



DISSIPATION, DISPERSION AND STABILITY OF
NUMERICAL SCHEMES FOR ADVECTION
AND DIFFUSION

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Title (and Subtitle) Dissipation, dispersion and stability properties of numerical schemes for advection and diffusion		
Abstract Advection and diffusion are fundamental processes in the atmosphere. They express the permanent balance between inertial and viscous forces. Some numerical treatments the equations, describing these processes, are presented. Three spatial discretization techniques, second order finite differences, linear finite element and pseudo-spectral, are tested in connection with a finite difference time integration. Dissipation, dispersion and stability of the numerical schemes for the linearized equations are investigated both theoretically and with the help of numerical simulations. Results with non-linear equations are also shown. In conclusion there is a presentation of the less conventional Monte Carlo method for diffusion.		
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DEFINITIONS

aliasing	in non-linear theory; misrepresentation by the grid of a not $\rightarrow$ resolvable wave. Its appearance is due to a non-linear interaction between two waves whose wavenumber lies near the limit of the $\rightarrow$ resolvability of the grid
aliasing error	in non-linear theory; the error due to an $\rightarrow$ aliasing
computational phase speed or diffusion coefficient	in linear theory; the coefficient needed to keep the advective or diffusive expression of the equation when the $\rightarrow$ elementary solution is substituted into the numerical scheme
conservation	a numerical scheme is conservative in regards to a physical invariant of the equation if the numerical expression of this invariant is conserved by the approximated equation
consistency	a numerical scheme is consistent if the approximation of derivatives approaches the derivative when the grid interval approaches zero
convergence	a numerical scheme is convergent if the error approaches zero when the grid interval approaches zero for any initial conditions. Remark: $\rightarrow$ consistency does not guarantee convergence.
dispersion	in linear theory; a numerical scheme is dispersive if the $\rightarrow$ computational phase speed or diffusion coefficient is a function of the wave number of the $\rightarrow$ elementary solution
dissipation	the inverse of $\rightarrow$ conservation
elementary solution	in linear theory, a wave solution of the advection or diffusion equation
error	the error of the numerical solution is the difference between the numerical and the true solution
linear stability	stability of the numerical scheme approximating the linearized equation
order of accuracy	lowest power of the grid interval that appears in the $\rightarrow$ truncation error
non-linear instability	in non-linear theory; instability due to the spurious energy flow associated by the $\rightarrow$ aliasing error
resolvability	property inherent to a discrete grid which expresses its ability to resolve wavelengths longer than two grid intervals (limit of resolvability)

¹ word also found in this list

DEFINITIONS, continuation

stability

a numerical scheme is stable if the error remains bounded as the time increases for any initial conditions

truncation error

additional term needed to keep the equations valid when the true solution is substituted into the numerical scheme and developed in Taylor series

1. METHODS OF DISCRETIZATION OF PARTIAL DIFFERENTIAL EQUATIONS

Three types of space discretization are considered.

1.1 Finite differences

The derivatives are approximated by finite difference quotients: difference between values of the variable at grid points over the grid interval, with the requirement that the approximation is consistent. Generally, the conditions of stability are then necessary and sufficient to ensure convergence (Arakawa, 1976).

The time derivatives are approximated by this method in the following study.

1.2 Finite elements

The variable is expanded by using a discrete series of piecewisely defined polynomial functions, called the basis functions.

Let us consider the one-dimensional problem

$$\frac{\partial \phi}{\partial t} + L\phi = 0 \quad \text{for } x \in \Omega = [x_1, x_M] \quad (1)$$

where L is a spatial differential operator.

To each point x_m of the grid is associated a basis function $\alpha_m(x)$

$$\alpha_m(x_n) = \delta_{m,n} \quad \left(\begin{array}{l} =1 \text{ if } m = n \\ =0 \text{ if } m \neq n \end{array} \right) \quad (2)$$

An approximation of $\phi(x,t)$ is:

$$\tilde{\phi}(x,t) = \sum_{n=1}^M \phi_n(t) \alpha_n(x)$$

with $\phi_n(t) = \phi(x_n, t)$

The procedure of discretization of the equation consists of substituting the approximated solution into the equation and orthogonalizing the residual to the basis functions (Galerkin procedure):

$$\int_{\Omega} \left(\frac{\partial \tilde{\phi}}{\partial t} - L\tilde{\phi} \right) \alpha_n dx = 0 \quad n=1, \dots, M \quad (3)$$

After time discretization, it remains to solve a system of M equations for M unknowns.

If L is a linear operator, one gets:

$$\sum_{m=1}^M \frac{d\phi_m}{dt} \int_{\Omega} \alpha_m \alpha_n dx = \sum_{m=1}^M \phi_m \int_{\Omega} \alpha_n L\alpha_m dx \quad n=1, \dots, M$$

The method has two characteristics (Cullen, 1979):

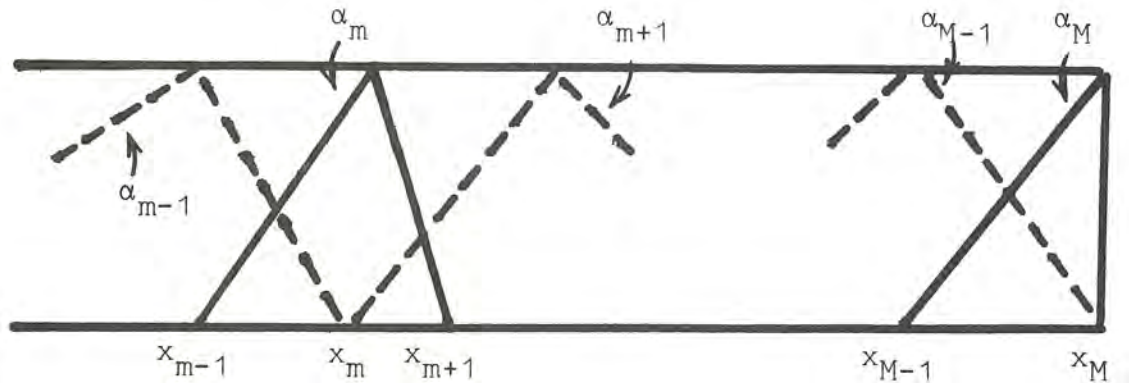
- the piecewise definition of the basis functions implies an almost orthogonality to one another (local interaction). This gives rise to a local spatial coupling between time derivatives (term $\int_{\Omega} \alpha_n \alpha_m dx$). The method is, by essence, an implicit method which needs the inversion of a sparse matrix each time step. The advantage consists of an improved description of the computational phase speed or diffusion coefficient and, in some case, of an increased order of accuracy (super convergence).
- The Galerkin integral guarantees aliasing free and conservative schemes. The effect of this integral is to prevent the appearance of a solution not resolvable by the basis function polynomial space. As the spectral method, the finite element method can be introduced as a least square approximation.

In all its generality, a finite element is the combination of

- a polynomial function space
- a set of points
- a geometric form

defined in such a way that the relation (2) permits a one-to-one relation between points and basis functions.

The simplest one-dimensional finite element is constituted by a linear polynomial defined on a segment:



The great flexibility of the method is due to the large freedom in the definition of the geometric form. Small elements can be concentrated where much information is desired, curved triangular or rectangular elements can be used to integrate with great precision the geometry of the boundaries (Johnson, 1980).

1.3 Pseudo-spectral method

The space derivatives at the grid points are calculated in wave number space. The variable ϕ is expanded by using a discrete series of globally defined trigonometric functions.

$$\phi(x,t) = \sum_k A(k,t) e^{i k x} \quad (4)$$

The amplitudes $A(k,t)$ are computed by the inverse relation of (4). The derivatives are then:

$$\frac{\partial \phi}{\partial x} = \sum_k i k A(k,t) e^{i k x}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \sum_k (-k^2) A(k,t) e^{i k x}$$

etc ...

The method has two characteristics (Merilees and Orszag, 1979).

- this evaluation of space derivatives may be considered as equivalent to the use of a certain finite differences scheme involving all the grid points, the weights of which are decreasing when the distance from the point under consideration increases.

For an infinitely differentiable variable, that leads to an infinite order of accuracy and, in reverse, to the problem of the remote influence of small perturbations.

- The calculation of the space derivatives in the spectral space makes the scheme essentially explicit. The stability conditions are furthermore restricted by the increasing space accuracy (of, for example, the stability condition for Leap Frog in Table I). It must be noticed that periodic boundary conditions and a regular grid are needed to apply the method.

If $M = 2N+1$, considerations of periodicity and resolvability give the resolvable wave numbers:

$$k_j = \frac{2\pi}{(2N+1)\Delta x} j \quad -N \leq j \leq N \quad \Delta x \text{ is the grid interval}$$

The transformation physical spectral space and its inverse are:

$$\phi(x_m, t) = \sum_{j=-N}^{+N} A(k_j, t) e^{i k_j x_m}, \quad 1 \leq m \leq 2N+1 \quad (4)$$

$$A(k_j, t) = \frac{1}{2N+1} \sum_{m=1}^{2N+1} \phi(x_m, t) e^{-i k_j x_m}, \quad -N \leq j \leq N \quad (5)$$

2. METHODS FOR INVESTIGATING LINEAR STABILITY AND ACCURACY OF NUMERICAL SCHEMES

2.1 Taylor development

The true solution is substituted into the numerical scheme and developed in Taylor series. The truncation error gives then the order of accuracy and, in some cases, the stability condition.

2.2 Fourier development or von Neumann's method

This method permits a systematic investigation of stability conditions and a study of the accuracy by examining the behaviour of the computational phase speed or diffusion coefficient.

Advection:

Let us consider

$$\boxed{\frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} = 0} \quad (6)$$

c is the physical phase speed, constant in time.

An elementary solution of (6) is

$$\phi(x,t) = \exp(-i k c t) \exp(i k x) \quad (7)$$

k is the wave number.

After time and space discretization,

$$\begin{aligned} \phi(m\Delta x, l\Delta t) &= \phi_m^l = \exp(-i k v l \Delta t) \exp(i k m \Delta x) \\ &= g^l \exp(i k m \Delta x) \end{aligned} \quad (8)$$

v is the computational phase speed, g is the amplification factor

$$g = |g| \exp(i\theta) = \exp(-i k v \Delta t) \quad (9)$$

The introduction of the expression (8) into the numerical scheme under consideration gives g as a function of c , Δt and Δx .

The stability criterion is obtained by

$$\boxed{|g(c, \Delta t, \Delta x)| \leq 1} \quad (10)$$

The behaviour of v in non-dimensional form is obtained from (9):

$$\boxed{\frac{v}{c} = -\frac{\theta}{R k \Delta x} + i \frac{\log|g|}{R k \Delta x}} \quad (11)$$

where $R = \frac{c\Delta t}{\Delta x}$

Remark. $k \Delta x$ varies from Π (the least resolvable wave length is $2\Delta x$) to 0 (wave degenerated into a constant)

Diffusion:

Let us consider

$$\boxed{\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial z} K \frac{\partial \phi}{\partial z} = K \frac{\partial^2 \phi}{\partial z^2} + \frac{dK}{dz} \frac{\partial \phi}{\partial z}} \quad (12)$$

K is the physical diffusion coefficient, constant in time.

An elementary solution of (12) is

$$\phi(x,t) = \exp \left[\left(i k \frac{dK}{dz} - k^2 K \right) t \right] \exp (i k z) \quad (13)$$

After time and space descretization,

$$\begin{aligned} \phi(m\Delta z, l\Delta t) &= \phi_m^l = \exp \left[\left(i k \frac{d\rho}{dz} - k^2 \rho \right) l\Delta t \right] \exp (i k m\Delta z) \\ &= g^l \exp (i k m\Delta z) \end{aligned} \quad (14)$$

ρ is the computational diffusion coefficient

g is the amplification factor

$$g = |g| \exp (i\theta) = \exp \left[\left(i k \frac{d\rho}{dz} - k^2 \rho \right) \Delta t \right] \quad (15)$$

The introduction of the expression (14) into the numerical scheme under consideration gives g as a function of K , $\frac{dK}{dz}$, Δt , Δz .

The stability criterion is obtained by

$$\boxed{\left| g(K, \frac{dK}{dz}, \Delta t, \Delta z) \right| \leq 1} \quad (16)$$

The behaviour of ρ and $\frac{d\rho}{dz}$ in non-dimensional form is obtained from (15):

$$\frac{\rho}{K} = - \frac{1}{S(k\Delta z)^2} \log |g| \quad (17)$$

$$\frac{d\rho/dK}{dz/dz} = \frac{\theta}{T(k\Delta z)} \quad (18)$$

where $S = \frac{K\Delta t}{\Delta z^2}$, $T = \frac{dK}{dz} \frac{\Delta t}{\Delta z}$

3. NUMERICAL SCHEMES FOR ADVECTION

Only the most widely used schemes are discussed here.

3.1 Linear theory

Table I recapitulates name, expression, order of accuracy, amplification factor and stability condition for all wave numbers of each scheme.

The symbol in parenthesis refers to the tables II, a through h, where the ratio v/c is presented depending on R and $k\Delta x$ following (11).

Relation (11) shows that $|g| < 1$ produces a complex computational phase speed which is a source of dissipation (only the real values are exhibited in table II).

Table II shows that all schemes, whose expression is not strictly symmetric in time and space are dissipative. Only Leap-Frog and Crank-Nicholson escape. The amount of damping is quite large for shorter wave lengths, especially for the wave length $2\Delta x$. A disadvantage lies in the fact that damping also depends, for a fixed Δx , on the time step Δt and the advection velocity c . However, we wish to choose Δt to give the best accuracy and stability properties, not to give the optimal amount of damping.

The Lax-Wendroff scheme is symmetric but a diffusion term is added in order to dissipate the shorter waves. The scheme can be rewritten explicitly as:

$$\frac{\psi_m^{l+1} - \psi_m^l}{\Delta t} + c \frac{\psi_m^{l+1} - \psi_m^{l-1}}{2\Delta x} = \frac{c^2 \Delta t}{2} \frac{\psi_{m+1}^l - 2\psi_m^l + \psi_{m-1}^l}{\Delta x^2}$$

The effect of introducing a dissipation in a Crank-Nicholson scheme by taking a backward time integration introduces very little change in the real part of the computational phase speed (compare IIb with IIc).

The amplification factor of a three-time-step scheme has two solutions. One gives the computational phase speed of the physical solution, the other one generates a spurious numerical solution, computational mode, whose amplitude changes sign every time-step (only the physical values are exhibited in Tables II). Nevertheless, for the same second order of accuracy, the computational phase speed of the physical solution is better described by a Leap-Frog scheme than by a Crank-Nicholson scheme (compare IIb with IIe).

The linear finite element technique is superior to the finite difference methods for all time integration schemes (compare IIb with IIc for Crank-Nicholson, IIe with IIg for Leap-Frog). The introduction of an increased order of spatial accuracy is paid for by a restriction on the stability condition for the Leap-Frog scheme: the upper boundary is 1 for a second order finite difference scheme, $1/\sqrt{3}$ for a linear finite element scheme, which is of fourth order and $1/\pi$ for a pseudo-spectral scheme of infinite order of accuracy. Another disadvantage is the large negative computational group speed at short wave lengths. The physical group speed c_g , which represents the velocity of transport of energy, is equal to the phase velocity for a constant phase speed according to the definition: (Holton, 1979, pp 151-152):

$$c_g = \frac{d(ck)}{dk} = c$$

The computational group speed is

$$v_g = \frac{d(vk)}{dk}$$

which is not equal to c because of the dispersive character of the numerical schemes under consideration, e.g. the fact that $v_g = v_g(k)$.

Looking at tables IIb and IIc, for example, the phase speed of wave-lengths $2\Delta x$ is zero, so the group speed can be approximated by:

$$v_g = \frac{d(vk\Delta x)}{d(k\Delta x)} \approx -v \quad (k\Delta x = \pi/2)$$

The energy propagates upstream in both cases but faster for the finite element scheme (IIc) than for the finite differences one (IIb). The improved computational phase speed at short wavelengths causes a deteriorated computational group speed.

It may be noticed that the pseudo-spectral scheme does not seem to be superior to the finite element one and that the computational phase speed exceeds for all R and $k\Delta x$ the physical one.

3.2 Numerical experiments

One-dimensional linear advection:

A Gaussian form given by

$$\phi(x,0) = 100 \exp \left(- \frac{(x-x_0)^2}{2} \right)$$

is advected on a 30 discretization points regular grid. The numerical solution is compared with the analytic one, $\phi(x,t) = \phi(x-ct,0)$.

Outflow boundary

Only the finite differences, **up-stream** and the finite element schemes have a prognostic equation for the boundary value ϕ_M .

For example: the linear finite element leap frog scheme

$$\frac{1}{3} \left(\frac{\phi_{M-1}^{\ell+1} - \phi_{M-1}^{\ell-1}}{2\Delta t} + 2 \frac{\phi_M^{\ell+1} - \phi_M^{\ell-1}}{2\Delta t} \right) + c \frac{\phi_M^{\ell} - \phi_{M-1}^{\ell}}{\Delta x} = 0$$

The other finite difference schemes need an additional condition like the no flux condition, $\frac{\partial \phi}{\partial x} = 0$, at the boundary. A special stability analysis must be performed to avoid spurious oscillations near the boundary.

