MODELING OF CLOUD MICROPHYSICS
Can We Do Better?

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Clouds are large ensembles of water droplets and/or ice crystals that from a distance seem suspended in the air. They typically form due to vertical air motion that leads to expansion and cooling. Latent heating associated with phase changes of the water substance (i.e., condensation, sublimation, and freezing) is a key element of cloud dynamics. Cycling of energy, water, and chemical species through Earth’s atmosphere is critically affected by the presence of clouds and accurate representation of clouds in numerical models of atmospheric flows is of paramount importance.

Atmospheric flows encompass an enormous range of scales, from the subcentimeter scale of atmospheric turbulence to nearly planetary-scale Hadley and Walker circulations in the tropics and synoptic weather systems in midlatitudes. Because of this range, incorporation of clouds and cloud processes in numerical models of atmospheric dynamics involves significant challenges. Small-scale models aim at representing clouds explicitly by coupling cloud and precipitation microphysical processes to the model-predicted cloud-scale flow. This allows the cloud and precipitation processes to directly affect buoyant circulations that are the key to cloud dynamics. Such models have been used in cloud physics research for the past 50 years (e.g., Ogura 1963; Orville 1965; Schlesinger 1975; Tapp and White 1976; Klemp and Wilhelmson 1978; Clark 1979; Lipps and Hemler 1982). Until about 20 years ago, weather and climate models were incapable of including clouds explicitly because the horizontal grid length of these models was much too coarse to resolve them. However, with steadily increasing computational power, it is now feasible to use cloud-scale models for simulating...
weather and climate. This is done either by a brute-force approach with global models applying horizontal grid lengths on the order of a few kilometers (e.g., Satoh et al. 2014 and references therein; see also http://nicam.jp/hiki) or by applying the so-called superparameterization approach (Grabowski and Smolarkiewicz 1999; Grabowski 2001; Khairoutdinov and Randall 2001; Randall et al. 2003). Hence, as far as weather and climate are concerned, cloud processes can now be studied with much more confidence, especially from the point of view of linking cloud-scale processes to large-scale atmospheric circulations (e.g., Bony et al. 2015).

The purpose of this paper is twofold. First, we review the progress of using increasingly sophisticated approaches to simulate cloud microphysics, focusing on cloud-scale models. We argue that continuing on this path brings significant challenges owing to numerical aspects and conceptual problems that are difficult to overcome. Second, we advocate an alternative approach to microphysical modeling that is gaining popularity in small-scale cloud models. We argue that this emerging approach deserves serious consideration for larger-scale models as well. The essence of this approach is to replace the standard Eulerian density-like variables for cloud and precipitation fields with a probabilistic Lagrangian approach that applies point particles to represent the formation, growth, and fallout of cloud droplets, raindrops, and ice particles.

The next section briefly reviews the evolution of microphysics scheme complexity in cloud-scale models, from simple bulk approaches to the most comprehensive bin (spectral) microphysics schemes, which are often considered the ultimate approach and are used as a “benchmark” for developing and testing simpler schemes. However, as discussed in the section on bin microphysics, there are significant issues concerning the bin approach that challenge this view. As an alternative, the section on the particle-based Lagrangian approach explains the benefits of this methodology. Prospects for expanding current applications of the Lagrangian method to more complex cloud systems are reviewed. A brief summary concludes the paper.

**EVOLUTION OF THE CLOUD MICROPHYSICS MODELING.** The growth of individual cloud and precipitation particles involves processes at subcentimeter scales, typically referred to as the cloud microscale. For instance, diffusional growth of a cloud droplet is driven by the molecular diffusion of water vapor and thermal energy between the droplet and its immediate environment. It follows that direct numerical simulation (DNS) is the only approach capable of explicitly simulating the growth of individual cloud particles in a turbulent cloud. DNS solves the Navier–Stokes equations and represents dissipative processes by using molecular transport coefficients. This requires grid lengths as small as the Kolmogorov length scale, on the order of 1 mm in Earth’s atmosphere. Hence, DNS allows computational domains of only a few cubic meters at most. Because of this limitation, DNS studies simulating individual cloud particles have focused on the impacts of small-scale turbulence on diffusional and collisional growth of cloud droplets [see the review of Grabowski and Wang (2013)].

