1 Vertical viscosity and diffusion operators in ROMS

The purpose of this document is to provide sufficient technical detail for the implicit solvers in ROMS code. Although the mathematical concepts are fairly standard – typically a Gaussian elimination procedure for tri-diagonal matrix problem – the practical implementation in ROMS always use high-computational-density "on fly" approach characterized by computing coefficients within the loops associated with elimination sweeps (hence it is not possible to apply a generic tri-diagonal solver without introducing additional temporal arrays), computation "in place" and reuse of provisional arrays (so the same FORTRAN object may be associated with different mathematical terms). This in its turn, makes it somewhat difficult to identify all mathematical steps in the actual code.

1.1 Implicit solution for vertical viscosity and diffusion terms using finite differences

Consider time-implicit, finite-difference discretization for advection-diffusion equation,

$$\frac{\partial q}{\partial t} = \mathrm{rhs}_q + \frac{\partial}{\partial z}\left[A\frac{\partial q}{\partial z}\right] \tag{1.1}$$

where q is a generic field, which may be either a tracer field, Θ, S, or horizontal momentum component, u, v. A is vertical diffusion coefficient, and rhs_q represents all other terms (advection, Coriolis, pressure gradient, lateral diffusion and viscosity, etc).

Assuming a set of vertical grid-boxes of height H_k, $k = 1, ..., N$, backward-Euler time stepping for viscous/diffusive terms, finite-difference approximation for vertical gradients, and overall finite-volume framework, the discretized form of the above becomes
$k = N$

$$H_N q_N^{n+1} = H_N q_N^n + \Delta t \,\cdot \mathrm{rhs}_N + \Delta t \,\cdot \mathit{SRFRC} - \Delta t\, A_{N-1/2}\frac{q_N^{n+1} - q_{N-1}^{n+1}}{\Delta z_{\,N-1/2}} \tag{1.2}$$

$k = 2, ..., N-1$

$$H_k q_k^{n+1} = H_k q_k^n + \Delta t \,\cdot \mathrm{rhs}_k + \Delta t\, A_{k-1/2}\frac{q_k^{n+1} - q_{k-1}^{n+1}}{\Delta z_{\,k-1/2}} - \Delta t\, A_{k+1/2}\frac{q_{k+1}^{n+1} - q_k^{n+1}}{\Delta z_{\,k+1/2}} \tag{1.3}$$

$k = 1$

$$H_1 q_1^{n+1} = H_1 q_1^n + \Delta t \,\cdot \mathrm{rhs}_1 + \Delta t\, A_{3/2}\frac{q_2^{n+1} - q_1^{n+1}}{\Delta z_{\,3/2}} \tag{1.4}$$

where SRFRC is surface forcing term: kinematic winds stress components, or air-sea interaction fluxes. The indexing rules are standard for ROMS: whole-integer k-indexed objects are placed inside grid boxes H_k, and typically should be interpreted as grid-box averages of the associate field, while half-integer $(k+1/2)$-indexed objects are defined at grid-box interfaces and are to be understood as instantaneous values at that locations. Vertical index $N+1/2$ indicates location exactly at the free surface, while $1/2$ exactly at the bottom [1].

The above can be rewritten as a tri-diagonal problem,

$$-\frac{\Delta t\, A_{N-1/2}}{\Delta z_{\;N-1/2}} q_{N-1}^{n+1} + \left(H_N + \frac{\Delta t\, A_{N-1/2}}{\Delta z_{\;N-1/2}} \right) q_N^{n+1} = H_N q_N^n + \Delta t\ \cdot \mathrm{rhs}_N + \Delta t\ \cdot \mathit{SRFRC} \tag{1.5}$$

$$-\frac{\Delta t\, A_{k-1/2}}{\Delta z_{\;k-1/2}} q_{k-1}^{n+1} + \left(H_k + \frac{\Delta t\, A_{k-1/2}}{\Delta z_{\;k-1/2}} + \frac{\Delta t\, A_{k+1/2}}{\Delta z_{\;k+1/2}} \right) q_k^{n+1} - \frac{\Delta t\, A_{k+1/2}}{\Delta z_{\;k+1/2}} q_{k+1}^{n+1} = H_k q_k^n + \Delta t\ \cdot \mathrm{rhs}_k \tag{1.6}$$

