# On the Choice of Relaxation Coefficients for Davies' Lateral Boundary Scheme for Regionál Weather Prediction Models 

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## Summary

Relaxation coefficients for Davies' lateral boundary scheme for limited-area numerical weather prediction models are constructed in such a way that, under idealized conditions, the unwanted partial reflection of outgoing waves (leaving the limited area) at the boundary is minimized.

## 1. Introduction

Regional weather prediction models need information about the state of the atmosphere outside their integration area (e.g. about cyclones entering the domain covered by the model). It is supplied to them by specifying lateral boundary conditions. However, several theoretical and practical issues arise (roughly speaking, boundary values should be prescribed only at boundaries where information is transferred into the model domain; however, this may be at different parts of the boundary for different Fourier components of the model's variables). That is why it has become common practice to overspecify the boundary values (by prescribing them at all lateral boundaries) and introduce a special zone near the boundary in which the model's variables are smoothly adjusted to the over-determined boundary values.

A technique frequently applied is the "flow relaxation scheme" proposed by Davies (1976). The basic idea is similar to that of "Newtonian nudging" in data assimilation: the differential
equations of the model are extended by a term that is proportional to the deviation of a certain model variable from the corresponding externally specified value and has such a sign that the model variable is forced towards the specified value. For the (one-dimensional) advection equation
$\frac{\partial u}{\partial t}+c \frac{\partial u}{\partial x}=0$.
this results in
$\frac{\partial u}{\partial t}+c \frac{\partial u}{\partial x}=-K(u-\tilde{u})$,
where $K=K(x)$ is the relaxation coefficient, which is non-zero only in the boundary zone, $\tilde{u}$ is an externally specified field, e.g. results of a global weather prediction model interpolated to the grid of the regional model.

We consider Eq. (1) here, because the linearized equations for the horizontal structure of the vertical eigenfunctions of a weather prediction model can be written in the form of shallow-water equations, which then may be recast in the compact characteristic form (1) (Davies, 1983).

If $\tilde{u}$ is prescribed consistently, it satisfies (1) itself (Davies, 1983),
$\frac{\partial \tilde{u}}{\partial t}+c \frac{\partial \tilde{u}}{\partial x}=0$,
so that, by subtracting (3) from (2), we obtain the following "error equation"
$\frac{\partial u^{\prime}}{\partial t}+c \frac{\partial u^{\prime}}{\partial x}=-K u^{\prime}$
for the deviation $u^{\prime}=u-\tilde{u}$.
As stated above, we prescribe the value $\tilde{u}$ for $u$ on the boundary itself, so that
$u^{\prime}=0$
on the boundary.
In the following, we simplify the notation by omitting the prime ' of $u$ '. Furthermore, we consider an integration area $x \in\left[x_{0}, \infty\right)$ with only one boundary $\left(x_{0}\right)$ covered by a grid $x_{0}, x_{1}, x_{2}, \ldots$ of constant grid width $\Delta x$.

Discretizing the spatial derivative in (4) by central differences, we obtain
$\frac{\partial u_{k}}{\partial t}+\frac{c}{2 \Delta x}\left(u_{k+1}-u_{k-1}\right)=-K_{k} u_{k}$
with the boundary condition (according to (5))
$u_{0}=0$,
where index $k$ indicates the corresponding value at grid point $x_{k}$.

We consider a boundary zone of width $s$, i.e.
$K_{k}>0$ for $k=1,2, \ldots, s$,
$K_{k}=0$ for $k \geqslant s+1$.
In order to complete the boundary relaxation scheme, we need values for $K_{1}, \ldots, K_{s}$. Usually they are determined by numerical experiments with the full model (e.g. Kållberg, 1977). Here we adopt a theoretical approach: Ideally, a wave impinging (from $+\infty$ ) upon the boundary zone should leave the model area without any interaction with the boundary zone. However, such a wave is partially reflected (Davies, 1983), i.e. an unwanted "computational mode" emerges. We determine $K_{1}, \ldots, K_{s}$ such that, for a prescribed range of wave velocities, the maximum possible reflection coefficient (ratio of the amplitudes of the reflected and impinging wave) is minimized. A numerical optimization algorithm is outlined in Section 3. An analytical solution for the "optimal" $K_{1}, \ldots, K_{s}$ is found for $s=2^{m}, m$ integer, in Section 4 (for a summary see subsection 4 H ). Both sections are based on an equation for the reflection coefficient that was published by H. C. Davies (1983)
and is rederived in Section 2. In Section 5, the relaxation coefficients obtained here are compared with the frequently-used K-values determined by the numerical experiments of Kållberg (1977); an application to a shallow-water model illustrates their "ability". The main results are summarized in Section 6.

## 2. Reflection by the Boundary Zone: Formula for the Reflection Coefficient

In order to simplify the subsequent computations, we consider an "extreme case" of a spatially well-resolved wave impinging on the boundary zone, namely a field of a constant value (corresponding to a wavelength $\infty$ or amplitude 0 ), i.e. we assume the initial condition
$u_{k}=\bar{u}=$ const. for $k=1,2, \ldots, t=0$,
$u_{0}=0$ (according to (7)).
During the integration, a reflected wave is generated within the boundary zone, which approaches a steady state. Because of (6) the steady-state solution satisfies the following equation:

$$
\begin{align*}
& \frac{c}{2 \Delta x}\left(u_{k+1}-u_{k-1}\right)=-K_{k} u_{k} \\
& \text { for } k=1,2, \ldots \tag{11}
\end{align*}
$$

For $k \geqslant s+1$ we have $K_{k}=0$ (see (9)) so that because of (11) we get
$u_{k+1}-u_{k-1}=0$
and consequently
$u_{k-1}=u_{k+1}$ for $k \geqslant s+1$.
This corresponds to a wave of wavelength $2 \Delta x$. In other words: the solution of (11) (for $k \geqslant s$ ) consists of the superposition of the physical solution $u=\bar{u}$ and a reflected wave of wavelength $2 \Delta x$. Let $|r|$ denote the corresponding reflection coefficient, so that $|r| \bar{u}$ is the amplitude of the reflected wave. Then we obtain:
$u_{s}=u_{s+2}=u_{s+4}=\cdots=\bar{u}+r \cdot \bar{u}$
$u_{s+1}=u_{s+3}=u_{s+5}=\cdots=\bar{u}-r \cdot \bar{u}$
and, with the abbreviation
$\mu:=\frac{u_{s+1}}{u_{s}}$,
it follows that
$\mu=\frac{1-r}{1+r}$
and thus

$$
\begin{align*}
r & =\frac{1-\mu}{1+\mu}  \tag{17}\\
|r| & =\left|\frac{1-\mu}{1+\mu}\right| \tag{18}
\end{align*}
$$

The ratio $\mu=u_{s+1} / u_{s}$ can be obtained from (11) ( $k=1, \ldots, s$ ) by successively eliminating $u_{1}, u_{2}, \ldots$ : We set
$K_{k}^{*}:=-\frac{2 K_{k} \Delta x}{c}$
(the minus sign assures $K_{k}^{*}>0$ for waves impinging on the boundary zone from the right, i.e. for $c<0$ ). Taking into account that $u_{0}=0$ (7), we can rewrite (11) in the form
$u_{2}-K_{1}^{*} u_{1}=0$
$u_{3}-K_{2}^{*} u_{2}-u_{1}=0$
$u_{4}-K_{3}^{*} u_{3}-u_{2}=0$
$u_{s+1}-K_{s}^{*} u_{s}-u_{s-1}=0$
Equation (20) yields
$u_{1}=\frac{1}{K_{1}^{*}} u_{2}$.
Substituting this in (21) and solving for $u_{2}$, we obtain
$u_{2}=\frac{1}{K_{2}^{*}+{\frac{1}{K_{1}^{*}}} u_{3}, ~}$
and analogously

$$
u_{3}=\frac{1}{K_{3}^{*}+\frac{1}{K_{2}^{*}+\frac{1}{K_{1}^{*}}}} u_{4},
$$

and finally

so that
$\mu=\frac{u_{s+1}}{u_{s}}=K_{s}^{*}+\frac{1}{K_{s-1}^{*}+\cdots+\frac{1}{K_{1}^{*}}}$.
Equations (18) and (24) are equivalent to Eqs. (29) and (30) of Davies (1983) (although we adopted a slightly different notation here). It is important to note that, under the assumptions made, they are independent of the scheme for the temporal integration of (6). These formulae for the reflection coefficient will be the basis for the subsequent search for "optimal" relaxation coefficients $K_{1}, \ldots, K_{s}$.

