Ninth GAMM-Conference on Numerical Methods in Fluid Mechanics, Lausanne, September 25–27, 1991

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

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Motivation

Sodium cooled fast breeder reactor
aim: passive decay heat removal by natural convection only

Water-experiments in 1:20 and 1:5 reactor models

Extrapolation to reactor conditions by computer codes

Problematic:

Calibration of statistical turbulence models for natural convection in liquid metals
(lack of experimental data)

$\Longrightarrow$ preparation of statistical turbulence data from direct numerical simulation (DNS)

Computer Code TURBIT

DNS and LES of turbulent channel flow

Solution of the 3D time dependent Navier Stokes equation and the thermal energy equation

Space discretization: finite differences

Time integration: explicit Euler-Leapfrog scheme

Stability criterion:

$$\Delta t \leq \Delta t_{max} = \frac{1}{\frac{|u_i|_{max}}{\Delta x_i} + 4 \frac{Max(\nu, a)}{\Delta x_i^2}}$$

liquid sodium: $Pr = \nu/a = 0.006$

temperature field: only large spatial structures

velocity field: contains very small spatial waves

increase of the time step width:
implicit treatment of the thermal diffusion terms

Semi-implicit time integration schemes for the thermal energy equation

Adams-Bashforth Crank-Nicolson (ABCN) scheme:

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

Leapfrog Crank-Nicolson (LFCN) scheme:

$$\frac{T^{n+1} - T^{n-1}}{2\,\Delta t} = -N^{n} + \frac{1}{2}\left(L^{n+1} + L^{n-1}\right)$$

$$L = a\nabla^2 T, \quad N = u\nabla T$$

Error: $O(\Delta t^2)$

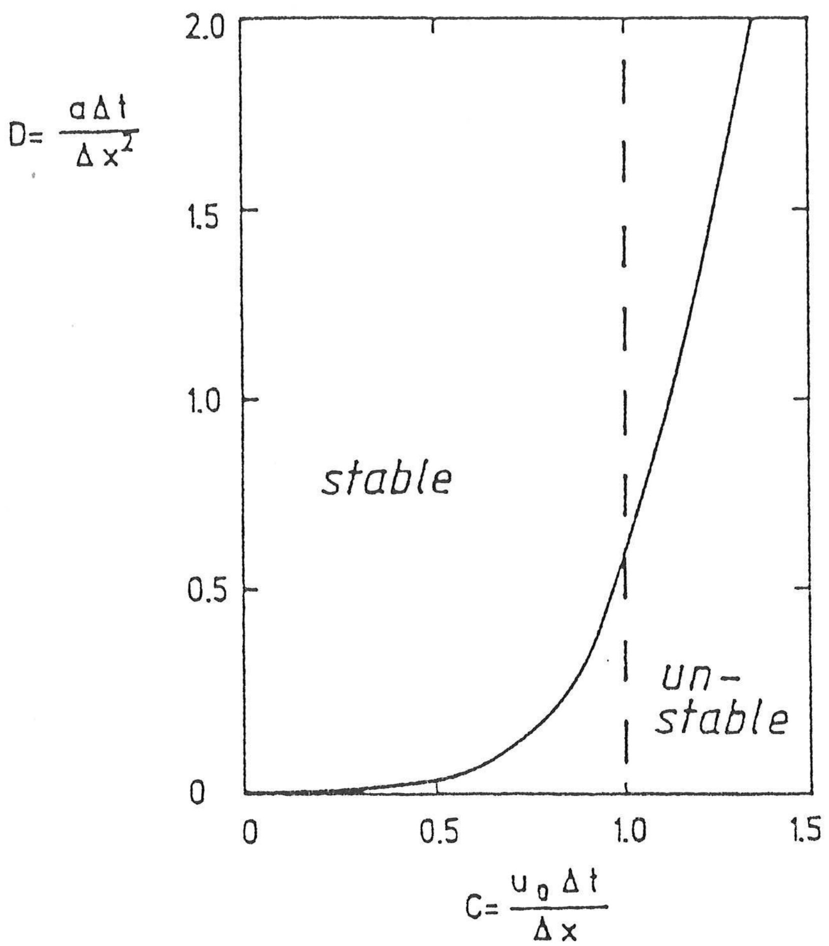
Von Neumann stability analysis

1D linear model equation:

$$\frac{\partial T}{\partial t} + u_0 \frac{\partial T}{\partial x} = a \frac{\partial^2 T}{\partial x^2} \qquad a, u_0 = \text{const.}$$