Models with coarser grids cannot represent individual cloud and precipitation particles because of their sheer number. For instance, 1 m$^3$ of cloudy air typically contains several tens of millions to a few billion cloud droplets. Thus, even high-resolution atmospheric models with grid lengths between a few to a few tens of meters, so-called large-eddy simulation (LES) models, predict selected features of the droplet population only within a grid cell (e.g., the size distribution). LES models have been applied in the past to cloud modeling (e.g., Grabowski and Clark 1993; Carpenter et al. 1998; Brown et al. 2002; Siebesma et al. 2003; Stevens et al. 2005) and more recently deep convective clouds (e.g., Bryan et al. 2003; Khairoutdinov et al. 2009; Lebo and Morrison 2015). The entire premise of the LES approach is that the mean features of the turbulent flow are determined by the behavior of large (energy containing) scales of motion, typically tens to hundreds of meters in the atmosphere, with smaller scales (down to the cloud microscale) slaved to the large eddies. Although such models typically feature quite sophisticated and physically well-posed subgrid-scale schemes to represent the impact of unresolved flow on the dynamics and transport, the effects of unresolved flow features on the growth of cloud particles are typically not considered. Cloud-system-resolving models (CSRMs), often called convection-permitting models, feature coarser horizontal grid lengths of 1–5 km but are still small enough so that the cloud buoyancy and nonhydrostatic pressure perturbations directly drive the model-resolved cloud-scale flow. Convection-permitting models are now commonly used for numerical weather prediction (NWP) and the sensitivity of forecasts to the representation of cloud microphysics in these models is well appreciated (e.g., Weisman et al. 2008; Lean et al. 2008; Clark et al. 2012; Stein et al. 2015).
Currently, most atmospheric models apply an Eulerian approach for the cloud and thermodynamic variables, not only for the temperature and water vapor, but also for cloud condensate and precipitation that in reality occur as sparsely distributed populations of drops and ice particles. The variables used are densities (i.e., total mass of particles per unit volume of air) or more often mixing ratios, the mass of particles per unit mass of dry air. This methodology has been the workhorse of cloud-scale modeling from its early days (e.g., Kessler 1969; Liu and Orville 1969; Murray 1970; Schlesinger 1973; Klemp and Wilhelmson 1978; Clark 1979). It is also the approach used in global and limited-area models for numerical weather prediction as well as in climate models.

The sophistication of microphysics parameterizations has been steadily increasing over the past several decades, which has been possible because of increasing computational resources. Figure 1 provides a schematic of various Eulerian approaches to represent cloud and precipitation microphysics in cloud-scale and mesoscale models. Early schemes in such models (e.g., Klemp and Wilhelmson 1978) adopted separate continuity equations for bulk cloud water and rain mass mixing ratios, based on the pioneering work of Kessler (1969). This approach was extended to include the ice phase in the 1980s, which added continuity equations for the bulk cloud and precipitating ice mass mixing ratios (e.g., Lin et al. 1983; Rutledge and Hobbs 1984). Many of these bulk schemes included two or more ice categories (e.g., cloud ice, snow, graupel, hail) to represent the wide variety of ice particle types that occur in nature. Conversion processes between the various ice categories were treated analogously to conversion between cloud and rain in the Kessler approach. In the past few decades multimoment bulk schemes (e.g., Ziegler 1985; Ferrier 1994; Milbrandt and Yau 2005) that evolve number and/or other distribution moments in addition to mass have come into wide use in both research and operational modeling. This includes schemes with several prognostic variables to smoothly represent the evolution of ice particle properties (Chen and Lamb 1994; Morrison and Grabowski 2008; Harrington et al. 2013; Morrison and Milbrandt 2015; Jensen et al. 2017).

The development of spectral bin microphysics schemes occurred during the 1960s and 1970s. Bin schemes predict the particle distributions on an Eulerian size or mass grid and, hence, explicitly evolve the distribution shape. Early development of bin schemes (e.g., Berry 1967; Bleck 1970; Clark 1973; Berry and Reinhardt 1974a,b,c) focused on methods for solving the kinetic equations for liquid drop growth by

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**Fig. 1.** General diagram of the increasing complexity of Eulerian microphysics schemes. Single-moment bulk microphysical schemes predict only mass mixing ratios q of various cloud and precipitation categories (cloud water, rain, cloud ice, snow, graupel). Double-moment bulk schemes predict the corresponding number mixing ratio N that together with q allows for the estimation of the mean particle size. Bin microphysical schemes represent a size distribution of each category as shown. If additional detail is needed (e.g., chemical composition of drops due to CCN, or ice crystal habits), then 2D (or even more dimensional) size distributions are required. The figure provides a broad summary of Eulerian microphysics schemes and there are many variations of the general schematic.
condensation and collision–coalescence, the latter involving the so-called stochastic collection equation (SCE). The SCE describes the evolution of the drop size distribution due to collisions between drops of different sizes, and in its generic form it is known as the Smoluchowski equation (Smoluchowski 1916).

As we argue below, numerical implementation continues to be a critical issue for bin schemes. Bin schemes have fewer assumptions than bulk schemes but apply several dozens of prognostic variables to represent the evolution of the size distributions and are thus at least an order of magnitude more computationally costly. Because of the cost, early work in the 1960s through the 1980s used bin schemes within idealized frameworks to study the evolution of drop size distributions (e.g., Berry and Reinhardt 1974a,b,c; Tzivion et al. 1989). With increasing computer power, studies since the early 1990s have used bin schemes coupled to two-dimensional and three-dimensional dynamical cloud models (e.g., Kogan 1991; Reisin et al. 1996; Stevens et al. 1998).

Another focus has been the inclusion of ice microphysics in bin schemes. The representation of various ice particle types is generally similar to bulk schemes; that is, it involves evolving size distributions for different categories (e.g., ice, graupel, hail; Fig. 1). Transfer of mass/number between categories—for example, from snow to graupel during riming—requires conversion processes similar to bulk schemes, which are an important source of uncertainty.

