Numerical solution of the Stochastic Collection Equation – Comparison of the Linear Discrete Method and the Method of Moments

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Abstract

The Linear Discrete Method (LDM; SIMMEL 2000; SIMMEL ET AL. 2000) is used to solve the Stochastic Collection Equation (SCE) numerically. Comparisons are made to the Method of Moments (MOM; TZIVION ET AL. 1999) which is suggested as a reference for numerical solutions of the SCE.

Simulations for both methods are shown for the GOLOVIN kernel (for which an analytical solution is available) and the hydrodynamic kernel after LONG (1974) as it is used by TZIVION ET AL. (1999). Different bin resolutions are investigated and the simulation times are compared. In addition, LDM simulations using the hydrodynamic kernel after BÖHM (1992b) are presented.

The results show that for the GOLOVIN kernel, LDM is slightly closer to the analytic solution than MOM. For the LONG kernel, the low resolution results of LDM and MOM are of similar quality compared to the reference solution. For the BÖHM kernel, only LDM simulations were carried out which show good correspondence between low and high resolution results.

Numerische Lösung der Gleichung für stochastisches Einsammeln – Vergleich der linearen diskreten Methode und der Methode der Momente

Zusammenfassung

Die lineare diskrete Methode (LDM; SIMMEL 2000; SIMMEL ET AL. 2000) wird dazu benutzt, die Gleichung für stochastisches Einsammeln (stochastic collection equation, SCE) numerisch zu lösen. Dabei werden Vergleiche gezogen zur Methode der Momente (Method of Moments, MOM; TZIVION ET AL. 1999), die als Referenz für numerische Lösungen der SCE vorgeschlagen wurde.

Simulationsrechnungen für beide Methoden werden für die Koaleszenzfunktion nach GOLOVIN (für die eine analytische Lösung existiert) und die hydrodynamische Koaleszenzfunktion nach LONG (1974) wie sie von TZIVION ET AL. (1999) verwendet wird, gezeigt. Verschiedene Klassenauflösungen werden untersucht und die Simulationszeiten verglichen. Zusätzlich werden LDM-Simulationen mit der hydrodynamischen Koaleszenzfunktion nach BÖHM (1992b) gezeigt.

Die Ergebnisse für die Koaleszenzfunktion nach GOLOVIN zeigen, daß die LDM der analytischen Lösung etwas näher kommt als MOM. Für die Koaleszenzfunktion nach LONG sind die Ergebnisse von LDM und MOM mit niedriger Auflösung von ähnlicher Qualität verglichen mit der Referenzlösung. Für die Koaleszenzfunktion nach BÖHM wurden nur Simulationen mit der LDM durchgeführt, die eine gute Übereinstimmung der Ergebnisse mit niedriger und hoher Auflösung zeigen.

1 Introduction

Collision and coalescence are important processes in cloud microphysics. They provide the major reason for cloud droplets to grow to rain drops. In bulk models, these processes are parameterized, whereas spectral or bin models are able to solve the governing equation, the stochastic collection equation (SCE), explicitly.

In literature there are various contributions to the numerical solution of the SCE (e. g., Kovetz and Olund 1969; Bleck 1970; Berry and Reinhardt 1974; Bott 1998; Tzivion et al. 1999). In addition, mathematical kernels were found, for which the SCE can be solved analytically (Golovin 1963; Scott 1968) when certain initial conditions are fulfilled. These analytical solutions are important for the evaluation of the different numerical schemes used in models.

For the hydrodynamic kernel, analytical solutions are not available. Therefore, theoretical considerations and comparisons between different numerical models are a good chance to evaluate the various methods. The high resolution solutions obtained by the Method of Moments (MOM) can be used as reference. This was proposed by Tzivion et al. (1999).

