CFD WI4011

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The stationary convection-diffusion equation in 1-D

Study the 1-D convection-diffusion equation:

$$(u\varphi)_{,x} = (\varepsilon\varphi_{,x})_{,x} + q(x) \;, \quad x \in \Omega \equiv (0,1) \;,$$

- Properties can be easily proved
- Both the continuous and discretized problem can be solved exactly

But the 1-D model has limited applicability ☹.
Note that we solve for φ for a given u !!!

The stationary convection-diffusion equation in 1-D

Analytical aspects:

- In the absence of a source term φ is determined only by the *boundary* 'inflow' (diffusive/convective).
- The choice of *boundary conditions* affects the *well-posedness* of the continuous problem for $Pe \gg 1$.
- The solution obeys a *maximum principle*.

The continuous convection-diffusion equation in 1-D (I)

Conservation form

$$\varphi_{,t} = L\varphi + q \;, \quad L\varphi \equiv (u\varphi)_{,x} - (\varepsilon\varphi_{,x})_{,x} = (u\varphi - \varepsilon\varphi_{,x})_{,x} \,.$$

Integrate over Ω:

$$\frac{d}{dt}\int_\Omega \varphi d\Omega = \int_\Omega L\varphi d\Omega + \int_\Omega q d\Omega.$$

Since

$$\int_\Omega L\varphi d\Omega = \left.(u\varphi - \varepsilon\varphi_{,x})\right|_0^1 ,$$

(where $f(x)|_a^b \equiv f(b) - f(a)$),

The continuous convection-diffusion equation in 1-D (II)

$$\frac{d}{dt}\int_\Omega \varphi d\Omega = (u\varphi - \varepsilon\varphi_{,x})|_0^1 + \int_\Omega q d\Omega.$$

If no transport through the boundaries $x = 0, 1$, and if $q = 0$, then

$$\frac{d}{dt}\int_\Omega \varphi d\Omega = 0\,.$$

Therefore $\int_\Omega \varphi d\Omega$ is *conserved*.
A differential operator L, whose integral over Ω reduces to an integral over the boundary, is said to be in *conservation form*.

The continuous convection-diffusion equation in 1-D (III)

Famous example of *nonlinear* convection equation: *Burgers equation*: Conservative form:

$$\varphi_{,t} + \frac{1}{2}\left(\partial\varphi^2\right)_{,x} = 0\,.$$

Non-conservative form:

$$\varphi_{,t} + \varphi\varphi_{,x} = 0\,.$$

In our case we only have *strong* solutions and no *weak* solutions, for which case it is essential to use the conservative form (Lax-Wendroff Theorem, see WI4212).

The exact solution of the *stationary* convection-diffusion equation in 1-D (I)

Start with the nondimensionalized form, with u en k constant.
This makes $u \equiv 1$ and $x \in \Omega \equiv (0, 1)$
Choose $\varepsilon = 1/\mathrm{Pe} \ll 1$ and $q = 0$.

$$\varphi_{,x} = \varepsilon \varphi_{,xx} \ , \quad x \in \Omega \equiv (0, 1) \ ,$$

The flow is from left to right...

The exact solution of the *stationary* convection-diffusion equation in 1-D (II)

Analytic solution: postulate $\varphi = C\mathrm{e}^{\lambda x}$.
This is a solution if

$$\lambda - \varepsilon\lambda^2 = 0\,, \quad \Rightarrow \quad \lambda = 0 \ \text{ or } \ \lambda = 1/\varepsilon\,.$$

General solution:

$$\varphi(x) = C_1 + C_2\mathrm{e}^{x/\varepsilon}\,.$$

Free constants C_1 and C_2 must follow from boundary conditions.
Two boundary conditions are needed...
Can we choose any two we like?

The exact solution of the *stationary* convection-diffusion equation in 1-D (II)

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The influence of boundary conditions on the well posedness of the problem (I).