$$\left(H_1 + \frac{\Delta t\, A_{3/2}}{\Delta z_{\;3/2}} \right) q_1^{n+1} - \frac{\Delta t\, A_{3/2}}{\Delta z_{\;3/2}} q_2^{n+1} = H_1 q_1^n + \Delta t\ \cdot \mathrm{rhs}_1 \tag{1.7}$$

where all unknowns, q_k^{n+1}, are collected in l.h.s., and all terms in r.h.s. are considered to be known. The above system has the property of *diagonal dominance*: the central coefficient, that is coefficient in front of q_k^{n+1} in kth equation is greater in its absolute value that the sum of absolute values of the other two coefficients, for q_{k-1}^{n+1} and q_{k+1}^{n+1}, as long as all $\Delta t\, A_{k+1/2} > 0$. This ensures well-posedness and stability of the problem, which can be solved by Gaussian elimination.

The procedure begins with converting the ($k = 1$)th equation into

$$q_1^{n+1} - c_{3/2}^* q_2^{n+1} = d_1^*\,, \quad \text{where} \quad \begin{cases} c_{3/2}^* = b^* \dfrac{\Delta t\, A_{3/2}}{\Delta z_{\;3/2}} \\ d_1^* = b^* \left(H_1 q_1^n + \Delta t\ \cdot \mathrm{rhs}_1 \right) \end{cases} \quad \text{and} \quad b^* = \frac{1}{H_1 + \dfrac{\Delta t\, A_{3/2}}{\Delta z_{\;3/2}}} \tag{1.8}$$

and, subsequently, transforming all other equations for $k = 2, ..., N-1$ one-by-one using the previously transformed ones to eliminate terms containing q_{k-1}^{n+1}. Thus, the pair of *transformed* ($k-1$)th and *old* kth equations

$$q_{k-1}^{n+1} \qquad -c_{k-1/2}^* \times \qquad q_k^{n+1} \qquad = d_{k-1}^*$$

$$-\frac{\Delta t\, A_{k-1/2}}{\Delta z_{\;k-1/2}} q_{k-1}^{n+1} + \left(H_k + \frac{\Delta t\, A_{k-1/2}}{\Delta z_{\;k-1/2}} + \frac{\Delta t\, A_{k+1/2}}{\Delta z_{\;k+1/2}} \right) q_k^{n+1} - \frac{\Delta t\, A_{k+1/2}}{\Delta z_{\;k+1/2}} q_{k+1}^{n+1} = H_k q_k^n + \Delta t\ \cdot \mathrm{rhs}_k$$

yields the *transformed* kth,

$$q_k^{n+1} - c_{k+1/2}^* q_{k+1}^{n+1} = d_k^* \qquad \text{where} \quad \begin{cases} c_{k+1/2}^* = b^* \dfrac{\Delta t\, A_{k+1/2}}{\Delta z_{\;k+1/2}} \\ d_k^* = b^* \left[H_k q_k^n + \Delta t\ \cdot \mathrm{rhs}_k + c_{k-1/2}^* d_{k-1}^* \right] \end{cases} \tag{1.9}$$

[1] Because indices in a `FORTRAN` code are always whole-integer, one must adopt an $1/2$-shift convention to map half-integer $k+1/2$. The standard convention in ROMS is start indexing of W-point-type variables from 0, so the mathematical range of $k + 1/2 \in \{1/2,\ 3/2,\ \dots, N + 1/2\}$ corresponds to `FORTRAN` range of `k` $\in$ (`0 : N`).

and the common multiplier $b^* = 1 \Big/ \left[H_k + \frac{\Delta t\, A_{k-1/2}}{Dz_{k-1/2}} \left(1 - c^*_{k-1/2}\right) + \frac{\Delta t\, A_{k+1/2}}{\Delta z_{\ k+1/2}} \right]$.