As computational power continues to increase, bin schemes have correspondingly become more complex by including more hydrometeor categories and increased Eulerian size or mass bin resolution with more prognostic variables, as well as additional process details. These schemes are now commonly employed within three-dimensional cloud models for simulating a variety of cloud regimes (e.g., Khain et al. 2015). Bin schemes have also been used as a “benchmark” for developing and testing the bulk schemes that remain the workhorses of climate and weather prediction models. Overall, these trends may suggest bin schemes are the ultimate approach to cloud microphysics and will converge toward the “truth” as they are further refined and developed. However, there are some conceptual and practical aspects that suggest otherwise, as detailed in the next section.

**IS BIN MICROPHYSICS THE ULTIMATE APPROACH?** Bin microphysics schemes explicitly model the evolution of particle size or mass distributions from various microphysical processes. Thus, it is generally accepted that bin schemes provide a more accurate, though computationally more expensive, means to simulate cloud and precipitation processes (e.g., Khain et al. 2015). However, recent studies have highlighted the large spread of model results using different bin microphysics schemes as discussed below. Thus, increasing the complexity of microphysics schemes has generally not led to a convergence of model results. Two examples are presented below.

First, vanZanten et al. (2011) compared LES simulations of a liquid shallow convective cloud field observed during the Rain in Cumulus over the Ocean (RICO; Rauber et al. 2007) field project using models with several different bulk and bin schemes. Significant variations of model results (e.g., order of magnitude for the precipitation rates; see Fig. 6 therein) occurred not only for bulk schemes but, perhaps surprisingly, for bin schemes as well. Although the bin schemes in this study were run with different dynamical LES models, vanZanten et al. (2011, p. 15) interpreted “this scatter as being the result of differences in the representation of cloud microphysical processes.” For bin schemes, variation in the representation of cloud microphysics must come from either different process rate formulations (e.g., owing to different collection or breakup kernels) or different numerical implementations and/or methods for solving the bin microphysical equations. Uncertainty in process rate formulations and microphysical parameters is relevant for all microphysics scheme types (bulk, bin, and Lagrangian), and sensitivity to these formulations and parameters has been documented in several studies (e.g., Stevens and Seifert 2008; Morrison et al. 2012; Xue et al. 2017). In addition to this uncertainty, bin microphysics schemes face unique challenges owing to numerical implementation issues. This specific aspect is discussed in the following subsection.

The above issues are even more problematic for ice microphysics. First, the complexity of ice formation and growth mechanisms (e.g., the dependence on environmental conditions and/or on ice crystal shape) means that process rate formulations are especially uncertain. In particular, evolving ice particle properties (shape, density, fall speed) during depositional, aggregation, and riming growth is a major challenge. This aspect is typically treated in bin schemes (as well as bulk) by partitioning ice into predefined categories of ice/snow and graupel/hail (see the previous section). This requires formulation of unphysical conversion rates and stepwise fall velocities (i.e., changing from slowly falling ice/snow and to fast-falling graupel/hail) once ice mass is moved from one category to the other.
These problems were highlighted in the recent study of Xue et al. (2017). They presented simulations of a squall-line event from the Midlatitude Continental Convective Clouds Experiment (Jensen et al. 2016) that applied three different state-of-the-art mixed-phase bin microphysics schemes coupled to the Weather Research and Forecasting (WRF) Model. All other aspects of the model setup were identical except for the microphysics. Figure 2 shows fields of observed and model-predicted reflectivity fields. We do not include in Fig. 2 specific details of the bin schemes as they are irrelevant to our argument [see Xue et al. (2017) for details]. The main point is that the schemes represent the best approach—in the developers’ judgments—for representing the evolution of cloud and precipitation particles. All three bin schemes produced a squall line with features resembling the observed storm characteristics, that is, with a leading edge of convective precipitation and trailing stratiform rain. However, there are significant differences in the details of the simulated convective systems. Xue et al. (2017) argue that the differences mainly come from different assumptions of the microphysical processes and physical properties, especially ice particle mass, density, and terminal velocity as a function of size. A key difference is how schemes treat conversion between ice categories—for example, between ice/snow and graupel/hail associated with riming—with attendant property changes as hydrometeors are converted from one category to another. Representation of melting is yet another challenge. These differences affect interactions between the microphysics and storm dynamics. As in the liquid cloud case from vanZanten et al. (2011), different numerical implementations and methods likely contributed to the spread among the model results as well.

Overall, these studies highlight the practical challenges of developing, implementing, and applying bin schemes in models. Numerical issues unique to bin
microphysics are elaborated upon next, after which we discuss two additional issues for bin schemes: the “curse of dimensionality” problem and the limitations of applying the Smoluchowski equation solved by bin schemes.