2 Equation for the moments

The coalescence process is described by the SCE (e. g. Pruppacher and Klett 1997). It can be written in the form

$$\begin{aligned}\frac{\partial n(x,t)}{\partial t} &= \frac{1}{2}\int_0^x n(x-y,t)n(y,t)K(x-y,y)dy \qquad (1)\\ &\quad -n(x,t)\int_0^\infty n(y,t)K(x,y)dy\end{aligned}$$

where $n(x,t)dx$ is the number of drops in the interval $[x, x+dx]$, measured per unit volume at time t and $K(x,y)$ is the collection kernel. A single drop of mass x belongs to bin k if

$$x_k \leq x < x_{k+1} \qquad (2)$$

with $x_{k+1} = px_k$ and $p = const > 1$. In the simulations presented $p = 2, 2^{1/2}, 2^{1/3}, 2^{1/4}$ and $x_1 = \frac{4}{3}\pi r_1^3 \rho_l$ with $r_1 = 1.5625$ μm and $\rho_l = 1000$ kg m^{-3} are used. The lth moment of the distribution function $n(x,t)$ in bin k is defined as

$$M_k^l = \int_{x_k}^{x_{k+1}} x^l n(x,t)dx \qquad (3)$$

After multiplying (1) with x^l and integrating over each bin k, a set of prognostic equations for the moments in each bin k is obtained:

$$\begin{aligned}\frac{dM_k^l(t)}{dt} &= \frac{1}{2}\int_{x_k}^{x_{k+1}}\int_{x_1}^{x} n(x-y,t)n(y,t)K(x-y,y)dy \qquad (4)\\ &\quad -\sum_{j=1}^{J_{MAX}}\int_{x_k}^{x_{k+1}} x^l n(x,t)dx\int_{x_j}^{x_{j+1}} n(y,t)K(x,y)dy\end{aligned}$$

with J_{Max} being the number of bins defined (36, 72, 108, 144 here). The first term on the right-hand side describes the gain of bin k due to collisions that result in drops belonging to bin k (gain term). The second term describes the loss of bin k caused by the collision of a drop of bin k with another drop (loss term). This set of equations is solved

case	golo1	golo3	long1	long3	böhm1	böhm3
M_0 (g/m^3)	1	3	1	3	1	3
x_0 (kg)	$3.33 \cdot 10^{-12}$	10^{-11}	$3.33 \cdot 10^{-12}$	10^{-11}	$3.33 \cdot 10^{-12}$	10^{-11}
kernel	GOLOVIN	GOLOVIN	LONG	LONG	BÖHM	BÖHM
time (min.)	20, 40	10, 15	20, 40	10, 15	20, 40	10, 15

Table 1: *Overview of all cases chosen. Two different initial distributions are combined with three kernels. For each case, several runs with different methods (MOM, LDM) and varying resolution are performed.*

numerically by the Linear Discrete Method (LDM; SIMMEL 2000; SIMMEL ET AL. 2000). The results are compared to the established and accurate MOM (TZIVION ET AL. 1987, 1999). For further information about the numerical methods used the reader is referred to the literature cited above.

3 Results and discussion

We present simulations using the numerical methods mentioned in the previous section. We conducted simulations for different resolutions ($p = 2$, $p = 2^{1/2}$, $p = 2^{1/3}$, and $p = 2^{1/4}$) for the GOLOVIN kernel (GOLOVIN 1963) and for the hydrodynamic kernels after LONG (1974) and BÖHM (1992b), respectively. As initial distribution we use the same exponential function as TZIVION ET AL. (1987, 1999)

$$n(x) = 4\frac{N_0 x}{x_0^2}\exp[-2x/x_0] \qquad , \tag{5}$$

with $N_0 = 3 \cdot 10^8$ m^{-3} and either $x_0 = 3.33 \cdot 10^{-12}$ kg or $x_0 = 10^{-11}$ kg (see Table 1). This corresponds to liquid water contents of 1 g m^{-3} and 3 g m^{-3}, respectively. Table 1 gives an overview over all runs performed and the parameters used. For all runs the water mass is conserved (except numerical inaccuracies).

3.1 Golovin kernel

Using the GOLOVIN kernel, the SCE can be solved analytically for various initial distributions (GOLOVIN 1963, SCOTT 1968). The GOLOVIN or "sum of mass" kernel is given as

$$K(x, y) = b(x + y) \tag{6}$$

with $b = 1.5$ m^3 s^{-1} kg^{-1} and x, y the mass of the colliding drops. Out of all kernels for which an analytical solution of the SCE is known, the GOLOVIN kernel is closest to the hydrodynamical kernel and therefore is a good test for the numerical method used.

