Numerical solution of convection-diffusion problems - difference schemes for steady problems.

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Outline

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1D Convection-diffusion problem.

Convection-diffusion problems have very much applications, e.g. the Navier-Stokes equations. Finite Difference schemes for these problems will be studied.

Consider the 1D model problem

$$Lu := -\epsilon u'' + b(x)u' + c(x)u = S(x) \quad \text{on } (0,1); \tag{1}$$

$$u(0) = u_L, \quad u(1) = u_R. \tag{2}$$

where $\epsilon > 0, b(x), c(x) \geq 0$.

The Péclet number is equal to $\text{Pe} = \frac{b}{\epsilon}$.

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Discretization of time.

We have a uniform mesh

$$x_j = jh, j = 0, \ldots, J, \quad x_0 = 0, x_J = 1,$$

such that $b_j = b(x_j), c_j = c(x_j), S_j = S(x_j)$ and

$$U_j \approx u(x_j).$$

The mesh Péclet number is equal to $\beta = bh/\epsilon = \text{Pe}h \geq 0$.

Standard difference notation:

$$\begin{aligned} \Delta_+ U_j &= U_{j+1} - U_j, & \Delta_- U_j &= U_j - U_{j-1}, \\ \delta^2 &= \Delta_+ - \Delta_- = \Delta_+ \Delta_-, & \Delta_0 &= \tfrac{1}{2}(\Delta_+ + \Delta_-), \\ D_\pm &= h^{-1} \Delta_\pm, & D_0 &= h^{-1} \Delta_0. \end{aligned} \quad (3)$$

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Well-known difference schemes.

Central difference scheme:

$$-\epsilon \frac{\delta^2}{h^2} U_j + b_j \frac{\Delta_0}{h} U_j + c_j U_j = S_j \tag{4}$$

Upwind scheme:

$$-\epsilon \frac{\delta^2}{h^2} U_j + b_j \frac{\Delta_-}{h} U_j + c_j U_j = S_j \tag{5}$$

Outline

OCI schemes.

In 1973 Collatz proposed the following schemes for $Lu = S$:

$$\sum_{\nu} p_{j,\nu} U_{j+\nu} = h^2 \sum_{\nu} q_{j,\nu} S_{j+\nu}. \quad (6)$$

The coefficients $\{p_{j,\nu}\}, \{q_{j,\nu}\}$ are to be determined by substituting polynomials $w(x)$ into the scheme:

$$\sum_{\nu} p_{j,\nu} w_{j+\nu} = h^2 \sum_{\nu} q_{j,\nu} w_{j+\nu}. \quad (7)$$

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Three-point OCI schemes.

A three-point scheme has five free parameters:

$$p_j^- U_{j-1} + p_j U_j + p_j^+ U_{j+1} = h^2[q_j^- S_{j-1} + q_j S_j + q_j^+ S_{j+1}]. \quad (8)$$

Normalisation: $q_j^- + q_j + q_j^+ = 1$.

Lemma

For any choice of $\{q_j^-, q_j, q_j^+\}$, the effect of adding the term $c(x)u$ to the operator $-\epsilon u'' + b(x)u'$ is accounted for by making the changes

$$p_j^- \to p_j^- + h^2 q_j^- c_{j-1}, p_j \to p_j + h^2 q_j c_j, p_j^+ \to p_j^+ + h^2 q_j^+ c_{j+1}.$$

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Derivation of standard scheme.

Truncation error

$$\begin{aligned} T_j &:= h^{-2}[p_j^- u_{j-1} + p_j u_j + p_j^+ u_{j+1}] \\ &- [q_j^-(Lu)_{j-1} + q_j(Lu)_j + q_j^+(Lu)_{j+1}] \\ &\equiv T_j^0 u_j + T_j^1 u_j' + \ldots + T_j^p u_j^{(p)} + O(h^{p-1}). \end{aligned}$$

$$T_j^0 = h^{-2}[p_j^- + p_j + p_j^+] \tag{9}$$

$$T_j^1 = h^{-1}[(-p_j^- + p_j^+) - h(q_j^- b_{j-1} + q_j b_j + q_j^+ b_{j+1}) \tag{10}$$

$$T_j^2 = \frac{1}{2}(p_j^- + p_j^+) + \epsilon - h(-q_j^- b_{j-1} + q_j^+ b_{j+1}) \tag{11}$$

$$T_j^m = \frac{h^{m-2}}{m!}[((-1)^m p_j^- + p_j^+) + m(m-1)\epsilon((-1)^m q_j^- + q_j^+) \tag{12}$$

$$- mh((-1)^{m-1} q_j^- b_{j-1} + q_j^+ b_{j+1})], \quad m \geq 3 \tag{13}$$

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Derivation of standard scheme.