When the above procedure – called *forward elimination* – reaches the $k = N$, it yields a 2×2 linear system for q_{N-1} and q_N,

$$
\begin{aligned}
q^{n+1}_{N-1} \qquad & -c^*_{N-1/2} \times \qquad q^{n+1}_N = d^*_{N-1} \\
-\frac{\Delta t\, A_{N-1/2}}{\Delta z_{\ N-1/2}} q^{n+1}_{N-1} & + \left(H_N + \frac{\Delta t\, A_{N-1/2}}{\Delta z_{\ N-1/2}} \right) q^{n+1}_N = H_N q^n_N + \Delta t\ \cdot \mathrm{rhs}_N + \Delta t\ \cdot \mathit{SRFRC}
\end{aligned}
\tag{1.10}
$$

which is solved directly

$$
q^{n+1}_N = \frac{H_N q^n_N + \Delta t\ \cdot \mathrm{rhs}_N + \Delta t\ \cdot \mathit{SRFRC} + \frac{\Delta t\, A_{N-1/2}}{\Delta z_{\ N-1/2}} d^*_{N-1}}{H_N + \frac{\Delta t\, A_{N-1/2}}{\Delta z_{\ N-1/2}} \left(1 - c^*_{N-1/2}\right)}
\tag{1.11}
$$

and, subsequently

$$
q^{n+1}_k = d^*_k + c^*_{k+1/2} q^{n+1}_{k+1} \qquad \forall\ k = N-1, N-2, \ldots, 1
\tag{1.12}
$$

which is *back-substitution* sweep. Note that by coefficients $c^*_{k+1/2}$ are all non-dimensional, and $0 < c^*_{k+1/2} < 1$ for all $k = 1, \ldots, N-1$, as the consequence of diagonal dominance property mentioned above. Also note that, once surface forcing is imposed as specified flux, the surface viscosity/diffusion coefficient $A_{N+1/2}$ does not participate in any computation: in fact, the updated values of q^{n+1}_k do not depend on it. As a consequence, for example, there is no singularity when $A_{N+1/2} = 0$ (as it happens in several turbulent closure schemes, where $A \to 0$ as z approaches free surface), even thought the underlying physical problem is singular and requires some kind of regularization (typically via a roughness length) to ensure a finite limit of A.

Alternatively one can start Gaussian elimination from surface,

$$
-a^*_{N-1/2} q^{n+1}_{N-1} + q^{n+1}_N = d^*_N \quad \text{where} \quad
\begin{cases}
a^*_{N-1/2} = b^* \cdot \frac{\Delta t\, A_{N-1/2}}{\Delta z_{\ N-1/2}} \\
d^*_N = b^* \cdot \left[H_N q^n_N + \Delta t\ \cdot \mathrm{rhs}_N + \Delta t\ \cdot \mathit{SRFRC} \right]
\end{cases}
\tag{1.13}
$$

and $b^* = 1 \Big/ \left[H_N + \frac{\Delta t\, A_{N-1/2}}{\Delta z_{\ N-1/2}} \right]$. Then proceed for all $k = N-1, \ldots, 2$, descending, as

$$
-a^*_{k-1/2} q^{n+1}_{k-1} + q^{n+1}_k = d^*_k \quad \text{where} \quad
\begin{cases}
a^*_{k-1/2} = b^* \cdot \frac{\Delta t\, A_{k-1/2}}{\Delta z_{\ k-1/2}} \\
d^*_k = b^* \cdot \left[H_k q^n_k + \Delta t\ \cdot \mathrm{rhs}_k + a^*_{k+1/2} d^*_{k+1} \right]
\end{cases}
\tag{1.14}
$$

along with $b^* = 1 \Big/ \left[H_N + \frac{\Delta t\, A_{k-1/2}}{\Delta z_{\ k-1/2}} + \frac{\Delta t\, A_{k+1/2}}{\Delta z_{\ k+1/2}} \cdot \left(1 - a^*_{k+1/2}\right) \right]$. When the bottom-most grid box is reached,

$$-a^*_{3/2} q_1^{n+1} + q_2^{n+1} = d_2^* \tag{1.15}$$

combined with the bottom boundary condition yields 2×2-matrix problem for q_1^{n+1} and q_2^{n+1}, for example no-flux (no-stress) bottom boundary condition

