Numerical Solution of Advection Diffusion Equations for Ocean Models

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Abstract: - The advection-diffusion equation is one of the important equations in oceanography that use in all hydro dynamical models. In this study "Pure Advection" equation that has been solved by several methods that accuracy of them was discussed. This article investigates a numerical scheme based on the high-order accurate method for solving diffusion equation. We discuss some finite difference techniques.
We compare numerical and exact solution and we find our numerical scheme is effective for solving diffusion equation.

Key-Words: - Finite difference schemes - Krylov subspace methods - Diffusion equation –Ocean Models – FTCS Method – BTCS method

1 Introduction

Several physical phenomena are modeled by diffusion equations. Problems of this type include chemical diffusion, heat conduction, medical science, biochemistry and certain biological processes.

There are two types of schemes for numerical solution of time-dependent diffusion problems, implicit and explicit schemes. The former has no restriction on its time stepping. But in each time step one has to solve a global system of equations. The implementation on parallel computer is not straightforward due to its global nature. The latter is easy to program and implement on parallel computer. However, it suffers the severely restricted time step size from stability requirement [3].

The diffusion equation with integral conditions has wide applications in heat transfer [1], control theory [2], thermo elasticity [3], medical engineering, and life sciences [4].

Parabolic initial-boundary value problems in one dimension which involve nonlocal boundary conditions are studied by several authors. A numerical solution of this problem by using Crank-Nicolson scheme is reported in [5].

Transfer of heat by conduction is also due to random molecular motions, and there is an obvious analogy between the two processes. This was recognized by Fick [], who first put diffusion on a quantitative basis by adopting the mathematical equation of heat conduction derived some years earlier by Fourier [2].

Differential diffusion has been modeled by a linear-eddy technique (Kerstein [3]), as well as by direct numerical simulation (DNS) of passive (Young and Pope [4]) and active (Merry field et al. [5]) scalars.

Kerstein [6] developed a novel modeling technique which resolves all relevant physical scales for Re up to $O(10^4)$, at the price of sacrificing the three-dimensionality of turbulent flows. The stirring effect of turbulent eddies on a scalar field is simulated by a one dimensional stochastic rearrangement process. Coupled with deterministic treatment of molecular diffusion according to Fick’s law, this linear-eddy model has been successful in capturing many features of mixing in a variety of laboratory flows. Kerstein [3] modified the original model for application to mixing in round jets, and predicted significant differential diffusion of H_2 and propane at $\mathrm{Re}_{jet} = 5000$, but not at $\mathrm{Re}_{jet} = 20000$. These predictions are in qualitative agreement with measurements by Bilger and Dibble [7], although quantitative discrepancies exist.

An alternate computational strategy for investigating differential diffusion is to resolve the dissipation scales of the relevant scalars directly in simulations of three-dimensional turbulence. With this “brute-strength” [7] approach, computational limitations impose compromise son either or both of the ranges of Re and Sc which can be addressed. Being motivated by laboratory diffusion flames, Yeung and Pope [4] considered only scalars with Sc ≤ 1, thus dramatically reducing spatial resolution requirements relative to calculations with Sc>>1, and allowing their 64^3 calculation to achieve a Taylor scale Reynolds number of $\mathrm{Re}_\lambda = 38$. In order to treat the oceanographically relevant case of the active scalars T and S which determine the density of seawater, and for which Prandtl number $Sc_T = \mathrm{Pr} = 7$ and $Sc_S = 700$, Merry field et al. [5] reduced the dimension of calculation to two. Two-dimensional simulations were able to achieve ranges of initial Reynolds number 10 ≤ Re ≤ 160 and Froude number 0.15 ≤ Fr ≤ 110 (Re = u l/ν and Fr = u/Nl, where N is the Brunt-Vaisala frequency and u and l are velocity and length scales characteristic of the field of turbulent kinetic energy which was supplied at t=0 and subsequently decayed). The simulations revealed a sizeable region of{Re, Fr} space in which the ratio of cumulative T- to S-flux was greater than 1, indicating preferential diffusion of T, while at the same time the T-flux magnitude was significantly larger than that caused by molecular diffusivity, indicating the action of turbulence, however weak. While suggestive, results from two-dimensional calculations are vulnerable to the criticism that two-dimensional turbulence has energy cascade properties which differ from those of three-dimensional turbulence, hence may not be applicable to the latter.