Results Figure 1 shows the good correspondence of the numerical LDM simulations for all resolutions with the analytical solution. `golo1` is on the left, `golo3` on the right. As expected, numerical solutions are closer to the analytical solution for higher resolution in both cases, but even for 36 bins, the LDM solution is pretty good.

Figure 2 compares the mass distribution function for LDM and MOM with 72 bins each to the analytical solution. LDM is closer to the analytical solution than MOM for both cases (`golo1` on the left and `golo3` on the right), but generally, they are in good agreement with the analytical solution. The drop growth tends to be overestimated by both methods for the GOLOVIN kernel.

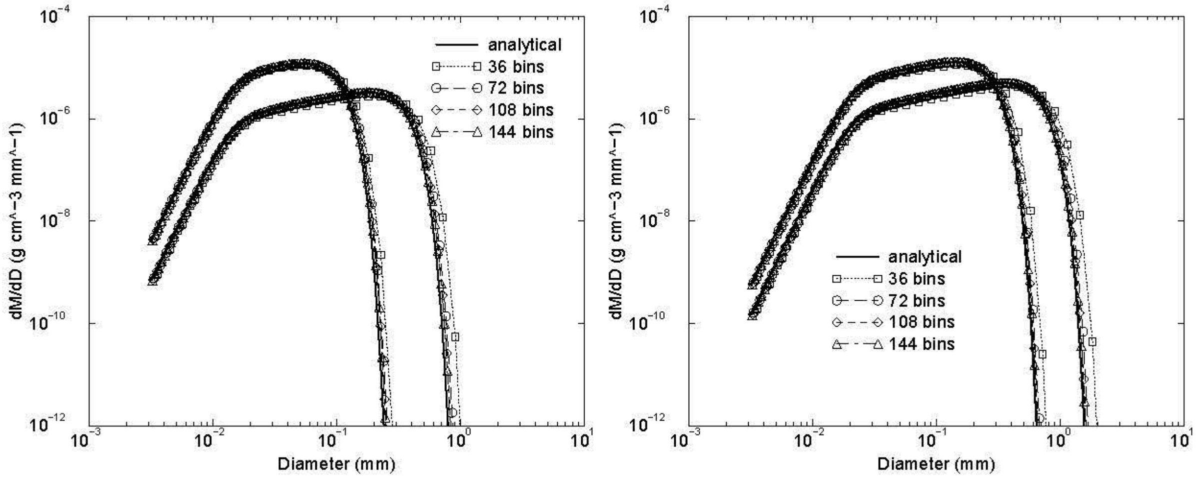

Figure 1: *Mass distribution for the* GOLOVIN *kernel using LDM with different resolutions compared to the analytical solution. Results are shown for the* `golo1` *(left) and* `golo3` *(right) cases, time step was 1 s.*

3.2 Hydrodynamic kernel

The hydrodynamic kernel of two interacting drops with masses x and y and radii r_x and r_y, respectively, is defined as

$$K(x, y) = \pi(r_x + r_y)^2 E(x, y)|v_x - v_y| \tag{7}$$

with the terminal fall velocities v_x and v_y and the collection efficiency $E(x, y)$, given as

$$E(x, y) = E_{coll}(x, y)E_{coal}(x, y) \quad . \tag{8}$$

Here, $E_{coll}(x, y)$ is the collision efficiency and $E_{coal}(x, y)$ the coalescence efficiency. In literature, different data from observations and theoretical investigations can be found. We choose one kernel after LONG (1974) and one after BÖHM (1992b). Using the first one, we can compare our results with those of TZIVION ET AL. (1999). The second one based more on theoretical considerations using boundary layer theory. It is valid

