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# ANALYSIS OF SEMI-IMPLICIT TIME INTEGRATION SCHEMES FOR DIRECT NUMERICAL SIMULATION OF TURBULENT CONVECTION IN LIQUID METALS

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## SUMMARY

Fully explicit time integration schemes are very inefficient for numerical simulation of diffusion dominated problems. In case of natural convection flow in liquid metals an implicit treatment of the thermal diffusion terms allows for the use of substantially increased time steps without involving loss of physically relevant information. Two suitable semi-implicit time integration schemes are investigated analytically by a Von Neumann stability analysis and a spectral analysis of the numerical error. Numerical solutions by the semi-implicit schemes are compared to the exact solution of a 1D linear test problem. The results show the crucial influence of the discretization ratio $\lambda = \Delta t/\Delta x$ on the accuracy of the numerical solutions. First 3D time dependent numerical simulations of natural convection in liquid metals with the semi-implicit time integration schemes confirm the theoretically estimated gain in the time step width and result in CPU-time savings up to a factor of 50 compared to the fully explicit scheme.

## 1. INTRODUCTION

New developments for sodium cooled fast breeder reactors aim at more inherent safety features. The decay heat, e.g., shall be removed by natural convection only. In this context many experiments with model fluids are performed. Computer codes using turbulence models are developed to extrapolate the experimentally based knowledge to reactor conditions. To improve and to calibrate the problematic turbulence models for pure natural convection in liquid metals we intend to provide statistical turbulence data from direct numerical simulations.

In the code TURBIT [1] the time dependent, three-dimensional Navier Stokes equations and the thermal energy equation are solved in simple channel geometries using a finite volume method. The time integration is done by an explicit Euler-Leapfrog scheme. TURBIT has been successfully used for direct numerical simulation of different heat transfer problems, as for example Rayleigh-Bénard convection in air [2] and natural convection in an internally heated fluid layer [3]. However, application of the code to natural convection in liquid metals leads to enormous CPU-time requirements. The inefficiency of the code for this type of flow is due to the fully explicit time integration scheme. For numerical stability it requires the use of much smaller time steps than would be physically necessary to resolve even the highest frequencies of turbulence in time. Similar problems arise in the numerical simulation of isothermal channel flow

with spectral methods [4]. Here very fine meshes have to be used near the walls to resolve the viscous boundary layers. In those cases the viscous diffusion terms are treated implicitly to avoid a physically irrelevant time step restriction.

In this paper we investigate two semi-implicit time integration schemes for the thermal energy equation. These are the Adams-Bashforth Crank-Nicolson scheme and the Leapfrog Crank-Nicolson scheme. In section 2 we will show that in case of direct numerical simulation of natural convection in liquid metals the strong time step restriction of explicit schemes is overcome by the implicit treatment of the thermal diffusion terms. In section 3 we will carry out a Von Neumann stability analysis and a spectral analysis of the numerical error. Comparison of numerical solutions of a one-dimensional linear test problem with the exact solution will be done in section 4. We will discuss the results in section 5 and make some remarks about the realization and practical experience with the semi-implicit schemes in TURBIT in section 6.

## 2. NECESSITY FOR SEMI-IMPLICIT TIME INTEGRATION

The stability criterion of the fully explicit time integration scheme used in TURBIT can be written, by using the summation convention, as

$$\Delta t \leq \left( \frac{|u_i|_{max}}{\Delta x_i} + 4 \frac{Max(\nu, a)}{\Delta x_i^2} \right)^{-1} . \qquad (1)$$

$U_i$ denotes the components of the velocity vector and $\nu$ and a the viscous and thermal diffusivity, respectively.