$$H_1 q_1^{n+1} = H_1 q_1^n + \Delta t\ \cdot \mathrm{rhs}_1 + \Delta t\, A_{3/2} \frac{q_2^{n+1} - q_1^{n+1}}{\Delta z_{\ 3/2}} \tag{1.16}$$

yields

$$q_1^{n+1} = \frac{H_1 q_1^n + \Delta t\ \cdot \mathrm{rhs}_1 + \dfrac{\Delta t\, A_{3/2}}{\Delta z_{\ 3/2}} \cdot d_2^*}{H_1 + \dfrac{\Delta t\, A_{3/2}}{\Delta z_{\ 3/2}} \cdot \left(1 - a^*_{3/2}\right)} \tag{1.17}$$

after which all other q_k^{n+1} are computed recursively (backsubstituted) via

$$q_k^{n+1} = d_k^* + a^*_{k-1/2} q_{k-1}^{n+1} \qquad \forall \quad k = 2, ..., N, \ \text{ ascending}. \tag{1.18}$$

In the case of Dirichlet (e.g., no-slip) boundary condition at bottom (1.16) is replaced with

$$H_1 q_1^{n+1} = H_1 q_1^n + \Delta t\ \cdot \mathrm{rhs}_1 + \Delta t\, A_{3/2} \frac{q_2^{n+1} - q_1^{n+1}}{\Delta z_{\ 3/2}} - \Delta t\, r_D q_1^{n+1} \tag{1.19}$$

where r_D is bottom drag coefficient. In the simplest case of resolved viscous boundary layer it can be approximated as $r_D = 2A_{1/2}/H_1$, which comes from the classical Poiseuille flow theory. However in most practical contexts r_D comes from a separate bottom boundary layer model, typically to thin to be adequately resolved in the discretized model, so r_D is not necessarily expressed in terms of $A_{1/2}$. The outcome is similar to (1.17), except that H_1 in denominator is replaced with $H_1 + 2\Delta t\, A_{1/2}/H_1$. It should be noted that the additional term $2\Delta t\, A_{1/2}/H_1$ may dominate H_1, which results in constraining q_1^{n+1} toward a small value. However, because q_1^{n+1} is defined as grid-box average within H_1, it would be not physical to set $q_1^{n+1} \to 0$ in the case of Dirichlet boundary.

1.2 Implicit viscosity and diffusion using parabolic-splines

The system (1.2)-(1.4) interprets q_k, $k = 1, ..., N$, as a set grid-box averaged values,

$$q_k^n = \frac{1}{H_k} \int_{+H_k/2}^{-H_k/2} q(z')\mathrm{d}z' \,, \tag{1.20}$$

while simultaneously using finite-differences to approximate vertical derivatives

$$\partial_z q\Big|_{k+1/2} = \left(q_{k+1} - q_k\right) / \Delta z_{\ k+1/2} \,. \tag{1.21}$$

Therefore, (1.3) can be viewed as a special case of a more general discrete equation,

$$H_k q_k^{n+1} = H_k q_k^n + \varDelta t \cdot \mathrm{rhs}_k + \varDelta t \cdot \left[A_{k+1/2} d_{k+1/2}^{n+1} - A_{k-1/2} d_{k-1/2}^{n+1} \right] \tag{1.22}$$

where $d_{k+1/2}$ are the values of vertical derivatives $\partial_z q$ at grid-box interfaces $z_{k+1/2}$. Both q_k^{n+1} and $d_{k+1/2}^{n+1}$ are considered as unknowns at this moment.