**The effects of numerical diffusion using bin microphysics.** A key challenge in bin microphysics schemes is the numerical diffusion across size or mass bins that occurs during growth calculations (collision–coalescence and condensation). Such diffusion can lead to numerical artifacts, namely, unphysical broadening of particle size distributions. Considerable effort has been made over the past 50 years to develop numerical methods for bin microphysics that minimize these artifacts. This includes the development of two-moment methods predicting mass and number in each bin, for both collision–coalescence (e.g., Tzivion et al. 1987) and condensation (e.g., Stevens et al. 1996), as well as methods that constrain multiple moments of the particle size or mass distributions during growth calculations (e.g., Liu et al. 1997; Khain et al. 2008). Numerical methods for bin schemes have typically been evaluated within simple box or parcel model frameworks for which analytic or quasi-analytic solutions are available for comparison. The studies above and others have shown considerable sensitivity of modeled particle spectra to different numerical methods and implementation details, with more sophisticated methods generally giving results that are closer to the analytic/quasi-analytic benchmarks.

Although considerable progress has been made in addressing numerical diffusion across bins for microphysical process calculations, another key challenge for bin schemes is the numerical diffusion of microphysical variables from advection in Eulerian physical space. This aspect has received much less attention, but was recently examined in detail by Morrison et al. (2018). They investigated droplet condensational growth using bin microphysics within two dynamical frameworks: a rising parcel and 1D vertical Eulerian flow. They showed that existing state-of-the-art numerical approaches for calculating droplet condensational growth have sufficient fidelity compared to benchmark analytic solutions for a rising parcel, particularly when a large number of bins is used. However, within the Eulerian 1D framework, numerical diffusion associated with vertical advection resulted in unphysical broadening of the drop size distributions even when the growth calculations themselves had little numerical diffusion. Figure 3 summarizes the results of Morrison et al. (2018) and illustrates differences between analytical and numerical solutions using bin microphysics in Eulerian models. Figure 3 also shows how this simple problem is represented in the particle-based Lagrangian approach discussed in the next section. The key point is that even if the growth in radius space when using bin microphysics has small errors, there is still broadening of particle distributions owing to numerical diffusion from advection in physical space (note that “advection” here refers to transport from air motion as well as particle sedimentation).

**The curse of dimensionality.** Another issue is the curse of dimensionality. Most bin schemes are one-dimensional in the sense that they predict distributions that are functions of droplet size (or mass). However, this is not always sufficient. For instance, solute composition, mass, and soluble fraction within cloud droplets may be needed; these affect the growth rate of small droplets and determine the properties of residual particles after droplets evaporate completely. This also includes physical properties such as the shape and density of ice particles. These measures provide detailed cloud particle properties and are referred to as attributes. Including attributes in bin microphysics schemes in a rigorous way requires additional dimensions for the distribution function. For instance, including solute mass as an additional cloud droplet attribute results in a distribution of solute masses for every drop mass; thus, the distribution function is two-dimensional (see Fig. 1). In general, if the number of attributes is \( d \), then the bin space is \( d \) dimensional. For \( d \) larger than 2, the problem becomes computationally intractable. We refer to this unfavorable feature as the curse of dimensionality. One solution is to calculate only mean attributes within a one-dimensional bin framework (e.g., Flossmann and Wobrock 2010; Morrison and Grabowski 2010). Although computationally more efficient (the cost is roughly proportional to \( d \) rather than the number of bins to the power of \( d \)), this approach requires many simplifications and approximations.

**Limitations of the Smoluchowski equation.** Bin microphysics schemes model collision–coalescence by solving the Smoluchowski equation, which is referred to as the “stochastic collection equation” in cloud physics. However, the Smoluchowski equation is deterministic, not stochastic. In contrast, collision–coalescence of cloud droplets is a stochastic process. As a result, some cloud droplets can undergo a series of unlikely collisions that make them grow faster than the average droplet. This effect has been proposed as being important for rapid
precipitation onset (e.g., Telford 1955; Kostinski and Shaw 2005; Wilkinson 2016). Bin microphysics schemes that rely on the Smoluchowski equation can capture only some aspects of this phenomenon (e.g., Bayewitz et al. 1974). Another limitation of the Smoluchowski equation comes from the assumptions necessary to derive it from the stochastic description (e.g., Gillespie 1972). On one hand, the volume of air in which collision–coalescence takes place needs to be large because only then is there a sufficiently large number of droplets in the volume so that the discreteness of individual droplets (i.e., their specific position in space) can be neglected. On the other hand, cloud droplets have to be assumed uniformly distributed within the volume. This assumption is appropriate for small volumes, but it becomes questionable for volumes as large as LES model grids because of unresolved subgrid-scale variability. In consequence, it is unclear how large the volume of air can be to model collision–coalescence through the Smoluchowski equation [see Dziekan and Pawlowska (2017) and references therein].