The fourth order standard OCI scheme is obtained by setting $T_j^0 = T_j^1 = T_j^2 = T_j^3 = T_j^4 = 0$ such that $T_j^5 = O(h^3)$. Because $q_j^+ - q_j^-$ and $p_j^+ - p_j^-$ are $O(h)$, it even follows that $T_j^5 = O(h^4)$.

It can be verified that for $q_j^- + q_j + q_j^+ = 1$

$$\begin{aligned} q_j^- : q_j : q_j^+ &= 6\epsilon^2 + (5b_j - 2b_{j+1}\epsilon h - b_j b_{j+1} h^2 \\ &: 60\epsilon^2 + 16(b_{j-1} - b_{j+1})\epsilon h - 4b_{j-1} b_{j+1} h^2 \\ &: 6\epsilon^2 + (2b_{j-1} - 5b_j)\epsilon h - b_{j-1} b_j h^2, \end{aligned} \tag{14}$$

while

$$\begin{aligned} p_j &= -(p_j^- + p_j^+) \\ p_j^- &= -\epsilon - \tfrac{1}{2} h(3q_j^- b_{j-1} + q_j b_j - q_j^+ b_{j+1}) \\ p_j^+ &= -\epsilon - \tfrac{1}{2} h(q_j^- b_{j-1} - q_j b_j - 3q_j^+ b_{j+1}). \end{aligned} \tag{15}$$

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Properties of standard OCI scheme.

Assume that $b(x) = b \geq 0$ is constant, so $\beta = bh/\epsilon$.
Characteristic equation:

$$p^+\lambda^2 + p\lambda + p^- = 0. \tag{16}$$

If $p = -(p^- + p^+)$ such that $T_j^0 = O(h)$,
$p^+\lambda^2 + p\lambda + p^- = p^+(\lambda - 1)(\lambda - \frac{p^-}{p^+})$. The root $\mu = \frac{p^-}{p^+}$ satisfies

$$\mu = \frac{24 + 12\beta - \beta^3}{24 - 12\beta + \beta^3}. \tag{17}$$

The scheme gets unwanted numerical oscillations for
$\beta > 2^{\frac{2}{3}}\left((3-\sqrt{5})^{\frac{1}{3}} + (3+\sqrt{5})^{\frac{1}{3}}\right) \approx 4.2.$

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Properties of central difference scheme.

Central difference scheme is also an OCI scheme satisfying $T_j^0 = T_j^1 = T_j^2 = 0$ and $q_j^+ = q_j^- = 0$. Then we get the coefficients: $p^- = -(1 + \frac{1}{2}\beta)\epsilon, p = 2\epsilon, p^+ = (-1 + \frac{1}{2}\beta)\epsilon, q = 1$. The root $\mu = \frac{p^-}{p^+}$ satisfies

$$\mu = \frac{2+\beta}{2-\beta}. \qquad (18)$$

Numerical oscillations occur for $\beta > 2$.
The truncation error satisfies $T_j^3 = \frac{1}{6}h^2 b$.

Properties of upwind scheme.

Upwind scheme is also an OCI scheme satisfying $T_j^0 = T_j^1 = 0, q_j^+ = q_j^- = 0$ and $p_j^+ = -\epsilon$. Now we get the coefficients: $p^- = -(1+\beta)\epsilon, p = (2+\beta)\epsilon, q = 1$. The root $\mu = \frac{p^-}{p^+}$ satisfies

$$\mu = 1 + \beta. \tag{19}$$

Numerical oscillations never occur because $\beta \geq 0$. However, the truncation error satisfies $T_j^2 = O(h)$.