With a pseudo-spectral technique, presupposing cyclic boundary values, the form advected out at the out-flow boundary is reintroduced at the in-flow boundary. To avoid this, Christensen and Prahm (1976) sacrifices the information on a few gridpoints near the out-flow boundary by artificially damping the solution.

In this case equation (6) becomes:

$$\frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} + \frac{\phi}{\tau} = 0$$

$$\tau = \frac{\Delta x}{c} \text{ is the e-folding time of the damping}$$

The comparison is made after advection through 12, 16 and 20 (out-flow boundary) gridpoints with $R = 0.25, 0.50$ and 0.75 . Figs Ia, b, c, d, e, f, g and h show the result for the corresponding numerical schemes.

It may be noticed:

- the intensive computational dissipation for asymmetric schemes, in space, the up-stream (Ia), in time Laasonen (Ic) and for the symmetric but intentionally dissipative Lax-Wendroff scheme (Id),

- the considerable reduction of noise in connection with the finite element technique (compare Ib with If for Crank-Nicholson and Ie with Ig for Leap-Frog).

Uniform rotation of a conical distribution

The analytical function describing the cone is given by

$$\phi(x,y,o) = \begin{cases} 100 \cos \left(\pi \frac{d}{2r} \right) & \text{if } d \leq r \\ 0 & \text{otherwise} \end{cases}$$

with $d^2 = (x-x_0)^2 + (y-y_0)^2$, (x_0, y_0) is the center of the cone
 r is the base radius of the cone

The uniform circular velocity field, centered at (x_1, y_1) (center of the grid) is given by: $\omega(-x + x_1, y - y_1)$, ω is the angular velocity. The grid has 30x30 discretization points separated by a constant interval Δs .

Fig IIa shows the evolution of the numerical solution of the rotation at an angle of 90° , 180° , 270° and 360° for $\omega \Delta t = 0.5^\circ$ and $r = 4\Delta s$.

Fig IIb shows the corresponding evolution of

- the maximal amplitude $\max_{m,n} (\phi_{m,n}^l)$, where $\phi_{m,n} = \phi(m\Delta s, n\Delta s, l\Delta t)$
- the sum of amplitudes $\frac{\sum_{m,n} \phi_{m,n}^l}{\sum_{m,n} \phi_{m,n}^0}$
- the sum of amplitudes squares $\frac{\sum_{m,n} (\phi_{m,n}^l)^2}{\sum_{m,n} (\phi_{m,n}^0)^2}$

The evolution of the two first quantities tests the conservative properties of the scheme under consideration, the evolution of the third tests the stability (an unstable scheme can conserve the sum of amplitudes).

Five schemes are tested:

finite differences/up-stream forward (Ia)
finite differences/Crank-Nicholson (Ib)
finite differences/Lax-Wendroff (Id)
linear finite element/Crank-Nicholson (If)
pseudo-spectral/Leap-Frog (Ih)

The results call for some comments:

- the up-stream scheme dissipates the maximal amplitude, the sum of amplitudes and the sum of amplitudes squares. Moreover the conical form expands itself with time,
- the finite differences/Lax-Wandroff and Crank-Nicholson show a tendency for a similar behaviour concerning the maximal amplitude and the conical form.
- the finite element/Crank-Nicholson and pseudo-spectral/Leap-Frog conserve exactly the sum of amplitudes and of amplitudes squares and nearly exactly the maximal amplitude and the form of the cone.

The computational times necessary to integrate the two-dimensional linear advection equation under consideration on a SAAB-UNIVAC 1100/21 computer with each of the five schemes are compared below:

the up-stream method acts as standard measure:

finite differences/up-stream forward (Ia)	1.
finite differences/Lax-Wandroff (Id)	1.4
finite differences/Crank-Nicholson (Ib)	3.5
linear finite element/Crank-Nicholson (If)	6.3
pseudo-spectral/Leap-Frog (Ih)	12.

The pseudo-spectral technique uses a FORTRAN Fast Fourier Transform elaborated by P. N. Swartzrauber at the NCAR (1978).

One-dimensional non-linear advection

The Burger equation:

$$\frac{\partial \phi}{\partial t} + \phi \frac{\partial \phi}{\partial x} = K \frac{\partial^2 \phi}{\partial x^2} \quad K \text{ constant}$$

together with the following initial condition:

$$\phi(x,0) = \frac{1}{2} (1 - \text{th} \frac{x}{4K})$$

has the analytic solution (Gazdag, 1973):

$$\phi(x,t) = \frac{1}{2} [1 - \text{th} (\frac{x-t/2}{4K})]$$

The true solution is compared with the computational one calculated on a 256 discretization points regular grid by means of the following schemes (for the diffusion schemes, see chapter 4)

- finite differences/up-stream forward

$$\frac{\phi_m^{\ell+1} - \phi_m^{\ell}}{\Delta t} + p \phi_m^{\ell} \frac{\phi_m^{\ell} - \phi_{m-p}^{\ell}}{\Delta x} = K \frac{\phi_{m+1}^{\ell+1} - 2\phi_m^{\ell+1} + \phi_{m-1}^{\ell+1}}{\Delta x^2}$$

$$\text{where } p = \begin{cases} +1 & \text{if } \phi_m^{\ell} > 0 \\ -1 & \text{if } \phi_m^{\ell} < 0 \end{cases}$$

- finite element/Laasonen

$$\begin{aligned} & \frac{\phi_{m-1}^{\ell+1} - \phi_{m-1}^{\ell}}{\Delta t} + 4 \frac{\phi_m^{\ell+1} - \phi_m^{\ell}}{\Delta t} + \frac{\phi_{m+1}^{\ell+1} - \phi_{m+1}^{\ell}}{\Delta t} + \\ & + \frac{1}{\Delta x} \left[(2\phi_m^{\ell} + \phi_{m+1}^{\ell}) \phi_{m+1}^{\ell+1} - (\phi_{m+1}^{\ell} - \phi_{m-1}^{\ell}) \phi_m^{\ell+1} - (2\phi_m^{\ell} + \phi_{m-1}^{\ell}) \phi_{m-1}^{\ell+1} \right] = \\ & = K \frac{\phi_{m+1}^{\ell+1} - 2\phi_m^{\ell+1} + \phi_{m-1}^{\ell+1}}{\Delta x^2} \end{aligned}$$

- pseudo-spectral/Adams-Bashforth

$$\frac{\phi_m^{\ell+1} - \phi_m^{\ell}}{\Delta t} + \phi_m^{\ell} \left(\frac{3}{2} \frac{\partial \phi_m^{\ell}}{\partial x} - \frac{1}{2} \frac{\partial \phi_m^{\ell-1}}{\partial x} \right) = K \left(\frac{3}{2} \frac{\partial^2 \phi_m^{\ell}}{\partial x^2} - \frac{1}{2} \frac{\partial^2 \phi_m^{\ell-1}}{\partial x^2} \right)$$

In order to satisfy to the cyclic boundary conditions, the domain of integration D is divided into two subdomains

$$\begin{cases} D_0 & \text{where } \phi \text{ is kept constant} \\ D_1 & \text{where the time integration is realized} \end{cases}$$

The numerical parameters are

$$\Delta x = 0.01, \Delta t = 0.001$$

$$D = [0., 2.55]$$

$$\text{in } D_0 = [0., 0.6], \quad \phi(x) = \begin{cases} 0 & 0 \leq x \leq 0.1 \\ 1 - \cos \frac{(x-0.1)\pi}{0.3} & 0.1 \leq x \leq 0.4 \\ 1 & 0.4 < x < 0.6 \end{cases}$$

$$\text{in } D_1 = 0.6, 2.55, \quad \phi(x,0) = \frac{1}{2} \left(1 - \tanh \frac{x-1}{4K} \right)$$

Fig III presents the computed and true profiles between $x = 1.20$ and $x = 1.60$ after 166 time-steps and for $K = 0.002, 0.005$ and 0.01 .

Table III exhibits the values in the transition domain between $x = 1.37$ and $x = 1.49$.

Finite element and pseudo-spectral techniques give nearly same result in good agreement with the true solution, while the finite differences technique both smoothes and retards exaggerately the computational solution.

4. NUMERICAL SCHEMES FOR DIFFUSION

Long (1975) has examined 8 different second order finite difference schemes for the diffusion equation. As for the advection only the most widely used schemes are presented here:

4.1 Linear theory

Table IV recapitulates name, expression, order of accuracy, amplification factor and stability conditions for all wave numbers of each scheme. The symbol in parenthesis refers to the table where the ratios ρ/K and $\frac{d\rho}{dz}/\frac{dK}{dz}$ are presented depending on s , T and $K\Delta z$ following (17), (18).

The decomposition of the diffusion into a K - and a $\frac{dK}{dz}$ -term is used for convenience. By this way the behaviour of ρ and $\frac{d\rho}{dz}$ can be examined separately.

The conventional form is obtained considering:

$$K = \frac{K_{m+1/2} + K_{m-1/2}}{2} \text{ and } \frac{dK}{dz} = \frac{K_{m+1/2} - K_{m-1/2}}{\Delta z}$$

For example, IVa becomes (see definition in table on next page)

$$\frac{\phi_m^{l+1} - \phi_m^l}{\Delta t} = \frac{1}{\Delta z^2} (K_{m+1/2} \phi_{m+1}^l - (K_{m+1/2} + K_{m-1/2}) \phi_m^l + K_{m-1/2} \phi_{m-1}^l)$$

If $\frac{dK}{dz} = 0$, relations (17), (18) become

$$\frac{\rho}{K} = - \frac{1}{s(K\Delta z)^2} \log |g| - i \frac{\theta}{s(K\Delta z)^2}$$

where g is real

$$\text{and } \theta = \begin{cases} 0 & \text{if } 0 < g \leq 1 \\ \Pi & \text{if } -1 \leq g < 0 \end{cases}$$

Remark:

$\theta = \Pi$ gives rise to a spurious $2\Delta t$ wave (cf (15)).

The condition on s to avoid the appearance of such a wave is:

numerical scheme	condition of positivity for g
finite differences forward (IVa)	$4s \leq 1$
finite differences trapezoidal (IVb)	$3s \leq 1$
finite differences (IVc)	$2s \leq 1$
finite differences Crank-Nicholson (IVd)	$2s \leq 1$
finite differences Laasonen (IVe)	$-\forall s$
finite differences Dufort-Frankel (IVf)	$1 \leq 2s$
linear finite element Laasonen (IVg)	$-\forall s$
pseudo-spectral Adams-Bashforth (IVh)	$s = 0$

Only the Laasonen method guarantees the absence of a $2\Delta t$ noise in the case of weak gradient of diffusion coefficient.

The adoption of a three-time-step scheme as Dufort-Frankel or Adams-Bashforth introduce two solutions: a physical one and a computational one (only the physical values are exhibited in table IV). Fortunately, the ratio ρ/K for the numerical solution goes to infinity when the wavelength increases. The computational mode is thus quickly damped.

Crank-Nicholson (IVd) is apparently better than Dufort-Frankel (IVf). The latter overestimates the shear $\frac{d\rho}{dz}$ at large s .

When $T (= \frac{dK}{dz} \cdot \frac{\Delta t}{\Delta z})$ increases, both ρ and $\frac{d\rho}{dz}$ decrease and underestimate K and $\frac{dK}{dz}$ for all schemes but for Laasonen. This one keeps the ratio ρ/K near one at least for large s (IVe).

The use of finite element in combination with the Laasonen time integration scheme improves the results at small s but amplifies the error at large S , that becomes troublesome at large T (compare IVe with IVg).

4.2 Numerical experiments

One-dimensional linear diffusion with constant coefficient

One considers the linear diffusion of an instantaneous point source

$$\phi(z,0) = 100 \delta(z_0)$$

where $\delta(z_0)$ is the Dirac function $\delta(z_0) = \begin{cases} 1 & z = z_0 \\ 0 & \text{otherwise} \end{cases}$

Considering $\frac{dK}{dz} = 0$ the solution of (12) is for the boundary conditions:
 $\frac{\partial \phi}{\partial z} = 0$ at infinity

$$\phi(z,t) = \frac{100}{\sqrt{4\pi Kt}} \exp \left[-\frac{(z-z_0)^2}{4Kt} \right]$$

The solution computed on a 30 discretization points regular grid with the help of the different schemes is compared with the Gaussian analytical solution after 3, 6 and 12 iterations with $S = 0.25, 0.50$ and 0.75 . Figs IVa, b, c, d, e, f, g and h present the result for the corresponding numerical schemes.

It may be noticed:

- the presence of a spurious $2\Delta z$ wave at some value of S for all the schemes except IVc, which is rather bad, and Laasonen IVe and IVg. This feature is particularly remarkable for Dufort-Frankel, IVf.
- the nearly equivalent description given by the finite element and the finite difference technique (compare IVe with IVg),
- the nearly similar results obtained with Crank-Nicholson, Laasonen and Dufort-Frankel for a weak gradient of diffusion coefficient ($T = 0.25$) and the superiority of the two-time-steps schemes Crank-Nicholson and Laasonen for strong gradient of diffusion coefficient ($T = 0.75$) (compare IVd, IVe and IVf).
- the unstable pseudo-spectral Adams-Bashforth scheme at $s = 0.25$ can be rendered stable by filtering the $2\Delta z$ wave, i.e. setting the amplitude of this wave equal to zero in the frequency space.

5. A STATISTICAL APPROACH TO THE DIFFUSION EQUATION

The previous chapter discussed diffusion from an Eulerian point of view, establishing the diffusion equation from a consideration of 'concentration' and flux at fixed points in space.

It is also possible to approach the diffusion problem from a Lagrangian point of view, focusing on the history of random movements executed by the diffusing particles. To get useful results, statistical properties of the random motions have to be considered.

A statistical treatment of the Brownian motion is performed by Csanady (1973). His approach can be generalized in the following way.

Let us consider the velocity field $u(t)$ of a diffusing particle (the space coordinates are omitted for simplicity).

Provided the physical process is stationary, it is convenient to define a time autocorrelation coefficient $r(\tau)$, and a Lagrangian integral scale I related to r by:

$$I_L = \int_0^{\infty} r(\tau) d\tau$$

The value of I_L is thus a rough measure of the time interval over which $u(t)$ is correlated with itself.

The conventional diffusion coefficient is related to the integral scale by (Tennekes and Lumley, 1972, p 225)

$$K = I_E \sigma^2$$

where σ^2 is the variance of the velocity field $u(t)$ and subscript E means an Eulerian property.

In the atmosphere turbulent surface boundary layer:

$$K = l_E \mu_*$$

where l_E is the mixing-length or size of the most energetic turbulent eddies

$\mu_* = \sigma$ is the friction velocity

From dimensional consideration one also has $I_E = \frac{l}{\mu_*}$

For e g $\ell = 5$ m, $\mu_* 0.25$ m/s, one gets $I_E = 20$ s.

It is reasonable to expect that all the integral scales associated with $\mu(t)$ are about the same, because they are determined by the scale of the physical processes that produces $\mu(t)$. I is also a measure of the time over which $\mu(t)$ is dependent on itself (Tennekes and Lumley, 1972).

It is thus possible to divide the total displacement of a particle into a number of (nearly) independent random steps, taking place over a time period Δt much larger than I : the particle is said to execute a 'random walk'.

The diffusion of a passive admixture is simulated by tracking a number of N particles, each representing a certain quantity Q . The motion of each particle of number i in one dimension z is described by the following equation:

$$z_i^{\ell+1} = z_i^{\ell} + \Delta t w^{\ell} + \Delta t p_i^{\ell}$$

where z^{ℓ} holds for $z(\ell\Delta t)$

w is the advection velocity in the z -direction

$\{p^{\ell}\}$ is a discrete random process, i e a sequence of mutually independent, identically distributed random variables

The transport due to diffusion is further related to the process $\{p^{\ell}\}$ by introduction of a scale of diffusion velocity $\underline{P}$:

$$p_i^{\ell} = \underline{P} v_i^{\ell}$$

where $\{v_i^{\ell}\}$ are random numbers between -1 and $+1$ chosen independently from a prescribed probability density function.

For a constant diffusion coefficient K , the diffusion velocity scale $\underline{P}$ is

$$\underline{P} = \left(\frac{6K}{\Delta t}\right)^{1/2} \quad (19)$$

But generally, the choice of $\underline{P}$ is entirely due to convenience.

The mean concentration ψ after a time t_0 in a segment of length Δz around z_0 is interpreted as the probability for a particle to be in the volume Δz around z_0 at time t_0 , i.e.:

$$\psi(z_0, t_0) = \frac{Q}{\Delta z} \sum_{i=1}^N \delta_i^{\Delta z}$$

where

$$\delta_i^{\Delta z} = \begin{cases} 1 & \text{if } z_0 - \frac{\Delta z}{2} < z_i(t_0) \leq z_0 + \frac{\Delta z}{2} \\ 0 & \text{otherwise} \end{cases}$$

The method described above is unconditionally stable, the only limitation lies in the choice of the time step $\Delta t \gg I$ and in the fact that the process has to be stationary.