In summary, although Eulerian bin schemes provide a comprehensive approach for simulating cloud microphysical processes, they face challenges difficult to overcome. The next section discusses the particle-based Lagrangian approach that not only eliminates most of the problems discussed above, but also provides additional benefits.
THE ALTERNATIVE: THE LAGRANGIAN PARTICLE-BASED APPROACH. The main idea behind the Lagrangian particle-based approach is to use a judiciously selected ensemble of Lagrangian point particles, often called superdroplets or superparticles, to represent the enormous number of aerosol, cloud, and precipitation particles typically present inside the grid cell of a cloud model. The superparticles are traced in physical space using the model-predicted flow field, and they grow or shrink as they move with the flow. Each superparticle represents a multitude of natural cloud particles and an additional parameter, the multiplicity, is used to describe the total number of real particles each superparticle represents. Figure 4 illustrates the superdroplet concept and puts it into the context of Eulerian bin approaches. Lagrangian particle-based microphysics has been gaining popularity over the last decade, starting from the pioneering works of Andrejczuk et al. (2008, 2010), Shima et al. (2009), Sölch and Kärcher (2010), and Riechelmann et al. (2012).

To illustrate the capabilities of the particle-based Lagrangian approach, we consider the classical problem of the droplet size distribution spectral width. Cloud observations show that the spectra are typically wide and often multimodal, and these features cannot be explained by growth of cloud droplets in adiabatic volumes rising from the cloud base [see references in Cooper (1989) and Lasher-Trapp et al. (2005), among many others]. Cooper (1989) argued that the key mechanism explaining the large spectral width involves droplets arriving at the same location within a turbulent cloud following different trajectories. Variability of the supersaturation along these trajectories results in broadening of the droplet distribution. The supersaturation variability comes from relatively large turbulent eddies (scales from meters to hundreds of meters), often resulting from cloud-edge instabilities and entrainment (Grabowski and Clark 1993). Lasher-Trapp et al. (2005) investigated this mechanism in realistic cumulus cloud simulations. They combined a 3D Eulerian LES cloud model with a Lagrangian trajectory model that included cloud condensation nuclei (CCN) activation and cloud droplet growth. The droplet distribution at a given location within the simulated cloud came from the superposition of distributions predicted by a large ensemble of back trajectories arriving at that location. The resulting droplet spectra were wide and quite realistic compared to the observations.

Fig. 4. Schematic of real droplets, superdroplets, and bin microphysics. (a) Cloud droplets with different sizes (horizontal axis) each containing a different CCN size (vertical axis). (b) The droplet ensemble can be represented by a two-dimensional number density function. (c) If CCN is of no interest, the ensemble can be represented by a one-dimensional number density function. If used in a cloud model, each bin in (b) and (c) needs to be advected in physical space and all bin combinations have to be considered in collision–coalescence calculations. (d) A superdroplet representation of the ensemble. Each symbol shows a single superdroplet on the same plane as in (a), with colors depicting an increasing multiplicity parameter from very low multiplicity (dark blue), through low to moderate multiplicity (green and yellow), to high multiplicity (red). Transport and growth of the real droplet ensemble in (a) is represented in a computationally tractable way by the orders-of-magnitude-smaller superdroplet ensemble in (d).
The methodology used in Lasher-Trapp et al. (2005) is cumbersome and requires additional assumptions when linking Eulerian bulk model fields to those experienced by the droplets along trajectories. In contrast, the particle-based Lagrangian approach allows direct simulation of droplet spectra and makes trajectory analyses straightforward (e.g., Sölch and Kärcher 2010). Figure 5 shows an example of results from the University of Warsaw Lagrangian Cloud Model (UWLCM; Dziekan et al. 2019) using a model setup similar to Lasher-Trapp et al. (2005). The spectra can be thought as analogous to observations by an aircraft flying through the simulated cloud. As Fig. 5 shows, the simulated spectra are wide and multimodal. The largest droplets are activated near the cloud base, but there are also smaller droplets that come from entrainment of environmental air above the cloud base and subsequent in-cloud droplet activation. As discussed by Lasher-Trapp et al. (2005), these features of the simulated spectra agree with numerous previous observations of droplet spectra in shallow cumuli.

Collision–coalescence is the computationally most demanding element of the Lagrangian approach because collisions between the two superparticles need to create a third one. This can lead to a rapid increase in the number of superparticles, making the problem intractable. Shima et al. (2009) developed a stochastic algorithm, referred to as the superdroplet method (SDM), that avoids this problem and scales linearly with the number of superparticles (rather than the usual number squared for binary collisions). In particular, SDM keeps the number of superparticles unchanged in its numerical implementation. Unterstrasser et al. (2017) and Dziekan and Pawlowska (2017) show that the SDM provides an efficient and accurate numerical algorithm for collision–coalescence. Li et al. (2017) also elucidated that the computational performance of the SDM is superior to Eulerian bin schemes, at least under the specific conditions they investigated.

Similar to the sensitivity of bin microphysics to the bin grid structure, SDM is sensitive to how superparticles are initialized. For collision–coalescence, it is sometimes preferable to sample rare but important particles more frequently to achieve better numerical convergence with respect to superparticle number (e.g., Unterstrasser et al. 2017; Dziekan and Pawlowska 2017). Furthermore, as pointed out in Grabowski et al. (2018), when there is large variability of multiplicity parameters among different superparticles, these sampling issues may lead to large statistical fluctuations when superparticles are advected from one grid to another. Unterstrasser and Sölch (2014) introduced a splitting and merging procedure to adaptively adjust the number of superparticles during the simulation that improved convergence; see also Schwenkel et al. (2018).