First try for b.c.:
Dirichlet and *Neumann* condition at $x = 0$:

$$\varphi(0) = a, \quad \varphi_{,x}(0) = b.$$

Information travels with the flow right?
Solution becomes:

$$\varphi(x) = a - \varepsilon b + \varepsilon b \mathrm{e}^{x/\varepsilon} \ .$$

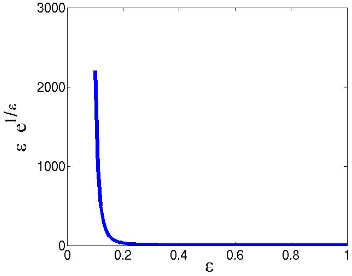
The influence of boundary conditions on the well posedness of the problem (II).

There appears to be something wrong with these boundary conditions

Perturbation of b by an amount $\delta b \;\Rightarrow$ perturbation in $\varphi(1)$:

$$\delta\varphi(1) = \delta b \cdot \varepsilon \mathrm{e}^{1/\varepsilon}\ .$$

$$\frac{|\delta\varphi(1)|}{|\delta b|} \gg 1 \quad \text{if} \quad \varepsilon \ll 1\ .$$



The influence of boundary conditions on the well posedness of the problem (II).

Ill-posed and well-posed:
Ill-posed: large sensitivity to perturbations of data: initial conditions, boundary conditions or coefficients
These perturbations are *always* present, due to representation with finite precision.
Cause: wrong choice for boundary conditions.

The influence of boundary conditions on the well posedness of the problem (III).

Dirichlet at $x = 0$ (inflow),
Neumann at $x = 1$ (outflow):

$$\varphi(0) = a, \quad \varphi(1)_{,x} = b.$$

Solution:

$$\varphi(x) = a + \varepsilon b(\mathrm{e}^{(x-1)/\varepsilon} - \mathrm{e}^{-1/\varepsilon}).$$

Mild sensitivity to perturbations of data.

The influence of boundary conditions on the well posedness of the problem (IV).

Dirichlet at $x = 0$ (inflow),
Dirichlet at $x = 1$ (outflow):

$$\varphi(0) = a, \qquad \varphi(1) = b.$$

Solution:

$$\varphi(x) = a + (b - a)\frac{\mathrm{e}^{x/\varepsilon} - 1}{\mathrm{e}^{1/\varepsilon} - 1}.$$

Again, mild sensitivity to perturbations of data.

The influence of boundary conditions on the well posedness of the problem (V).

To obtain a well-posed problem, the boundary conditions must be correct.
Elliptic PDE: give only one boundary condition at a boundary.
Convection-diffusion equation with $\varepsilon \ll 1$:
Do not prescribe Neumann at inflow boundary.

The maximum principle (I)

The solution of:

$$L[u] = (u\varphi)_{,x} - (\varepsilon\varphi_{,x})_{,x} = q(x), \quad q(x) \leq 0, \quad x \in \Omega = [a, b]$$

Can not have an *interior maximum*.
Local maxima can occur only *at the boundaries*. This is called the *Maximum Principle*
Certainly, not all PDE's fullfill this (hyperbolic PDE's, time-harmonic wave equation)
It is a property of the operator.

The maximum principle (II)

'The simple case': $q < 0$
Assume a local interior maximum at $c \in \langle a, b \rangle$:

$$\varphi(c)_{,x} = 0, \quad \varphi(c)_{,xx} < 0.$$

This leaves a contradiction with the PDE:
Incompressible flow $\Rightarrow u_{\alpha,\alpha} = 0$

$$\varphi(c)u(c)_{,x} - (\varepsilon\varphi(c)_{,x})_{,x} = 0$$

The maximum principle (II)

'The difficult case': $q \leq 0$

$$\tilde{L}[\varphi] = \varphi_{,xx} - \frac{u}{\varepsilon}\varphi_{,x} = -\frac{1}{\varepsilon}q(x) = \tilde{q(x)} \geq 0\,, \quad x \in \Omega\,. \qquad (1)$$

with u bounded on Ω.
Our previous proof of the maximum principle for $L[\varphi] < 0$ corresponds to $\tilde{L}[\varphi] > 0$

