mathrm{d}x + \frac{D}{h^2}\int_{x_i}^{x_{i+1}}\mathrm{d}x = \frac{2D}{h} \\ h_{i,i+1} &= -\frac{D}{h^2}\int_{x_i}^{x_{i+1}}\mathrm{d}x = -\frac{D}{h} \\ h_{i,i-1} &= h_{i,i+1} = -\frac{D}{h} \end{aligned}$$

From the above equations, it is possible to note that H is tridiagonal, symmetric and positive definite (SPD). Let us now compute the entries of the *convective matrix* B that arise from the first derivative of the unknown function. It is easily seen that the integral of ξ_i on a finite element containing node i is $h/2$. It is then obtained:

$$\begin{aligned} b_{ii} &= \int_0^L v_x\frac{\partial \xi_i}{\partial x}\xi_i\mathrm{d}x = \frac{v_x}{h}\int_{x_{i-1}}^{x_i}\xi_i\mathrm{d}x - \frac{v_x}{h}\int_{x_i}^{x_{i+1}}\xi_i\mathrm{d}x = 0 \\ b_{i,i+1} &= \int_0^L v_x\frac{\partial \xi_{i+1}}{\partial x}\xi_i\mathrm{d}x = \frac{v_x}{h}\int_{x_i}^{x_{i+1}}\xi_i\mathrm{d}x = \frac{v_x}{2} \\ b_{i,i-1} &= \int_0^L v_x\frac{\partial \xi_{i-1}}{\partial x}\xi_i\mathrm{d}x = -\frac{v_x}{h}\int_{x_{i-1}}^{x_i}\xi_i\mathrm{d}x = -\frac{v_x}{2} = -b_{i,i+1} \end{aligned}$$

The matrix B is then tridiagonal and emi-symmetric. Finally, the entries of the *capacity* *matrix* P arising from the time dependent term read:

$$\begin{aligned} p_{ii} &= \int_0^L \xi_i^2 \mathrm{d}x = \frac{1}{h^2}\int_0^h x^2 \mathrm{d}x + \frac{1}{h^2}\int_0^h (h-x)^2 \mathrm{d}x = \frac{h}{3}+\frac{h}{3} = \frac{2h}{3} \\ p_{i,i+1} &= \int_0^L \xi_i \xi_{i+1} \mathrm{d}x = \frac{1}{h^2}\int_0^h \left[x\left(h-x\right)\right] \mathrm{d}x = \frac{h}{6} \\ p_{i,i-1} &= \int_0^L \xi_i \xi_{i-1} \mathrm{d}x = p_{i,i+1} = \frac{h}{6} \end{aligned}$$

The P matrix is tridiagonal, and symmetric positive definite (SPD). The right-hand side $\mathbf{q}$ is completely null except the last n-th component where the Neumman condition is acting:

$$q_n = D\left.\frac{\partial c}{\partial x}\right|_{x=L} \xi_n\left(L\right) = \overline{q}$$

The resulting algebraic system reads:

$$\left(H+B\right)\mathbf{c} + P\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}t} - \mathbf{q} = 0 \tag{2}$$

where $\mathbf{c}$ is the vector of unknown nodal concentrations and the entries of the tridiagonal matrices H, B e P are those computed above. The Dirichlet boundary condition on the first node is enforced by substituing the first unknown c_1 with the imposed value $\overline{c}$ in the algebraic system arising from the time integration and updating accordingly the system matrix and the right-hand side, or by simply using the penalty method.

In the 2D case the convection-diffusion equation becomes:

$$\frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right) - v_x\frac{\partial c}{\partial x} - v_y\frac{\partial c}{\partial y} = \frac{\partial c}{\partial t} \tag{3}$$

with boundary conditions:

$$\begin{cases} c\left(x,y,t\right) = \overline{c}, & \forall\ \left(x,y\right)\in\partial\Omega_1 \\ D_x\dfrac{\partial u}{\partial x}n_x + D_y\dfrac{\partial u}{\partial y}n_y = \overline{q}, & \forall\ \left(x,y\right)\in\partial\Omega_2 \end{cases}$$

Let us discretize the Domain Ω with triangular finite elements. Let us use linear basis functions $\xi_i(x,y)$ and, defining $\hat{c}_n$ the approximate solution as a linear combination of the basis functions, let us apply the Galerkin method for $i = 1,\ldots,n$:

$$\int_\Omega\left[\frac{\partial}{\partial x}\left(D_x\frac{\partial \hat{c}_n}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial \hat{c}_n}{\partial y}\right)\right]\xi_i \mathrm{d}\Omega - \int_\Omega\left(v_x\frac{\partial \hat{c}_n}{\partial x} + v_y\frac{\partial \hat{c}_n}{\partial y}\right)\xi_i \mathrm{d}\Omega - \int_\Omega \frac{\partial \hat{c}_n}{\partial t}\xi_i \mathrm{d}\Omega = 0$$