Liquid metals are characterized by very low Prandtl numbers $Pr = \nu / a$ (e.g. $Pr = 0.025$ for mercury and $Pr = 0.006$ for liquid sodium) and thus by a very high ratio of thermal to viscous diffusivity. So the temperature field in natural convection of liquid metals is governed by a large thermal conductivity allowing only for large scale structures and thick thermal boundary layers. In contrast the velocity field has very small spatial structures and very thin boundary layers near walls. For direct numerical simulation of turbulence it is essential to choose a grid which resolves all physically relevant length scales of the flow. Therefore we are enforced by the velocity field for the use of very fine mesh cells $\Delta x_i$. Thus in the stability criterion (1) the diffusion type terms become dominant. Because of the very low Prandtl-number of liquid metals it is not the viscous, but the highly efficient thermal diffusion process which requires the use of very small time steps. This is really a kind of paradoxon since the temperature field does not show any rapid variations which would justify the use of such small time steps. Substantially larger time steps (typically of one to two orders of magnitude) can be reached when the thermal diffusivity is removed from the stability criterion (1). This can be achieved by treating the diffusive terms in the thermal energy equation implicitly and the convective terms and the complete momentum equation still explicitly.

## 3. ANALYTICAL INVESTIGATION OF SEMI-IMPLICIT SCHEMES

Two semi-implicit time integration schemes which are suitable for diffusion dominated problems are recommended e.g. in [5]. Both handle the diffu-

sive terms L = a$\nabla^2$T by the implicit Crank-Nicolson scheme, CN, whereas for the nonlinear convective terms N = u$\nabla$T the explicit Adams-Bashforth, AB, or the Leapfrog scheme, LF, is used, respectively:

$$ABCN-scheme: \quad \frac{T^{n+1} - T^n}{\Delta t} = -\frac{1}{2}\left(3N^n - N^{n-1}\right) + \frac{1}{2}\left(L^{n+1} + L^n\right), \tag{2}$$

$$LFCN-scheme: \quad \frac{T^{n+1} - T^{n-1}}{2\Delta t} = -N^n + \frac{1}{2}\left(L^{n+1} + L^{n-1}\right). \tag{3}$$

Here T denotes the temperature and n the time level. Both schemes are of second order in time and exhibit only small numerical diffusion.

For simplicity we consider the following one-dimensional linearized model for the thermal energy equation

$$\frac{\partial T}{\partial t} + u_o \frac{\partial T}{\partial x} = a \frac{\partial^2 T}{\partial x^2} \qquad a, u_o = const. \tag{4}$$

An exact solution is

$$T_{ex}(x,t) = e^{-ik(x - u_o t)} \cdot e^{-ak^2 t} \tag{5}$$

where i = $\sqrt{-1}$ and k is representing a wavenumber.

### 3.1 Von Neumann Stability Analysis

For both schemes the time step criterion for the linearized problem can be derived by a Von Neumann stability analysis. It's main idea is to carry out a Fourier decomposition of the error, leading to an amplification matrix and thus to the eigenvalues of the numerical scheme. Then the stability criterion results from the demand that the spectral radius of the amplification matrix has to be less equal unity. This ensures that no single harmonic component of the error may grow in time. Further details of the method are given in [6].

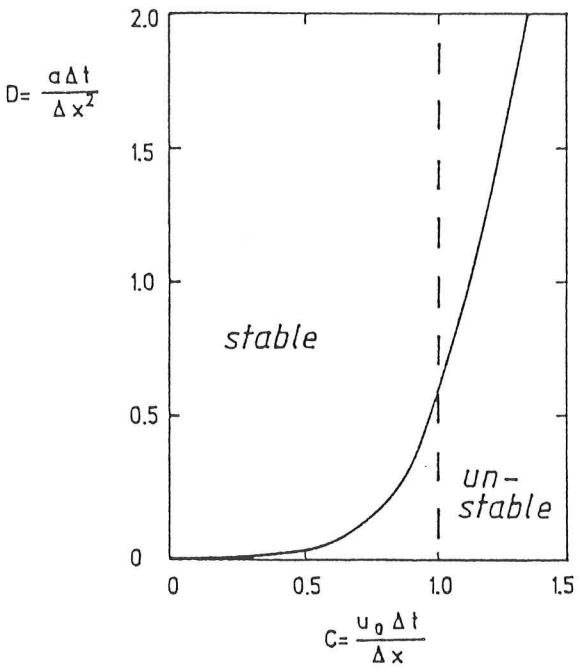



Fig. 1: Curves of stability for the ABCN-(solid line) and the LFCN-scheme (dashed line) according to [6].