A numerical experiment analogue to this described in 4.2 is performed: one considers N particles of coordinate $\{z_i\}$, the evolution of which is given by:

$$z_i^{\ell+1} = z_i^{\ell} + \Delta t \underline{v}_i^{\ell} \quad \text{initially } z_i^0 = z_0 \quad \forall i$$

P is related to $s = \frac{K\Delta t}{\Delta z^2}$ using (19):

$$P\Delta t = \Delta z(6s)^{1/2}$$

$$\text{and } \psi_m^{\ell} = \frac{100}{N\Delta z} \sum_{i=1}^N \delta_i^{\Delta z}$$

where

$$\delta_i^{\Delta z} = \begin{cases} 1 & (m - \frac{1}{2}) \Delta z \leq z_i^{\ell} \leq (m + \frac{1}{2}) \Delta z \\ 0 & \text{otherwise} \end{cases}$$

As before, the statistical solution is compared to the true solution after 3, 6 and 12 iterations in fig. V.

Δz is taken equal to 1.

The numbers $\{v_i^l\}$ are chosen independently from a rectangular probability density function and the number N is chosen as the minimal number of particles which gives an error of the statistical solution less than 10% in regard to the true solution after 12 iterations.

A systematic study shows that, on the mean:

for $S = 0.25$ $N = 120$

$S = 0.50$ $N = 60$

$S = 0.75$ $N = 30$

6. FILTERING TECHNIQUE

The numerical experiments with the advection and diffusion equations show the necessity of filtering spurious short waves, generally two time-step or space-interval waves.

The most usual filter is the so called Asselin filter (1972): if $\tilde{\psi}$ is the smoothed field, ψ the initial field, then

$$\tilde{\psi}_p = \psi_p + \frac{\nu}{2} (\psi_{p+1} - 2\psi_p + \psi_{p-1})$$

ν is the coefficient of the filter

p is a space or time gridpoint index

Table IVa gives the ratio $\tilde{\psi}/\psi$ depending on ν and the wavelength (Δs is the grid interval).

A filter much more efficient to damp the shorter waves while keeping unchanged the longer waves is used by Long et alii (1966):

$$(1-\nu)\tilde{\psi}_{p-1} + 2(1-\nu)\tilde{\psi}_p + (1-\nu)\tilde{\psi}_{p+1} = \psi_{p-1} + 2\psi_p + \psi_{p+1}$$

Table IVb indicates its performance. The method is time-consuming because of its implicit character.

As the pseudo-spectral method is concerned, the filtering is reduced to a setting of the amplitudes of the spurious waves to zero in the frequency space.

A selectively controlled filtering has, in all cases, a beneficial effect on the linear and non-linear stability.

7. CONCLUSION - OPTIMAL CHOICE OF A METHOD

To integrate a convection equation, several subjective factors guide the choice of a numerical scheme:

- a computational dissipation is desired or, on the contrary, good conservation properties are looked for.
- The boundary conditions require special attention.
- Precision is more important than computational integration time.

Some other factors have a more imperative character like:

- for the desired grid interval and time step, the stability condition must be fulfilled in regards to the advection velocity, the diffusion coefficient and its derivative,
- a compatibility must exist between the advection and the diffusion schemes as well as for the time integration scheme (two-or-three-time steps) in terms of accuracy in time and space.

Undoubtedly, the linear finite element/Crank-Nicholson scheme presents many good properties for modelling the advection equation: accuracy, conservation, unconditional linear and non-linear stability, good treatment of the boundaries, little dispersion of the computational phase speed. If desired, a controlled dissipation can be added by the introduction of a filter.

For modelling the diffusion equation, the finite differences technique seems to be superior in accuracy to the finite element one, as long as boundary conditions are out of consideration. The problem of non-linear instability which could justify an aliasing free method is not relevant in a diffusion problem where the shorter waves are filtered by the physical process itself as they appear. Some schemes, however, create and maintain a two-grid-interval noise. In this case, an additional selective filter must be used. Finally the finite differences/Laasonen scheme seems to be superior to the others: no spurious, two-grid-interval noise, unconditional linear stability and good accuracy speak in its favour.

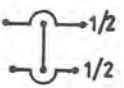
Comput. model	Name and expression	Order of accuracy	Amplification factor	Stability condition
Table 1 	finite differences up-stream forward or Euler (Ia) $\frac{\psi_m^{l+1} - \psi_m^l}{\Delta t} + c \frac{\psi_m^l - \psi_{m-1}^l}{\Delta x} = 0 \text{ for } c > 0$	$\Delta x, \Delta t$	$g = 1 + R(\cos k\Delta x - 1) - iR \sin k\Delta x$	$ R \leq 1$
	finite differences Crank-Nicholson (Ib) $\frac{\psi_m^{l+1} - \psi_m^l}{\Delta t} + \frac{c}{2} \left(\frac{\psi_{m-1}^{l+1} - \psi_{m-1}^l}{2\Delta x} + \frac{\psi_{m-1}^l - \psi_{m-1}^{l-1}}{2\Delta x} \right) = 0$	$\Delta x^2, \Delta t^2$	$g = \frac{1 - i \frac{R}{2} \sin k\Delta x}{1 + i \frac{R}{2} \sin k\Delta x}$	$\forall R$
	finite differences Crank-Nicholson backward or Laasonen (Ic) $\frac{\psi_m^{l+1} - \psi_m^l}{\Delta t} + c \frac{\psi_{m+1}^{l+1} - \psi_{m-1}^{l+1}}{2\Delta x} = 0$	$\Delta x^2, \Delta t$	$g = \frac{1}{1 + iR \sin k\Delta x}$	$\forall R$
	finite differences Lax-Wendroff (Id) (Gadd, 1974) $\frac{\psi_{m+1/2}^l - \frac{1}{2}(\psi_{m+1}^l + \psi_m^l)}{\frac{1}{2}\Delta t} + c \frac{\psi_{m+1}^l - \psi_m^l}{\Delta x} = 0$ $\frac{\psi_{m-1/2}^{l+1/2} - \frac{1}{2}(\psi_m^l + \psi_{m-1}^l)}{\frac{1}{2}\Delta t} + c \frac{\psi_m^l - \psi_{m-1}^l}{\Delta x} = 0$ $\frac{\psi_m^{l+1} - \psi_m^l}{\Delta t} + c \frac{\psi_{m+1/2}^{l+1/2} - \psi_{m-1/2}^{l+1/2}}{\Delta x} = 0$	$\Delta x^2, \Delta t^2$	$g = 1 + R^2(\cos k\Delta x - 1) - iR \sin k\Delta x$	$ R \leq 1$

Table 1, continuation

Comput. model	Name and expression	Order of accuracy	Amplification factor	Stability condition
	finite differences leap-frog (Ie) $\frac{\psi_m^{\ell+1} - \psi_m^{\ell-1}}{2\Delta t} + c \frac{\psi_{m-1}^{\ell} - \psi_{m+1}^{\ell}}{2\Delta x} = 0$	$\Delta x^2, \Delta t^2$	$g = \pm(1 - R^2 \sin^2 k\Delta x)^{1/2} - iR \sin k\Delta x$	$ R \leq 1$
	linear finite element Crank-Nicholson (If) $\frac{1}{6} \left(\frac{\psi_{m-1}^{\ell+1} - \psi_{m-1}^{\ell}}{\Delta t} + 4 \frac{\psi_m^{\ell+1} - \psi_m^{\ell}}{\Delta t} + \frac{\psi_{m+1}^{\ell+1} - \psi_{m+1}^{\ell}}{\Delta t} \right) +$ $+ \frac{c}{2} \left(\frac{\psi_{m+1}^{\ell+1} - \psi_{m-1}^{\ell+1}}{2\Delta x} + \frac{\psi_{m+1}^{\ell} - \psi_{m-1}^{\ell}}{2\Delta x} \right) = 0$	$\Delta x^4, \Delta t^2$	$g = \frac{\frac{2 + \cos k\Delta z}{3} - i \frac{R}{2} \sin k\Delta z}{\frac{2 + \cos k\Delta z}{3} + i \frac{R}{2} \sin k\Delta z}$	$\forall R$
	linear finite element leap-frog (Ig) $\frac{1}{6} \left(\frac{\psi_{m-1}^{\ell+1} - \psi_{m-1}^{\ell-1}}{2\Delta t} + 4 \frac{\psi_m^{\ell+1} - \psi_m^{\ell-1}}{2\Delta t} + \frac{\psi_{m+1}^{\ell+1} - \psi_{m+1}^{\ell-1}}{2\Delta t} \right) +$ $+ c \frac{\psi_{m+1}^{\ell} - \psi_{m-1}^{\ell}}{2\Delta x} = 0$	$\Delta x^4, \Delta t^2$	$g = \frac{\pm \left[\left(\frac{2 + \cos k\Delta x}{3} \right)^2 - R^2 \sin^2 k\Delta x \right]^{1/2} - iR \sin k\Delta x}{\frac{2 + \cos k\Delta x}{3}}$	$ R \leq \frac{1}{\sqrt{3}}$
	pseudo-spectral leap-frog (Ih) $\frac{\psi_m^{\ell+1} - \psi_m^{\ell-1}}{2\Delta t} + c \frac{\partial \psi_m}{\partial x} = 0$	$\Delta x^{\infty}, \Delta t^2$	$g = \pm(1 - R^2(k\Delta x)^2)^{1/2} - iR(k\Delta x)$	$ R < \frac{1}{\pi}$

Table 11a- finite differences up-stream forward

wave length $k\Delta x$	$2\Delta x$ π	$4\Delta x$ $\pi/2$	$6\Delta x$ $\pi/3$	$8\Delta x$ $\pi/4$
$R = 0.25$	0.	0.819	0.927	0.960
$R = 0.50$	0.	1.	1.	1.
$R = 0.74$	0.	1.060	1.024	1.013