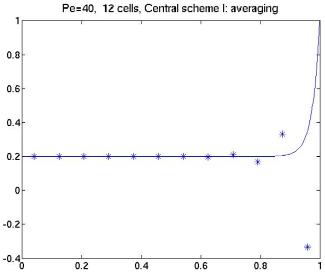
We will construct a solution $w(x)$ for this operator and see that an interior maximum for $w(x)$ would imply $L[w] < 0$ which is impossible ('The simple case').

The maximum principle (IV)

Assume $\varphi(x) \leq M$ in $\langle a, b \rangle$ and the maximum M is attained at interior point $c \in \langle a, b \rangle$ and there is a $d > c : \phi(d) < M$
Define $z(x)$ as

$$z(x) = e^{\alpha(x-c)} - 1 \tag{2}$$

with $\alpha > 0$, a constant to be determined later on.



The maximum principle (V)

$z(x)$ has the following properties:

$$z(x) \begin{cases} < 0 & ; \quad a \leq x < c \\ = 0 & ; \quad x = c \\ > 0 & ; \quad c < x \leq b \end{cases} \tag{3}$$

Substituting $z(x)$ gives:

$$\tilde{L}[z] = z" - \frac{u}{\varepsilon} z' = \alpha \left(\alpha - \frac{u}{\varepsilon} \right) e^{\alpha(x-c)} \tag{4}$$

u is bounded,choose $\alpha > \frac{u}{\varepsilon}$

The maximum principle (VI)

Define

$$w(x) = \phi(x) + \mu z(x), \mu \in \mathbb{R}^+ : \mu < \frac{M - \phi(d)}{z(d)} \qquad (5)$$

Since $\phi(d) < M$ and $z(d) > 0$, it is possible to find such a μ.
Using $z(x) < 0, \forall x \in \langle a, c \rangle$ and $\mu > 0$:

$$x < c \Rightarrow w(x) = \varphi(x) + \mu z(x) < \varphi(x) < M \qquad (6)$$

$$x = c \Rightarrow w(x) = \varphi(x) + \mu z(x) = \varphi(x) = = M \qquad (7)$$

$$x = d (> c) \Rightarrow w(x) = \varphi(x) + \mu z(x) < \varphi(x) + M - \varphi(d) = M \qquad (8)$$

This means $w(x)$ attains a maximum $\bar{M} \geq M$ in $\langle a, b \rangle$. But at the same time $\tilde{L}[w] = \tilde{L}[\phi] + \mu \tilde{L}[z] > 0$!!!.

The maximum principle (VII)

We started our discussion with the proof that when $L[z] < 0$ ($=$ $\tilde{L}[z] > 0$ ☺), z can not attain a maximum at an interior point, so we have a contradiction and the *only other* possibility is that $\phi \equiv M; x \in \langle a, b \rangle$.

So in general the solution φ of

$$L[\phi] = q, \quad q \leq 0$$

will not have internal maxima.

The maximum principle (VIII)

The absence of local internal maxima implies:

- The solution is *monotone*
- If our numerical solution will show oscillations *('wiggles')* these must be a numerical artifact (without even knowing the solution, the wiggles are definitely wrong !)

Important concept of *compatible schemes*, numerical methods that inherit properties of the underlying continuous operator:a Maximum Principle, conservation of energy and/or momentum, dymmetry etc.