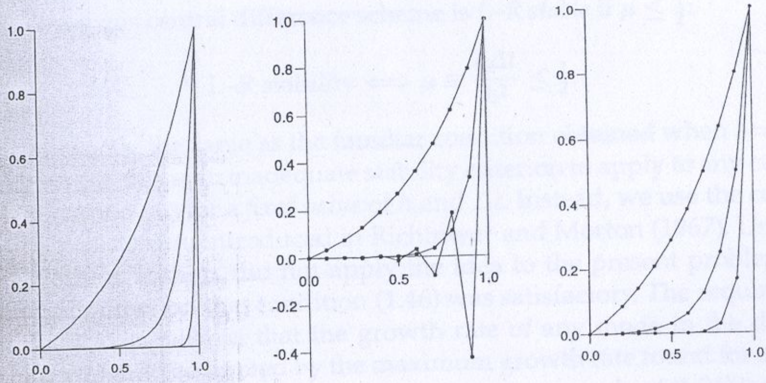

Figure 1.4. *Solutions of the model problem (1.20) with* $S \equiv 0$ *for* $\beta = 0.2, 1.0$ *and* 5.0*; exact (on the left) and approximations with a central (in the centre) and an upwind difference scheme (on the right)*

Adaptive upwind scheme.

$$-\frac{\epsilon}{h^2}\delta^2 U_j + \frac{b_j}{h}[(1-\alpha)\Delta_0 + \alpha\Delta_-]U_j = q_j^- S_{j-1} + (1-q_j^- - q_j^+)S_j + q_j^+ S_{j+1}, \tag{20}$$

where q_j^-, q_j^+ are free and

$$p^- = -\epsilon - \frac{1}{2}(1+\alpha)bh, \quad p^+ = -\epsilon + \frac{1}{2}(1-\alpha)bh. \tag{21}$$

For $\alpha = 0, 1$ we get the central and upwind scheme, respectively. There is no oscillatory solution if $p^+ \leq 0$ or

$$\alpha \geq 1 - 2/\beta. \tag{22}$$

Adaptive upwind scheme.

The scheme is second order if

$$T_j^2 = -bh(\frac{1}{2}\alpha - q^- + q^+) = 0.$$

This can be managed by setting $q^+ = 0, q^- = \frac{1}{2}\alpha, q = 1 - \frac{1}{2}\alpha$. To satisfy also (22) α should be chosen adaptively:

$$\alpha = \begin{cases} 0 & \text{if } \beta \leq 2 \\ 1 - \frac{2}{\beta} \in (0,1) & \text{if } \beta > 2 \end{cases} \tag{23}$$

Adaptive OCI scheme.

Lemma

An OCI scheme satisfies:

- *there are no numerical oscillations;*
- *the tridiagonal system is diagonally dominant;*
- *the scheme satisfies a discrete maximum principle.*

if $p_j^- < 0, p_j^+ \leq 0, p_j \geq -(p_j^- + p_j^+), q_j^- \geq 0, q_j \geq 0, q_j^+ \geq 0.$

Consider an OCI scheme such that

$$q_j^- : q_j : q_j^+ = 6+6\beta_j+3\beta_j^2+r_4\beta_j^3 : 60+30\beta_j+r_3\beta_j^2+r_4\beta_{j-1}\beta_j^2 : 6. \tag{24}$$

If $2b_j \geq \max(b_{j-1}, b_{j+1})$ r_3, r_4 reduce to

$$r_3 = \frac{3}{b_j}(4b_j - b_{j+1}) + \frac{1}{32b_j^2}(3b_{j+1} - 2b_j - b_{j-1})^2, \; r_4 = \frac{1}{2}\frac{r_3 b_j - 3b_{j-1}}{b_j + b_{j-1}}.$$

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Adaptive OCI scheme.

The other coefficients p_j, p_j^-, p_j^+ again satisfy

$$\begin{aligned} p_j &= -(p_j^- + p_j^+) \\ p_j^- &= -\epsilon - \tfrac{1}{2}h(3q_j^- b_{j-1} + q_j b_j - q_j^+ b_{j+1}) \\ p_j^+ &= -\epsilon - \tfrac{1}{2}h(q_j^- b_{j-1} - q_j b_j - 3q_j^+ b_{j+1}). \end{aligned} \quad (25)$$

Theorem

The resulting scheme is fourth order accurate as $h \to 0$ for fixed ϵ and satisfies the conditions of the previous lemma if $b(x)$ is sufficiently smooth.

The fourth order accuracy cannot be maintained uniformly for all ϵ and no error bound holds of the form Ch^δ with C independent of ϵ and $\delta > 0$.

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Introduction.