In the rest of this section, we explain how the bin microphysics problems highlighted in the previous section are addressed by the SDM and other Lagrangian particle-based approaches.

**Numerical diffusion of Lagrangian microphysics.** There is no numerical diffusion in the Lagrangian particle-based approach. This is because both the transport of superparticles in physical space and their growth...
are calculated individually using ordinary rather than partial differential equations. In simple terms, there is no need for spatial discretization (either in physical or radius–mass space), which is the cause of numerical diffusion in Eulerian bin schemes. This is illustrated in Fig. 3. Most Lagrangian particle-based approaches for collision–coalescence have no numerical diffusion either [see Unterstrasser et al. (2017)].

**The curse of dimensionality.** The Lagrangian particle-based approach can also relax the curse of dimensionality. As discussed in Shima et al. (2009), the SDM is more computationally efficient than a bin scheme when the number of attributes is larger than a critical number estimated to be in the range of 2–4. Jaruga and Pawlowska (2018) include eight attributes to study aqueous-phase oxidation of sulfur to sulfate occurring inside cloud droplets. Although, it should be noted that there is a cost of adding attributes because more superparticles are needed to cover the increased dimensionality of the attribute space without losing accuracy. Moreover, from a physical point of view, Lagrangian particle-based microphysics seems the simplest and most promising approach to cope with the complexity of ice particle habits and growth mechanisms by adding attributes for ice particle properties (e.g., density, aspect ratio, etc.). As argued in the previous section, traditional Eulerian bin microphysics schemes with separate categories for ice/snow and rimed ice (graupel or hail) are poorly suited to address this problem.

**SDM versus the Smoluchowski equation.** Modeling collision–coalescence in the SDM is based on the underlying stochastic process, not on the Smoluchowski equation. Therefore, SDM dispenses with the assumptions needed to derive the Smoluchowski equation (see “The limitations of the Smoluchowski equation” section). In consequence, as Dziekan and Pawlowska (2017) confirmed, SDM works well even with very small coalescence volumes for which the Smoluchowski equation cannot be assumed valid. Moreover, the SDM correctly represents fluctuations in collisional growth, albeit only in small-scale simulations (e.g., grid volume around 1 m$^3$). In coarser simulations, the SDM produces higher variability between different realizations than expected in nature because collision–coalescence is represented by a significantly smaller number of samples. In general, the stochastic (Kostinski and Shaw 2005; Wilkinson 2016) versus deterministic (Berry and Reinhardt 1974a,b,c) nature of rain onset in natural clouds remains controversial and should be further investigated in the future.

**THE WAY FORWARD.** What can be done using the Lagrangian particle-based approach that is difficult or simply impossible with traditional Eulerian bin schemes? In this section, we review possible applications of Lagrangian particle-based schemes and future research directions.

**Cloud–aerosol interactions.** We first discuss modeling cloud–aerosol interactions, such as the role of CCN [especially giant CCN (GCCN)] in rain formation, and aerosol processing by clouds. One-dimensional bin microphysics schemes exclude information about the CCN within cloud droplets and thus the impact of dissolved CCN on droplet diffusional growth cannot be considered. This is a critical omission as far as the impact of GCCN on precipitation development is concerned (Jensen and Nugent 2017). Moreover, aerosol processing by clouds can only be simulated using two-dimensional bin microphysics (see Figs. 1 and 4) because information about the CCN in each droplet is needed to simulate aerosol processing through the coalescence of droplets and removal through scavenging by raindrops.

Using the Lagrangian particle-based approach, all such interactions between clouds and aerosol particles can be simulated explicitly. Andrejczuk et al. (2010) applied a Lagrangian particle-based scheme to compare stratocumulus simulations with pristine and polluted aerosol conditions for a drizzling case. They simulated aerosol processing and noted distinct modification of the CCN size distribution. Jaruga and Pawlowska (2018) studied aerosol–cloud interactions in warm boundary layer clouds with a particular focus on the aqueous-phase oxidation of sulfur to sulfate occurring inside cloud droplets and the impact of this process on the size distribution of aerosol particles. They successfully reproduced the Hoppel gap (Hoppel et al. 1986, 1994), a feature of aerosol distributions resulting from processing of aerosols by clouds. These applications highlight the capability of the Lagrangian particle-based methodology.