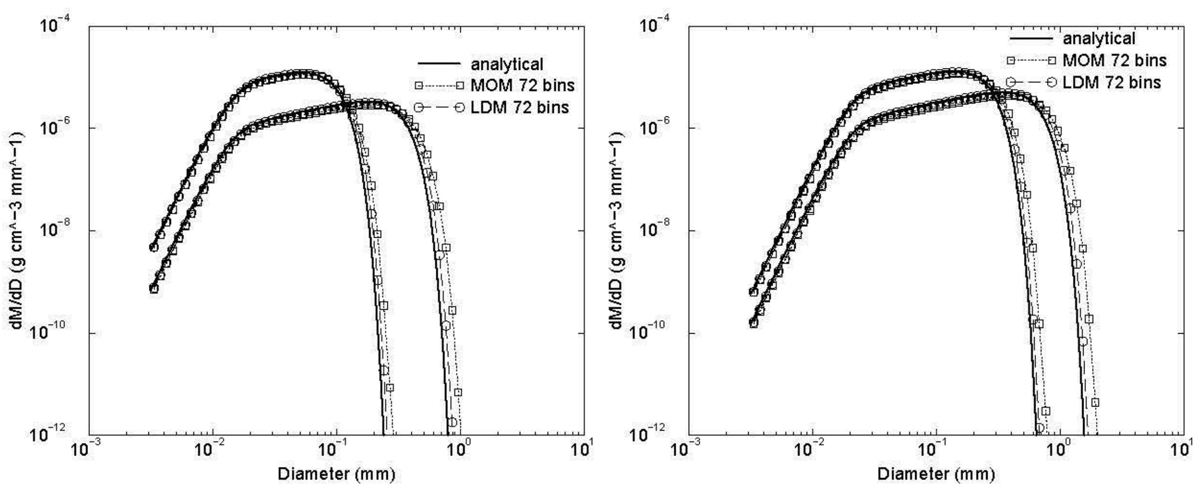

Figure 2: *Mass distribution for the* GOLOVIN *kernel using LDM and MOM with* $p = 2^{1/2}$ *compared to the analytical solution. Results are shown for the* `golo1` *(left) and* `golo3` *(right) cases, time step was 1 s.*

Diameter d_x (in μm)	α	β
< 79.37	$4.5795 \cdot 10^5$	$2/3$
79.37–800	$4.962 \cdot 10^3$	$1/3$
800–4031.74	$1.732 \cdot 10^3$	$1/6$
> 4031.74	$9.17 \cdot 10^2$	0

Table 2: *Coefficients for the velocity calculation following eq. (10).*

for hydrometeors that are regarded as porous spheroids moving in the orientation which offers the maximum drag to motion (BÖHM 1992a). The particles are described by four parameters: particle mass, semi axis of symmetry, equatorial radius, and the ratio of the effective over the circumscribed cross-sectional area. Therefore, the BÖHM theory can be applied not only to water drops but as well to different shapes of ice particles. This would lead to different kernels for the interaction of ice particles with drops or other ice particles.

3.2.1 Long kernel

The collision efficiency is approximated by

$$E_{coll}(x,y) = \begin{cases} 0 & \text{for} \quad r_x \leq 3\mu\text{m} \\ 1 & \text{for} \quad r_y \geq 50\mu\text{m} \\ 4.5 \cdot 10^4 r_y^2 (1 - 3 \cdot 10^{-4}/r_x) & \text{else} \end{cases} \tag{9}$$

The coalescence efficiency is assumed to be unity ($E_{coal}(x,y) = 1$). The collection kernel is calculated via eqs. (7) and (8) with the terminal velocity

$$v_x = \alpha x^\beta \tag{10}$$

using the coefficients α and β of Table 2. For all calculations concerning the LONG kernel cgs-units have to be used.

