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Analyzing numerics of bulk microphysics schemes in Community models: warm rain processes

I. Sednev and S. Menon

Dept. of Atmospheric Sciences, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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Correspondence to: I. Sednev (isednev@lbl.gov)

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Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

Abstract

In the last decade there has been only one study that discussed time integration scheme (TIS) applied to advance governing differential equations in bulk microphysics (BLK) schemes. Recently, Morrison and Gettelman (2008) examine numerical aspects of double-moment BLK scheme with diagnostic treatment of precipitating hydrometeors implemented into Community Atmosphere Model, version 3 (CAM) to find an acceptable level of accuracy and numerical stability. However, stability condition for their explicit non-positive definite TIS was not defined.

It is conventionally thought that the Weather Research and Forecasting (WRF) model can be applied for a broad range of spatial scales from large eddy up to global scale simulations if time steps used for model integration satisfy to a certain limit imposed mainly by dynamics. However, numerics used in WRF BLK schemes has never been analyzed in detail.

To improve creditability of BLK schemes we derive a general analytical stability and positive definiteness criteria for explicit Eulerian time integration scheme used to advanced finite-difference equations that govern warm rain formation processes in microphysics packages in Community models (CAM and WRF) and define well-behaved, conditionally well-behaved, and non-well-behaved Explicit Eulerian Bulk Microphysics Code (EEBMPC) classes.

We highlight that source codes of BLK schemes, originally developed for use in cloud-resolving models, implemented in Community models belong to conditionally well-behaved EEBMPC class and exhibit better performance for finer spatial resolutions when time steps do not exceed seconds or tenths of seconds. For coarser spatial resolutions used in regional and global scale simulations time steps are usually increased from hundredths up to thousands of seconds. This might lead to a degradation of conditionally well-behaved EEBMPCs ability to calculate the amount of precipitation as well as its spatial and temporal distribution since both stability and positive definiteness conditions are not met in the TIS. The correction through the so called

"mass conservation" technique commonly used in many models with bulk microphysics is a main characteristic of non-well-behaved EEBMPC, whose utilization leads to erroneous conclusions regarding relative importance of different microphysical processes. Moreover, surface boundary conditions for ocean, land, lake, and sea ice models are dependent on the precipitation and its spatial and temporal distribution. Uncertainties in calculations of temporal and spatial patterns of accumulated precipitation influence the global water cycle. In fact, numerics in non-well-behaved EEBMPCs, which are used in Community Earth System Model, act as a hidden climate forcing agent, if relatively long time steps are used for the host model integration.

By analyzing numerics of warm rain processes in EEBMPCs implemented in Community models we provide general guidelines regarding appropriate choice of integration time steps for use in these models.

1 Introduction

In the last decade there has been only one study (Morrison and Gettelman, 2008) (MG08) that discussed explicit time integration schemes (TIS) used to advance governing microphysical equations in bulk microphysics (BLK) scheme. MG08 implemented a two-moment BLK scheme with diagnostic treatment of precipitating hydrometeors in the Community Atmosphere Model (CAM) version 3 (Collins et al., 2006). To advance governing microphysical prognostic equations in MG08, time splitting is applied to separate between sedimentation and the rest of the microphysical processes, and rain and snow sedimentation are treated diagnostically similar to Ghan and Easter (1992). For cloud water and cloud ice sedimentation an upstream advection scheme and an explicit TIS are used. Courant-Friedrichs-Lewy (CFL) condition is always satisfied because the microphysical time step is sub-divided into smaller equal time steps. This procedure assures stability and positive definiteness. To advance other microphysical equations an explicit Eulerian (EE) TIS is used. Because stability and positive definiteness criteria are not defined, sometimes hydrometeors' mixing ratio and/or concentration might be negative. To prevent negative mixing ratios "mass conservation" technique is used to calculate artificially modified growth rates for some microphysical processes but time step remains unchanged. To keep positive concentrations additional artificial concentration adjustment is applied in MG08. This influences such cloud characteristics as effective radius, radar reflectivity, precipitation fluxes, and radiative cloud properties as well as cloud-aerosol interactions, amount of accumulated precipitation, and its spatial and temporal distributions. Moreover, if applied in Earth System Models on a global scale, non-stable and non-positive definite time integration schemes would influence the global water cycle providing artificial precipitation patterns that are used as surface boundary conditions for ocean, land, lake, and sea ice model. In fact, numerics in BLK schemes acts as a "hidden climate forcing agent" (HCFA) on a global scale.

In the Weather Research and Forecasting (WRF) model version 3 (Skamarock et al., 2008), both the single moment BLK schemes and the Morrison-Curry-Khvorostyanov double-moment BLK scheme (Morrison et al., 2005) (MCK05) share similar deficiencies of non-positive and unstable solutions in the autoconversion and accretion process if the microphysical time step used is greater than a few tenth of seconds. This feature of BLK schemes implemented in Community models (CAM and WRF) could lead to erroneous conclusions regarding the role of cloud microphysics and its influence on radiation or dynamics (amongst others) when relatively long time steps are used for integration.

To avoid highly uncertain performance of BLK microphysics schemes if relatively long time steps used for model integration and improve creditability of precipitation amount calculations we derive necessary condition (referred to as the SM-criterion) to keep the EE time integration scheme stable and positive definite. This imposes constrain on the time step permitted (like CFL condition for advection equation). We highlight that in addition to limitation on the time step imposed by dynamics there also exists a limitation due to the microphysics. We also define well-behaved, conditionally well-behaved, and non-well-behaved Explicit Eulerian Bulk Microphysics Code (EEBMPC) classes and show that source codes of BLK schemes, which were originally developed

GMDD
4, 1403–1434, 2011

for use in cloud-resolving models (CRM) and implemented in Community models, belong to conditionally well-behaved EEBMPC class. We also provide recommendations regarding integration time steps for prospective simulations with WRF and CAM.

The paper is organized as follows. The general considerations are given in Sect. 2. The growth rate calculation due to warm rain processes in BLK schemes are discussed in Sect. 3. The analytical and finite-difference solutions for the system of equation that governs warm rain formation in BLK schemes as well as stability analysis are presented in Sect. 4. Discussion and recommendations are provided in Sect. 5.

2 General consideration

We consider the following system of equations for bounded positive $X(t)$ and $X(t)$ with initial conditions $X(t=0)=X_0>0$ and $Y(t=0)=Y_0>0$ on time interval $0 \le t \le \tau$:

$$\frac{dX}{dt} = -F(X) - G(X,Y), \tag{1}$$

$$\frac{dY}{dt} = +F(X) + G(X,Y), \tag{2}$$

where $F(X)$ and $G(X,Y)$ are both positive and bounded, and positive τ is given.

We are looking for numerical solution for $X(n+1)$ and $Y(n+1)$ with initial conditions $X(n)=X_0$ and $Y(n)=Y_0$ that at each time step "n" satisfy the conservation equation

$$\frac{d[X+Y]}{dt} = 0 \tag{3}$$

as well as positiveness and boundness conditions

$$0 < X(n+1) \le X_0, \tag{4}$$

$$Y_0 \le Y(n+1) \le X_0 + Y_0, \tag{5}$$

where $X(n)$ and $Y(n)$ are X and Y at the beginning of time step "n".

GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

Explicit finite-difference scheme with time step τ is written as:

$$X(n+1) = X(n) - \tau[F(X(n)) + G(X(n),Y(n))] \tag{6}$$

$$Y(n+1) = Y(n) + \tau[F(X(n)) + G(X(n),Y(n))] \tag{7}$$

It is clearly seen that this solution conserves sum of X and Y. By adding expressions (6)–(7) we get finite-difference analog for the conservation equation given by Eq. (3):

$$X(n+1) + Y(n+1) = X(n) + Y(n)$$

The values of $X(n+1)$ and $Y(n+1)$ on the next time step are always bounded and positive only if

$$\tau_{\max} \leq \frac{X(n)}{F(X(n)) + G(X(n),Y(n))} \tag{8}$$

Expression (8) determines the time step permitted to keep the solution (6)–(7) bounded and positive. To solve the system we have to specify X, Y, $F(X)$, $G(X,Y)$, and τ as well as determine stability condition.

3 Warm rain processes in community models

Applying these general consideration to cloud physics and defining

$$\begin{aligned} X &= Q_c > 0 \\ Y &= Q_r > 0 \\ F(X) &= \text{PAUTO} > 0 \\ G(X,Y) &= \text{PACCR} > 0 \end{aligned}$$

GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

we get the following system of equations that governs the process of “warm” rain formation in prognostic BLK schemes:

$$\frac{\partial Q_c}{\partial t} = -(\text{PAUTO} + \text{PACCR}) \tag{9}$$

$$\frac{\partial Q_r}{\partial t} = +(\text{PAUTO} + \text{PACCR}) \tag{10}$$

where Q_c is cloud water mixing ratio, Q_r is rain water mixing ratio, and PAUTO and PACCR are their changes due to auto-conversion and accretion, respectively. By adding Eqs. (9) and (10), we get

$$\frac{\partial (Q_c + Q_r)}{\partial t} = 0 \tag{11}$$

Equation (11) has the simple physical meaning that is for the “warm” rain formation process total water mixing ratio $Q_t = Q_c + Q_r$ remains unchanged.

Different single-moment and double-moment BLK schemes used in CAM and WRF and referenced thereafter as RaschCAM (Rasch and Kristjansson, 1998) and KESSLER (Kessler, 1969), LIN (Lin et al., 1983), ETA (Ferrier, 1994), TAO (Tao et al., 2003), THOMPSON (Thompson et al., 2004), MORRISON (Morrison et al., 2005), and WSM6 (Hong and Lim, 2006) schemes, respectively, calculate auto-conversion and accretion growth rates using different analytical representation for functions PAUTO and PACCR. The system of non-linear differential Eqs. (9)–(10) is linearized and solved using explicit Eulerian (EE) time integration scheme. Our analysis of source codes of MG08 scheme in CAM and TAO, THOMPSON, MORRISON, and WSM6 schemes in WRF, respectively, reveals that positiveness criterion (SM-criterion) similar to inequality (8) and given by

$$\tau_{\max} \le \frac{Q_c}{\text{PAUTO} + \text{PACCR}} \tag{12}$$

is never checked.

GMDD
4, 1403–1434, 2011
Analyzing numerics of bulk microphysics schemes
I. Sednev and S. Menon

In our analysis of source codes for BLK schemes referred to above we use the following definitions of Explicit Eulerian Bulk Microphysics Code (EEBMPC). If SM-criterion has never been checked in EEBMPC, we define such codes as belonging to conditionally well-behaved EEBMPC class or non-well-behaved EEBMPC class as opposed to well-behaved EEBMPC, in which SM-criterion is always checked and satisfied (to the best of our knowledge there is no well-behaved EEBMPC implemented in Community models). The remarkable feature of well-behaved EEBMPC is that it assures a correct solution for governing differential equations.

The common feature of conditionally well-behaved EEBMPC and non-well-behaved EEBMPC is that both rely on so called "mass conservation" technique in an attempt to avoid negativeness of hydrometeors' mixing ratios and make EE TIS positive definite. Main characteristics of "mass conservation" technique are (a) inconsistency between published parameterization formulae for growth rates of microphysical processes and their representation in source code and (b) use of artificial reduced growth rates due to microphysical processes.

The distinguishable feature of conditionally well-behaved EEBMPC is that the SM-criterion is satisfied even if it has never been checked. As used in Cloud Resolving Models (CRM) or Large Eddy Simulation (LES) models with temporal resolution about a few seconds conditionally well-behaved EEBMPC provides a correct solution for governing differential equations because limitation on time step imposed by dynamics is more restrictive than that imposes by microphysics (SM-criterion), and, in fact, "mass conservation" technique is never applied. The transition between conditionally well-behaved EEBMPC and non-well-behaved EEBMPC is determined by the SM-criterion. If a time step used in a host model (CAM or WRF) is typical for regional scale and especially large scale simulations and SM-criterion is occasionally violated, a conditionally well-behaved EEBMPC would become non-well-behaved EEBMPC. The eventual feature of non-well-behaved EEBMPC is that it does not provide a correct solution for governing differential equations.

GMDD
4, 1403–1434, 2011

To avoid use of artificial "mass conservation" technique, mimic the utilization of well-behaved EEBMPC, and provide guidelines regarding time steps permitted for model integration for prospective CAM and WRF users we present maximal time steps for autoconversion and accretion processes as well as effective maximal time steps for both processes that are necessary to keep stability and positive definiteness of EE time integration scheme. These maximal time steps, which satisfy SM-criterion, are calculated for specified values of cloud water and rain water mixing ratios and two values of cloud droplet concentrations (N_c) for different BLK schemes and are shown in Table 1. The rightmost column in Table 1 shows maximal time step permitted if particular BLK scheme is chosen for simulation. The values in paretheness correspond to a different cloud droplet concentration (N_c) and indicate dependence of autoconversion or accretion on $N_c = 10(100)\,\text{cm}^{-3}$. For example, for KESSLER scheme representation of both autoconversion and accretion does not depend on N_c, and for the KESSLER row, values of time step are equal in each column. Non-dependence on N_c in autoconversion column manifests non-aplicability of KESSLER, LIN, and TAO schemes for cloud-aerosol interaction simulations whereas only THOMPSON scheme accounts for dependence of accretion on N_c. Except for this scheme, all other WRF BLK schemes under consideration can be used for regional scale simulations if time step in a host model does not exceed two to three hundreds seconds. However, it should be noted that this conclusion is valid only for specific $Q_c = 1.0\,\text{g}\,\text{kg}^{-1}$ and $Q_r = 0.5\,\text{g}\,\text{kg}^{-1}$ used to calculate maximal time steps presented in Table 1.