## 3. Optimal Relaxation Coefficients

Since $K_{k}^{*}, k=1, \ldots, s$, depend on the velocity $c$ of the impinging wave (see (19)), the corresponding reflection coefficient $|r|$ is also dependent on $c$ (cf. $(18)+(24))$. We express this by writing $|r(c)|$.

As pointed out by Davies (1983), there is a finite interval [ $c_{\text {min }}, c_{\text {max }}$ ] of $c$ values of interest: In the model, there is a mode with the largest phase velocity $c_{\text {max }}$; moreover, for an explicit integration scheme, an upper bound may be obtained from the stability criterion for the integration scheme. Furthermore, very slowly moving waves will not penetrate sufficiently into the boundary zone during the period $T$ of the integration to produce reflection, i.e. to pass the boundary of width $s \cdot \Delta x$ twice, which yields the estimate $c_{\text {min }} \geqslant 2 s \cdot \Delta x / T$.
It is our aim to choose the relaxation coefficients $K_{1}, \ldots, K_{s}$ such that $|r(c)|$ is "as small as possible" for $c$ within the range $\left[c_{\text {min }}, c_{\text {max }}\right.$ ] of interest. There are several ways of translating "as small as possible" into mathematical terms. For instance, we might require the mean reflection coefficient
$\frac{1}{c_{\text {max }}-c_{\text {min }}} \cdot \int_{c_{\text {min }}}^{c_{\text {max }}}|r(c)| d c$
to be minimal. However, by doing that, we could not exclude rather large values $|r(c)|$ for certain, possibly "important", wave velocities $c$. In order to avoid this effect, we require that the maximum $|r(c)|$ is as small as possible, i.e. we solve the optimization problem
$\min _{K_{1}, \ldots, K_{s}}\left\{\max _{c}\left\{|r(c)| \mid c_{\min } \leqslant c \leqslant c_{\max }\right\}\right\}$.

In order to simplify the subsequent computations, we introduce dimensionless variables:

$$
\begin{align*}
K_{k}^{+} & :=\frac{2 K_{k} \cdot \Delta x}{\sqrt{c_{\min } \cdot c_{\max }}}  \tag{27}\\
b & :=\frac{\sqrt{c_{\min } \cdot c_{\max }}}{|c|} \tag{28}
\end{align*}
$$

so that
$K_{k}^{*}=K_{k}^{+} \cdot b$
and
$b_{\text {min }}=\frac{\sqrt{c_{\text {min }} \cdot c_{\text {max }}}}{c_{\text {max }}}=\frac{1}{\beta}$
$b_{\text {max }}=\frac{\sqrt{c_{\text {min }} \cdot c_{\text {max }}}}{c_{\text {min }}}=\beta$
with
$\beta:=\sqrt{\frac{c_{\max }}{c_{\min }}}$.
Now the optimization problem (26) can be rewritten in the form

$$
\begin{equation*}
\min _{\mathbf{K}_{1}^{+}, \ldots, \mathbf{K}_{s}^{+}}\left\{\max _{b}\left\{|r(b)| \left\lvert\, \frac{1}{\beta} \leqslant b \leqslant \beta\right.\right\}\right\} \tag{33}
\end{equation*}
$$

where
$r(b)=\frac{1-\mu(b)}{1+\mu(b)}$
$\mu(b)=K_{s}^{+} b+\frac{1}{K_{s-1}^{+} b+\cdots+\frac{1}{K_{1}^{+} b}}$
(because of (18), (24), (29)).
Problem (33) can be solved by numerical optimization algorithms, e.g. by the standard method of steepest descent (e.g. Pshenichny and Danilin, 1978). However, here the values of the function to be minimized ( $\max _{b}\{|r(b)| \mid 1 / \beta \leqslant b \leqslant \beta\}$ ) are solutions of an optimization problem themselves. We computed them simply by discretizing the interval $[1 / \beta, \beta]$ (logarithmically, 1000 points), computing $|r(b)|$ at the resulting finite number of discretization points and searching for the largest of these values. The direction of the steepest descent is the solution of an optimization problem that can be transformed into a quadratic optimization problem (quadratic objective function, linear constraints) and then be solved by a corresponding algorithm (e.g. Fletcher, 1971). Results for $c_{\text {max }} / c_{\text {min }}=100$ are presented in Table 1.

## 4. Analytical Solution for Optimal Relaxation Coefficients

In the present chapter we derive (necessary) optimality conditions for the problem (33) and show that they can be used to determine an analytical solution for the optimal $K$ values for $s=2^{m}, m$ integer. In passing we note that the most widely applied schemes really use a relaxation zone of the

Table 1. Weights $\alpha_{k}\left(\alpha_{k}=2 \cdot K \cdot \Delta t /(1+2 \cdot K \cdot \Delta t)\right)$ of Externally Prescribed Values in a Boundary Zone of Width s and Corresponding Maximal Reflection Coefficient $r_{\max }$ of Out-Going Waves (for the range of Courant numbers $\left[\gamma_{\min }, \gamma_{\max }\right]$ indicated)

| $s$ | $\left[\gamma_{\text {min }}, \gamma_{\text {max }}\right]$ | Computed weights of external values in boundary zone |  |  |  |  |  |  |  | $r_{\text {max }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\alpha_{1}$ | $\alpha_{2}$ | $\alpha_{3}$ | $\alpha_{4}$ | $\alpha_{5}$ | $\alpha_{6}$ | $\alpha_{7}$ | $\alpha_{8}$ |  |
| Numerical solution according to Section 3: |  |  |  |  |  |  |  |  |  |  |
| 4 | [1/100, 1] | 0.498 | 0.176 | 0.0469 | 0.0095 |  |  |  |  | 0.07417 |
| 6 | [1/100, 1] | 0.580 | 0.313 | 0.1428 | 0.0591 | 0.0233 | 0.0063 |  |  | 0.01429 |
| 8 | [1/100, 1] | 0.629 | 0.404 | 0.2374 | 0.1284 | 0.0662 | 0.0335 | 0.01588 | 0.00475 | 0.00276 |
| Analytical solution according to Section 4: |  |  |  |  |  |  |  |  |  |  |
| 8 | [1/10, 1] | 0.701 | 0.537 | 0.4068 | 0.3004 | 0.2144 | 0.1443 | 0.08446 | 0.02857 | 0.00004 |
| 8 | [1/100, 1] | 0.629 | 0.404 | 0.2375 | 0.1284 | 0.0662 | 0.0335 | 0.01588 | 0.00474 | 0.00275 |
| 8 | [1/1000, 1] | 0.573 | 0.300 | 0.1305 | 0.0505 | 0.0186 | 0.0068 | 0.00252 | 0.00066 | 0.01713 |
| Kållberg ( $a=0.5$ ): |  |  |  |  |  |  |  |  |  |  |
| 8 | [ $1 / 10,1]$ |  |  |  |  |  |  |  |  | 0.04010 |
| 8 | [1/100, 1] | 0.538 | 0.238 | 0.0949 | 0.0360 | 0.0134 | 0.0049 | 0.00182 | 0.00067 | 0.04010 |
| 8 | [1/1000, 1] |  |  |  |  |  |  |  |  | 0.07634 |

width $s=8$ (e.g. Kållberg, 1977) or, less frequently, $s=4$ (e.g. Giorgi, 1990). Problem (33) has the standard form of problems in approximation theory. Applying the corresponding necessary optimality condition (Pšeničnyj, 1972, Theorem (5.3) to (33)), we obtain:

There exist $s+1$ values $b_{0}, \ldots, b_{s}$ (we assume $b_{0}<b_{1}<\cdots<b_{s}$ ) and $s+1$ non-negative real numbers $\lambda_{0}, \ldots, \lambda_{s}$ such that:
The function $|r()$.$| attains its maximal$
value ( $s+1$ times!) in $b_{0}, \ldots, b_{s}$,
consequently,
$\left|r\left(b_{0}\right)\right|=\left|r\left(b_{1}\right)\right|=\cdots=\left|r\left(b_{s}\right)\right|$
(of course, $|r|$ depends on $K_{1}^{+}, \ldots, K_{s}^{+}$, which is omitted in this notation); moreover
$\sum_{k=0}^{s} \lambda_{k} \cdot R_{k}=0$
$\sum_{k=0}^{s} \lambda_{k}=1$
where
$R_{k}:=\nabla_{K^{+}}\left|r\left(b_{k}\right)\right|:=\left(\frac{\partial|r|}{\partial K_{1}^{+}}\left(b_{k}\right), \ldots, \frac{\partial|r|}{\partial K_{s}^{+}}\left(b_{k}\right)\right)^{T}$.
Condition (36) may be explained verbally as follows: If we tried to solve (33) "by hand", we could proceed in the following way: We start with arbitrary values $K_{1}^{+}, \ldots, K_{s}^{+}$. Most probably, we would observe one single maximum of $|r|$, at some $b_{(0)}$. Now we try to adjust $K_{1}^{+}, \ldots, K_{s}^{+}$so that $\left|r\left(b_{(0)}\right)\right|$ is reduced (whereby $b_{(0)}$, defined as the $b$ value which yields the maximum of $|r()$.$| ,$ will be shifted itself). We may continue in this way until a second maximum $\left|r\left(b_{(1)}\right)\right|$ (of the same magnitude as $\left.\left|r\left(b_{(0)}\right)\right|\right)$ appears. Then we would try to reduce these two maxima simultaneously - this would impose one constraint on the $K^{+}$values we could choose (because one equality $\left|r\left(b_{(0)}\right)\right|=$ $\left|r\left(b_{(1)}\right)\right|$ has to be fulfilled). Then a third maximum appears, afterwards there will be two constraints on $K_{1}^{+}, \ldots, K_{s}^{+}$etc. Finally, we have found $s$ maxima and continue with $s-1$ constraints on the $K^{+}$values $\left(\left|r\left(b_{(0)}\right)\right|=\left|r\left(b_{(1)}\right)\right|=\cdots=\left|r\left(b_{(s-1)}\right)\right|\right)$, i.e. only one degree of freedom for choosing $K^{+}$ values remains. After finding an $(s+1)$-th maximum this process terminates. Theoretically, it would be possible to "gain" degrees of freedom for
choosing $K^{+}$during the above-described process if the reduction of all maxima but one would automatically bring about a reduction of the remaining maximum (at ( $b_{\left(i_{0}\right)}$, say), because the gradient $\nabla_{K^{+}}\left|r\left(b_{\left(i_{0}\right)}\right)\right|$ could be a linear combination (with non-negative weights) of the gradients $\nabla_{K^{+}}|r()$.$| at the remaining maxima. For the final$ solution, such a possibility is excluded by the conditions (38) and (39).

Since (36)-(39) is a necessary optimality condition, (36)-(37) alone is also (a weaker) one. The following considerations will be based on (36)-(37). We shall proceed in several steps:
(A) First, we slightly reformulate condition (36): It is equivalent to:

The function $r($.$) has s+1$ extrema
(maxima and minima) $b_{0}, \ldots, b_{s}$ in $\left[\frac{1}{\beta}, \beta\right]$.

For $b_{k} \in(1 / \beta, \beta)$ (i.e. in the interior of the interval $[1 / \beta, \beta]$ ) condition (41) has the consequence
$\frac{\partial r}{\partial b}\left(b_{k}\right)=0$.
It follows from (17) that

$$
\begin{align*}
\frac{\partial r}{\partial b} & =\frac{\left(-\frac{\partial \mu}{\partial b}\right)(1+\mu)-(1-\mu) \frac{\partial \mu}{\partial b}}{(1+\mu)^{2}} \\
& =-\frac{2 \frac{\partial \mu}{\partial b}}{(1+\mu)^{2}}, \tag{43}
\end{align*}
$$

so that (42) is equivalent to

$$
\begin{equation*}
\frac{\partial \mu}{\partial b}\left(b_{k}\right)=0 . \tag{44}
\end{equation*}
$$

(B) Next, we investigate the structure of $\mu$ (with the first goal to draw conclusions from (44)): The chain fraction $\mu$ may be converted into an ordinary fraction. Doing this step by step, we obtain intermediate results of the form

$$
\begin{equation*}
K_{k}^{+} b+\frac{1}{K_{k-1}^{+} b+\cdots+\frac{1}{K_{1}^{+} b}}=\frac{P_{k}(b)}{Q_{k}(b)}, \tag{45}
\end{equation*}
$$

(where $P_{k}$ and $Q_{k}$ are polynomials of $b$ ), starting
from
$K_{1}^{+} b=\frac{P_{1}(b)}{Q_{1}(b)}$,
i.e.
$P_{1}(b)=K_{1}^{+} b$,
$Q_{1}(b)=1$,
and ending with
$\mu(b)=\frac{P_{s}(b)}{Q_{s}(b)}$.
We note that the polynomials $P_{k}$ and $Q_{k}$ depend on $K_{1}^{+}, \ldots, K_{s}^{+}$and thus also on the boundary zone width $s$. That is why a complete notation for $P_{k}$ (and analogously $Q_{k}$ ) would be
$P_{k}^{s}\left(b ; K_{1}^{+}, \ldots, K_{s}^{+}\right)$.
In the following computations, we assume that $K_{1}^{+}, \ldots, K_{s}^{+}$are optimal values (in the sense of (36)-(37)) and omit the corresponding arguments in (50). Moreover, we omit the upper index if it is $s$ and replace it by a tilde ${ }^{\sim}$ (above $P$ ) if the lower and upper index are equal (i.e. for the "final" polynomials used for computing $\mu(b)$ in (49)), so that, for instance,
$P_{k}(b) \equiv P_{k}^{s}\left(b ; K_{1}^{+}, \ldots, K_{s}^{+}\right)$,
$\tilde{P}_{2 s}(b) \equiv P_{2 s}^{2 s}\left(b ; K_{1}^{+}, \ldots, K_{s}^{+}\right)$,
and
$\widetilde{P}_{s}(b)=P_{s}(b)$.
From (45) we obtain
$K_{k+1}^{+} b+\frac{1}{\frac{P_{k}(b)}{Q_{k}(b)}}=\frac{P_{k+1}(b)}{Q_{k+1}(b)}$,
i.e.
$\frac{K_{k+1}^{+} \cdot b \cdot P_{k}(b)+Q_{k}(b)}{P_{k}(b)}=\frac{P_{k+1}(b)}{Q_{k+1}(b)}$,
and consequently,
$P_{k+1}(b)=K_{k+1}^{+} \cdot b \cdot P_{k}(b)+Q_{k}(\mathrm{~b})$
$Q_{k+1}(b)=P_{k}(b)$.
Because of (55), we can recast (54) and (48) in the form

$$
\begin{align*}
& P_{k+1}(b)=K_{k+1}^{+} \cdot b \cdot P_{k}(b)+P_{k-1}(b) \\
& \quad \text { for } k \geqslant 1, \tag{56}
\end{align*}
$$

$$
\begin{equation*}
P_{0}(b)=1, \tag{57}
\end{equation*}
$$

and, according to (47),
$P_{1}(b)=K_{1}^{+} b$.
By straight-forward mathematical induction we can prove:
$P_{2 k}(b), k$ integer, is a polynomial of degree $2 k$, containing only even powers of $b$, e.g.

$$
\begin{align*}
P_{4}(b)= & K_{1}^{+} K_{2}^{+} K_{3}^{+} K_{4}^{+} b^{4}+\left(K_{1}^{+} K_{2}^{+}\right. \\
& \left.+K_{1}^{+} K_{4}^{+}+K_{3}^{+} K_{4}^{+}\right) b^{2}+1 \tag{59}
\end{align*}
$$

$P_{2 k+1}(b), k$ integer, is a polynomial of degree $2 k+1$, containing only odd powers of $b$, e.g.

$$
\begin{equation*}
P_{3}(b)=K_{1}^{+} K_{2}^{+} K_{3}^{+} b^{3}+\left(K_{1}^{+}+K_{3}^{+}\right) b . \tag{60}
\end{equation*}
$$

Again, straight-forward mathematical induction proves that, for even $s$, the coefficients in front of $b^{0}$ in $P_{s}(b)$ is 1 (because of $(57),(56)$ ).