**Ice microphysics.** Compared to liquid, our understanding of ice-phase microphysics is still poor owing to the complexity of ice crystal formation and growth, the diverse morphology of ice particles, the representation of ice melting, and the mechanisms of ice particle breakup (i.e., spontaneous, collisional, and rime splintering). Numerous efforts are under way to better understand the underlying physics, and recent efforts to develop Lagrangian particle-based ice-phase models have followed different paths. Sölch and Kärcher (2010) applied Lagrangian particle-based
ice microphysics to model cirrus. They grouped ice particles into several categories, such as hexagonal columns, bullet rosettes, and aggregates. The attributes they used to characterize ice particles were the mass and category. Brdar and Seifert (2018) developed McSnow, a Lagrangian model for riming and aggregation. They used four attributes: ice crystal mass, rime mass, rime volume, and the number of primary ice crystals. This is a multidimensional Lagrangian-based expansion of the Predicted Particle Properties (P3) bulk scheme (Morrison and Milbrandt 2015; Milbrandt and Morrison 2016). These models do not explicitly predict the shape of ice particles but rely on empirical mass–dimension and area–dimension relationships. Another strategy is to approximate ice particles as porous spheroids (e.g., Chen and Lamb 1994). Jensen and Harrington (2015) simulated the growth of single ice crystals and suggested that a smooth transition from unrimed ice to graupel through riming can be well modeled using the porous spheroid approximation. Shima et al. (2019, unpublished manuscript) employ this approach using the SDM to model mixed-phase cloud microphysics. However, more elaboration is still required to construct reliable models for mixed-phase clouds with Lagrangian particle-based approaches. We anticipate that this area will feature significant growth in the coming years.

Effects of cloud turbulence on growth of cloud particles. In modeling fluid flows, the role of unresolved scales of motion always needs to be considered. Lagrangian particle-based schemes are ideally suited to account for the influence of subgrid-scale (SGS) variability on the microphysics. For instance, broadening of the droplet size distribution due to cloud turbulence can be represented in a natural way. The key mechanism, referred to as eddy hopping [the term introduced in Grabowski and Wang (2013)], conjectures following Cooper (1989) that droplets arriving at a given location within a turbulent cloud follow different trajectories and the variability of supersaturation along these trajectories broadens the droplet distribution. This is illustrated in Fig. 6, which contrasts the smooth transport of droplets in an Eulerian model with that using the Lagrangian particle-based approach. The latter can directly incorporate an SGS scheme to impact both the particle motion (as in Sölch and Kärcher 2010) and its growth through SGS supersaturation fluctuations as in Grabowski and Abade (2017) and Abade et al. (2018). These fluctuations come from relatively large turbulent eddies (scales from meters to hundreds of meters) as these are capable of providing sufficiently large supersaturation fluctuations. Cloud droplets “hop” those eddies, moving from one large eddy to another due to the action of small-scale turbulence.

Fig. 6. CCN and droplet trajectories in (a) Eulerian and (b) Lagrangian cloud models. The color along the trajectories represents supersaturation experienced by droplets, with supersaturations below 0% colored black. In reality, the Eulerian model does not predict droplet trajectories, so (a) is a simple illustration of smooth advection and activation of CCN near the cloud base. Even if the Eulerian model represents unresolved subgrid-scale processes (e.g., cloud turbulence), these typically do not affect the motion or characteristics of individual droplets as only the evolution of the droplet spectra is predicted. In contrast, trajectories and growth histories of individual superdroplets are affected by unresolved turbulence in the Lagrangian particle-based microphysics with the supersaturation fluctuating as it is affected by the SGS processes. The difference between (a) and (b) is exaggerated for illustration.
eddies, and they grow in response to local fluctuations of the supersaturation.

Incorporation of eddy-hopping and entrainment into particle-based Lagrangian microphysics is relatively straightforward, as shown in Paoli and Shariff (2009), Grabowski and Abade (2017), Abade et al. (2018), and Hoffmann et al. (2019). For a homogeneous cloudy volume, supersaturation fluctuations are driven by SGS turbulence-induced vertical velocity fluctuations of the droplet-carrying air [see, for instance, Eq. (1) and its discussion in Grabowski and Wang (2013)]. This approximation has been used in many DNS studies of droplet condensation in turbulent environments (e.g., Vaillancourt et al. 2002; Lanotte et al. 2009; Sardina et al. 2015). For an inhomogeneous cloudy volume (e.g., containing a mixture of cloudy and cloud-free filaments), the droplet environment is modified not only by the air vertical velocity, but also through molecular diffusion between cloudy and cloud-free filaments. In both homogeneous and inhomogeneous cases, the superdroplet radius, its velocity fluctuation, and supersaturation fluctuation can be assumed stochastic superdroplet attributes. The time evolution is then governed by a set of Lagrangian stochastic differential equations, where SGS variability (in time and space, at different scales) can be introduced by adding random terms (“noise sources”) to the deterministic evolution equations. It follows that including SGS variability in Lagrangian microphysics schemes reduces to designing a physically based model of stochastic fluctuations experienced by individual droplets [see Hoffmann et al. (2019) for a specific albeit relatively complicated approach].