Table 11b- finite differences Crank-Nicholson

$R = 0.25$	0.	0.633	0.824	0.898
$R = 0.50$	0.	0.624	0.814	0.891
$R = 0.75$	0.	0.609	0.800	0.880

Table 11c- finite differences Laasonen

$R = 0.25$	0.	0.624	0.814	0.891
$R = 0.50$	0.	0.590	0.780	0.865
$R = 0.75$	0.	0.546	0.733	0.828

Table 11d- finite differences Lax-Wendroff

$R = 0.24$	0.	0.664	0.840	0.907
$R = 0.50$	0.	0.749	0.878	0.928
$R = 0.75$	0.	0.865	0.936	0.960

Table 11e- finite differences leap-frog

$R = 0.15$	0.	0.643	0.834	0.905
$R = 0.50$	0.	0.667	0.866	0.923
$R = 0.75$	0.	0.720	0.900	0.949

Table 11f- linear finite element Crank-Nicholson

$R = 0.25$	0.	0.944	0.987	0.995
$R = 0.50$	0.	0.914	0.971	0.985
$R = 0.75$	0.	0.870	0.946	0.970

Table 11g- linear finite element leap frog

$R = 0.25$	0.	0.979	1.004	1.004
$R = 0.50$	0.	1.080	1.044	1.025
$R = 0.75$	0.	/	1.138	1.067

Table 11h- pseudo-spectral leap frog

$R = 0.25$	1.150	1.028	1.012	1.007
$R = 0.50$	/	1.150	1.052	1.028
$R = 0.75$	/	/	1.150	1.069

$\frac{v}{c}$ / unstable

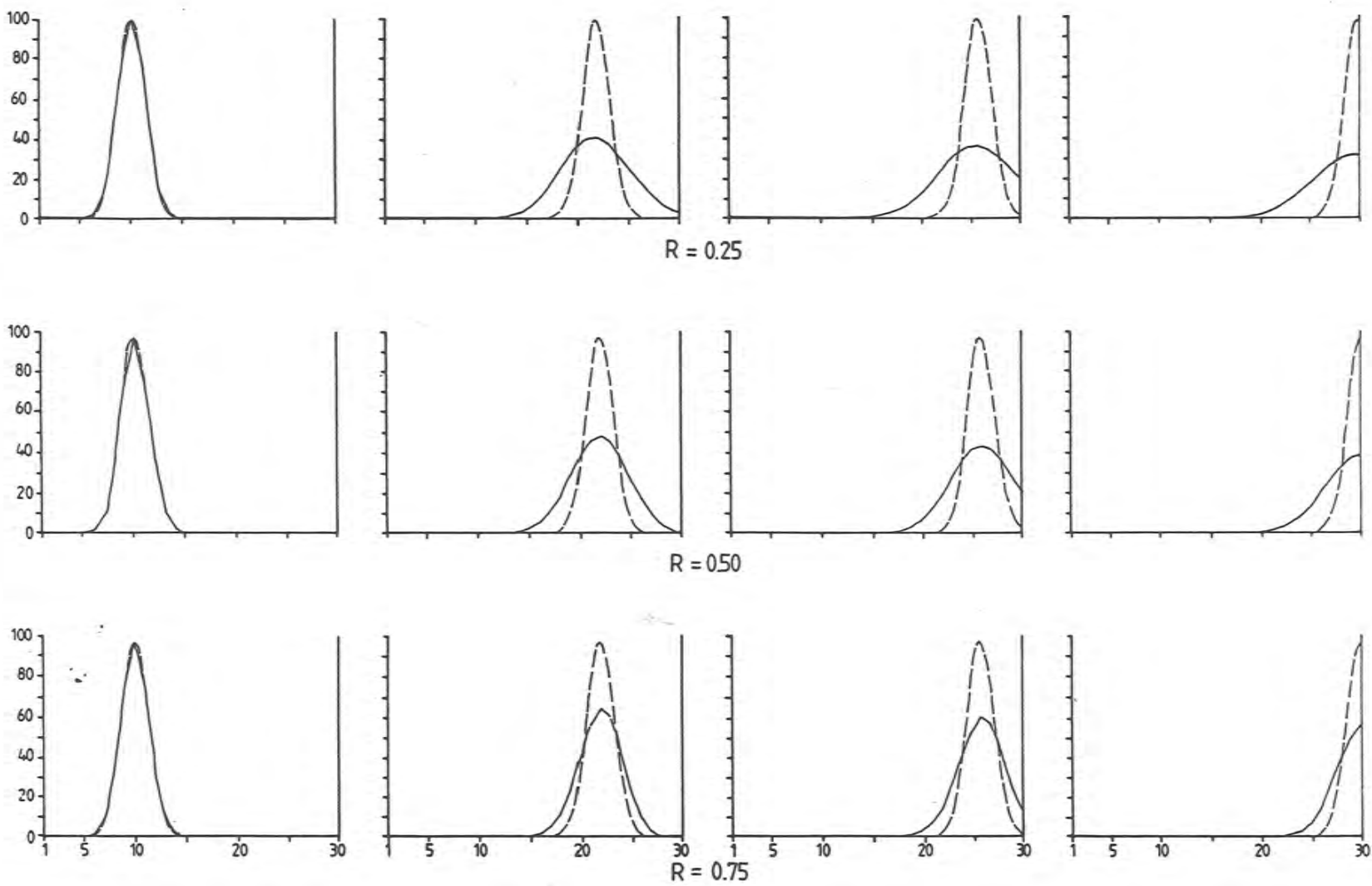


Figure 1a Finite differences up-stream forward

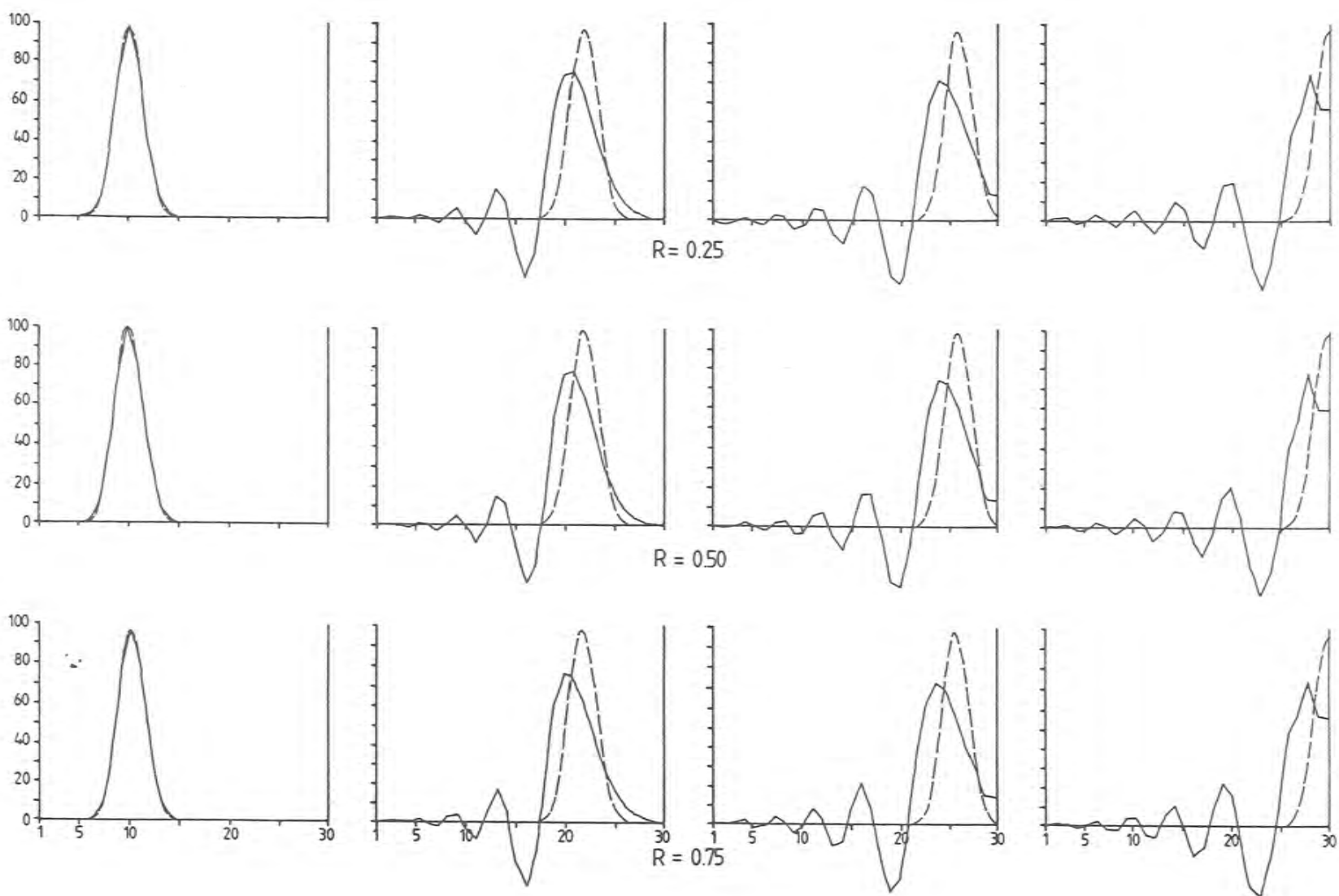
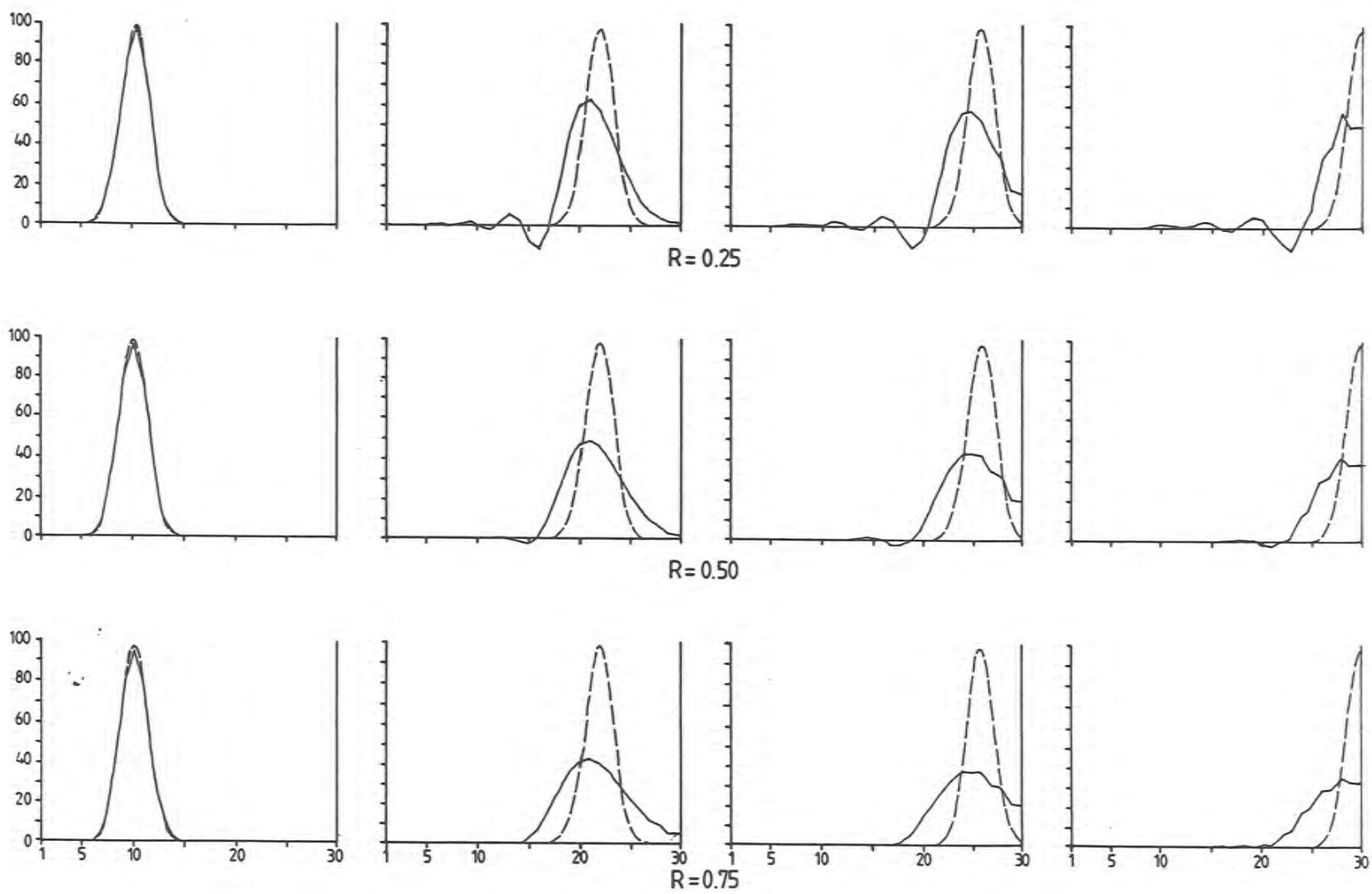