To demonstrate instantaneous dependences of effective maximal time step on typical cloud water mixing ratio and rain water mixing ratio for different cloud types we define SM-number (N_{sm}) as

$$N_{sm} = \frac{\tau(\text{PAUTO} + \text{PACCR})}{Q_c} \quad (13)$$

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

It should be noted that there is an obvious relation between SM-criterion and SM-number. SM-criterion is valid (EE finite-difference scheme is stable and positive definite) if

$$N_{sm} \leq 1 \tag{14}$$

Thus maximal time step permitted to keep EE time integration scheme stable and positive definite corresponds to

$$N_{sm} = 1 \tag{15}$$

Maximal time steps calculated according to expression (15) for TAO, THOMPSON, MORRISON, and WSM6 WRF BLK schemes as functions of Q_c and Q_r for two different droplet concentration $N_c = 10\,cm^{-3}$ and $N_c = 100\,cm^{-3}$, which are used as proxy for "maritime" and "continental" clouds, are shown on Figs. 1 and 2 and Figs. 3 and 4, respectively. For "maritime" clouds Fig. 1 shows instantaneous dependence of maximal time step on Q_c for $Q_r = 0.1\,g\,kg^{-1}$ (top left), $0.5\,g\,kg^{-1}$ (top right), $1.0\,g\,kg^{-1}$ (bottom left), and $3.0\,g\,kg^{-1}$ (bottom right), respectively, whereas Fig. 2 shows instantaneous dependence of maximal time step on Q_r for $Q_c = 0.1\,g\,kg^{-1}$ (top left), $0.5\,g\,kg^{-1}$ (top right), $1.0\,g\,kg^{-1}$ (bottom left), and $3.0\,g\,kg^{-1}$ (bottom right). Figures 3 and 4 replicate Figs. 1 and 2, respectively, for "continental" clouds.

The set of these four figures represents a simple yet powerful tool to analyze behavior of a BLK microphysics scheme. Because utilization of a single column model (SCM) is a conventional way to validate new microphysics parameterization, observations (vertical profiles of cloud water mixing ratio, rain mixing ratio, and cloud droplet concentration) and data from Figs. 1–4 can be used to analyze theoretical vertical profiles of SM-criterion. These vertical profiles provide thoughtful way for the appropriate choice of a time step used for SCM integration instead of arbitrary values as is conventionally done. Moreover, in the case of 2-D or 3-D simulations the vertical profiles of SM-criterion show additional limitations imposed on a time step used in a multidimensional host model. For example, limitation on a time step provided in the WRF User

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper

GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

Guide is given as

$$\tau_{\mathrm{wrf}} \leq 6\Delta X_{\mathrm{wrf}}, \tag{16}$$

where τ_{wrf} is the time step in seconds and ΔX_{wrf} is the spatial resolution in kilometers. However, this constrain does not account for additional restrictions due to microphysics imposed by SM-profiles that ensure EE scheme stability and positive definiteness and reliability of model output. In fact, for regional or large scale WRF simulations with a time step chosen according to inequality (16) violation of SM-criterion at different times, altitudes, and spatial locations leads to unstable and non-positive definite numerical solution for the governing warm rain differential equations.

Proof that SM-criterion is necessary condition for EE TIS stability and positive definiteness as well as consequences of using a "mass adjustment" technique are outlined in the next section.

4 Analytical and numerical solutions and stability analysis

Different single-moment and double-moment BLK schemes used in Community models formulate auto-conversion PAUTO and accretion PACCR growth rates in a variety of ways providing different non-linear functional dependences on Q_{c}, Q_{r}, and N_{c}. The system of nonlinear differential Eqs. (9)–(10) that governs the processes of warm rain formation can be solved only numerically using iterative methods. However, if some linearization is assumed, it could also be solved analytically.

4.1 Warm rain processes: analytical solution

For example, linearized on time interval $0 \leq t \leq \tau$ form can be used for both the auto-conversion growth rate PAUTO and accretion growth rate PACCR

$$\mathrm{AUTO} = C_{\mathrm{u}}^{0} Q_{\mathrm{c}}^{0} \tag{17}$$

$$\mathrm{ACCR} = C_{\mathrm{a}}^{0} Q_{\mathrm{r}}^{0} Q_{\mathrm{c}}^{0} \tag{18}$$

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

where C_u^0 and C_a^0 are given by

$$C_u^0 = \mathrm{PAUTO}(Q_c^0)[Q_c^0]^{-1} \tag{19}$$

$$C_a^0 = \mathrm{PACCR}(Q_c^0, Q_r^0)[Q_c^0]^{-1}[Q_r^0]^{-1} \tag{20}$$

With expressions (17)–(20) Eqs. (9)–(10) are as follows:

$$\frac{\partial Q_c}{\partial t} = -\mathrm{AUTO} - \mathrm{ACCR} = -C_u^0 Q_c^0 - C_a^0 Q_r^0 Q_c^0 \tag{21}$$

$$\frac{\partial Q_r}{\partial t} = +\mathrm{AUTO} + \mathrm{ACCR} = +C_u^0 Q_c^0 + C_a^0 Q_r^0 Q_c^0 \tag{22}$$

Solving for Q_c and Q_r on time interval $0 \le t \le \tau$ we get an analytical solution for linearized differential Eqs. (21)–(22):

$$Q_c = Q_c^0 - \tau(C_u^0 + C_a^0 Q_r^0)Q_c^0 \tag{23}$$

$$Q_r = Q_r^0 + \tau(C_u^0 + C_a^0 Q_r^0)Q_c^0 \tag{24}$$

It can be easily seen that solution (23)–(24) conserves mass. Analytical solution (23)–(24) is bounded and positive definite if and only if

$$0 \le Q_c^0 - \tau(C_u^0 + C_a^0 Q_r^0)Q_c^0 \le Q_c^0 \tag{25}$$

$$Q_r \le \tau(C_u^0 + C_a^0 Q_r^0)Q_c^0 + Q_r^0 \le Q_c^0 + Q_r^0 \tag{26}$$

These inequalities determine maximal time step permitted to keep a bounded and positive solution. Both are satisfied if SM-criterion is valid:

$$\tau \le \tau_{\max} = \frac{1}{C_u^0 + C_a^0 Q_r^0} \tag{27}$$

Thus SM-criterion determines sufficient and necessary positiveness condition for the analytical solution to the system of non-linear differential Eqs. (9)–(10) that governs the processes of warm rain formation regardless of specific formulations for autoconversion PAUTO and accretion PACCR growth rates. Condition (27) also determines applicability of linearization given by expressions (17)–(20).

