An Analysis of Two Schemes to Numerically Solve the Stochastic Collection Growth Equation

FAUSTO CARLOS DE ALMEIDA[1] AND ROGER D. DENNETT[2]

National Center for Atmospheric Research,[3] Boulder, CO 80307

(Manuscript received 24 July 1979, in final form 27 August 1980)

ABSTRACT

Two schemes for the numerical solution of the stochastic collection growth equation for cloud drops are compared. Their numerical approaches are different. One (the Berry/Reinhardt method) emphasizes accuracy; the other (the Bleck method) emphasizes speed. Our analysis shows that for applications where the number of solutions (time steps) does not exceed 10^4 the accuracy-oriented scheme is faster. For larger, repetitive applications, such as a comprehensive cloud model, an objective analysis can be made on the merits of exchanging accuracy for computational time.

1. Introduction

In attempting to theoretically understand the interactive processes occurring in the growth of a population of cloud droplets, whether for laboratory experimentation or the design of a cloud model, the numerical solution of the stochastic collection growth equation is one of the most important and perhaps most time-consuming computational tasks involved. With the more sophisticated cloud models (two- and three-dimensional with detailed microphysics) the computational time required to solve the stochastic collection growth equation is one of the major limiting factors. Several approaches have been suggested as general numerical methods for solving the stochastic collection growth equation (e.g., Berry, 1967; Berry and Reinhardt, 1974; Kovetz and Olund, 1969; Bleck, 1970; Egan and Mahoney, 1972) which should not be dependent on the initial conditions. Ochs and Yao (1978) have analyzed the Egan and Mahoney (1972) scheme adapted for the stochastic collection problem, and compared it to the Kovetz and Olund (1969) scheme as far as accuracy is concerned. In this paper, we will investigate the method proposed by Bleck (1970) and Berry (1967), as implemented in Berry and Reinhardt (1974). These two methods used in the literature by several authors (Almeida, 1977; Danielsen *et al.*, 1972; Takahashi, 1975; among others) have different characteristics, emphasizing different aspects of the numerical solution. The Berry/Reinhardt (1974) method (referred to here as the BR method) was designed for accuracy, with speed playing a secondary role, while the Bleck (1970) method (referred to here as the B method) was designed primarily for speed. An introduction to both schemes is presented to facilitate our discussion when the trade-offs between accuracy and speed are analyzed.

2. Methodological approach

In order to solve the stochastic collection growth equation numerically we first have to transform the continuous mass space into a quantized space. In general, the mass x is related to an integer J by

$$x(J) = x_s a^{b(J-1)}. \quad (1)$$

The relation between two adjacent mass categories, J and $J + 1$, using Eq. (1) is $x(J + 1) = x(J)a^b$. This defines a convenient logarithmic scale in which the total mass can be distributed. If we choose $a = 2$ and $b = 1$, we will define the mass resolution encountered in the most efficient form of Bleck's method; the mass doubling scheme. If we choose $a = 2$ and $b = \frac{1}{2}$, we will define the resolution commonly used in the Berry/Reinhardt method. Note that these choices of a and b are not arbitrary. Theoretically, other combinations can be used, such as $a = \sqrt{2}$ and $b = 1$, as long as the expression $\ln 2/b \ln a$ is an integer (Berry, 1967). Once the mass space has been quantized, the redistribution of mass among the defined categories (established by the physics of the problem) will depend on the method.

[1] Present affiliation: Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq, Instituto de Pesquisas Espaciais, INPE, C.P. 515, CEP 12.200, São José dos Campos, São Paulo, Brasil.

[2] Present affiliation: Department of Atmospheric Sciences, Georgia Institute of Technology, Atlanta, GA 30332.

[3] The National Center for Atmospheric Research is sponsored by the National Science Foundation.