In 1955 Allen and Southwell were developing methods to approximate incompressible viscous flow about a cylinder. They studied the next incompressible Navier-Stokes equations

$$\frac{\partial^2\psi}{\partial t^2} + \text{Re}\frac{\partial^2\psi}{\partial s^2} = \frac{\zeta}{\Delta^2} \tag{26}$$

$$\frac{\partial^2\zeta}{\partial t^2} + \frac{\partial\psi}{\partial s}\frac{\partial\zeta}{\partial t} + \left[\frac{1}{\text{Re}}\frac{\partial^2\zeta}{\partial s^2} - \frac{\partial\psi}{\partial t}\frac{\partial\zeta}{\partial s}\right] = 0. \tag{27}$$

The vorticity ζ is the solution of the 1D convection-diffusion

$$\frac{1}{\text{Re}}\frac{\partial^2\zeta}{\partial s^2} - \frac{\partial\psi}{\partial t}\frac{\partial\zeta}{\partial s} = S(s) \tag{28}$$

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Allen and Southwell scheme.

Consider the combination of the central and upwind schemes:

$$-\frac{\epsilon}{h^2}\delta^2 U_j + \frac{b_j}{h}[(1-\xi)\Delta_0 + \xi\Delta_-]U_j = S_j \tag{29}$$

with characteristic equation:

$$[1+\frac{1}{2}(\xi-1)\beta_j]\lambda^2 - [2+\xi\beta_j]\lambda + [1+\frac{1}{2}(\xi+1)\beta_j] = 0$$

and roots 1 and $\frac{p_j^-}{p_j^+}$. It the second root is equated to e^{β_j}, this implies that

$$\xi = \coth(\frac{1}{2}\beta_j) - \frac{2}{\beta_j}. \tag{30}$$

Exponentially fitted schemes.

Allen and Southwell scheme:

$$-\left(\frac{b_j}{2h}\coth(\frac{1}{2}\beta_j)\right)\delta^2 U_j + \frac{b_j}{h}\Delta_0 U_j = S_j. \qquad (31)$$

This scheme is first order accurate and satisfies an error bound Ch where C is independent of h and ϵ.

In 1978 El-Mistikawy and Werle proposed another exponentially fitted scheme:

$$p_j^- U_{j-1} + p_j U_j + p_j^+ U_{j+1} = h^2[q_j^- S_{j-1} + q_j S_j + q_j^+ S_{j+1}], \qquad (32)$$

which is second order accurate and also satisfies an error bound Ch^2 where C is independent of h and ϵ.

Both schemes satisfy the conditions of the previous lemma.

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Green's function.

$$(G_j f)(x) := \int_{x_{j-1}}^{x_{j+1}} G_j(x,\eta) f(\eta) d\eta. \tag{33}$$

Introduce the new variable:
$y(x) := u(x) - u_{j-1}\Phi_j^-(x) - u_{j+1}\Phi_j^+(x)$, where Φ_j^-, Φ_j^+ are linear Lagrange interpolation polynomials on $\{x_{j-1}, x_{j+1}\}$. Now y is the solution of a homogeneous BVP:

$$Ly = S - u_{j-1}L\Phi_j^- - u_{j+1}\Phi_j^+, y(x_{j-1}) = y(x_{j+1}) = 0.$$

Thus

$$y = G_j S - u_{j-1} G_j L\Phi_j^- - u_{j+1} G_j L\Phi_j^+.$$

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Locally exact schemes.

Let $G_j^0(.,.)$ be the Green's function for the operator $L - c$, then it also holds that

$$u - u_{j-1}\Phi_j^- - u_{j+1}\Phi_j^+ + G_j^0(L-c)(u_{j-1}\Phi_j^- + u_{j+1}\Phi_j^+) = G_j^0(S - cu). \quad (34)$$

Let G_{jj}^0 be the operator obtained from $G_j^0(x_j,.)$, we can derive:

$$\frac{u_j - u_{j-1}}{x_{j+1} - x_{j-1}}(x_{j+1} - x_j + G_{jj}^0 b) + \frac{u_j - u_{j+1}}{x_{j+1} - x_{j-1}}(x_j - x_{j-1} - G_{jj}^0 b) = G_{jj}^0(S - cu), \quad (35)$$

where $G_{jj}^0 b = [(x_j - x_{j-1})u^R(x_j) - (x_{j+1} - x_j)u^L(x_j)]/E$, while $u^L(x) = \int_{x_{j-1}}^{x} e^{\frac{\int b}{\epsilon}} ds$, $u^R(x) = \int_{x}^{x_{j+1}} e^{\frac{\int b}{\epsilon}} ds$ are the two solutions of $\epsilon u'' + bu' = 0$ with $u^L(x) + u^R(x) = E$.