The Von Neumann stability analysis of the ABCN- and LFCN-time integration schemes for the problem of equation (4) results in the curves of stability given in figure 1 where the Courant number $C = (u_o \Delta t)/\Delta x$ and the diffusion number $D = (a\,\Delta t)/(\Delta x^2)$ are used. The stability criterion of the LFCN-scheme is just the well known Courant-Friedrichs-Lewy (CFL) condition $C \leqq 1$. Thus the time step is, as desired, unaffected by the thermal diffusivity. In contrast the ABCN-scheme requires always a certain minimal diffusivity for numerical stability. On the other hand it is not limited to the CFL-condition for higher values of D. However, this is not an advantage compared with the LFCN-scheme since in TURBIT we have to meet the CFL-condition for reasons of numerical stability of the explicit integration of the momentum equations.

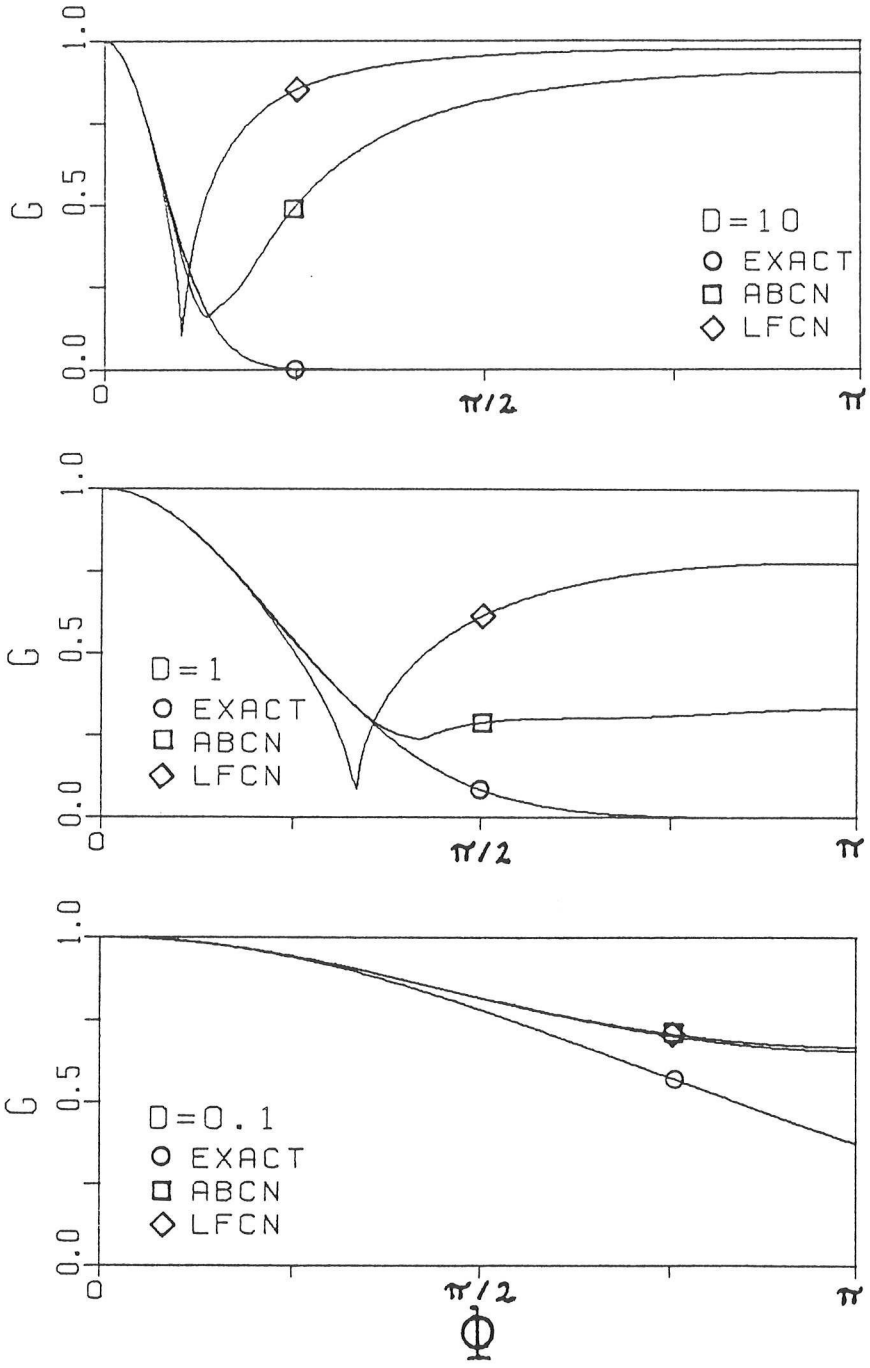



Fig. 2: Spectral analysis of the numerical error of ABCN- and LFCN-scheme for the Courant number C = 0.1 and three diffusion numbers.

### 3.2 Spectral Analysis of the Numerical Error

The damping in time of the amplitude of a spatial wave with wavenumber k follows from equation (5) to be

$$G_{ex} = \left| \frac{T(x, t + \Delta t)}{T(x, t)} \right| = e^{-a k^2 \Delta t} = e^{-D \phi^2} , \qquad (6)$$

where $\phi = k \Delta x$ is representing a phase angle. By a spectral analysis of the numerical error [6] this physical damping due to diffusion is compared to that of a numerical scheme, which is falsified by numerical diffusion, for a wide range of wavenumbers. The damping in time by a numerical scheme is characterized by the maximum of the absolute value of its complex eigenvalues.