4.2 Warm rain processes: explicit Eulerian time integration scheme

Finite-difference analog for the system of nonlinear differential Eqs. (9)–(10) that govern processes of warm rain formation can be given as:

$$\frac{q_c^{n+1} - q_c^n}{\tau} = -\text{PAUTO} - \text{PACCR} \tag{28}$$

$$\frac{q_r^{n+1} - q_r^n}{\tau} = +\text{PAUTO} + \text{PACCR} \tag{29}$$

where q_c^n and q_c^{n+1}, q_r^n and q_r^{n+1} are initial and new values of cloud water content and rain content, respectively. Time representations for auto-conversion and accretion growth rates are still not specified. In general, Eqs. (28)–(29) can be solved only using iterative numerical methods that need significant computational time. However, if some linearization is assumed, non-iterative computationally efficient numerical methods can be used. For example, in an explicit Eulerian scheme a linearized explicit form is used for both auto-conversion and accretion growth rates:

$$\text{PAUTO} = -C_u^n q_c^n \tag{30}$$

$$\text{PACCR} = -C_a^n q_r^n q_c^n \tag{31}$$

where C_u^n and C_a^n are given by

$$C_u^n = \text{PAUTO}(q_c^n)[q_c^n]^{-1} \tag{32}$$

$$C_a^n = \text{PACCR}(q_c^n, q_r^n)[q_c^n]^{-1}[q_r^n]^{-1} \tag{33}$$

Explicit representation means that both auto-conversion and accretion growth rates can be calculated at the beginning of the microphysical time step because q_c^n and q_r^n

GMDD

4, 1403–1434, 2011

I. Sednev and S. Menon

are known. With expressions (30)–(33) Eqs. (28)–(29) are as follows:

$$\frac{q_c^{n+1} - q_c^n}{\tau} = -C_u^n q_c^n - C_a^n q_r^n q_c^n \tag{34}$$

$$\frac{q_r^{n+1} - q_r^n}{\tau} = +C_u^n q_c^n + C_a^n q_r^n q_c^n \tag{35}$$

Solving for q_c and q_r we get a numerical solution for linearized differential Eqs. (9)–(10):

$$q_c^{n+1} = q_c^n - \tau(C_u^n + C_a^n q_r^n) q_c^n \tag{36}$$

$$q_r^{n+1} = q_r^n + \tau(C_u^n + C_a^n q_r^n) q_c^n \tag{37}$$

It is clearly seen that this solution conserves mass. By adding expressions (36)–(37) we get the finite-difference analog for mass conservation equation given by Eq. (11):

$$q_c^{n+1} + q_r^{n+1} = q_c^n + q_r^n$$

Despite the fact that solution (36)–(37) conserves mass, it is not positive definite. Whereas q_r^{n+1} is always positive, q_c^{n+1} sometimes might be negative. Numerical solution (36)–(37) is bounded and positive definite if and only if

$$0 \le q_c^n - \tau(C_u^n + C_a^n q_r^n) q_c^n \le q_c^n \tag{38}$$

$$q_r^{n+1} \le \tau(C_u^n + C_a^n q_r^n) q_c^n + q_r^n \le q_c^n + q_r^n \tag{39}$$

These inequalities determine maximal time step permitted to keep bounded and positive numerical solution. Both inequalities are satisfied if SM-criterion is valid:

$$\tau \le \tau_{\max} = \frac{1}{C_u^n + C_a^n q_c^n} \tag{40}$$

Thus SM-criterion provides necessary condition for the explicit Eulerian finite-difference scheme (34)–(35) to be positive definite regardless of parameterization formulae used for autoconversion and accretion growth rates (30)–(33). It should be noted that using a time step greater than that given by SM-criterion (40) leads to a violation of stability criteria for finite-difference scheme given by expressions (32)–(35).

GMDD
4, 1403–1434, 2011

4.3 Stability analysis: explicit Eulerian scheme

Numerical solution (36)–(37) is given by the matrix equation:

$$\begin{bmatrix} q_c^{n+1} \\ q_r^{n+1} \end{bmatrix} = \begin{pmatrix} 1-\tau(C_u^n + C_a^n q_r^n) & 0 \\ \tau(C_u^n + C_a^n q_r^n) & 1 \end{pmatrix} \times \begin{bmatrix} q_c^n \\ q_r^n \end{bmatrix}. \quad (41)$$

Matrix characteristic equation for system (41) has the following form:

$$\det \begin{pmatrix} 1-\tau(C_u^n + C_a^n q_r^n) - \lambda & 0 \\ \tau(C_u^n + C_a^n q_r^n) & 1-\lambda \end{pmatrix} = 0. \quad (42)$$

For the finite-difference scheme to be stable it is necessary that all roots $\lambda_{1,2}$ of its characteristic equation satisfy

$$|\lambda_{1,2}| \leq 1. \quad (43)$$

However, in the case

$$-1 \leq \lambda_{1,2} \leq 0, \quad (44)$$

the numerical solution (36)–(37) might oscillate. This fact contradicts the conditions of positiveness (38)–(39). Thus, instead of inequality (43) $\lambda_{1,2}$ must satisfy

$$0 \leq \lambda_{1,2} \leq 1. \quad (45)$$

To find stability conditions for the scheme given by expressions (32)–(35) all roots of matrix characteristic equation (42) have to be found. We then get the algebraic characteristic equation

$$\lambda^2 - [2-\tau(C_u^n + C_a^n q_r^n)]\lambda - [\tau(C_u^n + C_a^n q_r^n) + 1] = 0. \quad (46)$$

The solutions are as follows

$$\lambda_{1,2} = \frac{2-\tau(C_u^n + C_a^n q_r^n) \pm \tau(C_u^n + C_a^n q_r^n)}{2}. \quad (47)$$

GMDD
4, 1403–1434, 2011

The first root λ_1 is given by

$$\lambda_1 = 1, \tag{48}$$

and stability inequality (45) for λ_1 is always satisfied.

The second root λ_2 is given by

$$\lambda_2 = 1 - \tau(C_u^n + C_a^n q_r^n). \tag{49}$$

According to (45) it must satisfy the following inequality

$$0 \le 1 - \tau(C_u^n + C_a^n q_r^n) \le 1. \tag{50}$$

The right inequality is held unconditionally, but for the left inequality to be valid it is necessary that

$$\tau \le \tau_{max} = \frac{1}{C_u^n + C_a^n q_c^n}. \tag{51}$$

The condition given by expression (51) is necessary for computational stability of the finite-difference scheme given by expressions (32)–(35). Observation that conditions (40) and (51) coincide permits us to conclude that SM-criterion provides necessary condition for the explicit Eulerian finite-difference scheme given by Eqs. (34)–(35) to be stable and positive definite regardless of parameterization for autoconversion and accretion growth rates.

Because stability of EE time integration scheme for microphysical governing equations used in BLK schemes has never been discussed, an effect of violation of SM-criterion on EE TIS stability and positive definiteness is hidden. Because validation of SM-criterion is not reproduced in EEBMPCs used in Community models these codes belong to conditionally well-behaved EEBMPC class. Thus we conclude that if relatively long time steps are used for WRF integration and SM-criterion is occasionally violated, source code implementations of the TAO, THOMPSON, MORRISON, and WSM6 schemes in the official WRF distribution would belong to non-well-behaved

GMDD
4, 1403–1434, 2011
Analyzing numerics of bulk microphysics schemes
I. Sednev and S. Menon

EEBMPC that do not provide a correct numerical solution for governing differential equations.