A more thorough approach would be to reconstruct vertical profile of q as a continuous function of z, and use analytical differentiation to estimate derivatives $d_{k+1/2}$ at grid-box interfaces. The simplest reconstruction is to assume a parabolic distribution of concentration q within each grid box, and find its coefficients from some sort matching conditions at interfaces. The parabolic distribution can be expressed in terms of either interfacial values, $q_{k+1/2}$,

$$q(z') = q_k + \frac{q_{k+1/2} - q_{k-1/2}}{H_k} \cdot z' + 6 \left(\frac{q_{k+1/2} + q_{k-1/2}}{2} - q_k \right) \left(\frac{z'^2}{H_k^2} - \frac{1}{12} \right) \tag{1.23}$$

or interfacial derivatives, $d_{k+1/2}$,

$$q(z') = q_k + \frac{d_{k+1/2} + d_{k-1/2}}{2} \cdot z' + \frac{1}{2} \cdot \frac{d_{k+1/2} - d_{k-1/2}}{H_k} \left(z'^2 - \frac{H_k^2}{12} \right) \tag{1.24}$$

where z' in a local coordinate defined within each grid box H_k which has the same meaning as in (1.20). In both cases one can immediately verify that (1.20) holds regardless of the values of other coefficients, and $q(z') \to q_{k\pm1/2}$ if $z' \to \pm H_k/2$, in the first case, while in the second $\partial_z q(z') \to d_{k\pm1/2}$ if $z' \to \pm H_k/2$.

The interfacial values $q_{k+1/2}$ in (1.23) can be obtained from the condition that derivatives of distributions in adjacent grid boxes match each other at the interfaces,

$$\left. \frac{\partial q}{\partial z} \right|_{z'=\pm H_k/2} = \frac{q_{k+1/2} - q_{k-1/2}}{H_k} \pm \frac{6}{H_k} \left(\frac{q_{k+1/2} + q_{k-1/2}}{2} - q_k \right) = \begin{cases} \left(4q_{k+1/2} + 2q_{k-1/2} - 6q_k \right) / H_k \\ \left(6q_k - 4q_{k-1/2} - 2q_{k+1/2} \right) / H_k \end{cases}$$

hence

$$\frac{4q_{k+1/2} + 2q_{k-1/2} - 6q_k}{H_k} = \frac{6q_{k+1} - 4q_{k+1/2} - 2q_{k+3/2}}{H_{k+1}} \tag{1.25}$$

or

$$H_{k+1} q_{k-1/2} + 2(H_{k+1} + H_k) q_{k+1/2} + H_k q_{k+3/2} = 3 \left(H_{k+1} q_k + H_k q_{k+1} \right) \qquad k = 1, ..., N-1 \tag{1.26}$$

along with two appropriate boundary conditions to constrain the bottom and surface value $q_{1/2}$ and $q_{N+1/2}$.

Conversely, the interfacial derivatives $d_{k+1/2}$ in (1.24) are obtained from the continuity condition for q at grid box interfaces,

$$q\Big|_{z'=\pm H_k/2} = q_k \pm \frac{d_{k+1/2}+d_{k-1/2}}{4}\cdot H_k + \frac{d_{k+1/2}-d_{k-1/2}}{12}\cdot H_k = \begin{cases} q_k + \dfrac{H_k}{3} d_{k+1/2} + \dfrac{H_k}{6} d_{k-1/2} \\[2ex] q_k - \dfrac{H_k}{3} d_{k-1/2} - \dfrac{H_k}{6} d_{k+1/2} \end{cases}$$

resulting in

$$H_k d_{k-1/2} + 2\left(H_k + H_{k+1}\right) d_{k+1/2} + H_{k+1} d_{k+3/2} = 6\left(q_{k+1}-q_k\right)\,, \qquad k=1,...,N-1\,. \tag{1.27}$$

which in combination with two side boundary conditions for $d_{1/2}$ and $d_{N+1/2}$ comprises a well-posed problem for $d_{k+1/2}$, assuming that all q_k are known. In both cases, whether solving for interfacial values $q_{k+1/2}$, or derivatives $d_{k+1/2}$, the resultant reconstructed vertical profiles are equivalent to each other.