0022-4928/80/122707-05$05.25

3. Berry/Reinhardt solutions

Basically the Berry/Reinhardt method uses interpolation and integration schemes adapted to the problem of realistic collection kernels to obtain the best possible accuracy. One could view this approach as a straightforward numerical integration scheme for the stochastic collection growth equation. In order to achieve the best possible result, several interpolation schemes were tried (Reinhardt, 1972) in combination with improved integration schemes as compared with Berry's (1967) original solutions. This pursuit of accuracy rendered the process slower computationally. As opposed to the Bleck method, where speed was the defining factor, here accuracy predominated. For more details on the method see Berry and Reinhardt (1974).

4. Bleck's solution

With this method (Bleck, 1970) which may be characterized as a finite element method, the actual mass distribution within each category is replaced by a set of approximation functions that are chosen to substantially simplify the mechanics of the solution. In general, the method trades solution speed for accuracy; however, with judicious choice of the approximation functions (see Bleck, 1970) acceptable accuracy can be obtained without sacrificing solution speed.

The basis of the method as mentioned above, is to divide the total drop mass range into logarithmically related intervals or categories. Within each category, the actual distribution function is replaced by an approximation function. The replacement of the unknown "actual" distribution function with a "known" approximation function together with the logarithmic relationship of the categories allow much of the required calculation to be done once, beforehand, which substantially reduces the computation time per time-step solution. These approximations are also responsible for the increased numerical diffusion found in this approach.

For a detailed theoretical derivation see Bleck (1970). Also a manuscript report on the method, including a complete user oriented Fortran computer program is available (Dennett, 1979).

5. Solution conditions

The initial droplet distribution is characterized by a gamma-type function as used by Scott (1968). Since our comparison is made on the basis of accuracy and speed of the numerical solutions, an actively growing spectrum was chosen for the comparison. This choice not only guarantees many category interactions, but also redistribution of the total mass over a wide range of mass categories. Although many combinations of initial distributions and kernel functions can be used that satisfy the criteria above (Almeida, 1979b), the results shown are for an initial droplet distribution with the mean mass radius $R_0 = 12$ μm and the $e = 1$ cm^2 s^{-3} turbulent collision efficiency of Almeida (1979a). The comparisons were made using a category spacing of $a^b = 2$, as proposed by Bleck (1970) and powers of the $a^b = \sqrt{2}$ as published by Reinhardt (1972). While it would have been desirable to match the category spacing exactly, the BR scheme became unstable using $a^b = 2$ and the Bleck method would have had to be recoded so extensively that the revision was not feasible.

6. Results: Computational speed

As will be made clear later in this section, the B scheme has a very large overhead time for initialization. This contrasts with the very short set-up time required by the BR scheme. So, in order to make a meaningful comparison of computational speeds, we introduce the function

$$T = \frac{S + Nt}{N}, \tag{2}$$

where T represents the overall (average) computational time step for N time steps, S is the set-up time or time necessary to initialize the scheme (a constant for a given method), and t is the computational time per solution time step. Note that as $N \to \infty$, $T \to t$ and as $N \to 0$, $T \to S$; i.e., the function clearly indicates the set-up and the time-step computational times of the methods compared. To evaluate S, the same clock function was used in both program routines. The same computer system, the NCAR CDC 7600, was used for the comparisons. To evaluate t, the same clock function timed both the total computational time required per time step and the total computation time required for 1440 s of cloud life, i.e., t = (CPU time) $\times \Delta T/1440$, where ΔT is the time step used in seconds.

Note that at each time step, t has a different value, the reason being that as the droplet population develops, more and more categories enter in the interactive solution, therefore increasing t. This is true for the BR method, and it can be true for the B method, although most often it uses all categories at every time step regardless of the evolution of the droplet population. More about this will be said later. Because the factors deciding the mode of growth (Almeida, 1979b) are the same in both schemes, the calculated values of t represent the actual performance for each scheme. For the CDC 7600 NCAR operational system, the T functions [Eq. (2)], in seconds, for each method are given by