Figure 1b Finite differences Crank-Nicholson

Figure 1c Finite differences laasonen



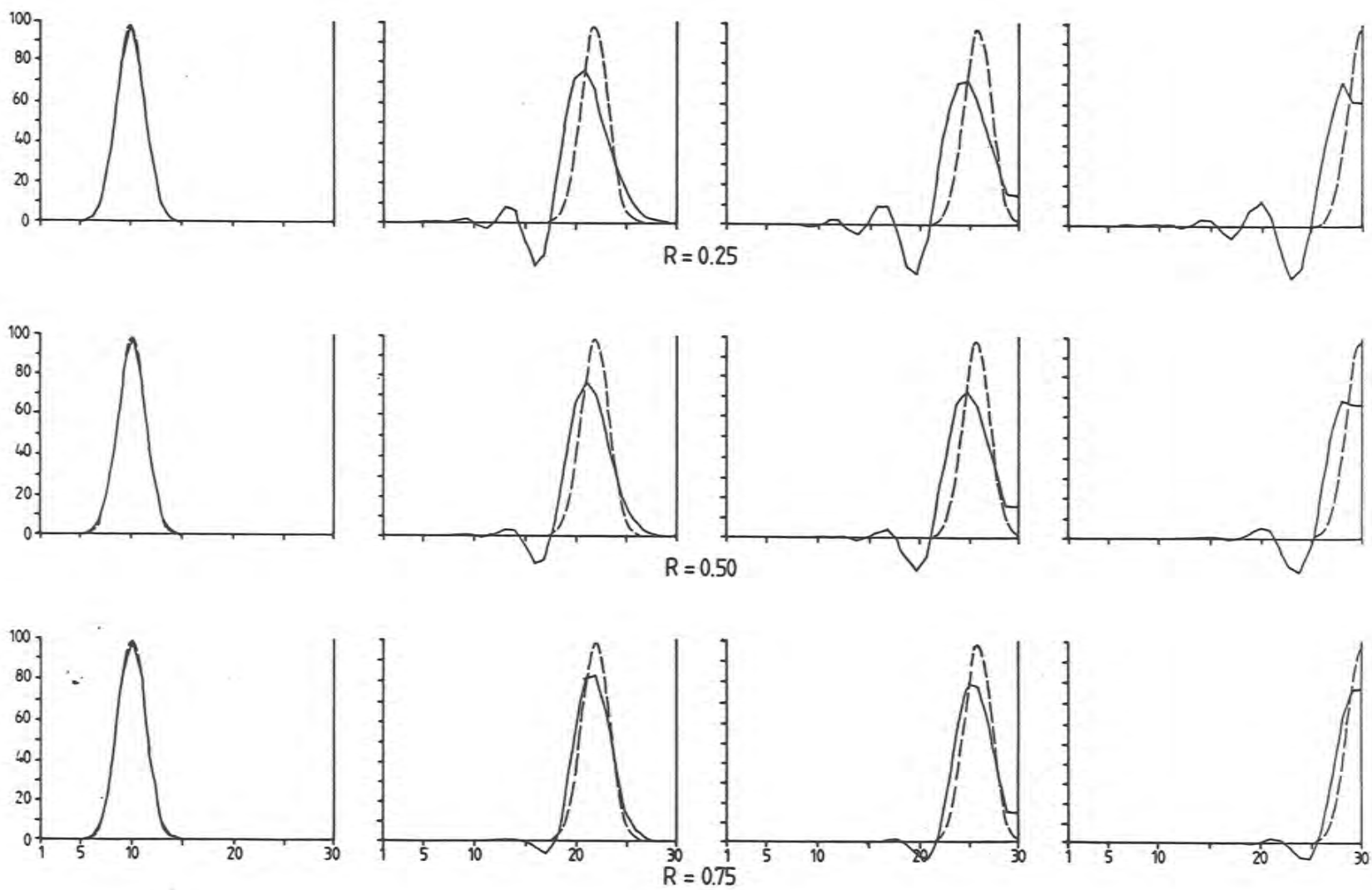


Figure 1d Finite differences Lax-Wendroff

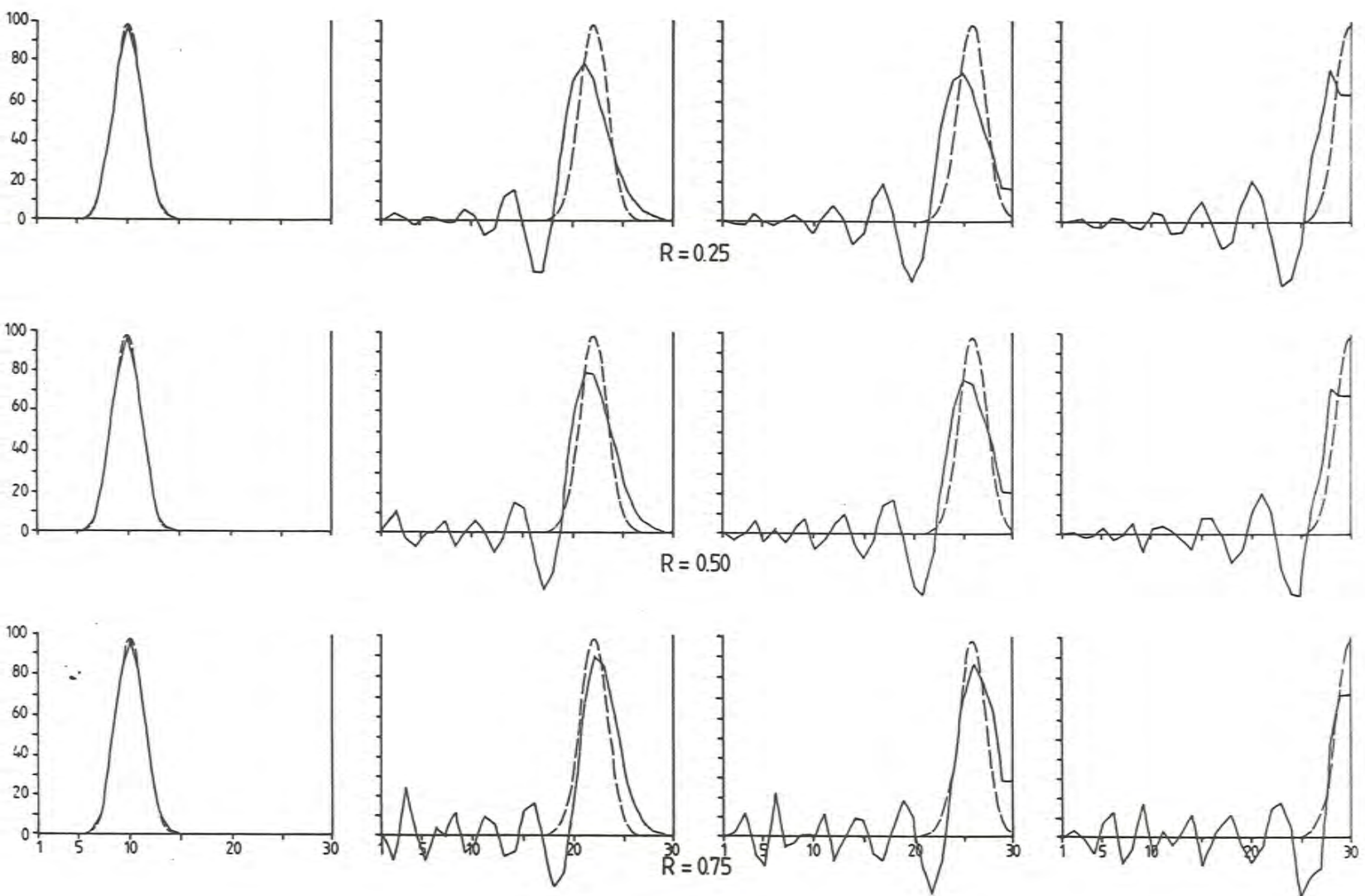


Figure 1e Finite differences leap frog

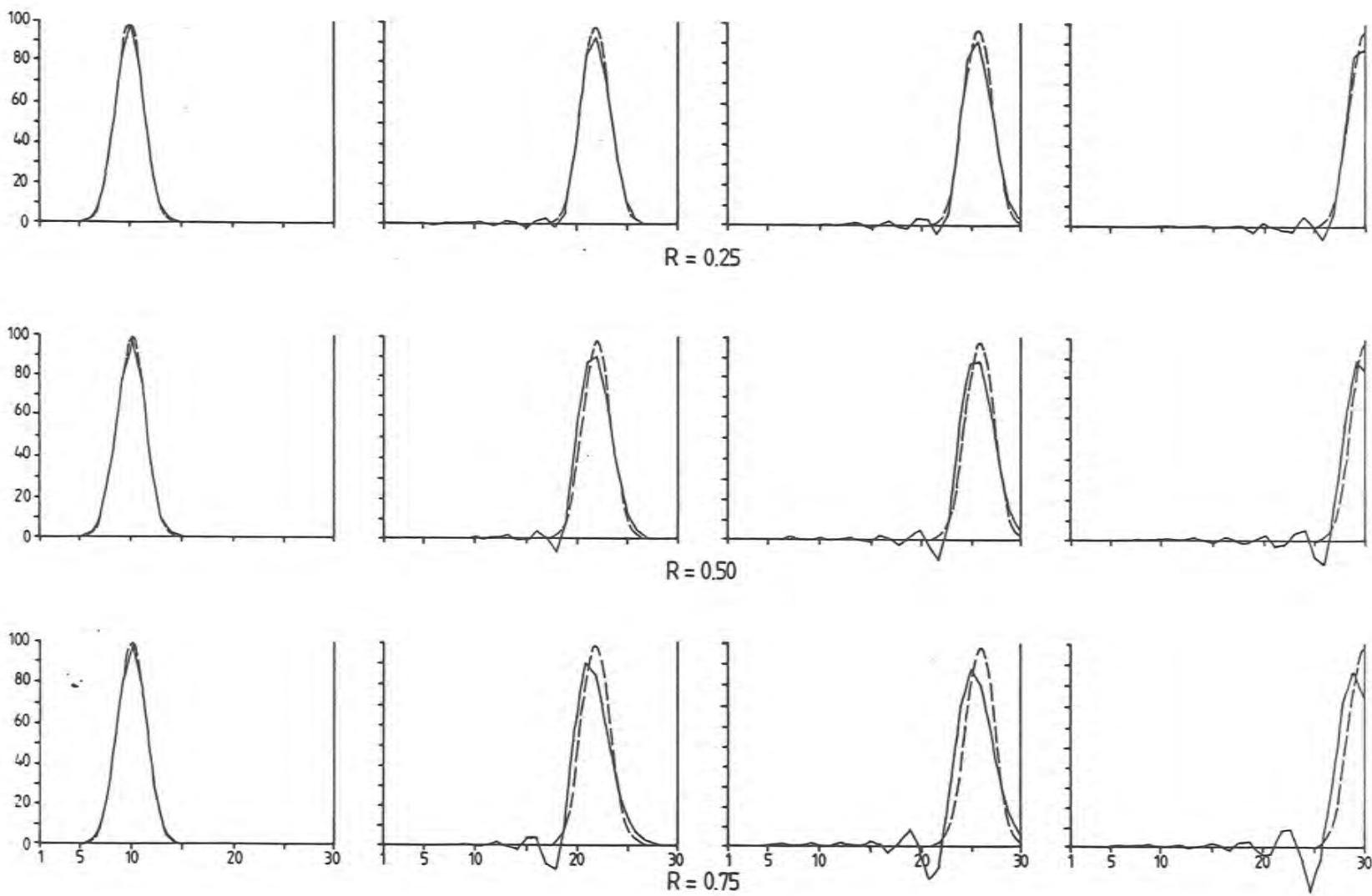


Figure 18 Linear finite element Crank-Nicholson

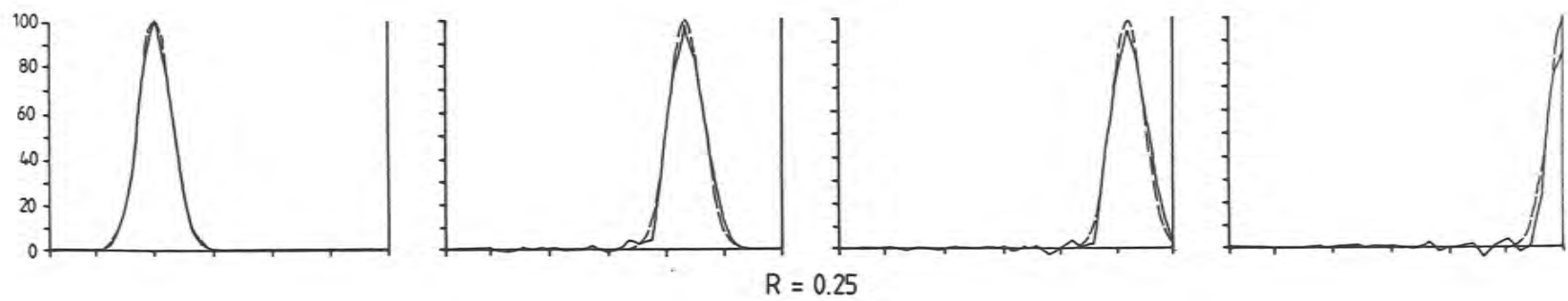
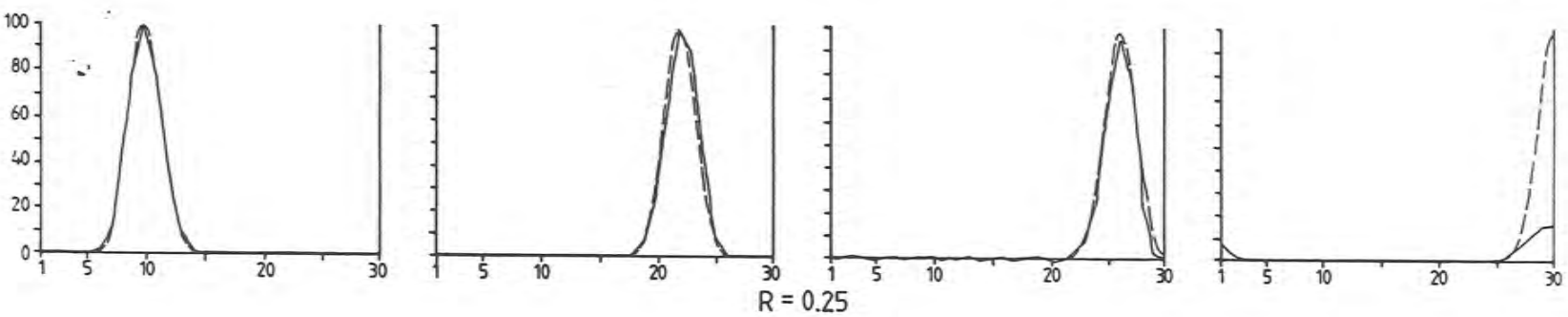
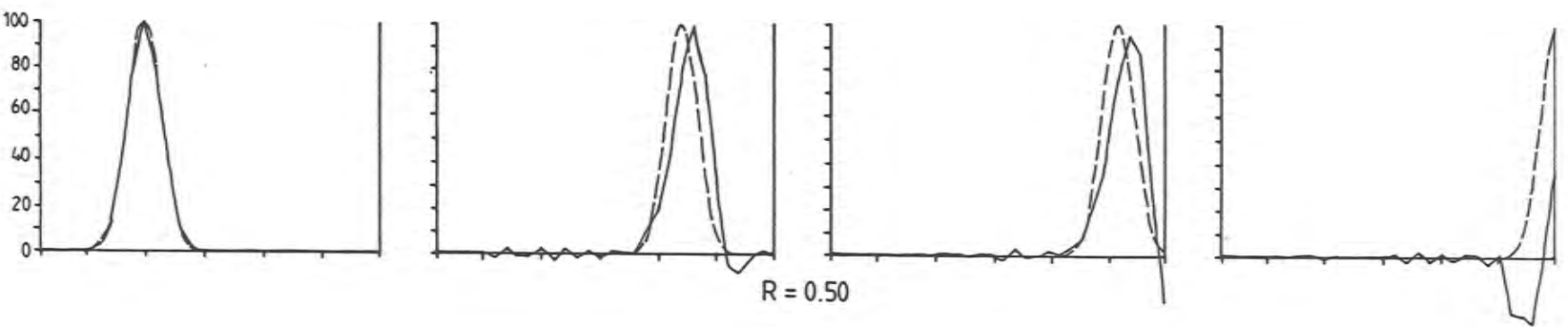
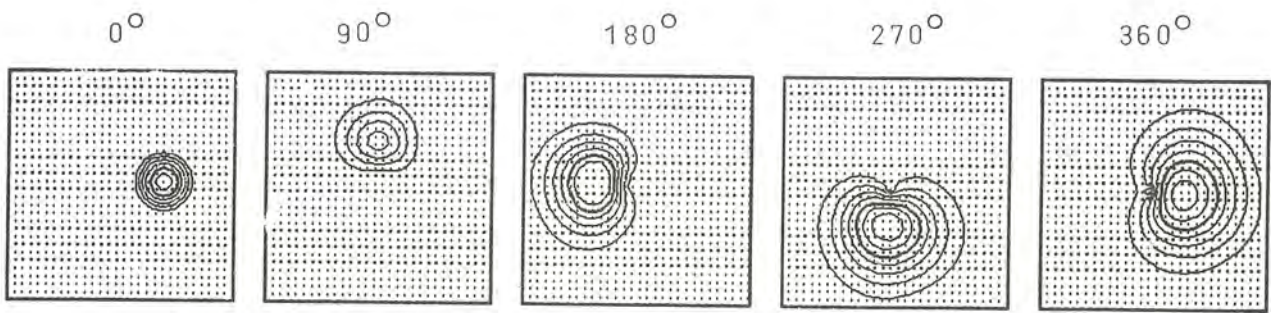
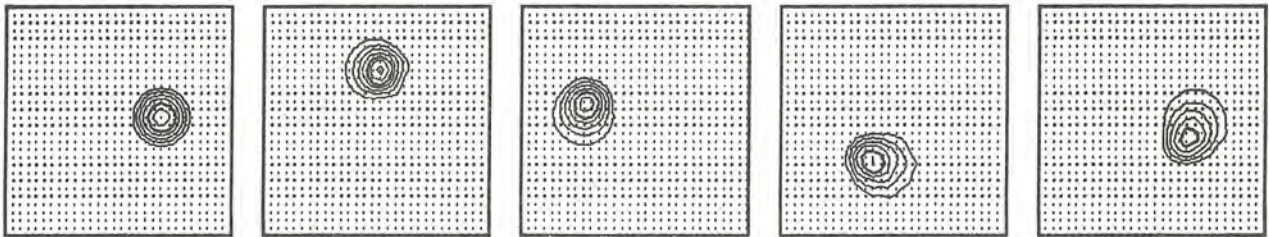


Figure 1g Pseudo-spectral leap frog

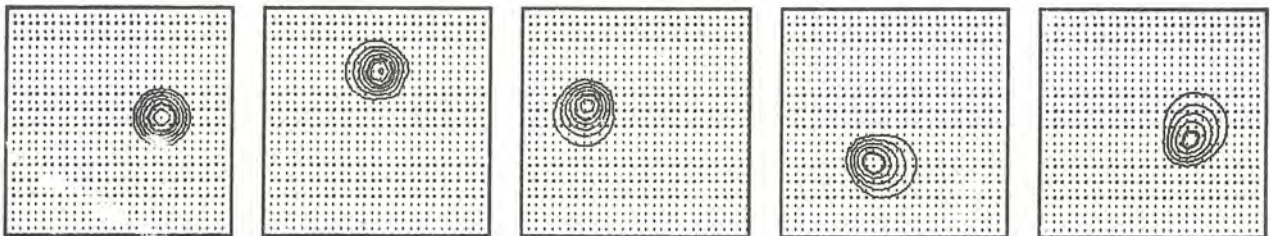
Figure 1h
Linear finite element
leap frog



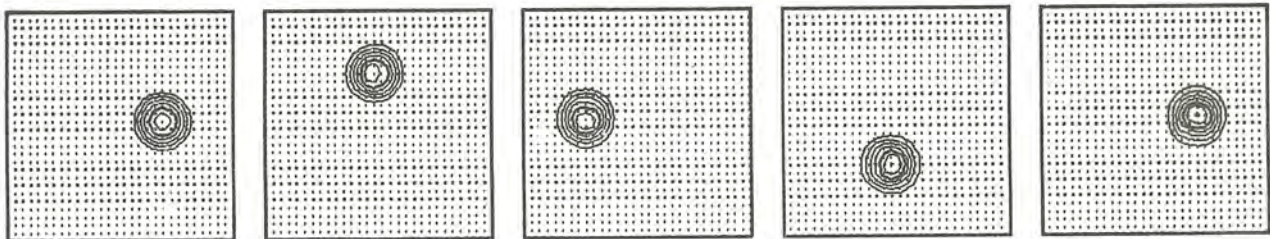
Finite differences up-stream



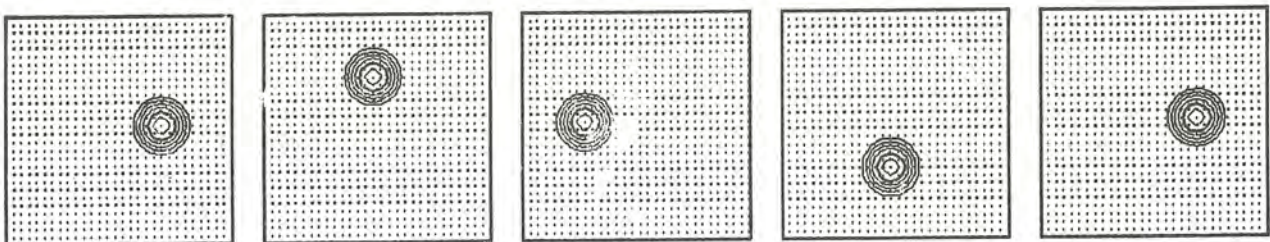
Finite differences Crank-Nicholson



Finite differences Lax-Wendroff



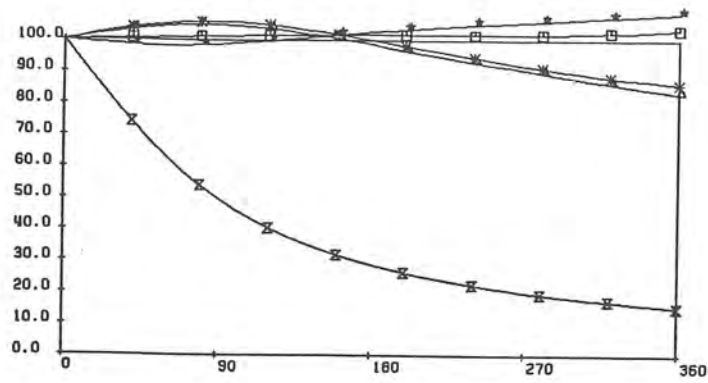
Linear finite element Crank-Nicholson



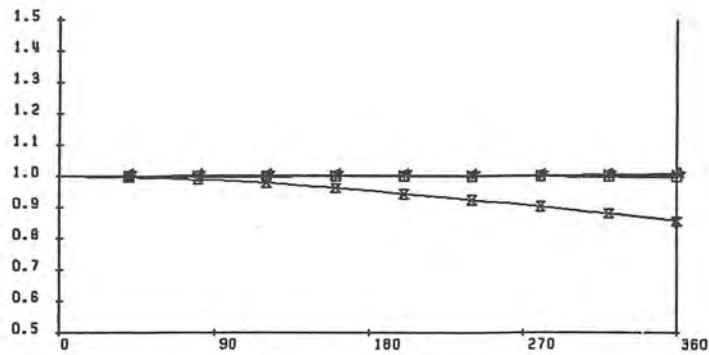
Pseudo-spectral leap-frog

Figure 11a Angle of rotation

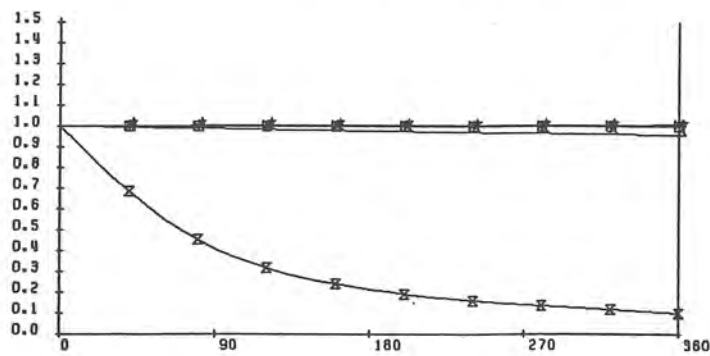
MAXIMAL AMPLITUDE



SUM OF AMPLITUDES

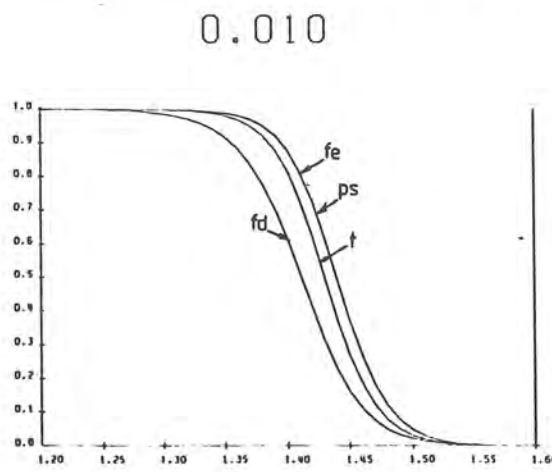
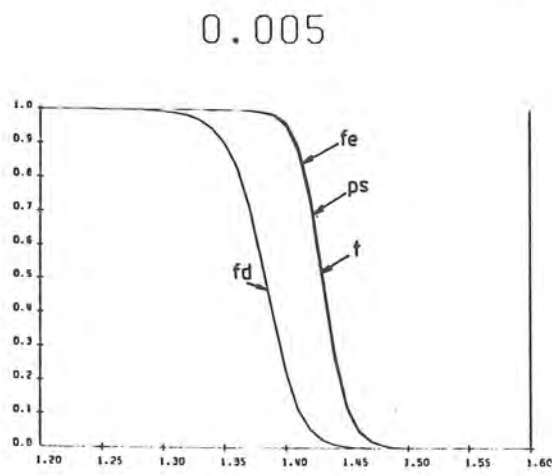
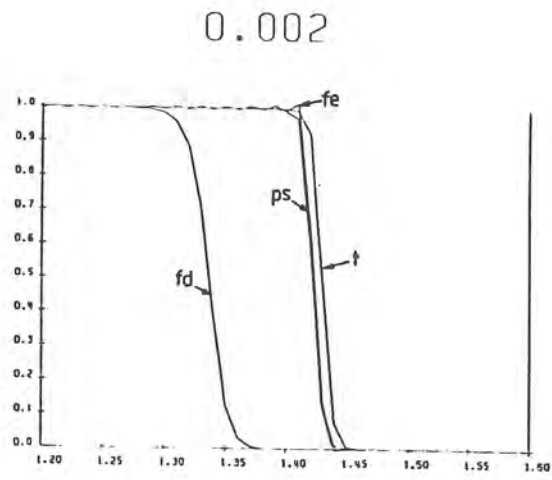


SUM OF AMPLITUDES SQUARES



- * linear finite element Crank Nicholson
- x finite differences Crank Nicholson
- + finite differences up-stream forwards
- Δ finite differences Lax-Wendroff
- ◻ pseudo-spectral leap frog

Figure 11b



t true
ps pseudo-spectral
fe finite element
fd finite differences

Figure III

Table III

K = 0.002				
x	t	ps	fe	fd
1.37	1.	1.007	0.999	0.007
1.38	1.	0.997	1.001	0.001
1.39	1.	1.008	0.999	0.
1.40	0.999	0.991	0.995	0.
1.41	0.993	0.969	1.014	0.
1.42	0.924	0.610	0.655	0.
1.43	0.5	0.128	0.139	0.
1.44	0.076	0.010	-0.03	0.
1.45	0.007	0.007	-0.01	0.
1.46	0.001	0.003	-0.01	0.
1.47	0.	0.001	0.	0.
1.48	0.	-0.001	0.	0.
1.49	0.	0.001	0.	0.