In the context of (1.22) both q_k^{n+1} and $d_{k+1/2}^{n+1}$ are unknown, however (1.27) makes it possible to exclude q_{k+1}^{n+1} and obtain a system for $d_{k+1/2}^{n+1}$ alone,

$$\begin{aligned} \left(\frac{H_k}{6} - \frac{\Delta t\, A_{k-1/2}}{H_k}\right) d_{k-1/2}^{n+1} + \left[\frac{H_k + H_{k+1}}{3} + \Delta t\, A_{k+1/2}\left(\frac{1}{H_k}+\frac{1}{H_{k+1}}\right)\right] d_{k+1/2}^{n+1} & \\ + \left(\frac{H_{k+1}}{6} - \frac{\Delta t\, A_{k+3/2}}{H_{k+1}}\right) d_{k+3/2}^{n+1} = q_{k+1}^n + \Delta t\,\cdot \mathrm{rhs}_{k+1} - q_k^n - \Delta t\,\cdot \mathrm{rhs}_k & \end{aligned} \tag{1.28}$$

for $k=1,...,N-1$. As before, two boundary conditions are needed: for $d_{N+1/2}^{n+1}$ at the surface, and $d_{1/2}^{n+1}$ at the bottom. However, it should be noted that, unlike in the previous case, these boundary conditions are now playing dual role: for physical reasons to apply forcing at surface and bottom, and, in addition to that, they are needed by the continuous profile reconstruction algorithm. These two goals can be matched in a well resolved situation, i.e., if there is a finite limit of $A_{N+1/2}$ at free surface, and it is not very small in comparison with, say, it value $A_{N-1/2}$ one grid box below, then it is natural to estimate the vertical derivative $d_{k+1/2}$ as the ratio of the forcing flux and the mixing coefficient at surface. However this cannot be done if $A_{N+1/2}$ is zero or is too small, because the resultant derivative becomes too large which may causes oscillations of the reconstructed profile. In this case $d_{k+1/2}$ must be limited, which effectively decouples it from the physical boundary condition. Same rationale should be applied to bottom, where a special treatment of the bottom-most grid box may be required in the case of unresolved bottom boundary layer. Once $d_{k+1/2}^{n+1}$ are computed from (1.28), all q_k are updated via (1.22) to compute q_k^{n+1}.

A practical Gaussian elimination algorithm begins with setting

$$d_{N+1/2}^{n+1} = SRFRC/A_{N+1/2} \tag{1.29}$$

which formally can be cast into

$$FC_{N-3/2}^{*} d_{N-3/2}^{n+1} + d_{N+1/2}^{n+1} = d_{N+1/2}^{*} \tag{1.30}$$

where $FC^*_{N-3/2} = 0$. This starts recursive procedure of elimination coefficient in from of $d^{n+1}_{k+3/2}$ in (1.28) starting from $k = N - 1$, and proceeding downward to $k = 3/2$ to convert it into

$$FC^*_{k-1/2} d^{n+1}_{k-1/2} + d^{n+1}_{k+1/2} = d^*_{k+1/2} \tag{1.31}$$

where the coefficients $FC^*_{k-1/2}$ and $d^*_{k+1/2}$ are obtained as follows: suppose the procedure already reached $k + 3/2$, so we have

$$FC^*_{k+1/2} d^{n+1}_{k+1/2} + d^{n+1}_{k+3/2} = d^*_{k+3/2} \tag{1.32}$$

where $FC^*_{k+1/2}$ and $d^*_{k+3/2}$ are known. Multiplying (1.32) by $\left(H_{k+1}/6 - \Delta t\, A_{k+3/2}/H_{k+1}\right)$ and subtracting it from (1.28) yields (1.31), where

$$\begin{aligned} FC^*_{k-1/2} &= b^* \cdot \left[\frac{H_k}{6} - \frac{\Delta t\, A_{k-1/2}}{H_k}\right] \\ d^*_{k+1/2} &= b^* \cdot \left[q^n_{k+1} + \Delta t\ \cdot \mathrm{rhs}_{k+1} - q^n_k - \Delta t\ \cdot \mathrm{rhs}_k - \left(\frac{H_{k+1}}{6} - \frac{\Delta t\, A_{k+3/2}}{H_{k+1}}\right) d^*_{k+3/2}\right] \end{aligned} \tag{1.33}$$

where

$$b^* = 1 \Big/ \left[\frac{H_k + H_{k+1}}{3} + \Delta t\, A_{k+1/2}\left(\frac{1}{H_k} + \frac{1}{H_{k+1}}\right) - \left(\frac{H_{k+1}}{6} - \frac{\Delta t\, A_{k+3/2}}{H_{k+1}}\right) \cdot FC^*_{k+1/2}\right]$$

for all $k = N - 1, ..., 1$ successively.