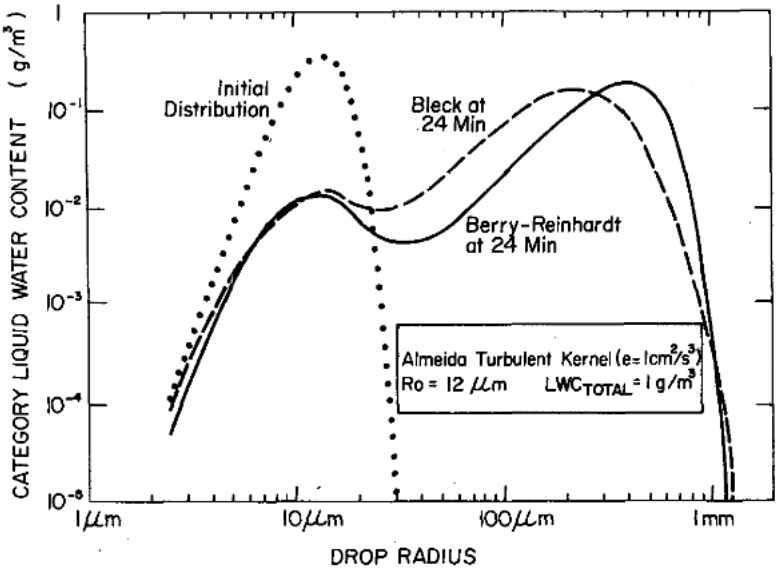

FIG. 1. Comparison of the computational speed for Bleck and Berry/Reinhardt methods. Conditions are as indicated. See text.

Berry/Reinhardt method $\rightarrow T$

$$= \frac{0.23 + 48.98 \times 10^{-3} N}{N}, \quad (3)$$

Bleck method $\rightarrow T$

$$= \frac{206.35 + 2.29 \times 10^{-3} N}{N}. \quad (4)$$

Observing Fig. 1, decisions can be made regarding the use of either method, as far as computational speed is concerned. For applications such as comparison studies where the system of equations has to be initialized several times and the number of solutions N does not exceed 10^4, clearly the BR method should be used. It is faster and more accurate. On the other hand, for applications where the initial conditions do not change during a set of calculations (such as in a cloud model application in which N is generally much larger than 10^4) the B method is much faster. For comparison purposes, the total computational time required for N number of time steps ($N \times T$) is indicated at the top of Fig. 1. Note that while the B method would require ~1 h for an application involving around a million time-step solutions, the BR method would require on the order of ~13 h of CDC 7600 time. This speed comparison may vary depending on the circumstances involved, but it would not change the main conclusions reached above.

It was brought to our attention at a later stage that Ochs and Yao (1978) had timed the modified Egan and Mahoney (1972) mass conserving technique and found that for a number of categories equal to 38, the CPU time for the CDC 7600 NCAR system (what it should be our t) was equal to 28.8 ms. Comparing this result with Eqs. (3) and (4), the modified Egan and Mahoney (1972) scheme, for the same number of categories, is somewhat faster than the BR scheme but still much slower than the B scheme.

Ochs and Yao (1978) did not clock the set-up time S defined in Eq. (2) for neither the Egan and Mahoney (1972) nor the Kovetz and Olund (1969) schemes. Therefore, we could not access the overall computational time step T; a quantity that can really show the total time a method takes to solve the stochastic growth equation for a number of N time steps.

7. Accuracy

Since no analytic solutions exist for realistic kernels, our comparison is limited to a plot of the result of each scheme. Independent tests of accuracy for each scheme have been done by Bleck (1970) and Reinhardt (1972). Because the liquid water content (LWC) of the distribution does not change with time in the collection drop growth process, the LWC could be used as a test of accuracy for the numerical solution of the stochastic collection equation. This is true for the BR method. Indeed, the variation in the LWC was within 0.04% for a total of 30 min of the drop population development, attesting to the accuracy of the method. For the B method, conservation of LWC is inherent and therefore cannot be independently checked. Fig. 2 compares the results from the two schemes. As mentioned before, because of the approximation functions used, the B method has a larger diffusion