Courant number: $C = u_0 \Delta t/\Delta x$

Diffusion number: $D = a\Delta t/\Delta x^2$



dashed line: LFCN-scheme $C \leq 1$

solid line: ABCN-scheme

Numerical Experiments

$$\frac{\partial T}{\partial t} + u_o \frac{\partial T}{\partial x} = a \frac{\partial^2 T}{\partial x^2}$$

$$u_o = 0.1, \quad a = 0.25, \quad 0 \leq x \leq L = \pi$$

Initial condition:

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

Boundary conditions:

$$T(0, t) = -\sin(k u_o t) \cdot e^{-k^2 a t}$$

$$T(L, t) = \sin[k(L - u_o t)] \cdot e^{-k^2 a t}$$

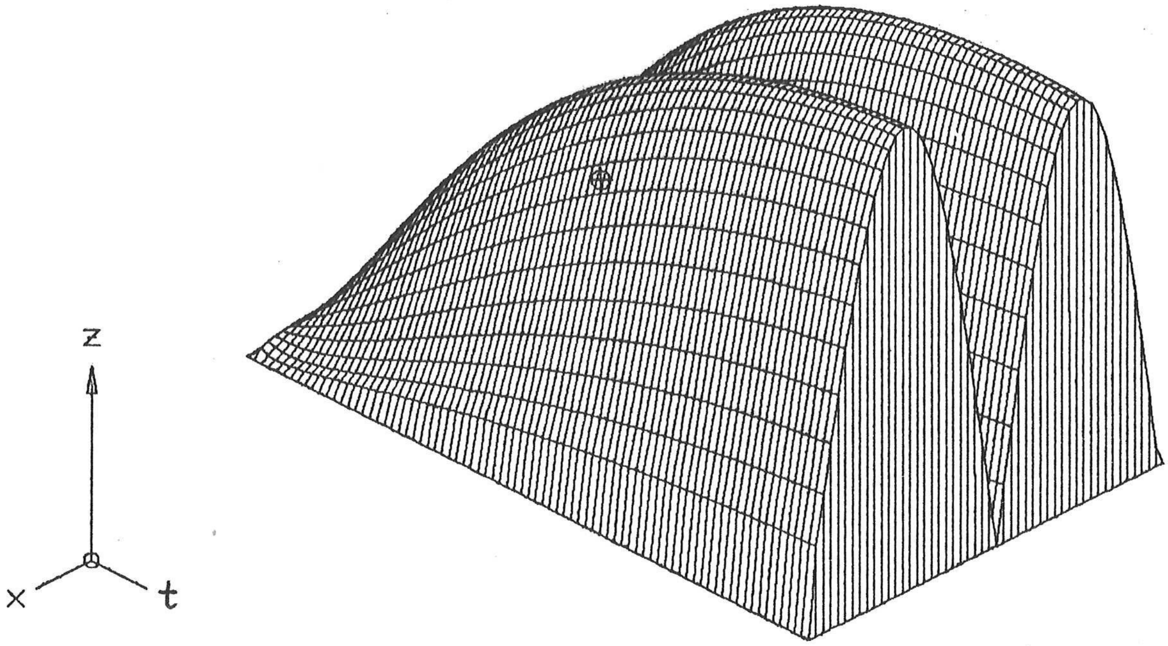
Exact solution:

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

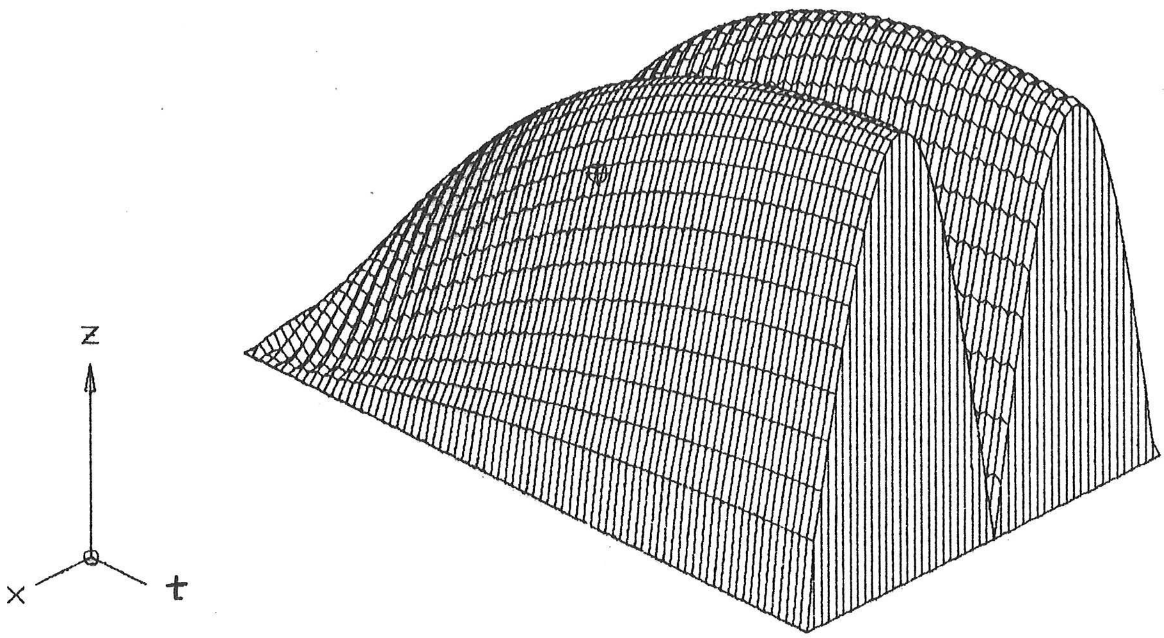
wavenumber:	$k = 2$
number of mesh cells:	$M = 50$
mesh cell width:	$\Delta x = L/M\text{-}1 \approx 0.064$
time step width:	Δt corresponding to discretization ratios $\lambda = \Delta t/\Delta x = 0.2, 1, 2$

Error: $z(x_i, t_j) = | T_{ex}(x, t) - T_{num}(x_i, t_j) |$

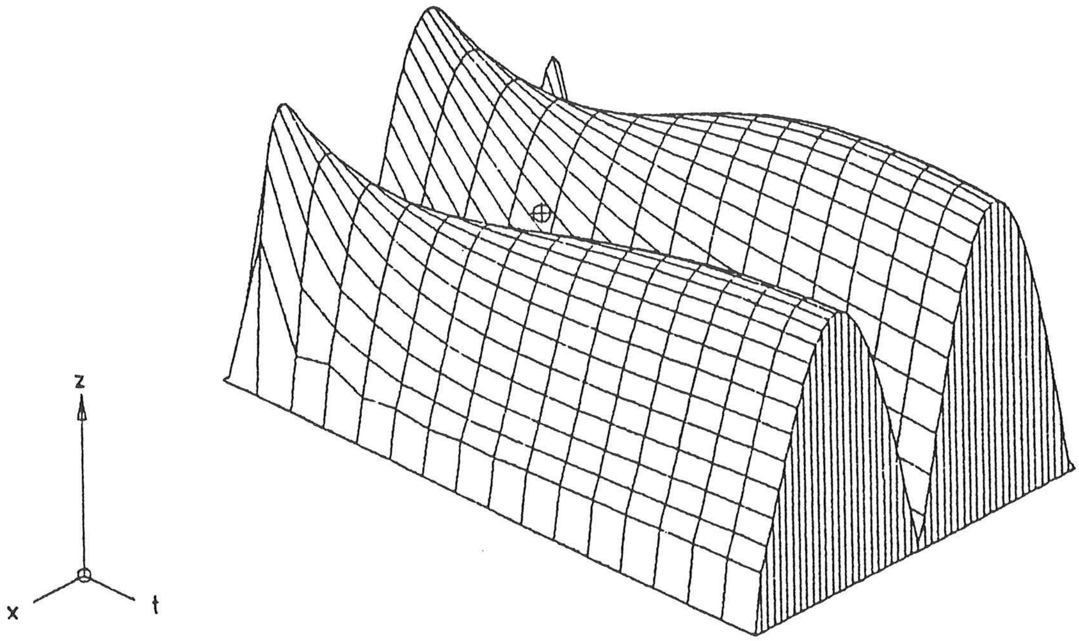
ABCN-scheme $(\lambda = 0.2)$: $z_{max} = 5.6 \cdot 10^{-4}$