Although source codes for these four schemes share the same deficiencies, in the following section we provide a detailed analysis of conditionally well-behaved EEBMPC for MORRISON scheme because it is implemented in both WRF (Morrison et al., 2005) and CAM (Morrison and Gettelman, 2008).

4.4 Warm rain processes in WRF: MCK05 numerical solution

It should be noted that finite-difference analog for the system of differential equations for double-moment BLK scheme is not presented and discussed in Morrison et al. (2005).

In this scheme warm rain formation processes are governed by the system of differential equations (Khairoutdinov and Kogan, 2000) (KK2000):

$$\frac{\partial q_\mathrm{c}}{\partial t} = -c_1[q_\mathrm{c}]^{2.47}[N_\mathrm{c}]^{-1.79} - c_3[q_\mathrm{c}]^{1.15}[q_\mathrm{r}]^{1.15} \quad (52)$$

$$\frac{\partial q_\mathrm{r}}{\partial t} = +c_1[q_\mathrm{c}]^{2.47}[N_\mathrm{c}]^{-1.79} + c_3[q_\mathrm{c}]^{1.15}[q_\mathrm{r}]^{1.15} \quad (53)$$

Using "reverse engineering", that is translating source code documented in WRF to scientific notation used in the theory of finite-difference schemes (TFDS), we reveal that finite-difference analog for the system (52)–(53) is used in the following form

$$\frac{q_\mathrm{c}^{n+1} - q_\mathrm{c}^n}{\tau} = -q_\mathrm{c}^n c_1[N_\mathrm{c}^n]^{-1.79}[q_\mathrm{c}^n]^{1.47} - q_\mathrm{c}^n c_3[q_\mathrm{c}^n]^{0.15}[q_\mathrm{r}^n]^{1.15} \quad (54)$$

$$\frac{q_\mathrm{r}^{n+1} - q_\mathrm{r}^n}{\tau} = +q_\mathrm{c}^n c_1[N_\mathrm{c}^n]^{-1.79}[q_\mathrm{c}^n]^{1.47} + q_\mathrm{c}^n c_3[q_\mathrm{c}^n]^{0.15}[q_\mathrm{r}^n]^{1.15} \quad (55)$$

where explicit representation for both PAUTO and PACCR is used:

$$\mathrm{PAUTO} = q_\mathrm{c}^n c_1[N_\mathrm{c}^n]^{-1.79}[q_\mathrm{c}^n]^{1.47} \quad (56)$$

$$\mathrm{PACCR} = q_\mathrm{c}^n c_3[q_\mathrm{c}^n]^{0.15}[q_\mathrm{r}^n]^{1.15} \quad (57)$$

GMDD
4, 1403–1434, 2011
Analyzing numerics of bulk microphysics schemes
I. Sednev and S. Menon

Explicit representation means that both auto-conversion and accretion growth rates can be calculated at the beginning of the microphysical time step because q_c^n and q_r^n are known.

Solving for q_c^{n+1} and q_r^{n+1} we get a numerical solution for the differential Eqs. (52)–(53):

$$q_c^{n+1} = q_c^n - \tau q_c^n \{c_1[N_c^n]^{-1.79}[q_c^n]^{1.47} + c_3[q_c^n]^{0.15}[q_r^n]^{1.15}\} \quad (58)$$
$$q_r^{n+1} = q_r^n + \tau q_c^n \{c_1[N_c^n]^{-1.79}[q_c^n]^{1.47} + c_3[q_c^n]^{0.15}[q_r^n]^{1.15}\}. \quad (59)$$

It is clearly seen that this solution conserves mass. By adding expressions (58)–(59) we get a finite-difference analog for the mass conservation equation given by Eq. (11):

$$q_c^{n+1} + q_r^{n+1} = q_c^n + q_r^n.$$

Although the solution (58)–(59) conserves mass, it is not positive definite. Whereas q_r^{n+1} is always positive, q_c^{n+1} sometimes might be negative because the positiveness condition given by SM-criterion

$$\tau \le \tau_{\max} = \frac{1}{\{c_1[N_c^n]^{-1.79}[q_c^n]^{1.47} + c_3[q_c^n]^{0.15}[q_r^n]^{1.15}\}} \quad (60)$$

where $\tau_{\max}$ is the time step permitted to keep positive solution, is not satisfied.

To avoid negative q_c^{n+1} similar to the approach usually employed in other BLK schemes (e.g., Reisner et al., 1998) reduced artificial auto-conversion AAUTO and accretion AACCR rates are used (through the "mass conservation" technique):

$$\mathrm{AAUTO} = \frac{q_c^n c_1[N_c^n]^{-1.79}[q_c^n]^{1.47}}{\tau\{c_1[N_c^n]^{-1.79}[q_c^n]^{1.47} + c_3[q_c^n]^{0.15}[q_r^n]^{1.15}\}} \quad (61)$$

$$\mathrm{AACCR} = \frac{q_c^n c_3[q_c^n]^{0.15}[q_r^n]^{1.15}}{\tau\{c_1[N_c^n]^{-1.79}[q_c^n]^{1.47} + c_3[q_c^n]^{0.15}[q_r^n]^{1.15}\}} \quad (62)$$

GMDD
4, 1403–1434, 2011

It is assumed that these artificial rates act during the time step τ provided by a host model. In fact, instead of the original KK2000 formulae for autoconversion and accretion growth rates (56)–(57) artificial "adjusted" growth rates (61)–(62) are accidentally used. It indicates that conditionally well-behaved EEBMPC (validation of SM-criterion is absent) for MORRISON scheme becomes non-well-behaved EEBMPC if SM-criterion is not satisfied and does not provide a correct numerical solution for differential Eqs. (52)–(53) that govern processes of warm rain formation. It is worth noting that output arrays of non-well-behaved EEBMPC passed to a host model contain artificial numbers that are chaotic at different times, altitudes, and geographical locations and should not be used for post-processing analysis in process oriented studies devoted to investigation of the relative importance of different microphysical processes or intercomparison of different formulations of auto-conversion and/or accretion processes.

To illustrate the problems accounted with utilization of artificial "mass conservation" technique we provide a simple example. Nowadays it is simply incorrect to use EE scheme with a time step Δt_{adv} for numerical solution for 1-D advection equation with positive constant velocity C_{adv} on equi-spaced grid ΔX_{adv} if CFL-condition given by

$$N_{\text{CFL}} = \frac{\Delta t_{\text{adv}} C_{\text{adv}}}{\Delta X_{\text{adv}}} \leq 1$$

is not satisfied. Thus maximal time step permitted to keep EE time integration scheme stable corresponds to

$$N_{\text{CFL}} = 1$$

and is determined by

$$\Delta t_{\max} = \frac{\Delta X_{\text{adv}}}{C_{\text{adv}}}. \tag{63}$$

Because both C_{adv} and ΔX_{adv} are constants and can not be changed, maximal time step permitted $\Delta t_{\max}$ is also known before numerical integration of 1-D advection equation. Any attempt to solve this equation using a time step that is longer than that given

GMDD
4, 1403–1434, 2011

by expression (63) results in an unstable solution. According to logics of "mass conservation" technique for condition (63) to be valid advection velocity C_{adv} has to be reduced, but time step Δt_{adv} remains unchanged. However, it is contrary to the definition of C_{adv} as a constant. In non-well-behaved EEBMPC for MORRISON scheme, utilization of reduced "adjusted" autoconversion (61) and accretion (62) growth rates instead of original KK2000 growth rates is similar to the reduction of constant advection velocity C_{adv}. The basic assumption of the "mass conservation" technique, that is applicability of reduced "adjusted" growth rates acting during unchanged microphysical time step (substep if any), contradicts the linearization used to derive finite-difference analog (30)–(31), in which autoconversion PAUTO and accretion PACCR are given by expressions (56)–(57) and are known at the beginning of each microphysical time step (substep if any).