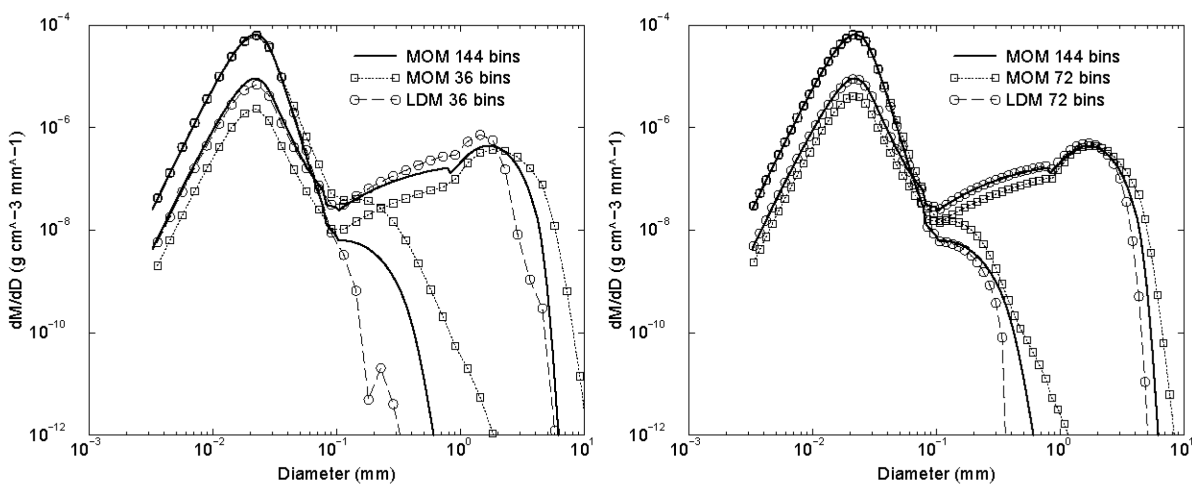

Figure 3: *Mass distribution for the* LONG *kernel using LDM and MOM with $p = 2$ (left) and $p = 2^{1/2}$ (right) compared to the reference solution (MOM with $p = 2^{1/4}$). Results are shown for the* `long1` *case, time step was 1 s.*

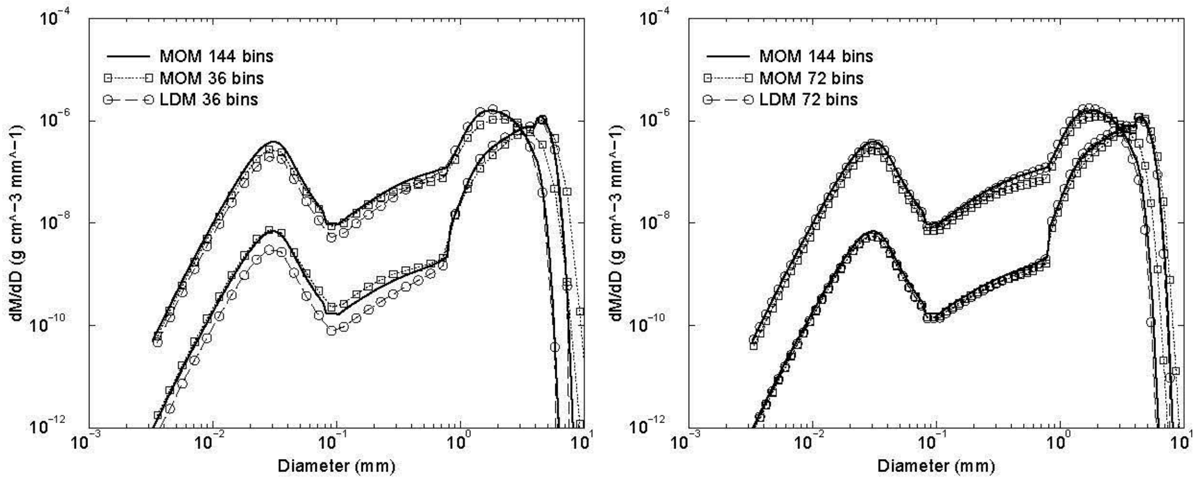

Figure 4: *Mass distribution for the* LONG *kernel using LDM and MOM with $p = 2$ (left) and $p = 2^{1/2}$ (right) compared to the reference solution (MOM with $p = 2^{1/4}$). Results are shown for the* `long3` *case, time step was 1 s.*

For the hydrodynamic kernel an analytic solution does not exist. Therefore, we use the MOM-solution with 144 bins ($p = 2^{1/4}$) as reference solution as it is proposed by TZIVION ET AL. (1999).