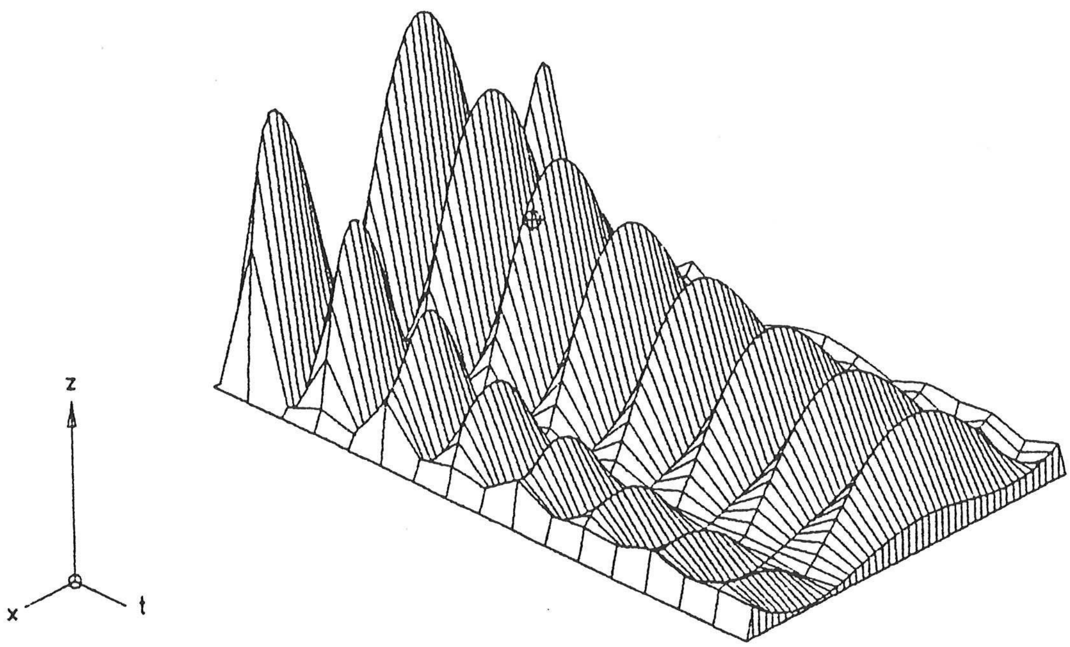
LFCN-scheme $(\lambda = 0.2)$: $z_{max} = 5.5 \cdot 10^{-4}$



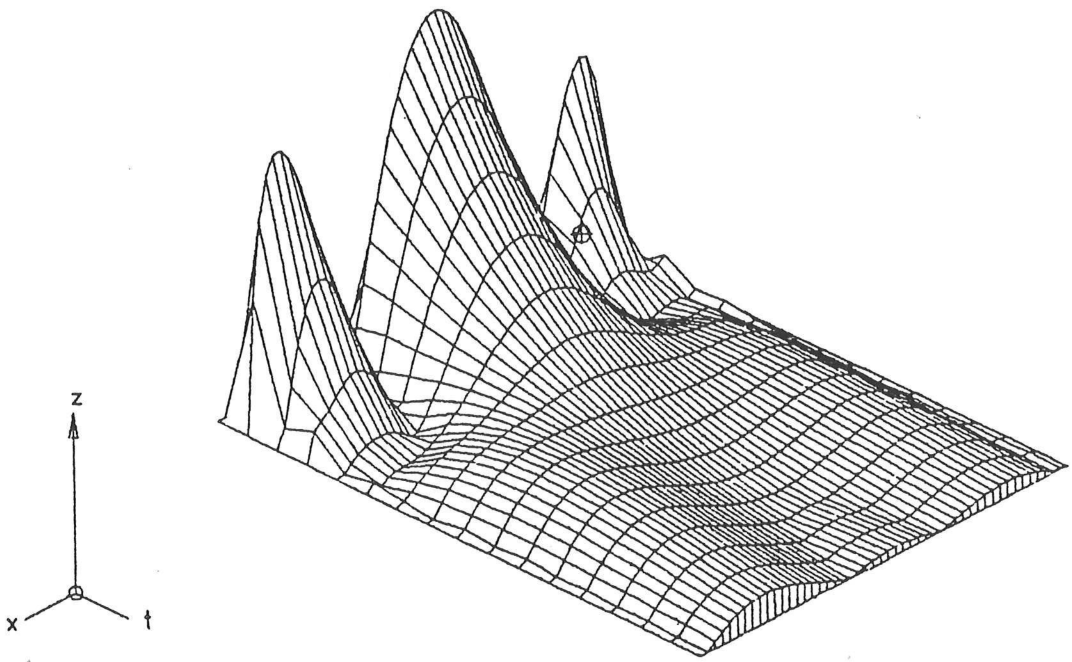
ABCN-scheme (λ = 1): $z_{max} = 4.1 \cdot 10^{-4}$