Note that, if we knew the polynomials $P_{s}$ and $Q_{s}\left(=P_{s-1}\right)$, we could determine $K_{1}^{+}, \ldots, K_{s}^{+}$: Equation (56) for $k=s-1$ is

$$
\begin{equation*}
P_{s}(b)=K_{s}^{+} \cdot b \cdot P_{s-1}(b)+P_{s-2}(b) \tag{61}
\end{equation*}
$$

Comparing the coefficients in front of $b^{s}$ in $P_{s}(b)$ and $K_{s}^{+} \cdot b \cdot P_{s-1}(b)$, we can determine $K_{s}^{+}$. Knowing $K_{s}^{+}$, we may obtain $P_{s-2}(b)$ from (61). Then we know $P_{s-1}$ and $P_{s-2}$ and can determine $K_{s-1}^{+}$in an analogous way etc. That is why we shall aim at determining $P_{s}\left(=\widetilde{P}_{s}\right)$ and $Q_{s}\left(=\widetilde{Q}_{s}\right)$.
(C) As a first step towards the construction of $\tilde{P}_{s}$ and $\tilde{Q}_{s}$, we apply the results of $(B)$ to an investigation of properties of $b_{0}, b_{1}, \ldots, b_{s}$. Because of (49), Eq. (44) is equivalent to

$$
\begin{align*}
& \frac{\partial \tilde{P}_{s}(b)}{\partial b} \cdot \tilde{Q}_{s}(b)-\tilde{P}_{s}(b) \cdot \frac{\partial \tilde{Q}_{s}(b)}{\partial b}=0 \\
& \quad \text { for } \quad b=b_{k} \in\left(\frac{1}{\beta}, \beta\right) \tag{62}
\end{align*}
$$

i.e., because of (55),

$$
\begin{align*}
& \frac{\partial \widetilde{P}_{s}(b)}{\partial b} \cdot P_{s-1}(b)-\widetilde{P}_{s}(b) \cdot \frac{\partial P_{s-1}(b)}{\partial b}=0 \\
& \text { for } b=b_{k} \in\left(\frac{1}{\beta}, \beta\right) \tag{63}
\end{align*}
$$

Because of the results of (B) we can summarize the following properties of the polynomials in Eq. (63):

Degree All powers of $b$ are (for $s$ even) (for $s$ odd)

| $\frac{\partial \widetilde{P}_{s}}{\partial b}$ | $s-1$ | odd | even |
| :--- | :--- | :--- | :--- |
| $P_{s-1}$ | $s-1$ | odd | even |
| $\widetilde{P}_{s}$ | $s$ | even | odd |
| $\frac{\partial P_{s-1}}{\partial b}$ | $s-2$ | even | odd |

It follows that

$$
\frac{\partial \widetilde{P}_{s}}{\partial b} P_{s-1}-\tilde{P}_{s} \frac{\partial P_{s-1}}{\partial b}
$$

has the degree $2(s-1)$ and contains only even powers of $b$, in other words: it is a polynomial of degree $s-1$ in $b^{2}$. That means that for every positive solution $b$ of (63) there exists a negative solution (of the same absolute value). It follows that (63) (and thus also the equivalent Eq. (42)) has at most $s-1$ positive solutions, i.e. there are at most $s-1$ extrema of $r$ in the interior of $[1 / \beta, \beta]$ (according to (A)). As there should be $s+1$ extrema in $[1 / \beta, \beta]$ (cf. (41)), we can conclude that two of them coincide with the end points of the interval $[1 / \beta, \beta]:$
$b_{0}=\frac{1}{\beta}$,
$b_{\mathrm{s}}=\beta$.
Furthermore, it follows that $r$ has exactly $s-1$ extrema in $(1 / \beta, \beta)$, namely $b_{1}, \ldots, b_{s-1}$. As maxima and minima alternate (for an increasing independent variable $b$ ), we obtain, taking (37) into account,
$r\left(b_{s}\right)=r\left(b_{s-2}\right)=\cdots=\bar{r}$,
$r\left(b_{s-1}\right)=r\left(b_{s-3}\right)=\cdots=-\bar{r}$
for some $\bar{r}$.
Let us define
$\bar{\mu}:=\mu\left(b_{s}\right)$,
then it follows immediately from (66) and (16) that
$\mu\left(b_{s}\right)=\mu\left(b_{s-2}\right)=\cdots=\bar{\mu}$.
Moreover,
$\bar{r}=\frac{1-\bar{\mu}}{1+\bar{\mu}} \quad$ (because of (17))
and

$$
\begin{aligned}
\mu\left(b_{s-1}\right) & =\frac{1-r\left(b_{s-1}\right)}{1+r\left(b_{s-1}\right)} \quad \text { because of }(16) \\
& =\frac{1+\bar{r}}{1-\bar{r}} \\
& =\frac{1+\frac{1-\bar{\mu}}{1+\bar{\mu}}}{1-\frac{1-\bar{\mu}}{1+\bar{\mu}}} \\
& =\frac{1}{\bar{\mu}}
\end{aligned}
$$

so that
$\mu\left(b_{s-1}\right)=\mu\left(b_{s-3}\right)=\cdots=\frac{1}{\vec{\mu}}$.
(D) We continue with the characterization of $b_{0}, b_{1}, \ldots, b_{s}$ :
Suppose, for the discussion in subsections (D) and (E) that $s$ is even, then (68) and (69) imply
$\mu\left(b_{0}\right)=\mu\left(b_{2}\right)=\cdots=\mu\left(b_{s}\right)=\bar{\mu}$,
$\mu\left(b_{1}\right)=\mu\left(b_{3}\right)=\cdots=\mu\left(b_{s-1}\right)=\frac{1}{\vec{\mu}}$.
Exploiting the representation (49) for $\mu(b)$ an (51), we can recast (70) and (71) in the form
$\tilde{P}_{s}(b)-\bar{\mu} \cdot \tilde{Q}_{s}(b)=0$ for $b=b_{0}, b_{2}, \ldots, b_{s}$,
$\tilde{P}_{s}(b)-\frac{1}{\mu} \cdot \tilde{Q}_{s}(b)=0$ for $b=b_{1}, b_{3}, \ldots, b_{s-1}$.

Differentiating the left-hand side of (73) with respect to $b$, we obtain
$\frac{\partial}{\partial b}\left(\tilde{P}_{s}(b)-\frac{1}{\bar{\mu}} \tilde{Q}_{s}(b)\right)=\frac{\partial \tilde{P}_{s}}{\partial b}-\frac{1}{\bar{\mu}} \frac{\partial \tilde{Q}_{s}}{\partial b}$.
For $b=b_{1}, b_{3}, \ldots, b_{s-1}$ we have
$\frac{1}{\bar{\mu}}=\mu(b)=\frac{\tilde{P}_{s}}{\widetilde{Q}_{s}}$
(because of (71) and (49)) and consequently

$$
\begin{align*}
\frac{\partial}{\partial b}\left(\tilde{P}_{s}(b)-\frac{1}{\mu} \tilde{Q}_{s}(b)\right) & =\frac{\partial \tilde{P}_{s}}{\partial b}-\frac{\tilde{P}_{s}}{\tilde{Q}} \frac{\partial \tilde{Q}_{s}}{\partial b} \\
& =0 \quad \text { because of }(62) \tag{75}
\end{align*}
$$