The results for a Courant number C = 0.1 and three different diffusion numbers D = 0.1, D = 1 and D = 10 are given in figure 2. The numerical schemes are working very well for small values of $\phi$. This means that the time characteristics of structures associated with large wavelengths are well approximated by both numerical schemes. In contrast figure 2 shows that small scaled spatial structures ($\phi = \pi$ corresponds to the lowest resolvable wavelength $2 \Delta x$) are damped too weakly by both schemes. Furthermore a clear tendency is outlined that the wavenumber range of which the time characteristic is well approximated becomes more and more limited as the diffusion number increases. The ABCN scheme works slightly better at high values of D than the LFCN scheme. Nevertheless it becomes evident that, with regard to the accuracy of the numerical results, a limitation with respect to the diffusion number will be necessary for both schemes.

However, one should keep in mind that we want to use these schemes for the solution of the thermal energy equation for turbulent natural convection in liquid metals. As stated above, for this type of flow the temperature field contains only large spatial structures. Thus both schemes may be expected to yield "physical" results.

## 4. NUMERICAL EXPERIMENTS

To get more information about the accuracy of the ABCN- and LFCN-scheme both are used for numerical solution of equation (4) on a domain $0 \leq x \leq L$. Corresponding to the initial condition

$$T(x, 0) = \sin(k \cdot x) \qquad (7)$$

and the boundary conditions

$$\begin{aligned} T(0, t) &= -\sin(k u_o t) \cdot e^{-k^2 a t} \\ T(L, t) &= \sin[k(L - u_o t)] \cdot e^{-k^2 a t} \end{aligned} \qquad (8)$$