Results Figure 3 shows the results for `long1` using MOM and LDM with $p = 2$ (left) and $p = 2^{1/2}$ (right) compared to the reference solution. For both resolutions, MOM tends to overestimate the growth, whereas LDM seems to underestimate the mass of the larger drops.

Figure 4 is the same but for `long3`. The deviations for `long3` are much smaller than for `long1`. Possibly, both numerical methods are not so sensitive to variations of the kernel for larger drops. The shorter overall integration time of `long3` is not the reason. The results are more accurate when the distributions are shifted to larger drops (compare 20 min. to 40 min. for `long1` and 10 min. to 15 min. for `long3`).

Compared to the GOLOVIN kernel, the errors for the hydrodynamic kernel are larger for both initial distributions and all resolutions. Nevertheless, we can state that if a model shows good results for the GOLOVIN kernel it will give good results for the hydrodynamic kernel as well.

3.2.2 Böhm kernel

The hydrodynamic kernel after BÖHM (1992b) is a semiempirical solution based on boundary-layer theory. It is in good agreement with measured coalescence efficiencies and other theories (Stokes', modified Oseen, superposition method). For drops of equal size and terminal velocity, non-vanishing kernels are predicted.

Results Figure 5 shows the results for the cases `böhm1` and `böhm3` for different resolutions using LDM. Only a slight retardation can be seen for low resolutions compared to the 144 bin-solution. Especially for `böhm3`, the results for the different resolutions are very close to each other. This supports the assumption that the growth process can be predicted more accurate for larger drops.

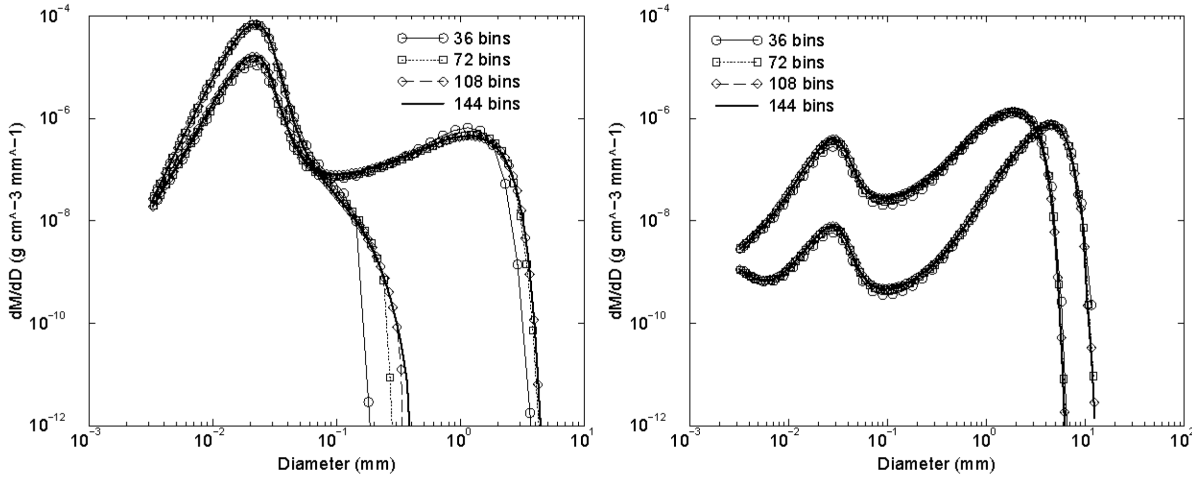

Figure 5: *Mass distribution for the* Böhm *kernel using LDM with different resolutions for the cases* `böhm1` *(left) and* `böhm3` *(right) with the averaging procedure. Time step was 1 s.*

3.3 Computation times

Table 3 shows the computation times for the runs with the Golovin (`golo1` and `golo3`) and the Long (`long1` and `long3`) kernel. Figure 6 shows the same for the `long1` and `golo1` cases on the left and the `golo3` and `long3` cases on the right. For high resolutions ($p = 2^{1/3}$, $p = 2^{1/4}$), LDM is much faster than MOM, whereas for low resolutions ($p = 2$), LDM seems to be somewhat slower, depending on the case. For MOM, `golo1` and `long1` need almost the same computation time, as well as `golo3` and `long3`. For LDM, the Golovin cases are faster than the corresponding Long cases (`golo1` vs. `long1` and `golo3` vs. `long3`).