(73) and (75) mean that $b_{1}, b_{3}, \ldots, b_{s-1}$ are roots of the polynomial $\tilde{P}_{s}-(1 / \bar{\mu}) \tilde{Q}_{s}$ and its derivative $\partial\left(\widetilde{P}_{s}-(1 / \bar{\mu}) \widetilde{Q}_{s}\right) / \partial b$. That means that $b_{1}, b_{3}, \ldots, b_{s-1}$ are two-fold roots of $\widetilde{P}_{s}-(1 / \bar{\mu}) \widetilde{Q}_{s}$. As $\widetilde{P}_{s}$ is a polynomial of degree $s$ (cf. (B)), it follows that these $s / 2$ two-fold roots are all roots of this polynomial; that is why it can be represented in the form

$$
\begin{equation*}
\tilde{P}_{s}-\frac{1}{\bar{\mu}} \tilde{Q}_{s}=A_{s} \cdot\left(b-b_{1}\right)^{2} \cdot\left(b-b_{3}\right)^{2} \cdot \ldots \cdot\left(b-b_{s-1}\right)^{2} \tag{76}
\end{equation*}
$$

with some real number $A_{5}$. Analogously we conclude that the $s / 2-1$ values $b_{2}, \ldots, b_{s-2}$ are twofold roots of $\tilde{P}_{s}-\bar{\mu} \tilde{Q}_{s}$ (and $b_{0}, b_{s}$ are simple roots) so that

$$
\begin{align*}
\tilde{P}_{s}-\tilde{\mu} \tilde{Q}_{s}= & B_{s} \cdot\left(b-b_{0}\right) \cdot\left(b-b_{2}\right)^{2} \cdot \ldots \\
& \cdot\left(b-b_{s-2}\right)^{2} \cdot\left(b-b_{s}\right) \tag{77}
\end{align*}
$$

with some real number $B_{s}$.
We recall that $\widetilde{P}_{s}$ contains only even powers of $b$, and $\tilde{Q}_{s}$ contains only odd powers of $b$. That is why a comparison of (76) and (77) yields: The coefficients in front of even powers of $b$ in
$A_{s} \cdot\left(b-b_{1}\right)^{2} \cdot\left(b-b_{3}\right)^{2} \cdot \ldots \cdot\left(b-b_{s-1}\right)^{2}$
and

$$
B_{s} \cdot\left(b-b_{0}\right) \cdot\left(b-b_{2}\right)^{2} \cdot \ldots \cdot\left(b-b_{s-2}\right)^{2} \cdot\left(b-b_{s}\right)
$$

coincide; the coefficients in front of odd powers differ by the factor $\bar{\mu} /(1 / \bar{\mu})=\bar{\mu}^{2}$. Thus, this comparison (of the coefficients in front of $b^{0}, b^{1}, \ldots, b^{s}$ ) yields $s+1$ equations (in particular, the comparison of the coefficient in front of $b^{s}$ yields $A_{\mathrm{s}}=B_{\mathrm{s}}$ ). Moreover, we know that the coefficient in front of $b^{0}$ is 1 (cf. (B)). So we have $s+2$ equations for the $s+2$ unknown variables $b_{1}, \ldots, b_{s-1}$, $A_{s}, B_{s}$, and $\bar{\mu}\left(b_{0}\right.$ and $b_{s}$ are already known according to (64) and (65)! ).

By the way, now the application of a standard algorithm for the solution of systems of nonlinear equations offers an alternative to the straightforward numerical minimization described at the end of Section 3 (for arbitrary even $s$ ). The slightly cumbersome task of expressing the coefficients in front of $b^{0}, \ldots, b^{s}$ by the variables $b_{0}, \ldots, b_{s}$ may be facilitated by applying Vieta's root theorem.
(E) For large $s$, the system of equations mentioned at the end of $(\mathrm{D})$ is rather complicated; however, we shall show that, knowing the solution for some $s$, we can construct a solution of the
corresponding system for $2 s$. Furthermore, we are not interested in $b_{1}, \ldots, b_{s-1}, A_{s}, B_{s}$ themselves, but only in the resulting $\widetilde{P}_{s}, \tilde{Q}_{s}$ (because they are sufficient for determining the optimal $K_{1}^{+}, \ldots, K_{s}^{+}-$ cf. (B)).

Now, suppose that we already know a solution $\hat{b}_{1}, \ldots, \hat{b}_{s-1}, A_{s}, B_{s}, \bar{\mu}_{s}$ of (76), (77) (the of $b_{i}$ and the index $s$ of $\bar{\mu}$ have been added in order to avoid confusion with the corresponding variables in the system for $2 s$; furthermore $A_{s}=B_{s}-$ cf. (D)):
$\tilde{P}_{s}-\frac{1}{\bar{\mu}_{\mathrm{s}}} \tilde{Q}_{s}=A_{s} \cdot\left(b-\hat{b}_{1}\right)^{2} \cdot\left(b-\hat{b}_{3}\right)^{2} \cdot \ldots \cdot\left(b-\hat{b}_{s-1}\right)^{2}$
$\tilde{P}_{s}-\bar{\mu}_{s} \tilde{Q}_{s}=A_{s} \cdot\left(b-\hat{b}_{0}\right) \cdot\left(b-\hat{b}_{2}\right)^{2} \cdot \ldots$ $\cdot\left(b-\hat{b}_{s-2}\right)^{2} \cdot\left(b-\hat{b}_{s}\right)$
$\hat{b}_{0}=\frac{1}{\beta}$
$\hat{b}_{s}=\beta$.
We seek a solution of the corresponding system for 2 s :

$$
\begin{align*}
& \tilde{P}_{2 s}-\frac{1}{\bar{\mu}_{2 s}} \tilde{Q}_{2 s}= \\
& A_{2 s} \cdot\left(b-b_{1}\right)^{2}  \tag{82}\\
& \cdot\left(b-b_{3}\right)^{2} \cdot \ldots \cdot\left(b-b_{2 s-1}\right)^{2} \\
& \tilde{P}_{2 s}-\bar{\mu}_{2 s} \tilde{Q}_{2 s}= A_{2 s} \cdot\left(b-b_{0}\right) \cdot\left(b-b_{2}\right)^{2} \ldots  \tag{83}\\
& \cdot\left(b-b_{2 s-2}\right)^{2} \cdot\left(b-b_{2 s}\right)  \tag{84}\\
& b_{0}=\frac{1}{\beta}  \tag{85}\\
& b_{2 s}=\beta .
\end{align*}
$$

By multiplying (78) and (79), we obtain

$$
\begin{align*}
& \left(\tilde{P}_{s}^{2}+\tilde{Q}_{s}^{2}\right)-\left(\bar{\mu}_{s}+\frac{1}{\bar{\mu}_{s}}\right) \tilde{P}_{s} \tilde{Q}_{s} \\
& =A_{s}^{2}\left(b-\hat{b}_{0}\right)\left(b-\hat{b}_{1}\right)^{2}\left(b-\hat{b}_{2}\right)^{2} \ldots \\
& \quad \cdot\left(b-\hat{b}_{s-1}\right)^{2}\left(b-\hat{b}_{s}\right) \tag{86}
\end{align*}
$$

Comparing (86) with (83), we observe that a possible solution of (83) might be the following:
$\tilde{P}_{2 s}=\tilde{P}_{s}^{2}+\tilde{Q}_{s}^{2}$
$\bar{\mu}_{2 s} \tilde{Q}_{2 s}=\left(\bar{\mu}_{s}+\frac{1}{\bar{\mu}_{\mathrm{s}}}\right) \tilde{P}_{s} \tilde{Q}_{s}$
$A_{2 s}=A_{s}^{2}$
$b_{2 k}=\hat{b}_{k}$ for $k=0, \ldots, s$.