All non-well-behaved EEBMPC calculate growth rates (tendencies) due to microphysical processes incorrectly. For warm rain processes in MORRISON scheme a sum of "adjusted" growth rates due to autoconversion (61) and accretion (62) multiplied by unchanged time step (or substep if in use) supplied by a host model τ_h is exactly equal to available cloud water mixing ratio that is all cloud water is completely depleted. However, it means that cloud water is depleted not during the time interval τ, which depends on a time step in a host model τ_h, but during the time interval, that is determined by SM-criterion, equal to $\tau_{\max}$ given by expression (60). Case $\tau > \tau_{\max}$ (necessity to apply "mass conservation") means that after microphysical calculations accumulated "real time" in a host model and microphysics are decoupled, and microphysics "lives its own life" not related to a "real time" in a host model.

Despite the fact that our analysis is focused on warm rain processes, we highlight that inclusion of ice phase into consideration makes SM-criterion more restrictive because additional solid hydrometeors compete for available cloud water. For example, source code implemented into CAM (Morrison and Gettelman, 2008) and GFDL AM3 GCM (Salzmann et al., 2010) uses diagnostic treatment of precipitating hydrometeors. However, the numerical treatment of cloud water generalized to include ice-phase

GMDD
4, 1403–1434, 2011
Analyzing numerics of bulk microphysics schemes
I. Sednev and S. Menon

remains similar to the one discussed above. To avoid numerical instability two equal time substeps are used, and to avoid non-positive definiteness "mass conservation" is applied to modify original growth rates due to numerous warm, ice, and mixed microphysical processes. Our simple analysis relevant to warm processes shows that these growth rates are affected if more restrictive criterion than SM-criterion is not satisfied when timesteps typical for GCM (10–20 min) are used for model integration, and transition from conditionally well-behaved EEBMPC to non-well-behaved EEBMPC is occurred. As a result, output of non-well-behaved EEBMPC contains artificially modified growth rates due to different microphysical processes used in post-processing to demonstrate their relative importance (see e.g., Salzmann et al., 2010, Figs. 10 and 11 for 30 min time step).

5 Discussion

To date, there are no studies that analyzed numerics of bulk microphysics schemes with prognostic treatment of precipitating hydrometeors implemented in WRF (TAO, THOMPSON, MORRISON, and WSM6). Moreover, finite-difference analog for each of these schemes has never been provided. Our analysis of source codes for these schemes in WRF reveals that non-positive definite explicit Eulerian time integration scheme is used to advance finite-difference microphysical equations. For warm rain processes we derive analytical condition (SM-criterion) that imposes constrain on time step permitted (like CFL condition for advection equation) and remains valid regardless of parameterization formulae used for autoconversion and accretion processes. We also prove that SM-criterion is a necessary condition of positive definiteness for linearized analytical solution as well as a necessary condition of stability and positive definiteness for explicit Eulerian time integration scheme.

Depending on the validation of SM-criterion in Explicit Eulerian Bulk Microphysics Code (EEBMPC), we introduce a definition for well-behaved EEBMPC, conditionally well-behaved EEBMPC, and non-well-behaved EEBMPC. In well-behaved EEBMPC, SM-criterion is always validated and satisfied, and a remarkable feature of

GMDD
4, 1403–1434, 2011
Analyzing numerics of bulk microphysics schemes
I. Sednev and S. Menon

well-behaved EEBMPC is an assurance of correctness of numerical solution for governing differential equations. If SM-criterion is never validated, EEBMPC is assigned to conditionally well-behaved EEBMPC class or non-well-behaved EEBMPC class, whose common feature is utilization of so called "mass conservation" technique.

As used in cloud resolving or large eddy simulations with a time step of a few seconds, conditionally well-behaved EEBMPC provides a correct numerical solution for governing differential equations despite the fact that validity of SM-criterion is never checked. Necessity of its validation is hidden, because limitation on time step imposes by dynamics is more restrictive than that imposed by microphysics. Thus SM-criterion is always satisfied, and "mass conservation" technique is never applied.

Because SM-criterion determines instantaneous transition between conditionally well-behaved EEBMPC and non-well-behaved EEBMPC, mechanistic extrapolation of applicability of conditionally well-behaved EEBMPC to regional (global) scales and utilization for WRF integration time steps of order of hundredths (thousandths) of seconds should be made with caution. As documented in the WRF User Guide limitation on time step permitted for model integration is imposed mainly by dynamics. However, this constrain does not account for additional restrictions due to microphysics imposed by SM-criterion that ensures explicit Eulerian time integration scheme stability and positive definiteness. Occasional violation of SM-criterion for this time step range determines the necessity of applying "mass conservation" technique to avoid negativeness of cloud water mixing ratio that makes conditionally well-behaved EEBMPC become non-well-behaved EEBMPC (explicit Eulerian time integration scheme becomes non-stable and non-positive definite). The eventual feature of non-well-behaved EEBMPC is that it does not provide a correct numerical solution for governing differential equations.

It is conventionally thought that WRF can be applied for a broad range of spatial scales from large eddy up to global scale simulations. However, in a prospective WRF run on regional or global scale, a time step chosen according to recommendation provided in User Guide can cause occasional violations of SM-criterion at different times, altitudes, and spatial locations. An inappropriate choice of a time step leads to unstable

GMDD
4, 1403–1434, 2011

and non-positive definite numerical solution for the governing differential equations and degradation of the ability of WRF to calculate precipitation amount and its spatial and temporal distribution. By introducing a concept of SM-criterion vertical profile we provide a simple yet powerful tool that permits a rough estimation of an additional limitation imposed on time step by microphysics and an appropriate choice of a time step for WRF simulations.

We highlight that utilization of "mass conservation" technique applied to warm rain processes in explicit Eulerian time integration framework is an incorrect attempt to avoid negativeness of cloud water mixing ratio. Additionally, this technique does not eliminate numerical instability that may arise if relatively long time steps are used. However, the most important issue is that the "mass conservation" approach is conceptually incorrect because it relies on assumption that "reduced" with respect to "original" autoconversion and accretion growth rates act during given time step, but this assumption contradicts a general rule used for derivation of explicit Eulerian finite-different representation for governing differential equations. In explicit Eulerian scheme for warm rain equations "original" growth rates are known constants calculated at the beginning of each time step and can not be changed.