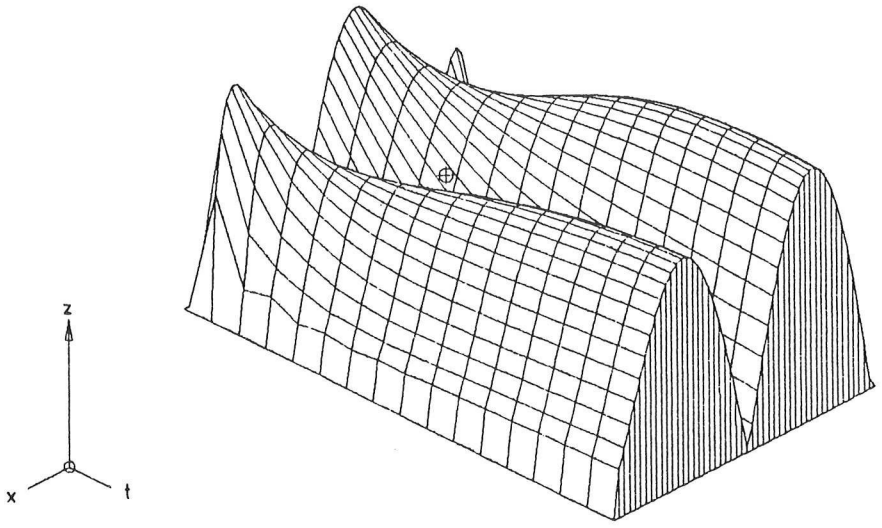
there exists the exact solution

$$T_{ex}(x, t) = \sin[k(x - u_o t)] \cdot e^{-k^2 a t} \qquad (9)$$

which can be used for comparison to the numerical solutions.

The LFCN- and ABCN-scheme are both three level schemes and thus a new time plane is calculated using values of two past time planes. Therefore both schemes cannot be used for the first integration step where only one time plane - corresponding to the initial condition - is available. Therefore a two level scheme has to be used for the first integration step. Here a semi-implicit Euler scheme is used which is only of first order in time. The results we present in this paper are gained using the following parameters: $u_o = 0.1$, $a = 0.25$, $L = \pi$ and $k = 2$. The number of mesh cells is $M = 50$ resulting in a mesh width $\Delta x = L/(M-1) \approx 0.064$. To judge on the accuracy of the numerical solutions the absolute value of their deviation from the exact solution will be shown in a three-dimensional representation dependent on space and time:

ABCN-scheme ($\lambda = 1$): $z_{max} = 4.1 \cdot 10^{-4}$




LFCN-scheme ($\lambda = 1$): $z_{max} = 3.9 \cdot 10^{-4}$

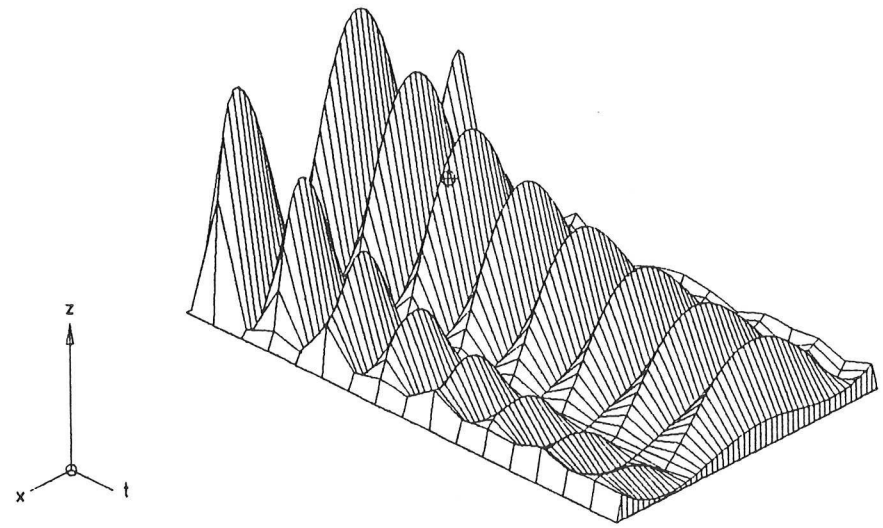
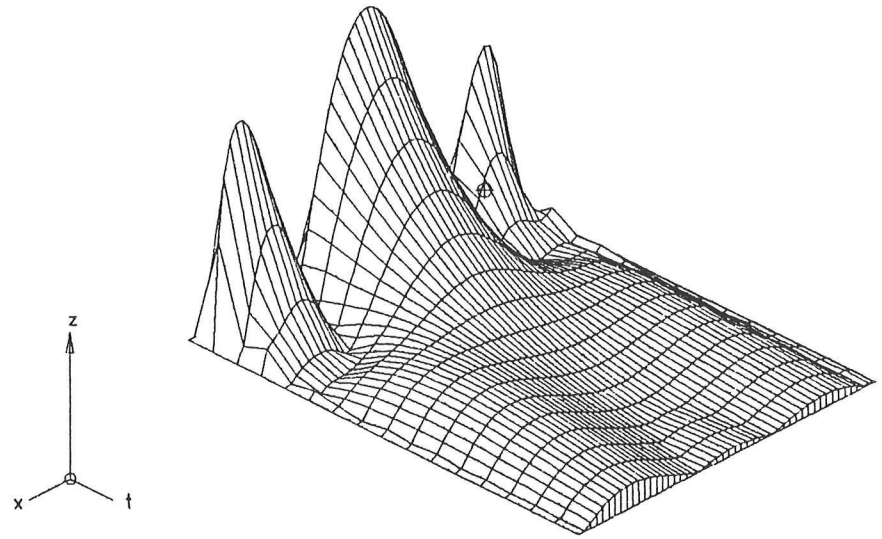