Numerical solution of the stationary convection-diffusion equation in 1D (I)

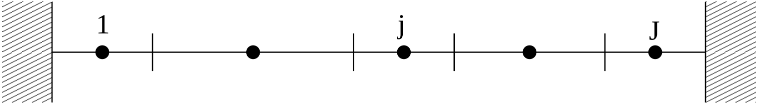
Problem to be solved numerically:

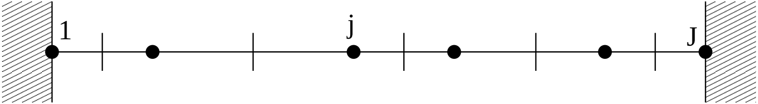
$$L\varphi \equiv (u\varphi)_{,x} - (\varepsilon\varphi_{,x})_{,x} = q, \quad x \in \Omega \equiv (0,1) \,. \quad (2.14)$$

Boundary conditions:
Assume $u(0) > 0, \quad u(1) > 0\,.$
Inflow: Dirichlet: $\varphi(0) = a$.
Outflow: Neumann: $d\varphi(1)/dx = b$,
or Dirichlet: $\varphi(1) = b$.

Numerical solution of the stationary convection-diffusion equation in 1D (II)

Finite volume method:
Subdivide Ω in cells Ω_j, $j = 1, \cdots, J$:
Using a *cell-centered* or a *vertex-centered* grid.





we will consider the *cell-centered* case...

Numerical solution of the stationary convection-diffusion equation in 1D (III)

$h_j = |\Omega_j|$, $\quad x_j$ is center of Ω_j. $x_{j\pm1/2}$ are boundaries of Ω_j.
Integrate over Ω_j :

$$\begin{aligned} \int\limits_{\Omega_j} L\varphi d\Omega &= \int\limits_{\Omega_j} [u\varphi - (\varepsilon\varphi_{,x})]_{,x} = \\ = F|_{j-1/2}^{j+1/2} &= \int\limits_{\Omega_j} q d\Omega \cong h_j q_j \ , \end{aligned}$$

$F|_{j-1/2}^{j+1/2} \equiv F_{j+1/2} - F_{j-1/2}, \quad F_{j\pm1/2} = F(x_{j\pm1/2}),$
$F(x) \equiv u\varphi - \varepsilon\varphi_{,x}.$
$F(x)$ is called the (numerical) *flux*.

Numerical solution of the stationary convection-diffusion equation in 1D (IV)

The resulting scheme can be written as

$$L_h\varphi_j \equiv F_{j+1/2} - F_{j-1/2} = h_j q_j \ , \quad j = 1, \cdots, J,$$

where the subscript h indicates L_h is a *discrete* operator working on a *gridfunction* φ_j.

Numerical solution of the stationary convection-diffusion equation in 1D (V)

The scheme is *conservative* when:

$$\sum_{j=1}^{J} L_h \varphi_j = \sum_{j=1}^{J} \left(F_{j+1/2} - F_{j-1/2} \right) = F_{J+1/2} - F_{1/2} \, .$$

Summation of the integration over all cells leads to a *telescoping sum*

The numerical scheme shares the property of conservation with the continuous operator: an example of *compatibility*

Numerical solution of the stationary convection-diffusion equation in 1D (VI)

Discretization of the flux:
Remember that we are mainly/only interested in using nonuniform grids !!
The value of the variable φ is not available on the cell interfaces, it has to be approximated.
Central scheme I:

$$(u\varphi)_{j+1/2} \cong \frac{1}{2} u_{j+1/2} \varphi_{j+1/2}, \quad \varphi_{j+1/2} = \frac{1}{2}(\varphi_j + \varphi_{j+1}) \,.$$

Here $\varphi_{j+1/2}$ is obtained by averaging, only (second order) accurate on a *uniform grid*, otherwise only first order accurate.

Numerical solution of the stationary convection-diffusion equation in 1D (VII)

One might think that (second order accurate) *linear interpolation* leads to a <u>more accurate solution</u>, this leads to **Central scheme II**

$$\varphi_{j+1/2} = \frac{h_j \varphi_{j+1} + h_{j+1} \varphi_j}{h_j + h_{j+1}} .$$

Surprise: this gives a *less* accurate solution.
This is a case where mathematical analysis can prove the engineer wrong ☺.