We note that (84), (85) are fulfilled because of (80), (81) and that $\widetilde{P}_{2 s}, \widetilde{Q}_{2 s}$ from (87), (88) satisfy the condition that $\widetilde{P}_{2 s}$ contains only even powers of $b$ and $\widetilde{Q}_{2 s}$ contains only odd powers of $b$. However, we still have to test whether (87)-(90) are consistent with (82), which now assumes the form
$\tilde{P}_{2 s}-\frac{1}{\bar{\mu}_{2 s}} \tilde{Q}_{2 s}=\left\{A_{s}\left(b-b_{1}\right) \cdot \ldots \cdot\left(b-b_{2 s-1}\right)\right\}^{2}$,
i.e. we have to prove that $(87)-(90)$ are consistent with the requirement that $\tilde{P}_{2 s}-\left(1 / \bar{\mu}_{2 s}\right) \tilde{Q}_{2 s}$ is the square of a polynomial of degree $s$ with $s$ different real roots $b_{1}, \ldots, b_{2 s-1}$ with
$b_{0}<b_{1}<b_{2}<\cdots<b_{2 s-2}<b_{2 s-1}<b_{2 s}$.
The left-hand-side of ( 91 ) can be rewritten (because of (87), (88)):
$\tilde{P}_{2 s}-\frac{1}{\bar{\mu}_{2 s}} \tilde{Q}_{2 s}=\tilde{P}_{s}^{2}+\tilde{Q}_{s}^{2}-\frac{\bar{\mu}_{s}+\frac{1}{\bar{\mu}_{s}}}{\bar{\mu}_{2 s}^{2}} \tilde{P}_{s} \tilde{Q}_{s}$.
The right-hand-side of (93) becomes a square of a polynomial of degree $s$, namely $\left(\widetilde{P}_{s}-\widetilde{Q}_{s}\right)^{2}$, for
$\frac{\bar{\mu}_{s}+\frac{1}{\bar{\mu}_{s}}}{\bar{\mu}_{2 s}^{2}}=2$.
Indeed, this choice ensures that also the require-
ment (92) is satisfied (cf. illustration in Fig. 1): For $\alpha=1 / \bar{\mu}_{s}$, the polynomial $\widetilde{P}_{s}-\alpha \widetilde{Q}_{s}$ has $s / 2$ (two-fold) roots, which are local minima. $\tilde{Q}_{s}$ has only positive coefficients (cf. (B)), and we consider positive $b$; consequently, $\tilde{Q}_{s}>0$. That is why all function values of $\widetilde{P}_{s}-\alpha \widetilde{Q}_{s}$ decrease for increasing $\alpha$. As a consequence, the two-fold roots of $\tilde{P}_{s}-\left(1 / \bar{\mu}_{s}\right) \tilde{Q}_{s}$ "split" into single ones, which separate more widely for increasing $\alpha$. The same arguments can analogously be applied to $\widetilde{P}_{s}-\alpha \tilde{Q}_{s}$ with $\alpha$ decreasing from $\alpha=\bar{\mu}_{s}$. (This discussion implies $1 / \bar{\mu}_{s}<\bar{\mu}_{s}$, i.e. $\bar{\mu}_{s}>1$, which follows, for even $s$, from (97) and, for $s=1$, from (105) in subsection (G)). Combining the above-mentioned facts, we can conclude that $\tilde{P}_{s}-\alpha \widetilde{Q}_{s}$ has $s$ single roots $b_{1}$, $b_{3}, \ldots, b_{2 s-1}$ with
$b_{0}<b_{1}<b_{2}<\cdots<b_{2 s-2}<b_{2 s-1}<b_{2 s}$
for $1 / \mu<\alpha<\mu$, i.e. especially for $\alpha=1$. Thus, we have constructed a solution of (82), (83) which satisfies all requirements. Now a mathematically strict treatment of the problem would require a discussion of the uniqueness of the solution of (82), (83). However, this is omitted here. We only mention that a comparison with the numerical results of Section 3 shows that we have found "the right" solution.
(F) In the steps (D), (E) we constructed $\tilde{P}_{2 s}, \tilde{Q}_{2 s}$ (under the assumption that $\tilde{P}_{s}, \widetilde{Q}_{s}$ are known) for even numbers $s$. The treatment of the case of odd


Fig. 1. Illustration to Section 4(E): Roots of $\tilde{P}_{s}-\alpha \tilde{Q}_{s}$ for $1 / \bar{\mu}<$ $\alpha<\bar{\mu}$
$s$ is quite similar: (78) and (79) assume the form
$\tilde{P}_{s}-\bar{\mu}_{s} \widetilde{Q}_{s}=A_{s} \cdot\left(b-\hat{b}_{1}\right)^{2} \cdot\left(b-\widehat{b}_{3}\right)^{2} \cdot \ldots$

$$
\begin{equation*}
\cdot\left(b-\hat{b}_{s-2}\right)^{2} \cdot\left(b-\hat{b}_{s}\right) \tag{95}
\end{equation*}
$$

$\tilde{P}_{s}-\frac{1}{\bar{\mu}_{s}} \tilde{Q}_{s}=A_{s} \cdot\left(b-\hat{b}_{0}\right) \cdot\left(b-\hat{b}_{2}\right)^{2} \cdot \ldots$

$$
\begin{equation*}
\cdot\left(b-\hat{b}_{s-3}\right)^{2} \cdot\left(b-\hat{b}_{s-1}\right)^{2} \tag{96}
\end{equation*}
$$

Multiplication of (95) and (96) yields again Eq. (86), and the discussion of the roots of $\widetilde{P}_{s}-\widetilde{Q}_{s}$ is similar to the case of even $s$.
(G) Equations (94), (87), (88) yield an algorithm for computing $\widetilde{P}_{2 s}, \widetilde{Q}_{2 s}$, and $\bar{\mu}_{2 s}$ if $\tilde{P}_{s}, \widetilde{Q}_{s}$, and $\bar{\mu}_{s}$ are known:
$\bar{\mu}_{2 s}=\sqrt{\frac{\bar{\mu}_{s}+1 / \bar{\mu}_{s}}{2}}$
$\tilde{P}_{2 s}=\tilde{P}_{s}^{2}+\tilde{Q}_{s}^{2}$
$\tilde{Q}_{2 s}=2 \bar{\mu}_{2 s} \tilde{P}_{s} \widetilde{Q}_{s}$.
Thus, we can determine (by successively doubling s) $\bar{\mu}_{s}, \widetilde{P}_{s}, \tilde{Q}_{s}$ for all $s=2^{m}, m$ integer. It only remains to find the starting values $\bar{\mu}_{1}, \widetilde{P}_{1}, \tilde{Q}_{1}$ : For $s=1$, Eqs. (95) and (96) assume the following form:
$\widetilde{P}_{1}-\bar{\mu}_{1} \tilde{Q}_{1}=A_{1} \cdot\left(b-b_{1}\right)$
$\tilde{P}_{1}-\frac{1}{\bar{\mu}_{1}} \tilde{Q}_{1}=A_{1} \cdot\left(b-b_{0}\right)$
with
$b_{0}=\frac{1}{\beta}$
$b_{1}=\beta$.
As $Q_{1}(b)=1$ (independently of $K_{1}^{+}$; see (48)), we have
$\tilde{Q}_{1}=1$.
Thus, we obtain from (100), (101) (by comparing the coefficients in front of $b$ and $b^{0}$ ):
$\tilde{P}_{1}=A_{1} b$
$\frac{1}{\bar{\mu}_{1}}=A_{1} \frac{1}{\beta}$.
Multiplying (103) and (104), we obtain $A_{1}=1$, so that finally:
$\bar{\mu}_{1}=\beta$
$\tilde{P}_{1}=b$
$\tilde{Q}_{1}=1$.
(H) We summarize the algorithm for computing the optimal $K_{1}, \ldots, K_{s}\left(s=2^{m}, m\right.$ integer $)$ :

- Input: estimates for maximum and minimum wave velocities: $c_{\max }, c_{\min }$; horizontal grid width: $\Delta x$.
- Set $\bar{\mu}_{1}=\sqrt{\frac{c_{\text {max }}}{c_{\text {min }}}}$ (real number),
$\tilde{P}_{1}=b, \tilde{Q}_{1}=1$ (polynomials in $b$ )
$((105)+(32),(106),(107))$.
- Knowing $\bar{\mu}_{s^{\prime}}, \tilde{P}_{s^{\prime}}, \tilde{Q}_{s^{\prime}}$ for some $s^{\prime}\left(s^{\prime}=2^{m^{\prime}}\right.$, $s^{\prime}<s$ ), compute $\bar{\mu}_{2 s^{\prime}}, \widetilde{P}_{2 s^{\prime}}, \widetilde{Q}_{2 s^{\prime}}$ :
$\bar{\mu}_{2 s^{\prime}}=\sqrt{\frac{\bar{\mu}_{s}^{\prime}+1 / \bar{\mu}_{s}^{\prime}}{2}}$
$\tilde{P}_{2 s^{\prime}}=\widetilde{P}_{s^{\prime}}^{2}+\tilde{Q}_{s^{\prime}}^{2}$
$\tilde{Q}_{2 s^{\prime}}=2 \bar{\mu}_{2 s^{\prime}}, \tilde{P}_{s^{\prime}} \tilde{Q}_{s^{\prime}}$
((97), (98), (99))
(Repeat this step until $\widetilde{P}_{s}, \widetilde{Q}_{s}$ are known.)
- Knowing $\tilde{P}_{s}, \tilde{Q}_{s}$, convert the fraction $\tilde{P}_{s} / \tilde{Q}_{s}$ into a chain fraction

$$
\frac{\tilde{P}_{s}}{\tilde{Q}_{s}}=K_{s}^{+} b+\frac{1}{K_{s-1}^{+} b+\cdots+\frac{1}{K_{1}^{+} b}}
$$

(cf. (61) and the corresponding text).