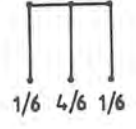
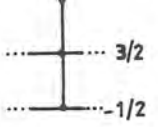
K = 0.005			
t	ps	fe	fd
0.998	0.998	0.999	0.717
0.993	0.994	0.996	0.560
0.982	0.984	0.988	0.382
0.953	0.957	0.964	0.224
0.881	0.891	0.898	0.116
0.731	0.750	0.752	0.055
0.5	0.525	0.523	0.025
0.269	0.289	0.288	0.011
0.119	0.131	0.129	0.005
0.047	0.053	0.050	0.002
0.018	0.020	0.018	0.001
0.007	0.008	0.006	0.
0.002	0.003	0.002	0.

K = 0.001			
t	ps	fe	fd
0.963	0.970	0.972	0.839
0.924	0.952	0.954	0.779
0.881	0.923	0.925	0.704
0.818	0.879	0.880	0.615
0.731	0.814	0.815	0.515
0.622	0.727	0.726	0.412
0.5	0.617	0.616	0.315
0.378	0.494	0.493	0.230
0.269	0.372	0.371	0.161
0.182	0.265	0.264	0.110
0.119	0.179	0.179	0.073
0.076	0.117	0.117	0.048
0.047	0.075	0.074	0.031

t	true	fe	finite element
ps	pseudo-spectral	fd	finite differences

Table IV

Name and expression	Order of accuracy	Amplification factor	stability condition	Comput. model
finite differences forward or Euler (IVa) (NMC large scale boundary layer model) $\frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} = \frac{K}{\Delta z^2} (\psi_{m+1}^\ell - 2\psi_m^\ell + \psi_{m-1}^\ell) + \frac{dK}{dz} \frac{\psi_{m+1}^\ell - \psi_{m-1}^\ell}{2\Delta z}$	$\Delta z^2, \Delta t$	$g = 1 + 2S(\cos k\Delta z - 1) + iT \sin k\Delta z$	$ T \leq 2S \leq 1$	
finite differences trapezoidal (IVb) (Mahrt, 1971) $\frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} = \frac{K}{\Delta z^2} (\psi_{m+1}^\ell - (\psi_m^{\ell+1} + \psi_m^\ell)) + \frac{dK}{dz} \frac{\psi_{m+1}^\ell - \psi_{m-1}^\ell}{2\Delta z}$	$\Delta z^2, \Delta t$	$g = \frac{1 + S(2 \cos k\Delta z - 1) + iT \sin k\Delta z}{1 + S}$	$S \leq 1$ and $T \leq 2S(S+1)$	
finite differences (IVc) $\frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} = \frac{K}{\Delta z^2} (\psi_{m+1}^\ell - 2\psi_m^{\ell+1} + \psi_{m-1}^\ell) + \frac{dK}{dz} \frac{\psi_{m+1}^\ell - \psi_{m-1}^\ell}{2\Delta z}$	$\Delta z^2, \Delta t$	$g = \frac{1 + 2S \cos k\Delta z + iT \sin k\Delta z}{1 + 2S}$	$T^2 \leq 2S(2S+1)$	
finite differences Crank-Nicholson (IVd) $\frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} = \frac{K}{2} \left(\frac{\psi_{m+1}^{\ell+1} - 2\psi_m^{\ell+1} + \psi_{m-1}^{\ell+1}}{\Delta z^2} + \frac{\psi_{m+1}^\ell - 2\psi_m^\ell + \psi_{m-1}^\ell}{\Delta z^2} \right) + \frac{1}{2} \frac{dK}{dz} \left(\frac{\psi_{m+1}^{\ell+1} - \psi_{m-1}^{\ell+1}}{2\Delta z} + \frac{\psi_{m+1}^\ell - \psi_{m-1}^\ell}{2\Delta z} \right)$	$\Delta z^2, \Delta t^2$	$g = \frac{1 + S(\cos k\Delta z - 1) + i \frac{T}{2} \sin k\Delta z}{1 - S(\cos k\Delta z - 1) - i \frac{T}{2} \sin k\Delta z}$	VS VT	

Name and expression	Order of accuracy	Amplification factor	Stability condition	Comput. model
finite differences Laasonen (IVe) $\frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} = \frac{K}{\Delta z^2} (\psi_{m+1}^{\ell+1} - 2\psi_m^{\ell+1} + \psi_{m-1}^{\ell+1}) + \frac{dK}{dz} \frac{\psi_{m+1}^{\ell+1} - \psi_{m-1}^{\ell+1}}{2\Delta z}$	$\Delta z^2, \Delta t$	$g = \frac{1}{1 - 2S(\cos k\Delta z - 1) - iT \sin k\Delta z}$	$\forall S$ $\forall T$	
finite differences Dufort-Frankel (IVf) $\frac{\psi_m^{\ell+1} - \psi_m^{\ell-1}}{2\Delta t} = \frac{K}{\Delta z^2} (\psi_{m+1}^\ell - (\psi_m^{\ell+1} + \psi_m^{\ell-1}) + \psi_{m-1}^\ell) + \frac{dK}{dz} \frac{\psi_{m+1}^\ell - \psi_{m-1}^\ell}{2\Delta z}$	$\Delta z^2, \Delta t$	g is solution of $g^2(1+2S) - 2g(2S \cos k\Delta z + iT \sin k\Delta z) - 1+2S = 0$	$ T \leq 1$	
finite linear element Laasonen (IVg) $\frac{1}{6} \left(\frac{\psi_{m-1}^\ell - \psi_{m-1}^{\ell-1}}{\Delta t} + 4 \frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} + \frac{\psi_{m+1}^{\ell+1} - \psi_{m+1}^\ell}{\Delta t} \right) = \frac{K}{\Delta z^2} (\psi_{m+1}^{\ell+1} - 2\psi_m^{\ell+1} + \psi_{m-1}^{\ell+1}) + \frac{dK}{dz} \frac{\psi_{m+1}^{\ell+1} - \psi_{m-1}^{\ell+1}}{2\Delta z}$	$\Delta z^2, \Delta t$	$g = \frac{2 + \cos k\Delta z}{2 + \cos k\Delta z - 6S(\cos k\Delta z - 1) - i3T \sin k\Delta z}$	$\forall S$ $\forall T$	
pseudo-spectral Adams-Bashforth (IVh) (Christensen and Prahm, 1976) $\frac{\psi_m^{\ell+1} - \psi_m^\ell}{\Delta t} = K \left(\frac{3}{2} \frac{\partial^2 \psi_m}{\partial z^2} - \frac{1}{2} \frac{\partial^2 \psi_m^{\ell-1}}{\partial z^2} \right) + \frac{dK}{dz} \left(\frac{3}{2} \frac{\partial \psi_m^\ell}{\partial z} - \frac{1}{2} \frac{\partial \psi_m^{\ell-1}}{\partial z} \right)$	$\Delta z^\infty, \Delta t$	g is solution of $g^2 - g(1 - \frac{3}{2} S(k\Delta z)^2 + i \frac{3}{2} T(k\Delta z)) - \frac{1}{2} S(k\Delta z)^2 + i \frac{1}{2} T(k\Delta z) = 0$	$\pi^2 S \leq 1$ and $ T \pi \leq 2S$	

wave length $k\Delta z$	$2\Delta z$ π	$4\Delta z$ $\pi/2$	$6\Delta z$ $\pi/3$	$8\Delta z$ $\pi/4$
T = 0.25				
S = 0.25	∞	0.943	0.903	0.891
	2.	1.183	1.073	1.040
S = 0.50	0.	1.124	1.107	1.025
	0.	4.	1.561	1.248
S = 0.75	/	0.314	1.345	1.148
	/	-1.181	2.736	
T = 0.50				
S = 0.25	∞	0.562	0.525	0.513
	1.	1.	1.	1.
S = 0.50	0.	0.562	0.754	0.762
	0.	2.	1.363	1.181
S = 0.75	/	0.187	0.843	0.889
	/	-1.	2.	1.433
T = 0.75				
S = 0.25	∞	0.168	0.029	/
	0.667	0.834	0.909	/
S = 0.50	0.	0.233	0.363	0.400
	0.	1.333	1.165	1.092
S = 0.75	/	0.056	0.441	0.560
	/	-0.834	1.532	1.286

Table IVa - finite differences forward

T = 0.25				
S = 0.25	0.652	0.743	0.730	0.726
	0.	0.819	0.814	0.809
S = 0.50	0.223	0.800	0.698	0.670
	0.	1.181	0.814	0.741
S = 0.75	0.045	0.964	0.653	0.605
	0.	2.	0.814	0.683
T = 0.50				
S = 0.25	0.652	0.530	0.501	0.491
	0.	0.749	0.780	0.790
S = 0.50	0.223	0.610	0.583	0.571
	0.	1.	0.780	0.726
S = 0.75	0.045	0.617	0.576	0.549
	0.	1.410	0.780	0.671
T = 0.75				
S = 0.25	0.652	0.266	0.172	0.134
	0.	0.667	0.733	0.761
S = 0.50	0.223	0.413	0.419	0.418
	0.	0.834	0.733	0.703
S = 0.75	0.045	0.429	0.466	0.461
	0.	1.060	0.733	0.653

Table IVb - finite differences trapezoidal

ρ/K
 $\frac{dp}{dz}/\frac{dK}{dz}$ / unstable

wave length $k\Delta z$	$2\Delta z$ π	$4\Delta z$ $\pi/2$	$6\Delta z$ $\pi/3$	$8\Delta z$ $\pi/4$
$T = 0.25$				
$S = 0.25$	0.445	0.608	0.611	0.611
	0.	0.624	0.655	0.661
$S = 0.50$	∞	0.537	0.506	0.496
	2.	0.624	0.548	0.526
$S = 0.75$	0.217	0.479	0.424	0.410
	0.	0.624	0.470	0.436
$T = 0.50$				
$S = 0.25$	0.445	0.476	0.458	0.452
	0.	0.590	0.637	0.651
$S = 0.50$	∞	0.471	0.452	0.445
	1.	0.590	0.537	0.520
$S = 0.75$	0.217	0.435	0.398	0.386
	0.	0.590	0.463	0.433
$T = 0.75$				
$S = 0.25$	0.445	0.296	0.229	0.203
	0.	0.546	0.610	0.634
$S = 0.50$	∞	0.381	0.368	0.364
	0.667	0.546	0.520	0.511
$S = 0.75$	0.217	0.375	0.355	0.348
	0.	0.546	0.453	0.428

Table IVc - finite differences

$T = 0.25$				
$S = 0.25$	0.445	0.814	0.906	0.944
	0.	0.674	0.837	0.903
$S = 0.50$	∞	0.869	0.920	0.949
	-2.	0.836	0.878	0.917
$S = 0.75$	0.217	0.993	0.944	0.957
	0.	1.362	0.955	0.943
$T = 0.50$				
$S = 0.25$	0.445	0.775	0.875	0.922
	0.	0.661	0.826	0.896
$S = 0.50$	∞	0.811	0.886	0.927
	-1.	0.801	0.864	0.910
$S = 0.75$	0.217	0.870	0.905	0.934
	0.	1.181	0.935	0.934
$T = 0.75$				
$S = 0.25$	0.445	0.717	0.827	0.888
	0.	0.641	0.810	0.884
$S = 0.50$	∞	0.734	0.834	0.892
	-0.667	0.754	0.844	0.897
$S = 0.75$	0.217	0.745	0.846	0.897
	0.	1.013	0.905	0.920

Table IVd - finite differences Crank-Nicholson

ρ/K

$\frac{dp}{dz} \frac{dK}{dz}$ /unstable

wave length $k\Delta z$	$2\Delta z$ π	$4\Delta z$ $\pi/2$	$6\Delta z$ $\pi/3$	$8\Delta z$ $\pi/4$
$T = 0.25$				
$S = 0.25$	0.281	0.680	0.868	0.962
	0.	0.421	0.655	0.779
$S = 0.50$	0.223	0.568	0.758	0.863
	0.	0.317	0.548	0.692
$S = 0.75$	0.187	0.498	0.690	0.803
	0.	0.254	0.470	0.622
$T = 0.50$				
$S = 0.25$	0.281	0.743	1.021	1.181
	0.	0.410	0.637	0.762
$S = 0.50$	0.223	0.586	0.812	0.950
	0.	0.312	0.537	0.680
$S = 0.75$	0.187	0.506	0.717	0.851
	0.	0.251	0.463	0.613
$T = 0.75$				
$S = 0.25$	0.281	0.838	1.250	1.515
	0.	0.394	0.610	0.736
$S = 0.50$	0.223	0.615	0.896	1.085
	0.	0.305	0.520	0.661
$S = 0.75$	0.187	0.518	0.759	0.925
	0.	0.247	0.453	0.599

Table IVe - finite differences Laasonen

$T = 0.25$				
$S = 0.25$	0.445	0.891	0.934	0.939
	0.	0.746	0.924	0.966
$S = 0.50$	∞	1.124	1.107	1.025
	2.	4.	1.561	1.248
$S = 0.75$	0.217	0.315	0.672	0.990
	0.	4.	3.297	2.361
$T = 0.50$				
$S = 0.25$	0.445	0.891	0.817	0.793
	0.	0.784	0.946	0.975
$S = 0.50$	∞	0.562	0.754	0.762
	1.	2.	1.363	1.181
$S = 0.75$	0.217	0.201	0.409	0.580
	0.	2.	1.763	1.521
$T = 0.75$				
$S = 0.25$	0.445	0.891	0.574	0.506
	0.	0.889	0.980	0.989
$S = 0.50$	∞	0.233	0.363	0.400
	0.667	1.333	1.165	1.092
$S = 0.75$	0.217	0.095	0.189	0.266
	0.	1.333	1.258	1.190

Table IVf - finite differences Dufort-Frankell

ρ/K

$$\frac{dp}{dz} / \frac{dK}{dz}$$

/unstable

wave length $k\Delta z$	$2\Delta z$ π	$4\Delta z$ $\pi/2$	$6\Delta z$ $\pi/3$	$8\Delta z$ $\pi/4$
$T = 0.25$				
$S = 0.25$	0.562	0.944	1.028	1.066
	0.	0.538	0.753	0.850
$S = 0.50$	0.394	0.752	0.881	0.946
	0.	0.379	0.615	0.748
$S = 0.75$	0.311	0.640	0.792	0.876
	0.	0.293	0.519	0.667
$T = 0.50$				
$S = 0.25$	0.562	1.044	1.227	1.324
	0.	0.516	0.726	0.828
$S = 0.50$	0.394	0.778	0.949	1.047
	0.	0.371	0.600	0.732
$S = 0.75$	0.311	0.651	0.824	0.930
	0.	0.289	0.510	0.656
$T = 0.75$				
$S = 0.25$	0.562	1.188	1.517	1.713
	0.	0.485	0.688	0.795
$S = 0.50$	0.394	0.817	1.051	1.133
	0.	0.359	0.577	0.709
$S = 0.75$	0.311	0.667	0.875	1.014
	0.	0.283	0.496	0.639