Numerical solution of the stationary convection-diffusion equation in 1D (IIX)

Third alternative: one-sided interpolation (first order accurate).
Upwind scheme:

$$
\begin{aligned}
(u\varphi)_{j+1/2} &\cong \frac{1}{2}(u_{j+1/2} + |u_{j+1/2}|)\varphi_j \\
&+ \frac{1}{2}(u_{j+1/2} - |u_{j+1/2}|)\varphi_{j+1} \ .
\end{aligned}
$$

Biased in upstream direction.

Numerical solution of the stationary convection-diffusion equation in 1D (IX)

Fourth alternative: higher order interpolation.
A one parameter family, the so-called κ-scheme (assume $u_{j+1/2} \geq 0$):

$$(u\varphi)_{j+1/2} \cong$$
$$u_{j+1/2}\left\{\frac{(\varphi_j+\varphi_{j+1})}{2}+\frac{1-\kappa}{4}\left(-\varphi_{j-1}+2\varphi_j-\varphi_{j+1}\right)\right\}, \quad u_{j+1/2} \geq 0$$

Scheme	κ
Central	1
QUICK	$\frac{1}{2}$
Second order upwind	-1
Third order upwind	$\frac{1}{3}$

QUICK=Quadratic Upstream Interpolation for Convective Kinematics (Leonard, 1979)

Numerical solution of the stationary convection-diffusion equation in 1D (X)

The diffusive flux:

$$(\varepsilon\varphi_{,x})_{j+1/2} \cong \varepsilon_{j+1/2}(\varphi_{j+1} - \varphi_j)/h_{j+1/2}\,,$$

$$h_{j+1/2} = \frac{1}{2}(h_j + h_{j+1})\;.$$

Numerical solution of the stationary convection-diffusion equation in 1D (XI)

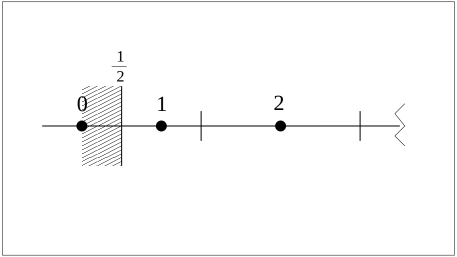
Boundary conditions at the upstream boundary

Diffusive flux at $x_{1/2}$:

$$(\varepsilon\varphi_{,x})_{1/2} \cong \varepsilon_{1/2}(\varphi_1 - \varphi_0)/h_{1/2}\,,$$

Difficulty: φ_0 is outside the domain.

Use the boundary condition to eliminate the contribution of φ_0.



Numerical solution of the stationary convection-diffusion equation in 1D (XII)

Boundary conditions at the upstream boundary
Boundary $x = 0$: Dirichlet:
We know $\varphi_{1/2} = a$

$$(\varepsilon\varphi_{,x})_{1/2} \cong 2\varepsilon_{1/2}(\varphi_1 - a)/h_1 \ .$$

This asymmetric approximation might impair the accuracy. To be investigated later.
Convective flux:

$$(u\varphi)_{1/2} \cong u_{1/2}a \ .$$

Note that despite the Dirichlet boundary condition, no degrees of freedom can be eliminated

Numerical solution of the stationary convection-diffusion equation in 1D (XIII)

Boundary conditions at the downstream boundary

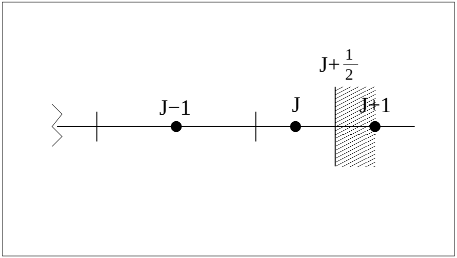
Boundary $x = 1$: Neumann:

Diffusive flux given directly by the boundary condition

$$(\varepsilon\varphi_{,x})_{J+1/2} \cong \varepsilon_{J+1/2} b.$$

For convective flux $u\varphi$, use extrapolation, with $\varphi_{,x}(1) = b$:

$$\varphi_{J+1/2} \cong \varphi_J + h_J b/2\ .$$



Numerical solution of the stationary convection-diffusion equation in 1D (XIV)

The numerical scheme

$$
\begin{aligned}
F_{j+1/2} &= \beta_j^0 \varphi_j + \beta_{j+1}^1 \varphi_{j+1}, \quad j = 1, \cdots, J-1 \,, \\
F_{1/2} &= \beta_1^1 \varphi_1 + \gamma_0 \,, \quad F_{J+1/2} = \beta_J^0 \varphi_J + \gamma_1 \,.
\end{aligned}
$$

$$
L_h \varphi_j = F_{j+1/2} - F_{j-1/2} \quad \Rightarrow (2.31):
$$

$$
L_h \varphi_j = \alpha_j^{-1} \varphi_{j-1} + \alpha_j^0 \varphi_j + \alpha_j^1 \varphi_{j+1} = \tilde{q}_j, \quad j = 1, \cdots, J \,,
$$

with $\alpha_1^{-1} = \alpha_J^1 = 0$.
This is called the numerical or finite volume scheme.

Numerical solution of the stationary convection-diffusion equation in 1D (XV)

General form of a linear scheme:

$$L_h \varphi_j = \sum_{k \in K} \alpha_j^k \varphi_{j+k} = \tilde{q}_j \ ,$$

with K some index set; in our case

$$K = \{-1, \ 0, \ 1\}$$

Stencil $[L_h]$ of the operator L_h:

$$[L_h]_j = [\ \alpha_j^{-1} \quad \alpha_j^0 \quad \alpha_j^1\ ]\ .$$

Numerical solution of the stationary convection-diffusion equation in 1D (XVI)

$$Ay = b\,, \quad y = \begin{bmatrix} \varphi_1 \\ \vdots \\ \varphi_J \end{bmatrix}, \quad b = \begin{bmatrix} \tilde{q}_1 \\ \vdots \\ \tilde{q}_J \end{bmatrix},$$

A is tridiagonal matrix:

$$A = \begin{bmatrix} \alpha_1^0 & \alpha_1^1 & 0 & \cdots & 0 \\ \alpha_2^{-1} & \alpha_2^0 & \alpha_2^1 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & \alpha_{J-1}^{-1} & \alpha_{J-1}^0 & \alpha_{J-1}^1 \\ 0 & \cdots & 0 & \alpha_J^{-1} & \alpha_J^0 \end{bmatrix}.$$

Numerical solution of the stationary convection-diffusion equation in 1D (XVII)

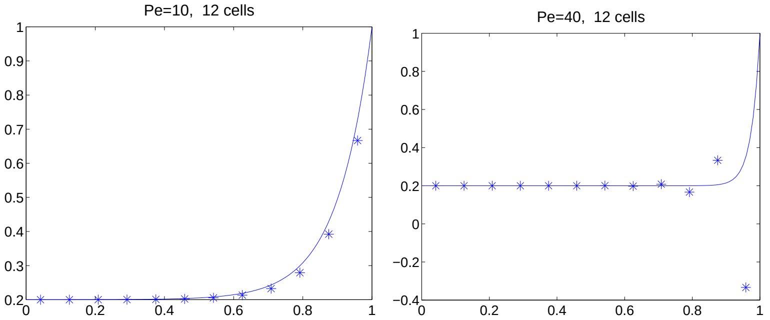
Two important questions

• How well does the numerical solution approximate the exact solution?

• How accurately and efficiently can we solve the linear algebraic system?

Numerical solution of the stationary convection-diffusion equation in 1D (XIIX)

Numerical experiments on uniform grid



Exact solution (—) and numerical solution (*).
Why the *wiggles* for $\mathrm{Pe} = 40$?