Generally, empty bins are not taken into account to save computation time. Therefore, underestimation of the growth saves computation time whereas overestimation leads to longer computation times. These effects should be negligible.

4 Conclusions

A new spectral model LDM for a numerical solution of the SCE was compared to the well-known MOM whose 144-bin numerical solution was proposed as a reference for the numerical solution of the SCE.

For different kernels, simulations with varying resolution were carried out. For the Golovin kernel, the results were compared to the analytical solution, too. For the hydrodynamic kernel, no analytical solution is available. For the Böhm kernel, the solutions

	$p = 2$		$p = 2^{1/2}$		$p = 2^{1/3}$		$p = 2^{1/4}$	
	MOM	LDM	MOM	LDM	MOM	LDM	MOM	LDM
`golo1`	2.62 s	2.46 s	22.28 s	9.57 s	63.28 s	20.18 s	159.18 s	36.81 s
`golo3`	1.04 s	1.59 s	7.79 s	4.60 s	22.76 s	11.82 s	62.10 s	15.63 s
`long1`	2.54 s	4.61 s	22.32 s	17.98 s	62.02 s	37.44 s	169.53 s	57.88 s
`long3`	1.00 s	2.68 s	7.85 s	7.45 s	21.75 s	16.33 s	60.19 s	27.06 s

Table 3: *Run times of the runs performed on an IBM RS6000. For* `golo1` *and* `long1` *the integration time was 40 min., for* `golo3` *and* `long3` *it was 15 min.*

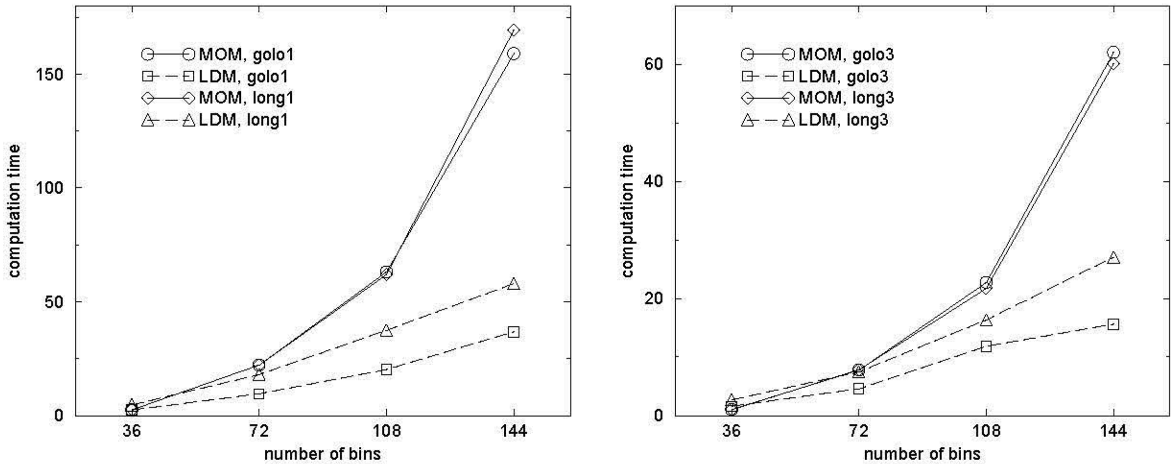

Figure 6: *Run times for the cases* `golo1` *and* `long1` *on the left and* `golo3` *and* `long3` *on the right for MOM (solid line) and LDM (dashed line).*

using different resolution are very close to each other which means that LDM gives good results even when using low resolution.

Especially for high resolutions, LDM needs less computation time than MOM without being less accurate. Considering both, accuracy and integration time, LDM is a good choice for the numerical solution of the SCE and therefore, for a spectral model.

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