However Gargett, Merry field and Hollowa [8] have recently reported results from fully three-dimensional simulations that confirm the presence of significant differential diffusion at values of Re and Fr typical of the stably stratified ocean interior, where turbulence (as revealed by those oceanic variables such as temperature dissipation rate χ_T and kinetic energy dissipation rate ε which we are routinely able to measure) appears to be weak and sporadic. In the ocean, diapycnal mixing of density is actually a process of mixing of two variables, heat (or temperature T) and salt (or salinity S), both of which contribute to the density of ocean water. All numerical ocean models presently parameterize unresolved interior diapycnal fluxes as a turbulent diffusivity K times a mean property gradient normal to isopycnals. Most models also use $\mathrm{K} = K_T = K_S$, i.e.[9]

In this paper we developed a new family of group explicit scheme for solution of diffusion equations. The presented scheme is based on domain decomposition concept and using asymmetric Saul'yev schemes for internal nodes of each sub-domain and Evan's group explicit method [11] for sub-domain's boundary nodes.

The rest of this paper is organized as follows. In the next section, we construct the scheme and describe details of implementation. In Section 3 the stability analysis is presented and in Section 4, some numerical examples are given to show the stability and accuracy of presented scheme.

2 The Diffusion equation

Diffusion is the process by which matter is transported from one part of a system to another as a result of random molecular motions.[2]

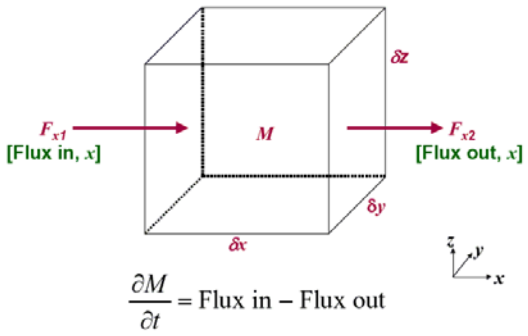

Fig.1. Element of volume

$$\frac{\partial M}{\partial t} = [F_{x1}\delta y\,\delta z - F_{x2}\delta y\,\delta z] + [F_{y1}\delta x\,\delta z - F_{y2}\delta x\,\delta z]$$
$$+[F_{z1}\delta x\,\delta y - F_{z2}\delta x\,\delta y] \qquad (2.1)$$

$$\frac{1}{\delta x\,\delta y\,\delta z}\frac{\partial M}{\partial t} = \frac{[F_{x1} - F_{x2}]}{\delta x} + \frac{[F_{y1} - F_{y2}]}{\delta y} + \frac{[F_{z1} - F_{z2}]}{\delta z} \quad (2.2)$$

$$\frac{1}{V}\frac{\partial M}{\partial t} = -\nabla.F = \frac{\partial C}{\partial t} \qquad (2.3)$$

Advection flux, FA

$$\mathrm{FA} = \mathrm{u}C \qquad (2.4)$$

$$\left[\frac{L}{T}\right]\left[\frac{M_s}{L^3}\right] \sim \left[\frac{M_s}{L^2 T}\right] \Rightarrow Flux \; (2.5)$$

Diffusive flux, FD

$$F_{Dx} \propto \frac{\partial C}{\partial x}$$

$$F_{Dx} = -k\,\frac{\partial C}{\partial x}$$

$$F_D = -k\nabla C$$

$$\frac{\partial C}{\partial t} = -\nabla.(\mathrm{F}_A + \mathrm{F}_D) = -\nabla.(UC) + \mathrm{k}\nabla^2 C$$

$$\nabla.(UC) = \mathrm{C}\nabla U + (\mathrm{U}.\nabla)C = (\mathrm{U}.\nabla)C = u\frac{\partial C}{\partial x} + \upsilon\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z}$$

$$\frac{dC}{dt} = k\nabla^2 C$$

Molecular diffusivity of heat is in water. In this case, a table [11] can be consulted to find that $k \approx 0.001cm^2/s$.

However, the ocean is turbulent, so that this value is irrelevant except at small scales where the motion is laminar (i.e., motions on scales of centimetres or less).

For turbulent motions, we must replace this value by the so-called eddy diffusivity.

These values are generally many orders of magnitude larger than the molecular values (i.e. as high as $10^8\,cm^2/\sec$ for horizontal motions).