Applying the first Green's identity to the diffusive component, a weak formulation including the Neumman boundary condition as well:

$$\int_\Omega\left(D_x\frac{\partial \hat{c}_n}{\partial x}\frac{\partial \xi_i}{\partial x} + D_y\frac{\partial \hat{c}_n}{\partial y}\frac{\partial \xi_i}{\partial y}\right)\mathrm{d}\Omega + \int_\Omega\left(v_x\frac{\partial \hat{c}_n}{\partial x} + v_y\frac{\partial \hat{c}_n}{\partial y}\right)\xi_i \mathrm{d}\Omega + \int_\Omega \frac{\partial \hat{c}_n}{\partial t}\xi_i \mathrm{d}\Omega = \int_{\partial\Omega_2}\overline{q}\xi_i \mathrm{d}S \tag{4}$$

Substituting $\hat{c}_n$ with its definition:

$$\hat{c}_n = \sum_{j=1}^{n} c_j\left(t\right)\xi_j\left(x,y\right)$$

and computing all the integrals, the differential linear system (2) is obtained that becomes an algebraic system after integration in time through finite differences. This system becomes non-singular after the imposition of Dirichlet boundary conditions on the nodes belonging to $\partial\Omega_1$. The local contributions of the element e on the entries h_{ij} of the stiffness matrix H and p_{ij} of the capacity matrix P read:

$$\begin{aligned} h_{ij}^{(e)} &= \int_{\Delta_e}\left(D_x\frac{\partial\xi_i^{(e)}}{\partial x}\frac{\partial\xi_j^{(e)}}{\partial x}+D_y\frac{\partial\xi_i^{(e)}}{\partial y}\frac{\partial\xi_j^{(e)}}{\partial y}\right)\mathrm{d}x\mathrm{d}y = \frac{D_x b_i b_j + D_y c_i c_j}{4\Delta_e} \\ p_{ij}^{(e)} &= \int_{\Delta_e}\xi_i^{(e)}\xi_j^{(e)}\mathrm{d}x\mathrm{d}y = \begin{cases}\Delta_e/6 & i=j\\ \Delta_e/12 & i\neq j\end{cases}\end{aligned}$$

where b_i, b_j, c_i e c_j are computed using the triangle e coordinates. If i is a node belonging to the Neumman boundary $\partial\Omega_2$, the contribution to the i-th right-hand side component arises from (4):

$$q_i^{(e)} = \int_{\partial\Omega_2^{(e)}}\overline{q}\xi_i^{(e)}\mathrm{d}S = \overline{q}\frac{l^{(e)}}{2} \tag{5}$$

with $l^{(e)}$ the length of the side a triangle belonging to $\partial\Omega_2$ and having the node i as vertex.

The b_{ij} entry of the convective matrix B is given by:

$$b_{ij} = \int_{\Omega}\left(v_x\frac{\partial\xi_j}{\partial x}+v_y\frac{\partial\xi_j}{\partial y}\right)\xi_i\mathrm{d}x\mathrm{d}y \tag{6}$$

Swapping i and j, eq. (6) is changed thus B is non-symmetric, as already pointed out for the 1D case. Assuming v_x and v_y constant over the element e, the local contribution to matrix B is given by:

$$b_{ij}^{(e)} = \int_{\Delta_e}\left(v_x\frac{\partial\xi_j^{(e)}}{\partial x}+v_y\frac{\partial\xi_j^{(e)}}{\partial y}\right)\xi_i^{(e)}\mathrm{d}x\mathrm{d}y = \frac{v_x b_j + v_y c_j}{2\Delta_e}\int_{\Delta_e}\xi_i^{(e)}\mathrm{d}x\mathrm{d}y = \frac{v_x b_j + v_y c_j}{6} \tag{7}$$

It is immediately seen that $b_{ij}^{(e)} \neq b_{ji}^{(e)}$. Very often, the two velocities v_x e v_y are known on the same nodes of the computational grid used to solve the convection-diffusion equation. In such a case, a better approximation than (7) can be obtained by considering the velocities as linear funcions over the triangle e;

$$\begin{aligned} v_x^{(e)} &= v_{x,i}\xi_i^{(e)}\left(x,y\right)+v_{x,j}\xi_j^{(e)}\left(x,y\right)+v_{x,m}\xi_m^{(e)}\left(x,y\right)\\ v_y^{(e)} &= v_{y,i}\xi_i^{(e)}\left(x,y\right)+v_{y,j}\xi_j^{(e)}\left(x,y\right)+v_{y,m}\xi_m^{(e)}\left(x,y\right)\end{aligned}$$

After substituing in (7) and integrating:

$$b_{ij}^{(e)} = \frac{\left(2v_{x,i}+v_{x,j}+v_{x,m}\right)b_j+\left(2v_{y,i}+v_{y,j}+v_{y,m}\right)c_j}{24}$$

After the assembly of all the local contribution in the global matrices H, P, B and right-hand side $\mathbf{q}$, the non-symmetrix differential system (2) is obtained and then integrated in time.