Locally exact schemes.

Let $G_j^0(.,.)$ be the Green's function for the operator $L-c$, then it also holds that

$$u-u_{j-1}\Phi_j^- - u_{j+1}\Phi_j^+ + G_j^0(L-c)(u_{j-1}\Phi_j^- + u_{j+1}\Phi_j^+) = G_j^0(S-cu). \tag{34}$$

Let G_{jj}^0 be the operator obtained from $G_j^0(x_j,.)$, we can derive:

$$\frac{u_j-u_{j-1}}{x_{j+1}-x_{j-1}}(x_{j+1}-x_j+G_{jj}^0 b)+\frac{u_j-u_{j+1}}{x_{j+1}-x_{j-1}}(x_j-x_{j-1}-G_{jj}^0 b) = G_{jj}^0(S-cu), \tag{35}$$

where $G_{jj}^0 b = [(x_j-x_{j-1})u^R(x_j)-(x_{j+1}-x_j)u^L(x_j)]/E$, while $u^L(x)=\int_{x_{j-1}}^{x} e^{\frac{\int b}{\epsilon}} ds$, $u^R(x)=\int_{x}^{x_{j+1}} e^{\frac{\int b}{\epsilon}} ds$ are the two solutions of $\epsilon u''+bu'=0$ with $u^L(x)+u^R(x)=E$.

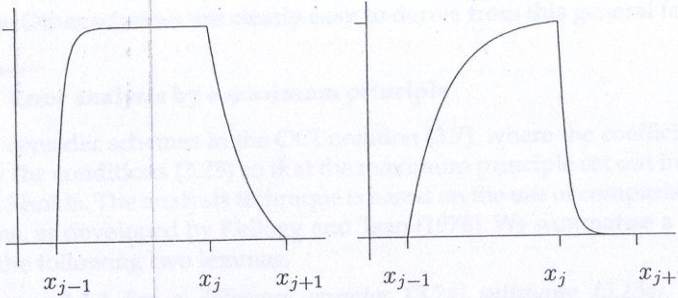

Figure 3.2. *The Green's function* $G_j^0(x_j, \eta)$ *for constant* b *corresponding to* $\beta = 10$ *in* (x_{j-1}, x_j) *and* $\beta = 5$ *in* (x_j, x_{j+1})*, on the left; the values of* β *are interchanged, on the right*

Locally exact scheme.

It is possible to rewrite the locally exact scheme as

$$(u_j-u_{j-1})\frac{\epsilon u^R}{u^R E^L + u^L E^R}+(u_j-u_{j+1})\frac{\epsilon u^L}{u^R E^L + u^L E^R} = \frac{G^0_{jj}(S-cu)}{G^0_{jj}(1)}, \tag{36}$$

where

$$u^L = \frac{\epsilon}{b_j^-}(1-e^{-\beta_j^-}), \qquad u^R = \frac{\epsilon}{b_j^+}(e^{\beta_j^+}-1)$$
$$E^L = \frac{\epsilon h_j^-}{b_j^-}\left[1-\frac{1}{\beta_j^-}(1-e^{-\beta_j^-})\right], \quad E^R = \frac{\epsilon h_j^+}{b_j^+}\left[\frac{1}{\beta_j^+}(e^{\beta_j^+}-1)-1\right]. \tag{37}$$

Locally exact schemes.

The term $G^0_{jj}(S - cu)$ can be approximated by the G^0_j-weighted trapezoidal method:

$$q_j^- = \frac{1}{2}\frac{u^R E^L}{u^R E^L + u^L E^R}, q_j^+ = \frac{1}{2}\frac{u^L E^R}{u^R E^L + u^L E^R}. \qquad (38)$$

This scheme is equivalent to the El-Mistikawy and Werle scheme, but the Allen and Southwell scheme can also be derived.

Outline

2D convection-diffusion problem.

General multi-dimensional convection-diffusion problems require the use of flexible meshes, which is best accomplished by finite element or finite volume formulations.