Fig. 3: Error $z(x_i, t_i) = |T_{ex}(x,t) - T_{num}(x_i, t_i)|$ for the test problem of equation (4) for $u_o = 0.1$, $a = 0.25$, $0 \leqq x \leqq L = 3.14$ and $0 \leqq t \leqq 1.025$. The exact solution $T_{ex}$ is given by equation (9) for $k = 2$. The discretization ratio used is $\lambda = \Delta t/\Delta x = 1$.

$$z(x_i, t_i) = |T_{ex}(x, t) - T_{num}(x_i, t_i)|. \qquad (10)$$

The main result of the numerical tests is the crucial influence of the discretization ratio $\lambda = \Delta t/\Delta x$ on the accuracy of the numerical solutions. Calculations done with $\lambda = 0.2$ show nearly identical error characteristics for the LFCN- and ABCN-scheme whereas they are clearly different if a larger time step corresponding to $\lambda = 1$ is used (Fig. 3). The results of the LFCN-scheme are more accurate not only as regards to the magnitude of the error but also with respect to statistical data of the solution. The reason is that the LFCN-scheme yields an alternating over- and underestimation of the exact solution whereas the ABCN-scheme does not show a change of sign in the deviation from the exact solution at a fixed spatial position for long times.

ABCN-scheme ($\lambda = 2$): $z_{max} = 1.5 \cdot 10^{-3}$




LFCN-scheme ($\lambda = 2$): $z_{max} = 1.7 \cdot 10^{-3}$

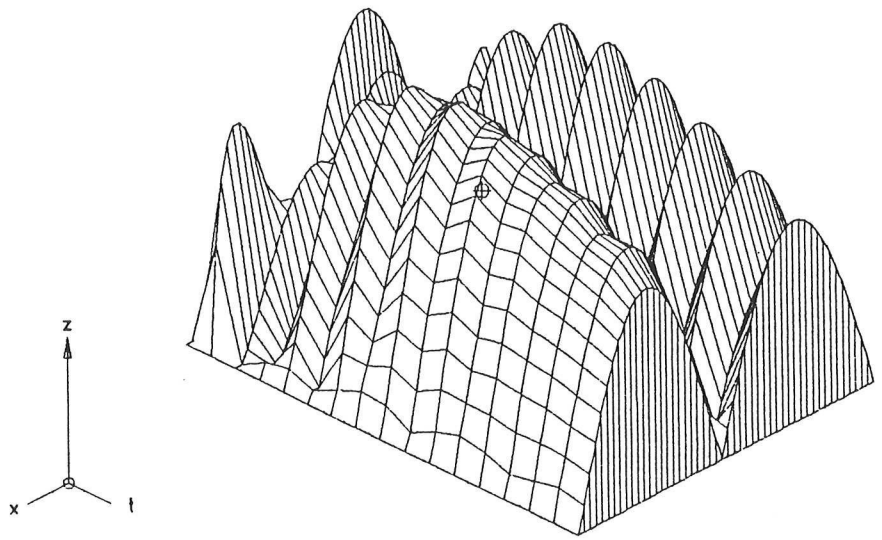



Fig.4: Error behaviour of test problem as in Fig. 3, but with discretization ratio $\lambda = \Delta t/\Delta x = 2$ and for $0 \leqq t \leqq 2.05$.

The error characteristics given in figure 4 result from a discretization ratio $\lambda = 2$. Now the solution of the ABCN-scheme is clearly superior to that of the LFCN-scheme. The latter exhibits strong oscillations in the error characteristic which are only weakly damped in time. To analyze this tendency towards $2\Delta t$ oscillations we consider the LFCN-scheme which can be written as:

$$\left[\left(2 + \frac{1}{D}\right) T_i - \left(T_{i+1} - T_{i-1}\right)\right]^{n+1} = -\frac{C}{D}\left(T_{i+1} - T_{i-1}\right)^n + \left[\left(T_{i+1} - T_{i-1}\right) - \left(2 - \frac{1}{D}\right) T_i\right]^{n-1} . \tag{11}$$

It becomes evident that for small values of the mesh Peclet number

$$Pe_{\Delta x} = \frac{C}{D} = \frac{u_o \, \Delta x}{a} \tag{12}$$

neighbouring time planes are only weakly coupled. This is the explanation why, once a time oscillation appeared, this will be damped only weakly.