Our analysis shows that source code implementation of single moment (TAO, THOMPSON, and WSM6) schemes and double-moment MORRISON scheme with prognostic treatment of precipitating hydrometeors in WRF use "mass conservation" technique and belong to conditionally well-behaved EEBMPC class if used for cloud-resolving or large-eddy simulations, but they can become non-well-behaved EEBMPC for regional and large scale simulations. Additional artificial manipulations used to keep positive concentration in two-moment BLK scheme in CAM (Morrison and Gettelman, 2008) and MORRISON scheme in WRF, as well as in some other double-moment WRF BLK schemes (e.g., Lim and Hong, 2010) decrease creditability of these schemes as well as their ability to represent warm rain processes in clouds.

It should be noted that one of the most important aspects of numerical modeling is solving governing differential equations using appropriate numerical methods. If

GMDD
4, 1403–1434, 2011

governing differential equation are used, it is obvious that milestones of applied mathematics in general and the theory of finite-difference schemes (TFDS) in particular, developed in the past and under development nowadays, should not be violated. The TFDS is a branch of science that provides definitions for stability and positive definiteness of finite-difference schemes (among many others). Our analysis of EEBMPCs in CAM and GFDL AM3 GCM reveals that these extremely important issues are not recognized as essential and crucial. For example, both CAM (Gettelman et al., 2008) and GFDL AM3 GCM (Salzmann et al., 2010) utilize diagnostic equations for precipitating hydrometeors, but numerical treatment of cloud water remains similar to that used in EEBMPC with prognostic equations, which is discussed above. Additionally, both codes use a mechanistic approach that is utilization of equal time substeps because long time steps are used for the host model integration. A remarkable feature of these codes is that as a minimum two substeps are used even if stability and positiveness condition is occasionally satisfied. It makes this approach extremely computationally inefficient. Moreover, even in a case of a few substeps, stability and positive definiteness conditions (SM-criterion) can be violated at different times, altitudes, and spatial locations, and necessity to apply "mass conservation" to "correct" negative hydrometeors' mixing ratios results in highly uncertain calculations of temporal and spacial patterns of accumulated precipitation.

Treatment of precipitation formation processes in the non-well-behaved EEBMPC in CAM and GFDL AM3 GCM influences the global water cycle providing artificial precipitation patterns that are in turn used as surface boundary conditions for ocean, land, lake, and sea ice model. In fact, numerics in double-moment bulk microphysics scheme (Morrison and Gettelman, 2008) in CAM and GFDL AM3 GCM acts as a hidden climate forcing agent on a global scale.

Despite the fact that our analysis is focused on warm rain processes, we highlight that inclusion of ice phase into consideration makes SM-criterion even more restrictive because additional solid hydrometeors compete for available cloud water.

GMDD
4, 1403–1434, 2011

In our forthcoming paper we will describe positive definite mass conserving Adaptive SubStepping (ADSS) time integration scheme suitable for use in bulk microphysics scheme implemented in atmospheric models of different scales.

It should be clear that our analysis is focused on numerics of bulk microphysics schemes, e.g. stability and positive definiteness of finite-difference explicit Eulerian scheme used to advanced governing differential microphysical equations for warm rain process used in Community models. However, even if governing differential equations can be solved using stable and positive definite finite-difference scheme we would highlight the necessity to reevaluate validity of utilization of relatively long time steps in bulk microphysics schemes because of non-linear dependence of the growth rates of microphysical process on cloud characteristics. It is difficult to expect that linearization of these growth rates remains valid for periods of time significantly longer than time steps routinely used in cloud-resolving models.

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GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

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GMDD

4, 1403–1434, 2011

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GMDD

4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

Table 1. Maximal time steps permitted to keep explicit Eulerian time integration scheme stable and positive definite for autoconversion, accretion, and due to both processes in CAM and WRF bulk microphysics schemes. For comparison, the same values for Beheng (1994), Seifert and Beheng (2001), and Seifert and Beheng (2006) parameterizations are presented in gray. Maximal time steps shown for $Q_c = 1.0\,\mathrm{g\,kg^{-1}}$, $Q_r = 0.5\,\mathrm{g\,kg^{-1}}$, $N_c = 10(100)\,\mathrm{cm^{-3}}$.

	Time step, s		
SCHEME	AUTOCONVERSION	ACCRETION	EFFECTIVE
RaschCAM	487(1050)	375(375)	212(277)
KESSLER	1000(1000)	351(351)	260(260)
LIN	1000(1000)	418(418)	295(295)
TAO	208(208)	418(418)	139(139)
THOMPSON	133(105e2)	315(321)	93(312)
MORRISON	1174(724e2)	263(263)	215(262)
WSM6	660(1423)	418(418)	256(323)
BEHENG	36(381e2)	333(333)	33(330)
SIEFERT	161(161e2)	348(348)	110(341)
SIEFERTnew	492(492e2)	381(381)	215(378)

GMDD
4, 1403–1434, 2011

I. Sednev and S. Menon

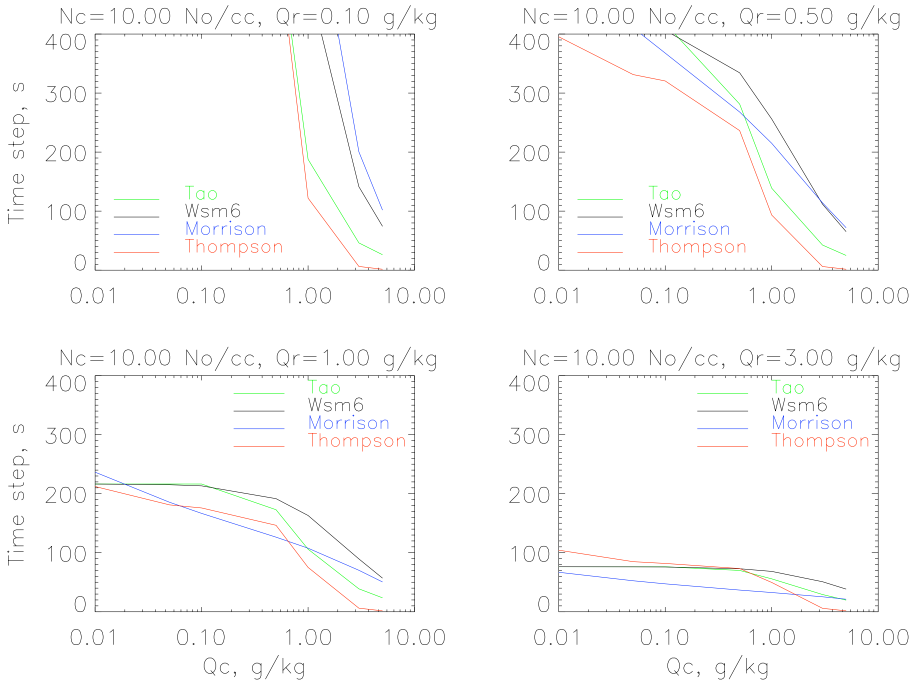

Fig. 1. Maximal time step dependence on Q_c and Q_r for $N_c = 10\ \mathrm{cm}^{-3}$.