ρ/K

$$\frac{d\rho}{dz}/\frac{dK}{dz}$$

/ unstable

Table IVg - linear finite element Laasonen

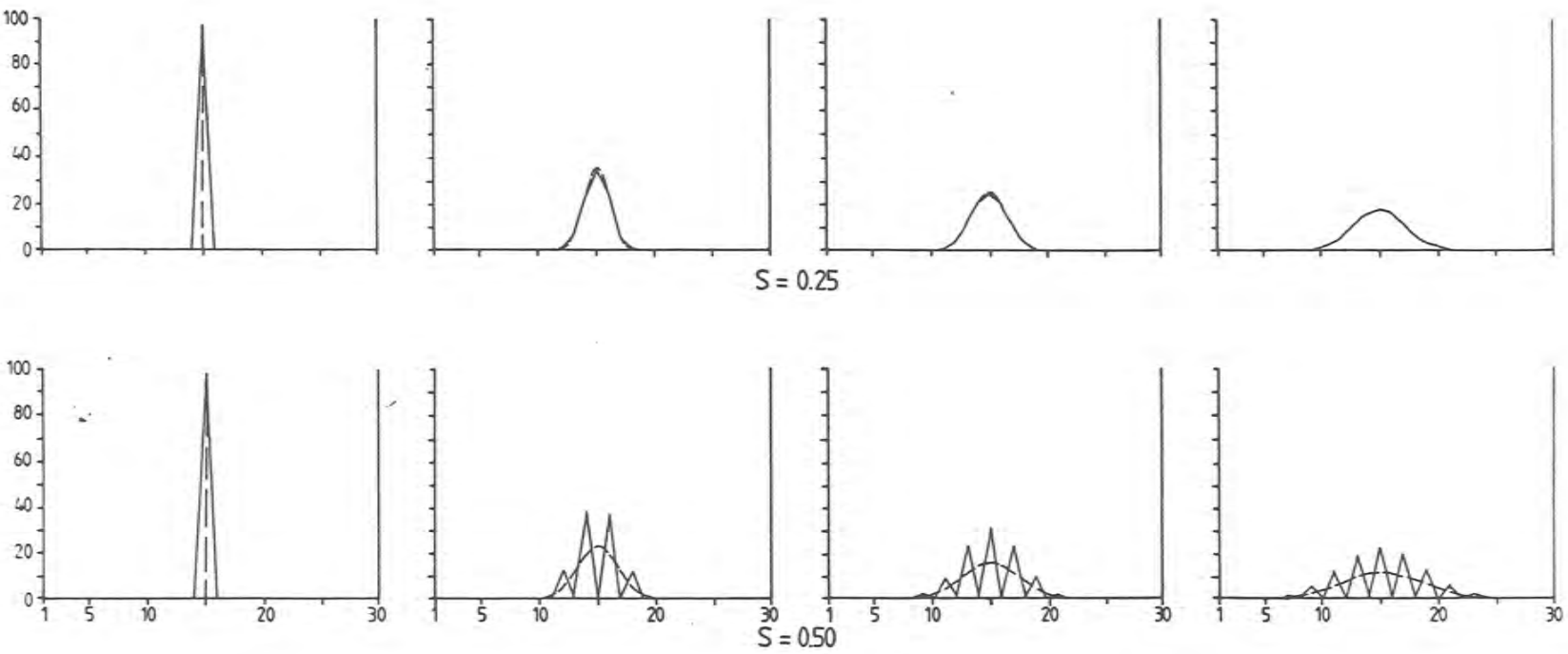


Figure 1Va Finite differences forward

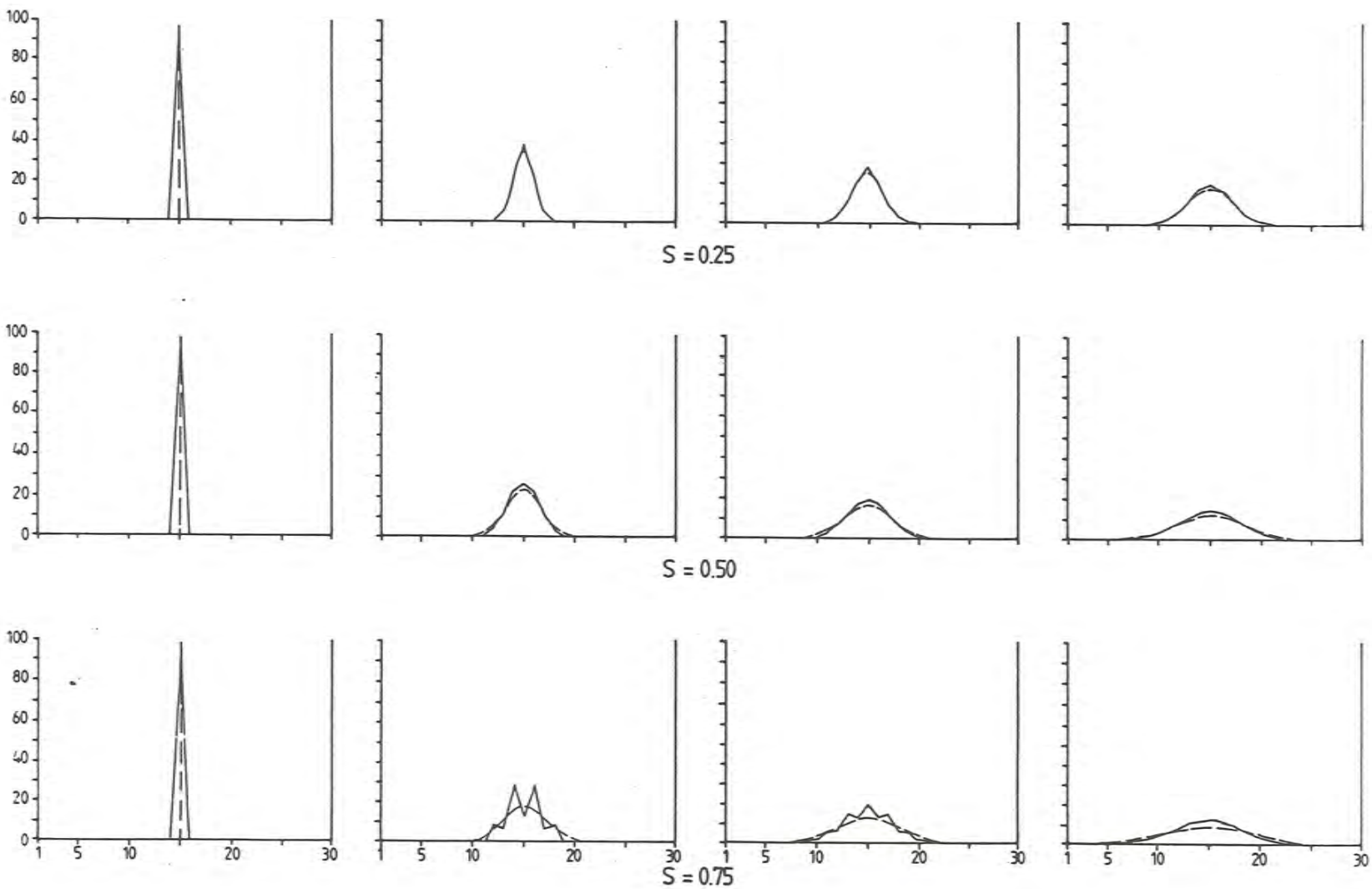


Figure 1Vb Finite differences trapezoidal

Figure IVc Finite differences

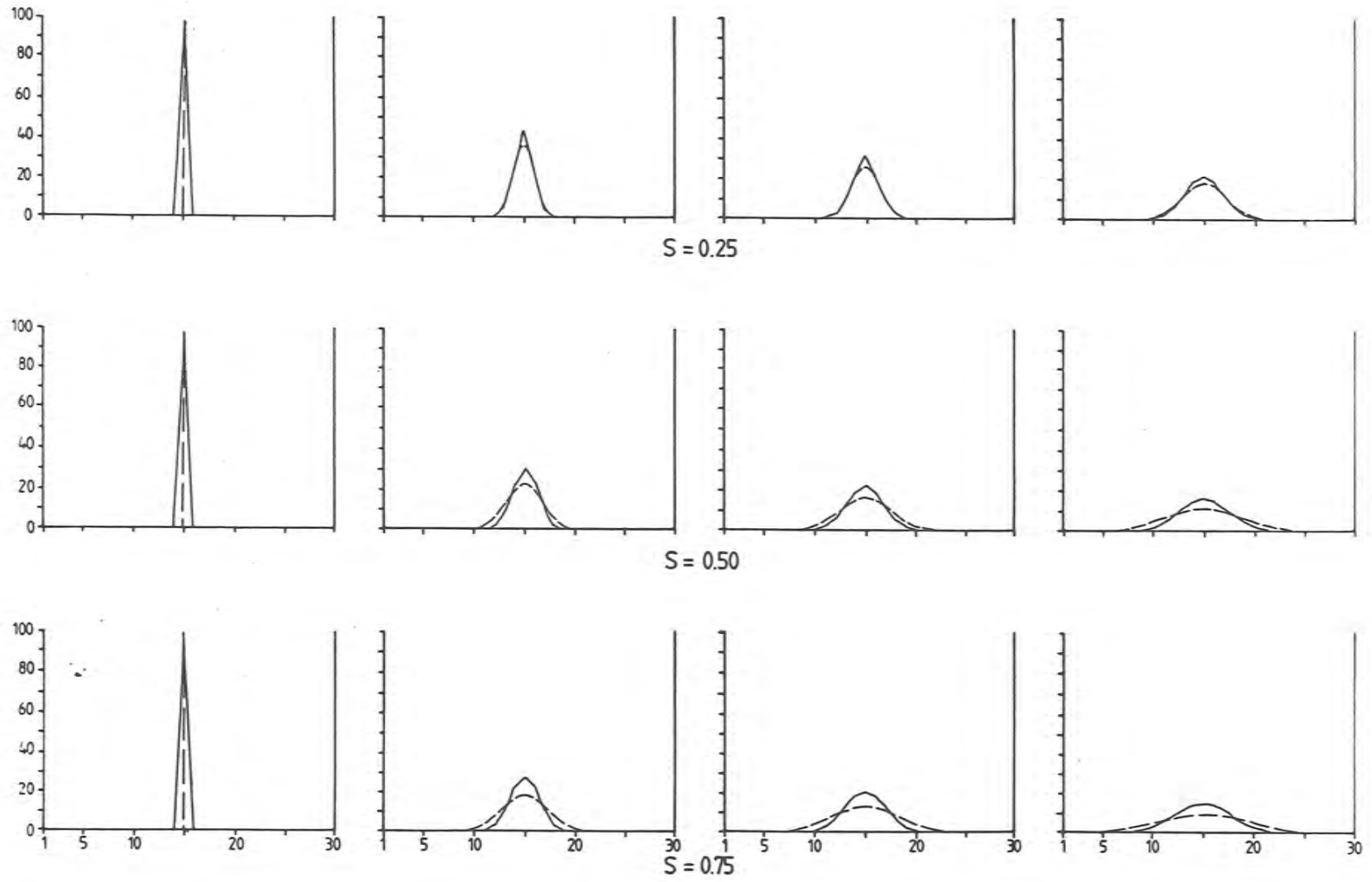


Figure 1Vd Finite differences Crank-Nicholson

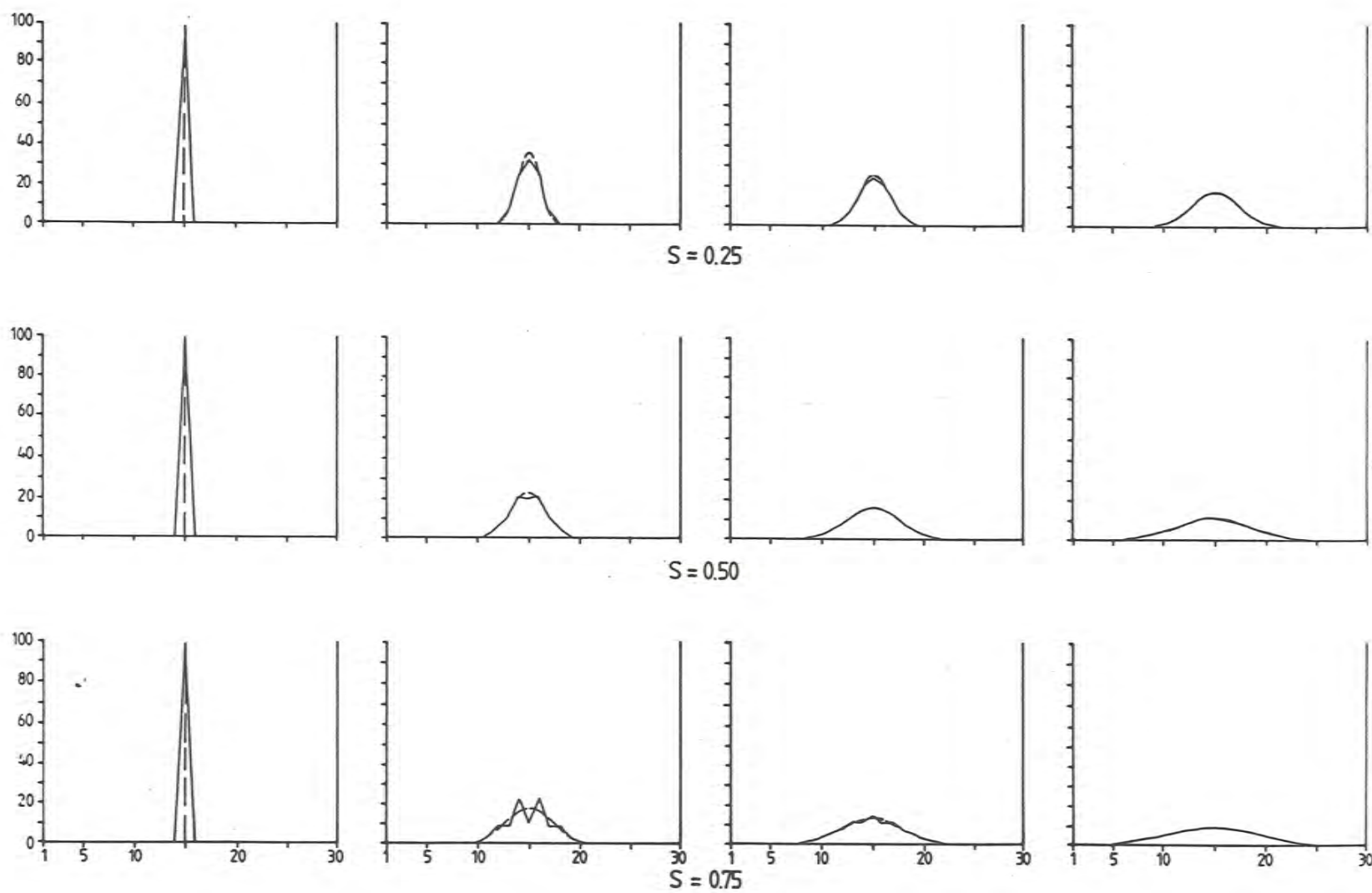
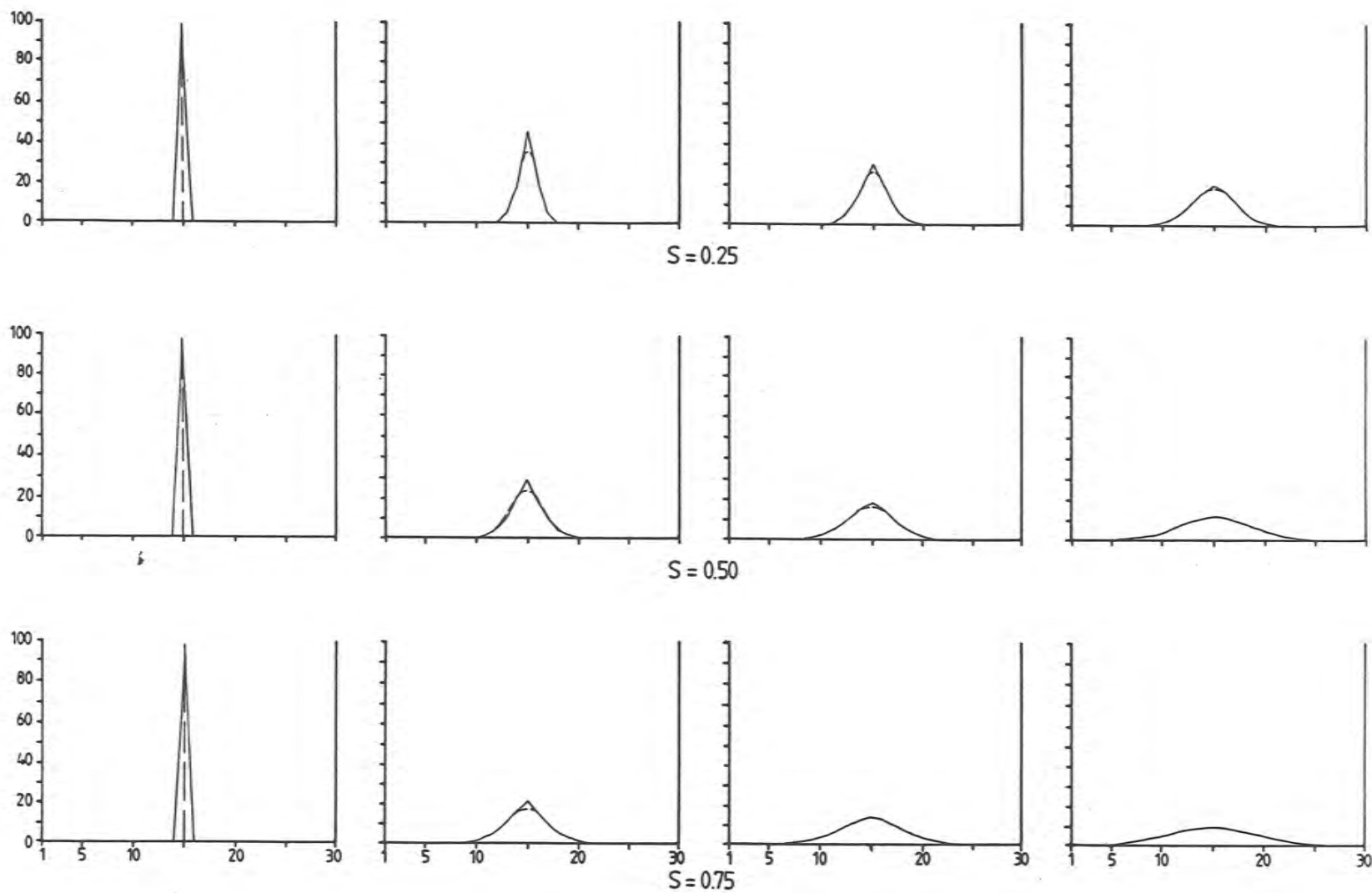