In the general case, for irregular grids and non-uniform velocity field, the B matrix is not exactly emi-symmetric. However, it is very important to emphasize that while matrices H and P are SPD, the transport matrix has different characteristics being close to an emi-symmetric matrix. Let us recall that the eigenvalues of an SPD matrix are real and positive numbers, while those related to an emi-symmetric matrix are null or imaginary conjugate. Let us observe that any matrix A can always be additively split into a symmetrix A_s and emi-symmetric A_{-s} part:

$$A_s = \frac{A + A^T}{2}, \qquad A_{-s} = \frac{A - A^T}{2}$$

The non-symmetric part A_{-s} has a negative impact on the perfomance of the algorithms used to solve the corresponding linear systems. In particular, the iterative methods may converge slowlier, or even fail to converge, if the relative weight of A_{-s} on A is high. In the case of direct methods, non-symmetry may cause numerical instability. For the above reasons, the convection-diffusion equation will be subject to these downside as much as the B component becomes heavier than than H and P.

Finally, let us briefly outline matrices H, P e B in 3D convection-diffusion problems discretized with tetrahedral finite elements. The basis functions $\xi_i^{(e)}(x,y,z)$ associated to node i:

$$\xi_i^{(e)}(x,y,z) = \frac{a_i + b_i x + c_i y + d_i z}{6V_e}$$

where V_e is the signed volume of the element:

$$V_e = \frac{1}{6} \det \begin{bmatrix} 1 & x_i & y_i & z_i \\ 1 & x_j & y_j & z_j \\ 1 & x_k & y_k & z_k \\ 1 & x_m & y_m & z_m \end{bmatrix}$$

and the other entries are:

$$a_i = \det \begin{bmatrix} x_j & y_j & z_j \\ x_k & y_k & z_k \\ x_m & y_m & z_m \end{bmatrix}, \qquad b_i = -\det \begin{bmatrix} 1 & y_j & z_j \\ 1 & y_k & z_k \\ 1 & y_m & z_m \end{bmatrix},$$

$$c_i = \det \begin{bmatrix} 1 & x_j & z_j \\ 1 & x_k & z_k \\ 1 & x_m & z_m \end{bmatrix}, \qquad d_i = -\det \begin{bmatrix} 1 & x_j & y_j \\ 1 & x_k & y_k \\ 1 & x_m & y_m \end{bmatrix}$$

The local contrinutions to the stiffness, capacity and transport read:

$$
\begin{aligned}
h_{ij}^{(e)} &= \int_{V_e} \left(D_x \frac{\partial \xi_i^{(e)}}{\partial x} \frac{\partial \xi_j^{(e)}}{\partial x} + D_y \frac{\partial \xi_i^{(e)}}{\partial y} \frac{\partial \xi_j^{(e)}}{\partial y} + D_z \frac{\partial \xi_i^{(e)}}{\partial x} \frac{\partial \xi_j^{(e)}}{\partial z} \right) \mathrm{d}V = \frac{D_x b_i b_j + D_y c_i c_j + D_z d_i d_j}{36 \left| V_e \right|} \\
p_{ij}^{(e)} &= \int_{V_e} \xi_i^{(e)} \xi_j^{(e)} \mathrm{d}V = \begin{cases} \left| V_e \right| / 10 & i = j \\ \left| V_e \right| / 20 & i \neq j \end{cases} \\
b_{ij}^{(e)} &= \int_{V_e} \left(v_x \frac{\partial \xi_j^{(e)}}{\partial x} + v_y \frac{\partial \xi_j^{(e)}}{\partial y} + v_z \frac{\partial \xi_j^{(e)}}{\partial z} \right) \xi_i^{(e)} \mathrm{d}V = \frac{\left| V_e \right| \left(v_x b_j + v_y c_j + v_z d_j \right)}{24 V_e}
\end{aligned}
$$

The source term $f(x, y, z, t)$ gives the following contribution to the right-hand side:

$$
\int_{V_e} f \xi_i^{(e)} \mathrm{d}V = \frac{|V_e|}{4} \overline{f}^{(e)}
$$

where $\overline{f}^{(e)}$ is the mean value of f over e, and the diffusive flux enforced along the Neumman boundary $\overline{q}$:

$$
\int_{\Gamma_e} \overline{q} \xi_i^{(e)} \mathrm{d}\Gamma = \overline{q}^{(e)} \frac{\Delta_e}{3}
$$

with Γ_e the triangular face of element e belonging to the Neumman boundary and Δ_e its area.