For the turbulent case, due to the possibility that horizontal and vertical diffusion are different due to different processes, the diffusive flux must be rewritten as

$$k\nabla^2 C \to k_x\frac{\partial^2 C}{\partial x} + k_y\frac{\partial^2 C}{\partial y} + k_z\frac{\partial^2 C}{\partial z}$$

2.1 Molecular Diffusion in the Ocean

At very small length scales, oceanic motions are laminar. Recall that for Reynolds numbers less than about 3000, the flow is laminar. Thus,

$$\mathrm{Re} \sim \frac{UL}{\nu} \le 3000 \Rightarrow L \le \frac{3000\nu}{U} = \frac{3000\times 0.001}{3} = 1cm$$

Thus, on centimetre scales, true molecular diffusion might occur.

Note that (molecular values)

$$K_S \approx 10^{-5}cm^2/\mathrm{Sec}$$

$$K_T \approx 10^{-3}cm^2/\mathrm{Sec}$$

2.2 Turbulent Diffusion (Stirring) in the Ocean

In this case, clearly vertical and horizontal diffusivities are not the same. Diffusivity is difficult to measure, and can only be estimated. Various methods have been devised to do this.

$$\frac{dT}{dt} = \frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} + w\frac{\partial T}{\partial z}$$
$$= \frac{\partial}{\partial x}\left(k_x\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z\frac{\partial T}{\partial z}\right)$$

$$u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \nabla.(\mathrm{u}_H\mathrm{T}) \Rightarrow \iint \nabla.(\mathrm{u}_H\mathrm{T})dxdy = 0$$

$$\iint\left[\frac{\partial}{\partial x}\left(k_x\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y\frac{\partial T}{\partial y}\right)\right]dxdy = 0$$

We then arrive at a simplified heat balance for the world ocean:

$$w\frac{\partial T}{\partial z} = \frac{\partial}{\partial z}\left(k_z\frac{\partial T}{\partial z}\right) \Rightarrow \frac{\partial^2 T}{\partial z^2} - \left(\frac{w}{k_z}\right)\frac{\partial T}{\partial z} = 0$$

If k_z is constant. In general, both w and k_z might be functions of depth. However, let's examine the result if they are constants, so that

$$\frac{w}{k_z} = \lambda = \text{constant}$$

$$\frac{\partial^2 T}{\partial z^2} - \lambda\frac{\partial T}{\partial z} = 0$$

3 Construction of numerical scheme

In this section the numerical solution of the following problem is considered:

$$\begin{cases} u_t = ku_{xx}, & (x,t)\in \mathrm{W} \\ \mathrm{u}(\mathrm{x},0) = \delta(\mathrm{x}), & a \le x \le b, \\ \mathrm{u}(0,\mathrm{t}) = \mathrm{u}(1,\mathrm{t}) = \alpha, & 0 \le \mathrm{t} \le \mathrm{T} \end{cases}$$

Where $W = [a,b]\times[0,T]$, $\delta(x)$ initial condition and α is prescribed constant boundary condition. The domain $[a,b]\times[0,T]$ will be divided into a $M\times N$ mesh with spatial step size $\Delta x = b - a/M$ in x direction and the time step size $\Delta t = T/N$ respectively. Grid points (x_i,t_n) are given by

$x_i = i\Delta x$, i = 0,1,2, . . . ,M, and $t_n = n\Delta t$, n = 0,1,2, . . . ,N, in which M and N are positive integers. We use u_i^n to denote the finite difference approximations of $u(i\Delta x, n\Delta t)$.

4 Numerical experiments

The solution to the 1D diffusion equations: [10]

$$c(x,t) = \sum_{n=1}^{\infty} c_n(x,t) = \sum_{n=1}^{\infty} B_n\, \mathrm{e}^{-\lambda_n^2 t}\, \mathrm{Sin\,n}\frac{\pi}{L}x$$

Initial condition:

$$c(x,0) = \sum_{n=1}^{\infty} B_n\, \mathrm{Sin\,n}\frac{\pi}{L}x = f(x)$$

$$B_n = \frac{2}{L}\int_0^L f(x) Sin\, n\frac{\pi}{L}x dx$$

$$c(0,t) = c(L,t) = 0$$

Length of the bar: $L = 80cm$

Sinusoidal initial conditions:

$$f(x) = 100Sin\frac{\pi}{80}x, B_1 = 100, B_2 = B_3 = ... = 0$$

$$k = 1.158, \quad \lambda_n = n\frac{k\pi}{L} \Rightarrow \lambda_1^2 = 0.001758$$