The appearence of a first error oscillation can be explained by the Euler scheme which is used to calculate the first time plane out of the initial condition. Due to the decoupling of neighbouring time planes in case of a low mesh Peclet number, the first LFCN-step will also mainly use the data given by the initial condition for calculation of the second time plane. However, the error involved by the second order LFCN-scheme will be lower than that of the first order Euler-scheme. Especially the use of larger time steps $\Delta t$, or larger $\lambda = \Delta t/\Delta x$ respectively, will introduce quite different errors in the first two time planes and thus is leading to a first oscillation.

## 5. DISCUSSION

In the previous sections it has been shown that a decision between both schemes depends at least on the problem of interest. The ABCN-scheme works very well for diffusion dominated problems over the whole range of discretization ratios $\lambda = \Delta t/\Delta x$ investigated. Difficulties may arise due to numerical stability for more convection dominated problems. The main advantage of the LFCN-scheme is its superior numerical stability. However, in case of low mesh Peclet numbers it shows a tendency to time oscillations and should not be used with time steps corresponding to a discretization ratio $\lambda = \Delta t/\Delta x > 1$.

In TURBIT typical values of the discretization ratio $\lambda$ may be expected to range between 0.1 and 1 when a semi-implicit solution scheme for the thermal energy equation is used. Thus application of both schemes is possible. However, since we use a Leapfrog scheme for the integration of the momentum equations it may be reasonable to use a Leapfrog-type scheme in the energy equation too, i.e. the LFCN- instead of the ABCN-scheme. By this the possibility of phase errors between the velocity- and the temperature field seems avoidable. These may be introduced by the use of such different schemes as explicit Euler-Leapfrog- and semi-implicit ABCN- scheme are representing. We took the decision to implement the ABCN-scheme in TURBIT too, since later on the necessity may arise to solve the momentum equation also semi-implicitly. Then time steps corresponding to $\lambda > 1$ become possible and therefore the ABCN-scheme has to be used for both, for the momentum and for the energy equation.