- Set $K_{k}=K_{k}^{+} \cdot \frac{\sqrt{c_{\text {min }} \cdot c_{\text {max }}}}{2 \cdot \Delta x}$
for $k=1, \ldots, s$.
Sometimes it is more convenient to work with the Courant number $\gamma=c \cdot \Delta t / \Delta x$ instead of $c$, $\Delta x$, and $\Delta t$ separately. Then the above-mentioned equations for $\bar{\mu}_{1}$ and $K_{k}$ can easily be transformed into the following ones:
$\bar{\mu}_{1}=\sqrt{\frac{\gamma_{\text {max }}}{\gamma_{\text {min }}}}$
$2 \cdot K_{k} \cdot \Delta t=K_{k}^{+} \cdot \sqrt{\gamma_{\text {min }} \gamma_{\text {max }}}$.
(The latter quantity will be needed in this form for the temporal integration of the differential equation by the leap-frog method - cf. Section 5).

The algorithm described above can easily be carried out "by hand" for $s=2$ (cf. subsection (I)) and $s=4$, but a computer code should be applied
for $s \geqslant 8$. The corresponding FORTRAN subroutine is given in the Appendix.
(I) We illustrate the algorithm of subsection (H) by carrying it out explicitly for $s=2$ :
$\bar{\mu}_{1}=\sqrt{\frac{c_{\text {max }}}{c_{\text {min }}}}$
$\tilde{P}_{1}=b$
$\tilde{Q}_{1}=1$
$\bar{\mu}_{2}=\sqrt{\frac{\bar{\mu}_{1}+1 / \bar{\mu}_{1}}{2}}$
$\tilde{P}_{2}=b^{2}+1$
$\tilde{Q}_{2}=2 \bar{\mu}_{2} b$
$\frac{\tilde{P}_{2}}{\tilde{Q}_{2}}=\frac{b^{2}+1}{2 \bar{\mu}_{2} b}$

$$
\begin{equation*}
=\frac{1}{2 \bar{\mu}_{2}} b+\frac{1}{2 \bar{\mu}_{2} b} \tag{108}
\end{equation*}
$$

which yields
$K_{2}^{+}=\frac{1}{2 \bar{\mu}_{2}}$,
$K_{1}^{+}=2 \bar{\mu}_{2}$,
$K_{k}=K_{k}^{+} \cdot \frac{\sqrt{c_{\text {min }} \cdot c_{\text {max }}}}{2 \cdot \Delta x}, \quad k=1,2$.

## 5. Comparison with Kållberg's Coefficients

In the present section we shall compare the "optimal" relaxation coefficients with Kållberg's coefficients (1977). In order to introduce the latter ones, we assume that some model (e.g. (1)) is integrated by the leap-frog method, i.e.
$u^{\tau+1}=u^{\tau-1}+2 \cdot \Delta t \cdot D u^{\tau}$
where the superscripts denote time levels and $D u^{\tau}$ is the tendency of $u$. Since the boundary relaxation term $-K(u-\tilde{u})$ may be large, it should be integrated implicitly (Kållberg, 1977; Davies, 1983).

The above-mentioned scheme together with an implicit integration of the relaxation term yields (we add a "hat"" in order to distinguish the solution from that of (109)):

$$
\begin{equation*}
\hat{u}^{\tau+1}=u^{\tau-1}+2 \cdot \Delta t \cdot\left[D u^{\tau}-K\left(\hat{u}^{\imath+1}-\tilde{u}^{\tau+1}\right)\right] . \tag{110}
\end{equation*}
$$

Subtracting (109) from (110), we obtain
$\hat{u}^{\tau+1}-u^{\tau+1}=-2 K \cdot \Delta t\left(\hat{u}^{\tau+1}-\tilde{u}^{\tau+1}\right)$
$\hat{u}^{\tau+1}=(1-\alpha) u^{\tau+1}+\alpha \tilde{u}^{\tau+1}$
where
$\alpha:=\frac{2 K \cdot \Delta t}{1+2 K \cdot \Delta t}$,
i.e. the boundary relaxation scheme produces a linear combination of the model variables (without boundary relaxation) and the corresponding externally prescribed values. $K$, and thus $\alpha$, may (and usually do) depend on the distance $k$ of a grid point from the boundary itself. The external values should get more "weight" ( $\alpha \approx 1$ ) close to the boundary, whereas the model-generated values should dominate ( $\alpha \approx 0$ ) further away from the boundary. Kållberg (1977) suggested the following $\alpha$-profile:
$\alpha_{k}=1-\tanh (a \cdot k)$
where $a$ is a constant, usually $a=0.5$. The corresponding $K$-profile is
$K_{k}=\frac{\alpha_{k}}{1-\alpha_{k}} \cdot \frac{1}{2 \Delta t}$ because of (113)

$$
=\frac{1-\frac{e^{a k}-e^{-a k}}{e^{a k}+e^{-a k}}}{\frac{e^{a k}-e^{-a k}}{e^{a k}+e^{-a k}}} \cdot \frac{1}{2 \Delta t} \quad \text { because of (114) }
$$

$$
=\frac{1}{e^{2 a k}-1} \cdot \frac{1}{\Delta t},
$$

i.e.
$K_{k}=\frac{1}{e^{k}-1} \cdot \frac{1}{\Delta t}$ for $a=0.5$.
Equation (115) shows that Kållberg's $K_{k}$ depends on the time step $\Delta t$. This has a paradoxical effect: If we reduce $\Delta t$ (usually in order to reduce the time-integration error, which should result in improved internally-generated values $u^{\tau+1}$ in the boundary zone), we automatically increase $K$ and thus produce a stronger forcing towards the externally prescribed values. According to Eq. (27) in Section $4(\mathrm{H}), K$ should be inversely proportional to the grid width $\Delta x$ instead of the time step $\Delta t$. (The dependence of $K$ on $\Delta x$ is not so "paradoxical", since the artificial waves, especially of wavelength
$2 \Delta x$, which shall be damped by the boundary relaxation scheme [cf. Section 2], depend on $\Delta x$ themselves.) However, in practical applications the above-mentioned problem may be of minor importance if $\Delta t$ and $\Delta x$ are fixed at the same time in such a way that the Courant number $\gamma:=c \cdot \Delta t / \Delta x$ falls within a certain prescribed interval (usually, $\gamma \leqslant 1$ to guarantee the stability of explicit integration schemes), i.e. $\Delta t$ and $\Delta x$ are chosen proportionally to each other.

In Table 1 we compare the relaxation coefficients (more precisely, the dimensionless weights $\alpha$-cf. (113)) according to Kållberg (1977) with those of the present study.

$$
\text { Optimal Relaxation Coefficients }\left(\gamma_{\min }=1 / 100, \gamma_{\max }=1\right) \text { : }
$$



## Kallberg:



Fig. 2. Illustration to Section 5: Divergence $\left[10^{-9} \mathrm{~s}^{-1}\right]$ after 1 h of model time

Table 2. Maximum of Perturbation of Geopotential and Divergence after 1 h of Integration (within $40 \times 40$ grid points)

| $s$ | $\left[\gamma_{\min }, \gamma_{\max }\right]$ | Perturbation of <br> geopotential <br> $[\%$ of initial | Divergence <br> $\left[10^{-9} \mathrm{~s}^{-1}\right]$ |
| :--- | :--- | :--- | :--- |
|  | perturbation $]$ |  |  |


| "Optimal" relaxation coefficients: |  |  |  |
| :--- | :--- | :--- | ---: |
| 4 | $[1 / 100,1]$ | 0.290 |  |
| 8 | $[1 / 10,1]$ | 0.005 | 15.46 |
| 8 | $[1 / 100,1]$ | 0.017 | 0.62 |
| 8 | $[1 / 1000,1]$ | 0.076 | 2.07 |
| Kållberg $(a=0.5)$; |  | 7.30 |  |
| 8 |  | 0.117 |  |

In order to illustrate the ability of the new coefficients, we apply them to an example almost identical to the first test experiment of Kållberg (1977): The shallow-water equations are integrated on $40 \times 40$ grid points ( $\Delta x=10 \mathrm{~km}, \Delta t=10 \mathrm{~s}$ ), starting from initial conditions with zero winds and a Gaussian perturbation of the geopotential in the centre of the integration area. The lateral boundary conditions are constant in time: zero winds and a constant geopotential. Results are contained in Table 2 and illustrated in Fig. 2: We chose the perturbation of the geopotential and the divergence of the wind field as indicators for the noise generated by wave reflection in the boundary zone.