$$c(x,t) = 100e^{-0.001785t} Sin\frac{\pi}{80}x$$

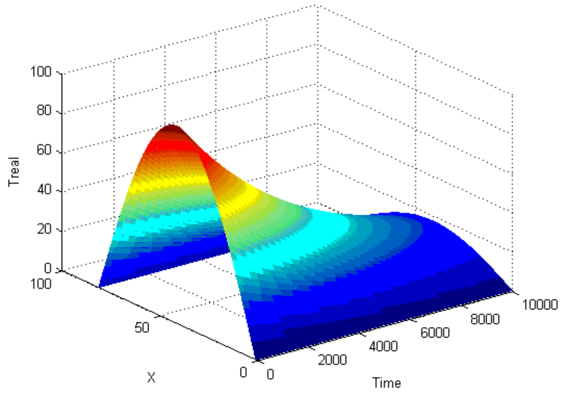

Fig.3. Space-time graph of the exact solution

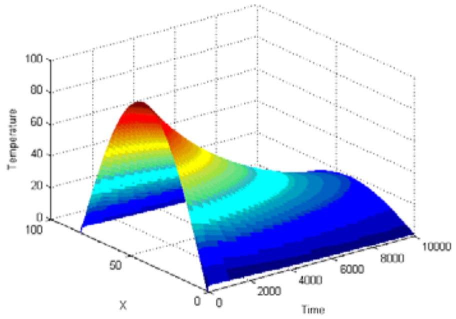

Fig.5. Space-time graph of the numerical Solution (BTCS Bicgstab)

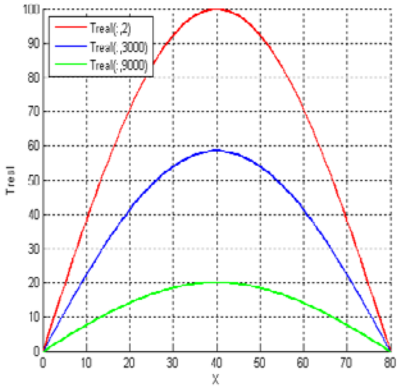

Fig.6. The exact solution

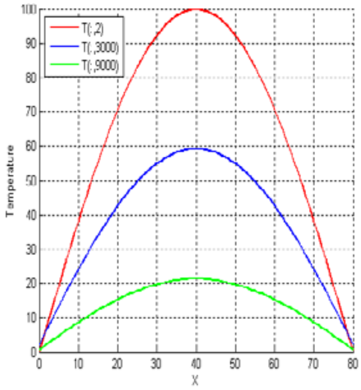

Fig.8. The Numerical solution (BTCS Bicgstab)

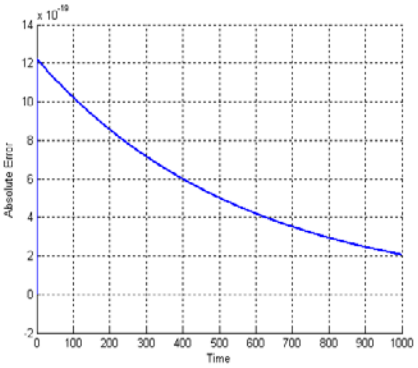

Fig.9. Absolute Error of the Numerical solution (FTCS)

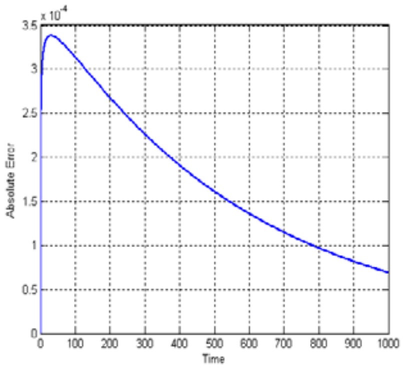

Fig.10. AbsoluteError of the Numerical solution (BTCS Bicgstab)

5 Conclusion

In this paper, we discussed FTCS method and BTCS methods (with Krylov subspace methods such as BICG, BICGSTAB, CGM) and we compare numerical scheme with exact solution then we find both of numerical scheme are good for solving diffusion equation but FTCS method have constraint because the stability of that is limited and BTCS method is stable but for use BTCS method we need more time for solving because is implicit and maximum of absolute error of Krylov subspace method (BICG, BICGSTAB , CGM) are same and all of them are good for use in BTCS method. Error of FTCS method is less than of BTCS method and processing time of FTCS is less than BTCS methods.

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