Once this procedure reaches $k = 1$, hence $FC^*_{1/2}$ and $d^*_{3/2}$ are known, combined with bottom boundary condition, this leads a 2×2 matrix problem for $d_{1/2}$ and $d_{3/2}$. Suppose we are solving for velocity component u, and no-slip boundary conditions are needed at bottom. Then, at the bottom-most grid box the parabolic distribution (1.24) should yield 0 when $z' \to -H_1/2$, i.e.,

$$u^{n+1}_1 - \frac{H_1}{3} d^{n+1}_{1/2} - \frac{H_1}{6} d^{n+1}_{3/2} = 0 \tag{1.34}$$

at the same time

$$u^{n+1}_1 = u^n_1 + \Delta t\ \left[A_{3/2} d^{n+1}_{3/2} - A_{1/2} d^{n+1}_{1/2}\right] \tag{1.35}$$

and, from the Gaussian elimination above, also

$$FC^*_{1/2} d^{n+1}_{1/2} + d^{n+1}_{3/2} = d^*_{3/2}. \tag{1.36}$$

There are three unknowns, u^{n+1}_1, $d^{n+1}_{1/2}$, and $d^{n+1}_{3/2}$. Excluding u^{n+1}_1 first, and solving 2×2 problem for $d^{n+1}_{1/2}$ and $d^{n+1}_{3/2}$, we find the bottom-most derivative,

$$d^{n+1}_{1/2} = \frac{u^n_1 - d^*_{3/2} \cdot \left(\dfrac{H_1}{6} - \dfrac{\Delta t\, A_{3/2}}{H_1}\right)}{\dfrac{H_1}{3} - \dfrac{\Delta t\, A_{1/2}}{H_1} - FC^*_{1/2} \cdot \left(\dfrac{H_1}{6} - \dfrac{\Delta t\, A_{3/2}}{H_1}\right)} \tag{1.37}$$

after which all others are obtain recursively from (1.31),

$$d_{k+1/2}^{n+1} = d_{k+1/2}^{*} - FC_{k-1/2}^{*} d_{k-1/2}^{n+1} \tag{1.38}$$

for $k = 1, ..., N-1$, ascending. Once derivatives $d_{k+1/2}^{n+1}$ become known, q^{n+1} is updated via (1.22),

$$H_k q_k^{n+1} = H_k q_k^n + \Delta t \cdot \mathrm{rhs}_k + \Delta t \cdot \left[FLX_{k+1/2} - FLX_{k-1/2} \right] \tag{1.39}$$

where $FLX_{N+1/2} = SRFRC$ and $FLX_{k+1/2} = A_{k+1/2} d_{k+1/2}^{n+1}$ for $k = 2, ..., N-1$. For simplicity, above we also assume that the bottom-most derivative and viscous coefficient remain finite (and resolved), so this applies to $k = 0$ as well. In a more general case computation of bottom-most flux requires a special consideration. We should also note that the surface derivative condition (1.29) is applicable only for non-vanishing $A_{N+1/2}$. If $A_{N+1/2}$ is too small (as in the case of unresolved viscous boundary layer), the derivative may be too large in comparison with the derivative one grid-box below, resulting in oscillation of the reconstructed profile. To prevent it, (1.29) should be modified into

$$d_{N+1/2}^{n+1} = SRFRC / \max \left\{ A_{N+1/2} \, , \alpha \cdot A_{N-1/2} \right\} \tag{1.40}$$

where α is a non-dimensional constant chosen to be not too small, say $\alpha = 1/3$. This essentially decouples physical surface boundary condition from reconstruction (i.e, $FLX_{N+1/2} = SRFRC$ still holds, but $d_{N+1/2}^{n+1}$ is no longer proportional to $SRFRC$) as it should be in the case of unresolved boundary layer.