Figure IVe Finite differences Laasonen



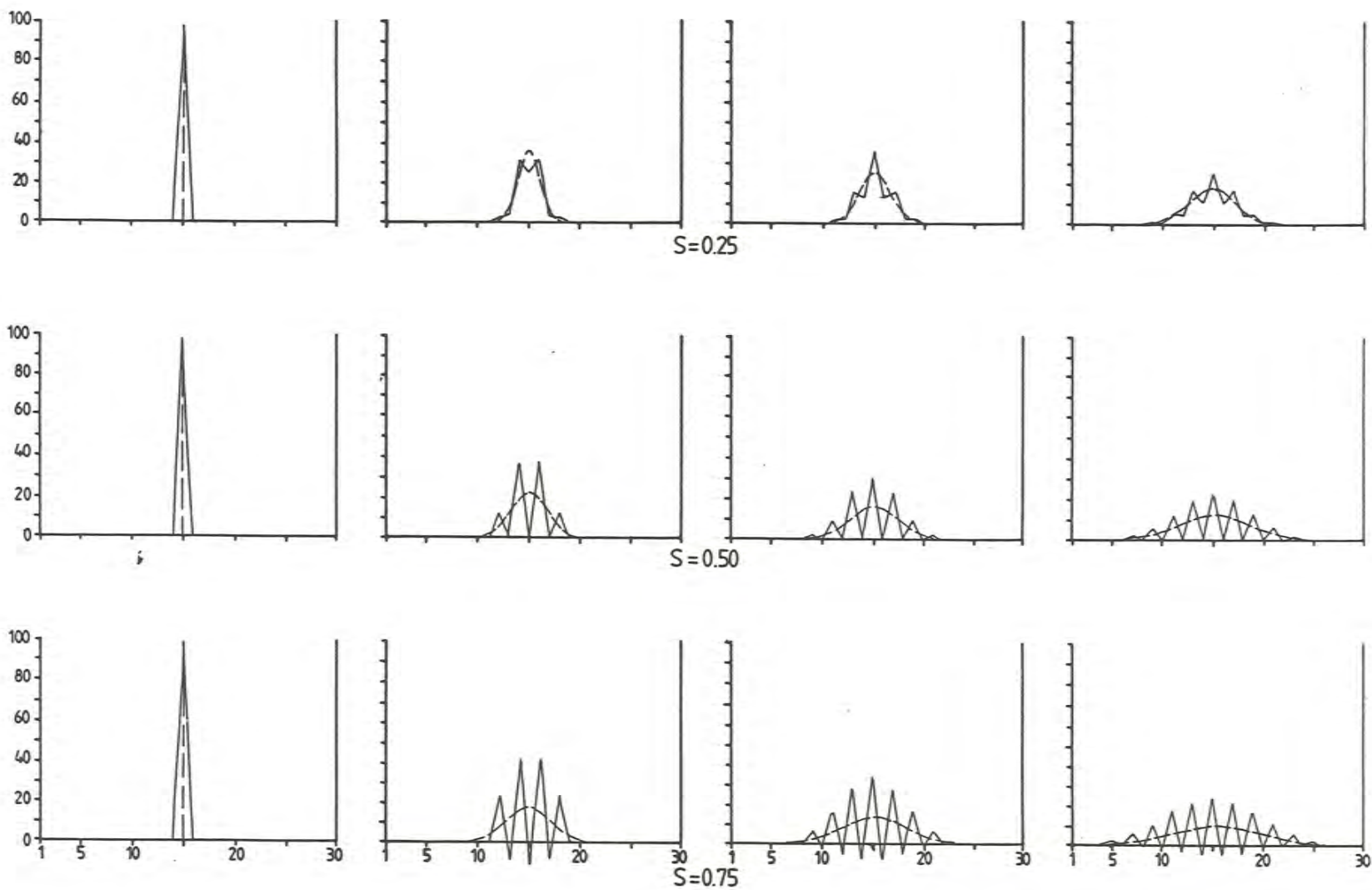


Figure IV.6 Finite differences Dufort-Frankel

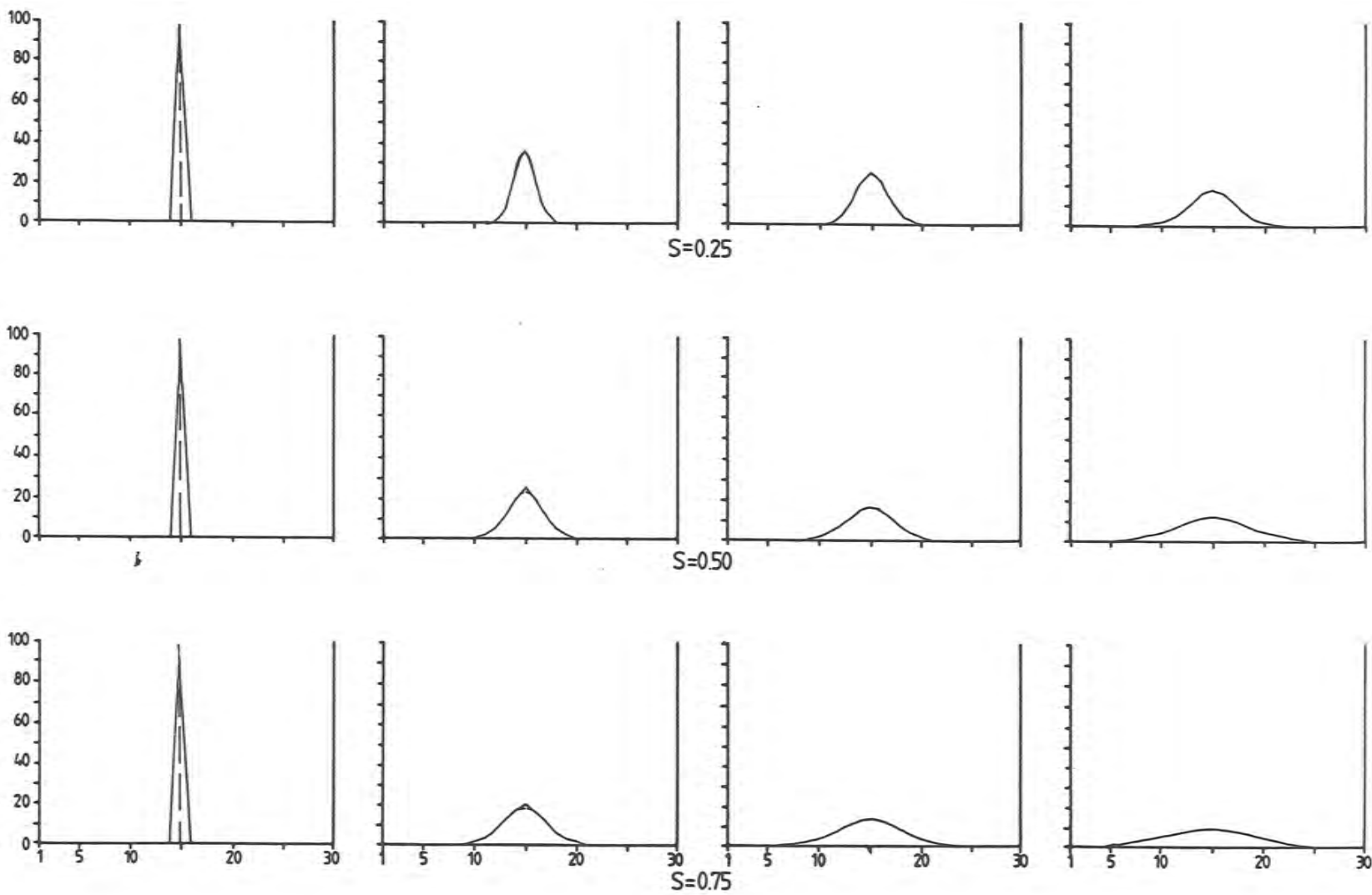


Figure 1Vg Linear finite element laasonen

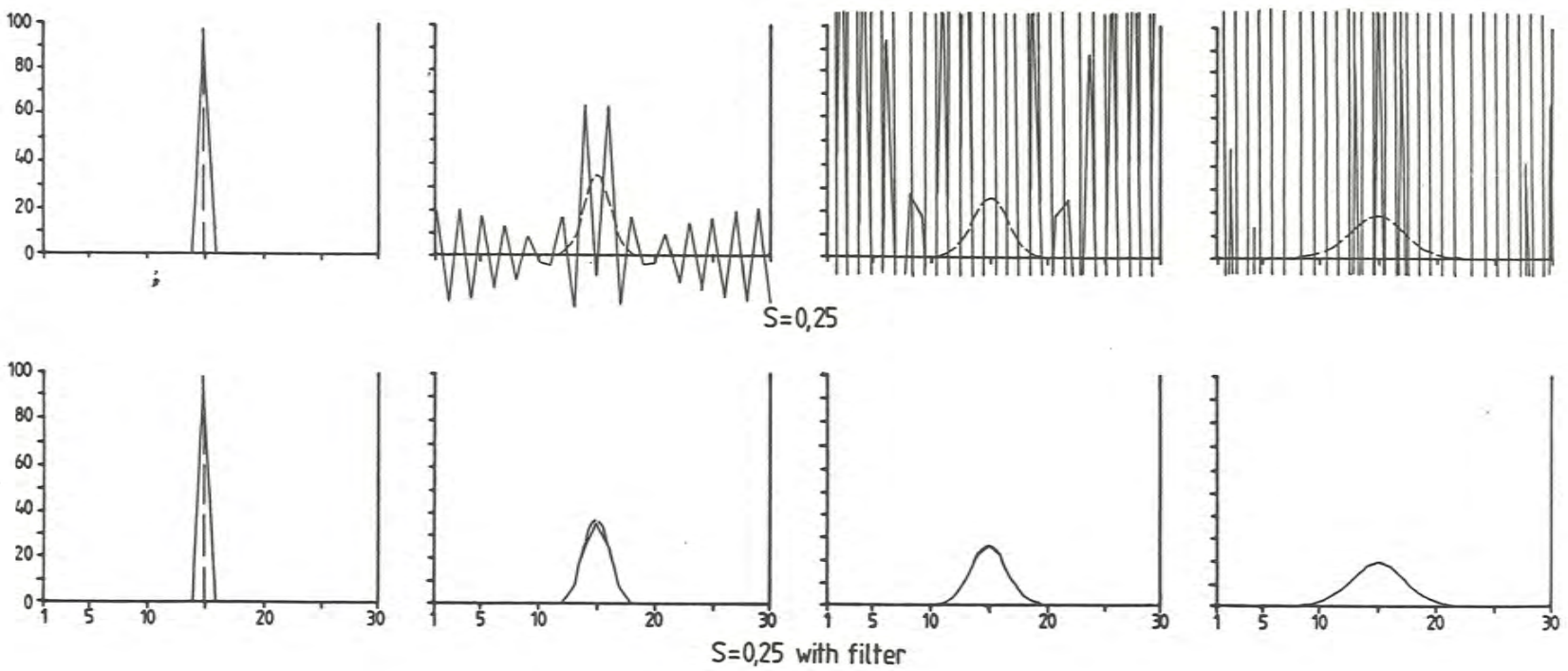
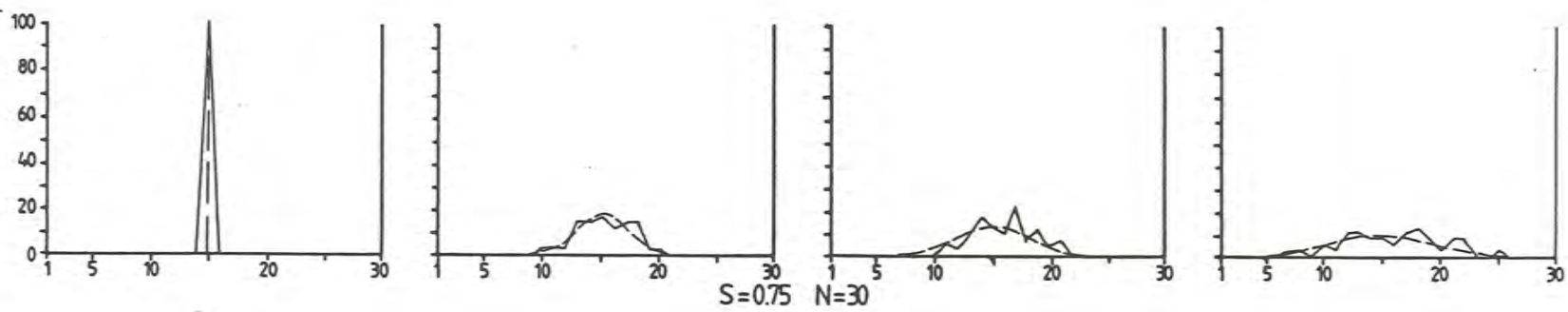
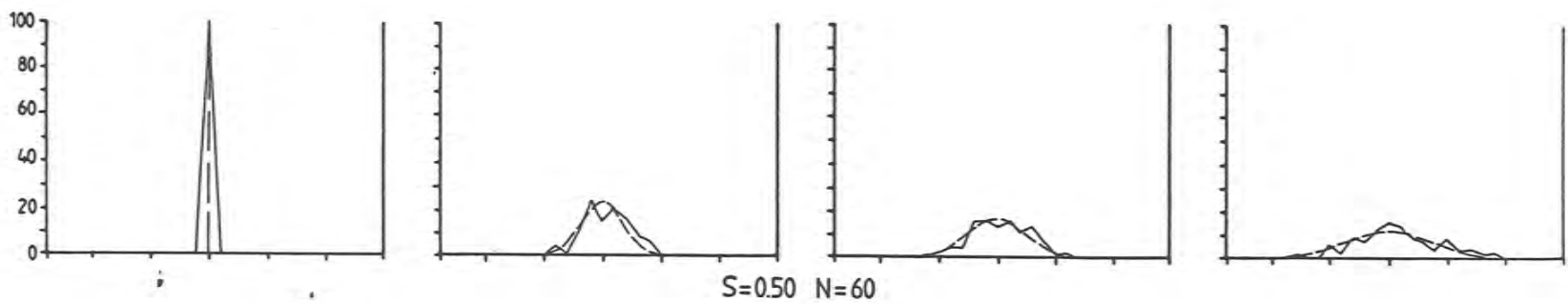
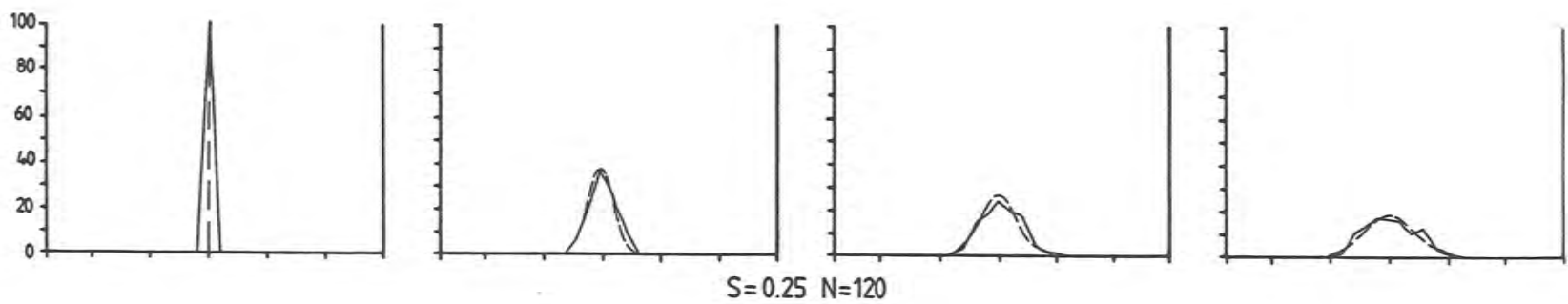


Figure 1h Pseudo-spectral Adams-Bashforth

Figure V Random Walk



Wave length	$2\Delta s$	$4\Delta s$	$6\Delta s$	$8\Delta s$
$\nu = 0.005$	0.990	0.995	0.997	0.998
$\nu = 0.05$	0.9	0.95	0.975	0.985
$\nu = 0.5$	0.	0.5	0.75	0.853
$\nu = 1$	-1.	0.	0.5	0.707

Table VIa Asselin filter

$\nu = 0.01$	0.	0.990	0.996	0.998
$\nu = 0.05$	0.	0.952	0.983	0.991
$\nu = 0.1$	0.	0.909	0.967	0.983
$\nu = 0.25$	0.	0.8	0.923	0.959
$\nu = 1.$	0.	0.5	0.75	0.853

Table VIb Long filter

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