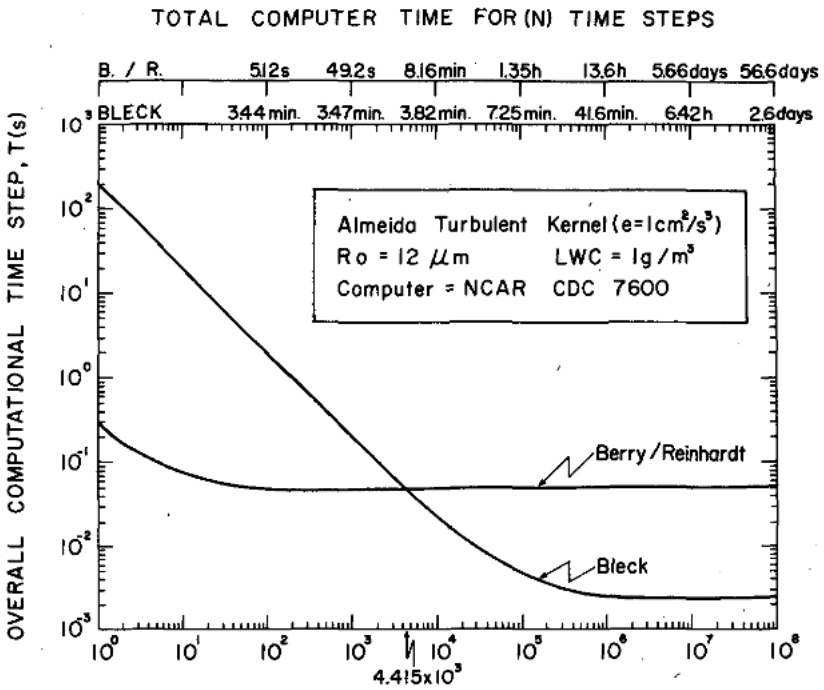

FIG. 2. Comparison of the computational accuracy for Bleck and Berry/Reinhardt methods. See text.

for large-radius categories, although this numerical diffusion is generally within the errors present in most cloud models applications.

8. Comments

Since the BR method calculates a mass distribution function in a category and the Bleck method calculates only the total mass in a category, it was necessary to transform the BR results to the Bleck equivalent. For our comparison a parabolic interpolation was used.

For either method, one way to cut the computational time without appreciable change in accuracy is to limit the number of categories interacting during each time step. To achieve this time savings, we varied the value of the smallest amount of mass being considered in each category, or G_{lim}. Trials for the BR scheme showed that with $10^{-70} \leq G_{\text{lim}} \leq 10^{-15}$ g cm^{-3}/ln$R$, the deviations in the LWC were within 0.09%. For values of $G_{\text{lim}} > 10^{-15}$ g cm^{-3}/ln$R$, this deviation starts to be noticeable, changing the growth behavior of the droplet population (a numerical error). When G_{lim} was increased from 10^{-70} to 10^{-15} g cm^{-3}/ln$R$ (the maximum advisable), the computational times per time-step solution t decreased from 48.98 to 37.65 ms, a 23% savings in time. In our comparison we used a value of 10^{-70} for G_{lim}. For the Bleck method, using a gravitational kernel (Almeida, 1979a) and $R_0 = 12$ μm, t varied from 1.20 to 2.38 ms when the LWC threshold was varied from 10^{-20} to 10^{-200} g cm^{-3}/ln$R$. The difference is due to very small amounts of mass in the larger categories. For the comparisons, a value of 10^{-50} was used.

Another possibility for saving time in the BR scheme would be to transfer some of the computations, in the sense of Bleck's scheme, from t to S [Eq. (2)]. In essence, this attempt would be the same as transforming the BR code into a B code equivalent, what the authors did not do.

Note that no attempt was made to optimize the Fortran code of the BR method. Our purpose was to run in this comparison study the same program as that published by Reinhardt (1972).