GMDD
4, 1403–1434, 2011

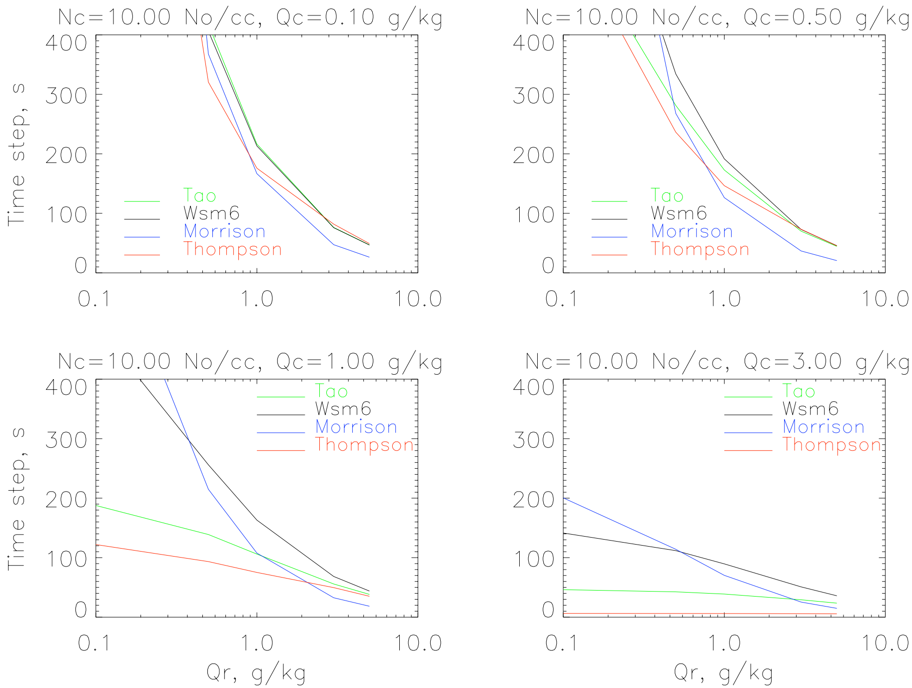

Fig. 2. Maximal time step dependence on Q_r and Q_c for $N_c = 10\ \mathrm{cm}^{-3}$.

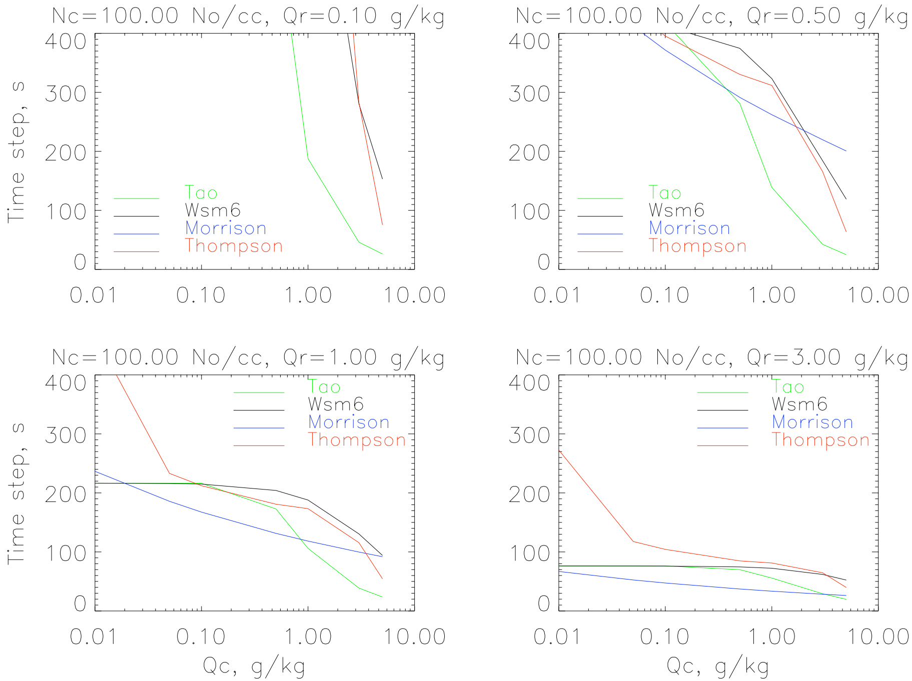

Fig. 3. Maximal time step dependence on Q_c and Q_r for $N_c = 100\ \mathrm{cm}^{-3}$.

GMDD
4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

Title Page
Abstract | Introduction
Conclusions | References
Tables | Figures
◀| |▶
◀ ▶
Back | Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion

GMDD
4, 1403–1434, 2011

Analyzing numerics of bulk microphysics schemes

I. Sednev and S. Menon

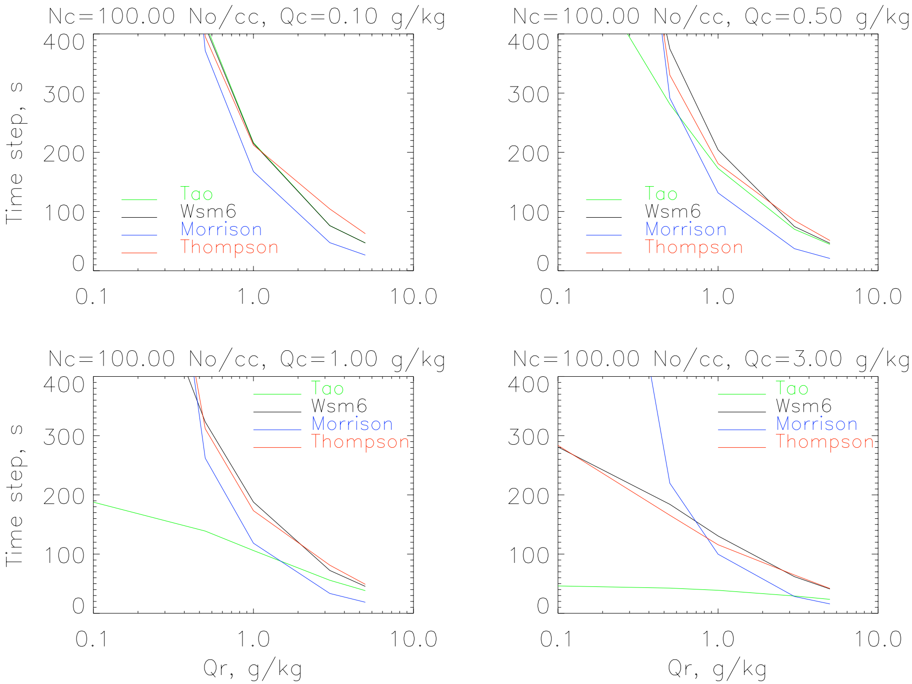

Fig. 4. Maximal time step dependence on Q_r and Q_c for $N_c = 100\ cm^{-3}$.