In analogy to Davies (1983) we assume that the range of wave velocities relevant to the boundary scheme is $c_{\max }: c_{\min } \approx 100$, which motivates the choice of the interval $\gamma \in[1 / 100,1]$ of Courant numbers for the present scheme (results for $\gamma \in$ $[1 / 10,1]$ and $\gamma \in[1 / 1000,1]$ and also for the smaller relaxation zone width $s=4$ are given for comparison). It turns out that, in the present example, the results obtained with the "optimal" relaxation coefficients are superior to those of the Kållberg scheme.

## 6. Conclusions

One common method of supplying boundary values to limited-area numerical weather prediction models consists in specifying all variables at all boundary points. This deliberate overspecification provokes an unwanted partial reflection of outgoing waves. In order to mitigate this effect, Davies (1976) suggested a (Newtonian)
relaxation technique: In a boundary zone all variables are smoothly adjusted to the prescribed boundary values. Up to now the coefficients of this scheme (corresponding to "weights" of the internally computed variables and the externally prescribed values in the boundary zone) have mostly been determined ad hoc and "confirmed" by numerical experiments. The present paper describes a way of computing these coefficients, starting from the requirement that, under idealized conditions, the unwanted partial reflection of outgoing waves is minimal. More precisely: For a prescribed range of wave velocities (or, equivalently, Courant numbers), the maximum (wave-velocity-dependent!) reflection coefficient is minimized. This work is based on an equation for the reflection coefficient originally presented by Davies (1983) (for linearized shallow-water equations) and re-derived here under the additional assumption of steady state.

The complete algorithm for computing the relaxation coefficients can be found in Section $4(\mathrm{H})$. These coefficients have the following properties:

- They are optimal in a clearly identified sense.
- They depend on the grid width $\Delta x$, thus allowing adequate modifications if the grid width is changed.
- They depend on a prescribed range of wave velocities (or, equivalently, Courant numbers), for which the coefficients are required to be optimal. This additional degree of flexibility can be an advantage (e.g. when the model is modified) or may cause problems (if too little is known about the wave velocities in the model); but, in any case, the free parameters of the scheme have a clear physical meaning.

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## Appendix

FORTRAN Subroutine for Computing Optimal
Relaxation Coefficients (for $s=\mathbf{2}^{\boldsymbol{m}}$ )

|  | subroutine relax (s, gammin, gammax, alpha) |
| :---: | :---: |
| c | Input: s........... width of boundary relaxatio |
| c | zone (power of 2) |
| c | gammin..... minimal Courant number |
| c | gammax......maximal Courant number |
| c | (for which "optimal" |
| c | relaxation coefficients shall be determined) |

c kk
130
$\mathrm{q}(\mathrm{i})=\mathrm{qq}(\mathrm{i})$
$\mathrm{n}=2 * \mathrm{n}$
if ( n . lt. s) goto 1000
if ( n. ne. s ) write $(6, *)^{\prime}!\mathrm{s}$ is not a power of 2 !'
*** Computation of $\mathrm{K}+$ and alpha:
c $\mathrm{p}(.) \ldots \ldots . . . .$. coefficients of polynomial $\mathrm{P}_{\mathrm{A}} \mathrm{i}$ (b)
c $\quad \mathrm{q}(.) \ldots \ldots \ldots . .$. coefficients of polynomial $\mathrm{P}_{\mathrm{i}}-1$ (b)
kk..............K +
c $\quad \mathrm{kdt} 2 \ldots \ldots \ldots \ldots .2 \mathrm{~K}$ dt
Output: alpha (.)....weights of externally specified values in the boundary zone (corresponding to "optimal" relaxation coefficients)
parameter $(s m a x=16, s \max 2=\operatorname{smax} * 2)$
(We need smax $>\mathrm{s}$ !)
implicit real $* 8$ ( $\mathrm{a}-\mathrm{h}, \mathrm{o}-\mathrm{z}$ )
integer s
dimension alpha (s)
dimension $\mathrm{p}(0: \mathrm{smax}), \mathrm{q}(0: \mathrm{smax})$
dimension pp ( $0: \mathrm{smax} 2$ ), qq $(0: \operatorname{smax} 2)$
real*8 my, kk, kdt2
*** Computation of $\mathrm{P}(),. \mathrm{Q}():$.
$\mathrm{p}($.$) ............coefficients of polynomial \mathrm{P}(\mathrm{b})$
$\mathrm{q}(.) \ldots \ldots \ldots .$. coefficients of polynomial $\mathrm{Q}(\mathrm{b})$
$\mathrm{pp}(),. \mathrm{qq}($.$) .... auxiliary variables for computation$ of $\mathrm{p}(),. \mathrm{q}($.
n................s'
"Initialization" for $\mathrm{n}=1$ :
$\mathrm{n}=1$
$\mathrm{p}(0)=0$.
$\mathrm{p}(1)=1$.
$\mathrm{q}(0)=1$.
$q(1)=0$.
my $=\operatorname{sqrt}($ gammax $/$ gammin $)$
Begin of main loop (Step from n to $2 * \mathrm{n}$ ):
$\mathrm{my}=\mathrm{sqrt}((\mathrm{my}+1 . / \mathrm{my}) / 2$.
do $109 \mathrm{i}=0, \mathrm{n}+\mathrm{n}$
$\mathrm{pp}(\mathrm{i})=0$.
qq $(\mathrm{i})=0$.
do $119 \mathrm{i}=0$, n
do $119 \mathrm{j}=0, \mathrm{n}$
$\mathrm{pp}(\mathrm{i}+\mathrm{j})=\mathrm{pp}(\mathrm{i}+\mathrm{j})+\mathrm{p}(\mathrm{i}) * \mathrm{p}(\mathrm{j})+\mathrm{q}(\mathrm{i}) * \mathrm{q}(\mathrm{j})$
$\mathrm{qq}(\mathrm{i}+\mathrm{j})=\mathrm{qq}(\mathrm{i}+\mathrm{j})+2 . * \mathrm{my} * \mathrm{p}(\mathrm{i}) * \mathrm{q}(\mathrm{j})$
do $129 \mathrm{i}=0, \mathrm{n}+\mathrm{n}$
$\mathrm{p}(\mathrm{i})=\mathrm{pp}(\mathrm{i})$
do $139 \mathrm{i}=\mathrm{n}, 1,-1$
$\mathrm{kk}=\mathrm{p}(\mathrm{i}) / \mathrm{q}(\mathrm{i}-1)$
do $149 \mathrm{j}=\mathrm{i}, 1,-1$
$\mathrm{xxx}=\mathrm{q}(\mathrm{j})$
$\mathrm{q}(\mathrm{j})=\mathrm{p}(\mathrm{j})-\mathrm{kk} * \mathrm{q}(\mathrm{j}-1)$
$\mathrm{p}(\mathrm{j})=\mathrm{xxx}$
$\mathrm{xxx}=\mathrm{q}(0)$
$\mathrm{q}(0)=\mathrm{p}(0)$
$\mathrm{p}(0)=\mathrm{xxx}$
$\mathrm{kdt} 2=\mathrm{kk} * \mathrm{sqrt}($ gammin $*$ gammax $)$
alpha $(\mathrm{i})=\mathrm{kdt} 2 /(1 .+\mathrm{kdt} 2)$
REMARK: This alpha corresponds to the leap-frog scheme, whereas kdt2 is independent of the integration scheme.
return
end

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