As mentioned before, the value of t varies depending on the initial distribution used and the kernel function chosen for the computations. For gravitational kernels (Davis and Sartor, 1967; Almeida, 1979a) and for droplet distributions with $8 \leq R_0 \leq 14$ μm, we found, taking the BR method as an example, that $23.26 \leq t \leq 50.45$ ms. For turbulent cases (Almeida, 1979a), due to the active participation of more mass categories in each time step, t now varies from 27.88 ms, corresponding to $R_0 = 8$ μm, up to 55.83 ms, corresponding to $R_0 = 14$ μm.

These results serve to illustrate the fact that the more categories a numerical scheme has to take into account, the more attractive a faster method becomes, even though some accuracy is lost. Note that for the comparisons illustrated in Figs. 1 and 2, as mentioned in Section 5, the same initial distribu-

tion and the same kernel function were used in both model computations.

9. Conclusions

Our recommendation is that the Berry/Reinhardt method be used where parameter investigations such as kernel comparisons are being made ($N < 10^4$ solutions) and that the Bleck method be used where large numbers of similar solutions are required, as in a cloud model with detailed microphysics. The Berry/Reinhardt solutions can also be useful in tuning the Bleck method for best accuracy. Thus, a judgement can be made (Figs. 1 and 2) for each application, and the importance of speed, accuracy, or a combination of both will dictate the choice. In other words, both methods, each with a different philosophy of design, have their place and should be used in conjunction rather than competition, until a combination Bleck-Berry/Reinhardt code is developed or an entire new approach is devised.

REFERENCES

Almeida, F. C. de, 1977: Collision efficiency, collision angle and impact velocity of hydrodynamically interacting cloud drops: A numerical study. *J. Atmos. Sci.*, **34,** 1286–1292.

——, 1979a: The collisional problem of cloud droplets moving in a turbulent environment—Part II. Turbulent collision efficiencies. *J. Atmos. Sci.*, **36,** 1564–1576.

——, 1979b: The effects of small-scale turbulent motions on the growth of a cloud droplet spectrum. *J. Atmos. Sci.*, **36,** 1557–1563.

Berry, E. X, 1967: Cloud droplet growth by collection: *J. Atmos. Sci.*, **24,** 688–701.

——, and R. L. Reinhardt, 1974: An analysis of cloud drop growth by collection: Part I. Double distributions. *J. Atmos. Sci.*, **31,** 1814–1824.

Bleck, R., 1970: A fast approximative method for integrating the stochastic coalescence equation. *J. Geophys. Res.*, **75,** 5165–5171.

Davis, M. H., and J. D. Sartor, 1967: Theoretical collision efficiencies for small cloud droplets in Stokes flow. *Nature*, **215,** 1371–1372.

Danielsen, E. F., R. Bleck and D. A. Morris, 1972: Hail growth by stochastic collection in a cumulus model. *J. Atmos. Sci.*, **29,** 135–155.

Dennett, R., 1979: Report on the Bleck method of solving the stochastic collection—Results, codes and extensions. NCAR/1201-79/1, 149 pp.

Egan, B. A., and J. R. Mahoney, 1972: Numerical modeling of advection and diffusion of urban area source pollutants. *J. Appl. Meteor.*, **11,** 312–322.

Kovetz, A., and B. Olund, 1969: The effects of coalescence and condensation on rain formation in a cloud of finite vertical extent. *J. Atmos. Sci.*, **26,** 1060–1065.

Ochs, H. T., and C. S. Yao, 1978: Moment conserving techniques for microphysical computations, Part I: Numerical techniques. *J. Atmos. Sci.*, **35,** 1947–1958.

Reinhardt, R. L., 1972: An analysis of improved numerical solutions of the stochastic collection equation for cloud droplets. Ph.D. thesis, University of Nevada, 111 pp.

Scott, W. T., 1968: Analytic studies of cloud drop coalescence I. *J. Atmos. Sci.*, **25,** 54–65.

Takahashi, T., 1975: Tropical showers in an axisymmetric cloud model. *J. Atmos. Sci.*, **32,** 1318–1330.