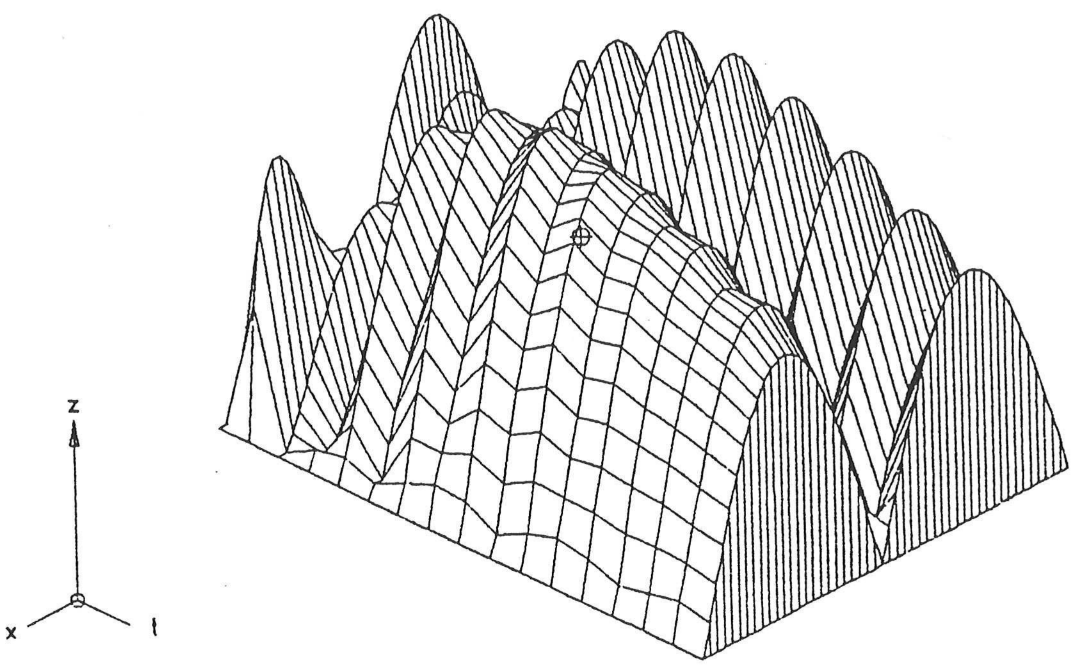
LFCN-scheme (λ = 1): $z_{max} = 3.9 \cdot 10^{-4}$



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



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



LFCN-scheme:

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

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

mesh Peclet number:

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

$Pe_{\Delta x} << 1$: decoupling of neighbouring time planes

first error oscillation:

t_o	$\longrightarrow$	t_1:	semi-implicit Euler-scheme	$O(\Delta t)$
t_o, t_1	$\longrightarrow$	t_2:	LFCN-scheme	$O(\Delta t^2)$
t_1, t_2	$\longrightarrow$	t_3:	LFCN-scheme	$O(\Delta t^2)$

Discussion

ABCN-scheme:

- \+ works well for diffusion dominated problems for the whole range of discretization ratios investigated ($0.2 \leq \lambda \leq 2$)
- \- difficulties may arise due to numerical stability for more convection dominated problems

LFCN-scheme:

- \+ superior numerical stability
- \- tendency towards $2\Delta t$ oscillations in case of low $Pe_{\Delta x}$ and $\lambda > 1$

TURBIT: $\lambda \leq 0.5$
Implementation of both schemes

Realisation in TURBIT and practical experience

- semi-implicit time integration

  $\Longrightarrow$ set of linear equations

- solution method:

  modified direct FFT-based Poisson solver

  additional CPU-time per time-plane:

  10 - 20% compared to the fully explicit scheme

- increase of the time step width:

$$\frac{\Delta t_{impl}}{\Delta t_{expl}} \approx 20 - 50$$

- upper limit for Δt:

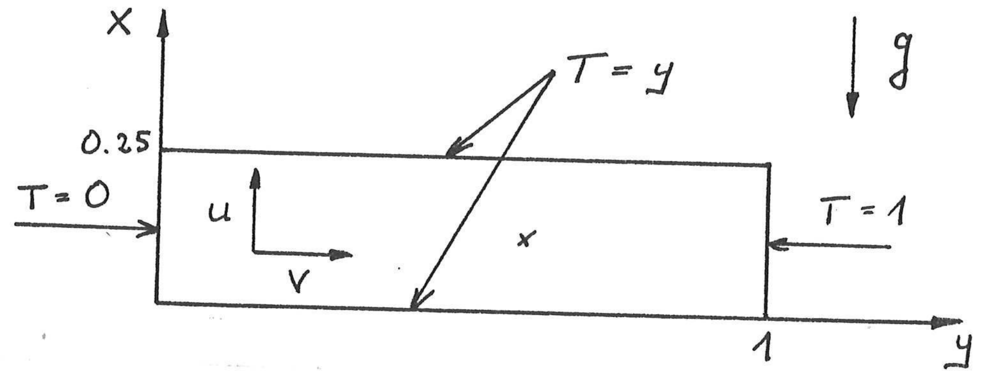
$$D = \frac{a\,\Delta t}{\Delta x_{min}^{2}} \leq D_{max} = 4$$

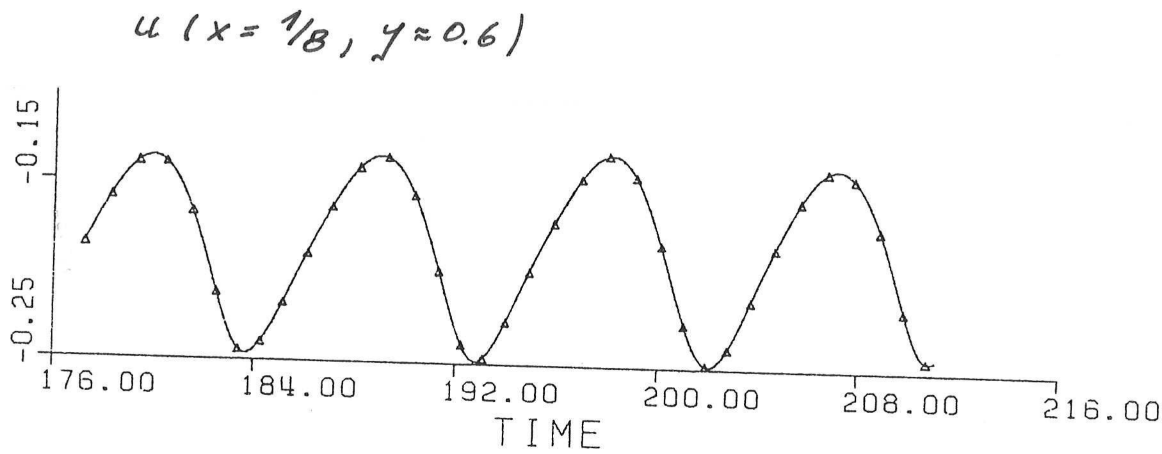
GAMM Benchmark Marseille 1988

on

"Numerical Simulation of Oscillatory Convection in Low-Pr Fluids"

2D, Pr = 0.015, Gr = 40 000





Code (time integration scheme)	grid	Δt	t_{max}	CPU-time [min]	U^*_{max}	f
Reference-Code [10]	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

Conclusions

DNS of natural convection in liquid metals

fully explicit time integration:

- strong restriction of Δt

implicit treatment of thermal diffusion terms:
- substantially increase of Δt
- no loss of physically relevant information

Analysis of semi-implicit schemes:

	$\lambda = \Delta t/\Delta x < 1$	$\lambda > 1$
ABCN-scheme:	+	+ +
LFCN-scheme:	+ +	- -
		(2Δt oscillations)

in practice:

time step increase: $\Delta t_{impl.}/\Delta t_{expl.} \leq 50$

$\Longrightarrow$ DNS of turbulent convection in liquid metals with justifiable computational expense