Model problem:

$$Lu := -\epsilon \nabla u + \mathbf{b} \cdot \nabla u + cu = S \quad \text{on } \Omega \subset \mathbb{R}^2; \tag{39}$$

$$u = u_B \text{ on } \partial\Omega_D, \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega_N. \tag{40}$$

Operator decomposition:

$$Lu = L^{(x)}u + L^{(y)}u,$$

with

$L^{(x)}u := -\epsilon \frac{\partial^2 u}{\partial x^2} + b^{(x)} \frac{\partial u}{\partial x} + \frac{1}{2} cu$, $L^{(y)}u := -\epsilon \frac{\partial^2 u}{\partial y^2} + b^{(y)} \frac{\partial u}{\partial y} + \frac{1}{2} cu$.

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Typical difference schemes.

For decomposed operator $L = L^{(x)} + L^{(y)}$ each part can be approximated by an 1D difference scheme, e.g.

$$-\epsilon \nabla_h^2 U_P + b_P^{(x)} D_{x-} U_P + b_P^{(y)} D_{y-} U_P + c_P U_P = S_P \qquad (41)$$

where $\nabla_h^2 U_P := \frac{1}{(\Delta x)^2} \delta_x^2 U_P + \frac{1}{(\Delta y)^2} \delta_y^2 U_P$.

A rectangular grid gets difficulties with boundary conditions at a non-rectangular domain. For the Neumann boundary conditions one can use the approximation

$$U_N - U_P = 0$$

but it is better to use:

$$\frac{U_N - U_P}{\Delta y} \cos(\theta) + \frac{U_P - U_W}{\Delta x} \sin(\theta) = 0.$$

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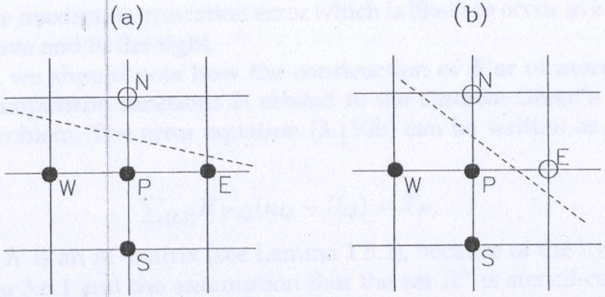

Figure 3.3. *Typical mesh configurations at a Neumann boundary: (a) with one exterior point; (b) with two exterior points*

Crosswind diffusion.

Consider the scheme:

$$-\epsilon\nabla_h^2 U_P + b_P^{(x)}\left[(1-\alpha^{(x)})D_{x0} + \alpha^{(x)}D_{x-}\right]U_P \\ + b_P^{(y)}\left[(1-\alpha^{(y)})D_{y0} + \alpha^{(y)}D_{y-}\right]U_P = 0 \qquad (42)$$

with truncation error
$T_P = -\frac{1}{2}\left[\alpha^{(x)}b^{(x)}\Delta x\frac{\partial^2 u}{\partial x^2} + \alpha^{(y)}b^{(y)}\Delta y\frac{\partial^2 u}{\partial y^2}\right]_P + O(h^2)$. Consider the coordinate system with ξ, η the flow and crosswind directions, respectively.

Crosswind diffusion.

If $b^{(x)} = b\cos(\theta), b^{(y)} = b\sin(\theta)$ and $\Delta x = \Delta y = h$,

$$\begin{aligned} T_p &= -\tfrac{1}{2}bh(\alpha^{(x)}\cos^3(\theta) + \alpha^{(y)}\sin^3(\theta))\tfrac{\partial^2 u}{\partial \xi^2} \\ &+ bh\cos(\theta)\sin(\theta)(\alpha^{(x)}\cos(\theta) - \alpha^{(y)}\sin(\theta))\tfrac{\partial^2 u}{\partial \xi \partial \eta} \\ &- \tfrac{1}{2}bh\cos(\theta)\sin(\theta)(\alpha^{(x)}\sin(\theta) + \alpha^{(y)}\cos(\theta))\tfrac{\partial^2 u}{\partial \eta^2} + O(h^2). \end{aligned} \tag{43}$$

If $\alpha^{(x)} > 0, \alpha^{(y)} > 0$ to damp the numerical oscillations, it gives also an enhanced crosswind diffusion expressed by the $\partial^2 u/\partial \eta^2$ term. This is worst when the flow is diagonal to the mesh. The skew upstream differencing scheme of Raithby (1976) tries to avoid this problem.

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- Central and upwind schemes
- Operator Compact Implicit schemes
- Numerical oscillations
- Green's functions
- Locally exact schemes
- 2D steady convection-diffusion problem
- Crosswind diffusion

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