## 6. REALISATION IN TURBIT AND PRACTICAL EXPERIENCE

An important aspect according to semi-implicit time integration is the efficient solution of the arising linear equation system. The set of linear equations arising from the implicit treatment of the thermal diffusion terms is similar to that of a discretized Poisson equation [7]. Therefore in TURBIT we use a modified version of a direct FFT-based Poisson solver [8] for the solution of this set of equations. The additional CPU-time per time step of the semi-implicit scheme is about 10 to 20 percent compared to the fully explicit scheme. This is contrasted by a gain in the time step width of one to two orders of magnitude.

In case of direct numerical simulation of Rayleigh-Bénard convection in liquid sodium with the LFCN-scheme time steps can be used which are up to a factor of 50 larger than those allowed for the fully explicit scheme. However, in some of these applications numerical instability of both the ABCN- and the LFCN-scheme was observed in case of high diffusion number. Although the Von Neumann analysis is predicting numerical stability even for an infinite diffusion number this instability is not surprising due to the results of the spectral analysis of the numerical error discussed above. Further on one should mention that a stability criterion derived by the linearized version of a nonlinear problem can only give approximative results. To avoid these stability problems we restrict the diffusion number to a maximum value of $D_{max} = a\Delta t/(\Delta x_{min}^2) = 4$ and thus set an upper limit for the time step width.

In table 1 we present results for the 2D GAMM Benchmark [1, 9] on "Numerical Simulation of Oscillatory Convection in Low-Pr Fluids" calculated by the semi-implicit schemes on a Siemens VP 400 computer. Compared to calculations on a 30·4·64 grid with the explicit scheme the use of the ABCN-scheme results in a factor of 37 for the increase of the time step width. Furthermore with the LFCN-scheme calculations on a 50·4·102 grid could be realized, while these were impracticable with the fully explicit scheme. This mesh refinement results in a clear improvement of the requested results (see Table 1), namely the maximum horizontal velocity amplitude $U^*_{max}$ and the frequency of oscillation f.

Table 1 Requested results for 2D GAMM Benchmark [1, 9] Case C, Gr = 40000, Pr = 0.015, R-R. (Remark: TURBIT is a 3D-code in which one has to use at least 4 mesh cells in the third direction even for a 2D problem)

| Code (time integration scheme) | grid | $\Delta t$ | $t_{max}$ | CPU-time [min] | $U^*_{max}$ | f |
|---|---|---|---|---|---|---|
| Reference-Code [9] | 81·321 | - | - | - | 1.093 | 21.76 |
| TURBIT (explizit [1]) | 30·4·64 | $2.6 \cdot 10^{-4}$ | 72.1 | 1089 VP 50 | 0.987 | 22.35 |
| TURBIT (semi-implicit ABCN) | 30·4·64 | $9.8 \cdot 10^{-3}$ | 228.1 | 90 VP 400 | 0.991 | 22.00 |
| TURBIT (semi-implicit LFCN) | 50·4·102 | $4.2 \cdot 10^{-3}$ | 103.4 | 217 VP 400 | 1.026 | 21.86 |

## 7. CONCLUSIONS

Direct numerical simulation of natural convection in liquid metals using fully explicit time integration schemes results in strong time step restrictions. This is enforced by the numerical stability of the thermal diffusion process and can be overcome by semi-implicit time integration of the thermal energy equation. Two semi-implicit time integration schemes - the Adams-Bashforth Crank-Nicolson scheme and the Leapfrog Crank-Nicolson scheme, respectively - have been investigated analytically and numerically. For both schemes an increase of the time step width becomes possible without loosing physically relevant information. Dependent on the Prandtl number time steps can be used that are up to a factor of 50 larger than that allowed for fully explicit schemes. Since the arising set of linear equations is efficiently solved by an adapted direct FFT-based Poisson solver this time step increase results in a CPU-time saving of nearly the same magnitude. Results for a Benchmark problem [1, 9] gained by semi-implicit time integration show the validity of the new method. Thus direct numerical simulations of turbulent natural convection in liquid metals at moderate Rayleigh numbers become feasible with justifiable computational expense.

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