One disadvantage of using the Lagrangian particle-based approach is its computational cost. This is mostly because initially the entire computational domain needs to be filled with aerosol particles and only a small fraction of these are activated to form cloud droplets. Moreover, CCN deliquescence (humidification) and eventual activation requires short time steps in its numerical implementation, at least an order of magnitude shorter than needed to simulate the flow. However, if CCN processing is of secondary importance, a significant reduction of computational cost is possible by applying the Twomey activation approach (Grabowski et al. 2018). The idea is to create superdroplets only when CCN is activated and to remove them when there is complete evaporation of the droplet (i.e., CCN deactivation), as is typically done in Eulerian bin microphysics and in analogy to ice formation in cirrus simulations using Lagrangian microphysics (e.g., Sölch and Kärcher 2010). Thus, no superparticles exist outside of clouds. Because clouds occupy a small fraction of the computational domain volume, the Twomey superdroplet method provides a significant computational advantage when compared to the standard Lagrangian particle-based approach. Moreover, other formulations of droplet activation could be applied in the case of a low vertical resolution LES model, for instance, linking the concentration of activated cloud droplets to the local updraft speed. This paves the way for using Lagrangian particle-based microphysics in lower-resolution models targeting, for instance, deep convection and mesoscale processes.

**SUMMARY.** Representing the formation and evolution of cloud and precipitation particles is a key element of numerical cloud modeling. Since the very beginning of cloud dynamics modeling about a half century ago, the populations of drops and ice particles in natural clouds have been typically represented by continuous-in-time-and-space density-like (i.e., Eulerian) variables representing particle mass or number within a grid volume. The “grid volume” represents either the volume in physical space for bulk schemes or the volume in physical space combined with the volume in the particle mass space (and other attributes, if needed) for bin schemes. The Eulerian methodology, justified by the sheer number of cloud and precipitation particles typically present in a grid volume, has been the workhorse of cloud-scale modeling as well as climate and weather prediction models that until recently have not been able to directly simulate cloud-scale dynamics.

With increasing computational resources, there is a clear trend to move from simplified bulk approaches to more comprehensive and arguably better physically posed bin schemes. For instance, only 11 papers published in all American Meteorological Society journals for the period between 1980 and 1989 included the phrase “bin microphysics” in their titles; that number increased about an order of magnitude for papers published between 2000 and 2009. Bin schemes have been considered the ultimate approach to cloud modeling as they allow the particle size or mass distributions to evolve freely, and have been used in the past to derive process rates for bulk schemes (e.g., Khairoutdinov and Kogan 2000; Kogan 2013). However, some fundamental problems challenge the ultimacy of the bin approach. For warm-rain microphysics, one-dimensional bin schemes cannot accurately represent CCN processing unless an even more costly multidimensional bin approach is used. The complexity of ice particle shapes and forms makes
formulation of ice processes especially challenging in bin ice schemes. Finally, there is a fundamental problem with the Smoluchowski equation that is used to evolve the number (and/or mass) density function in time because it neglects statistical fluctuations of the droplet population. Beyond these aspects, it is also challenging to solve numerically the bin scheme equations accurately. Morrison et al. (2018) showed that the typical approach of separately calculating advection in physical space and advection in size (or mass) space to represent particle growth leads to an unphysical broadening of the simulated particle size distribution. In summary, we feel that continuing on the current path of microphysical modeling (i.e., with a focus on an Eulerian approach) brings challenges that are difficult to overcome, and the advancement of an alternative methodology would be beneficial.

We argue that Lagrangian particle-based microphysics is a good alternative methodology. The key is to dispense with the Eulerian continuous number or mass density representation and instead apply a judiciously selected ensemble of Lagrangian point particles, called superdroplets or superparticles, to represent the formation, growth, and motion of cloud and precipitation particles. Each superparticle has a multiplicity parameter to represent the total number of particles with the same properties. The advantage comes from replacing partial differential equations describing the density function evolution with an approach solving ordinary differential equations for the transport and growth. The latter eliminates the numerical diffusion of the Eulerian approach but requires confident assessment of errors arising from having a limited number of superparticles affordable in a given simulation. We also emphasize that the underlying physics of many processes and parameters remains poorly understood (e.g., drop breakup), and this represents an important uncertainty in all microphysics schemes including Lagrangian particle-based approaches.

The Lagrangian approach is relatively well established for warm microphysics, where the largest challenge has been the development of accurate and computationally efficient algorithms to simulate collision–coalescence (see Unterstrasser et al. 2017). Arabas and Shima (2013) document the sensitivity of a precipitating shallow convective cloud field observed during RICO to details of the LES model with Lagrangian particle-based microphysics and show reasonable agreement with the observations. Although there have been recent attempts to apply Lagrangian schemes to simulations of ice-bearing clouds (e.g., Sölch and Kärcher 2010; Unterstrasser and Sölch 2010; Brdar and Seifert 2018), Lagrangian ice modeling for mixed-phase clouds is in its infancy. This is partly because of significant gaps in our knowledge of ice processes (details of ice initiation being an essential one), but also because of the wide variety of ice particle shapes and types and more complicated paths from pristine ice crystals to precipitation that can involve both diffusional and accretional growth.

Ice processes are required to simulate deep convection as well as cloud systems associated with most extratropical weather systems. Modeling clouds that span the entire troposphere requires numerical models to apply vertical resolutions insufficient to resolve cloud-base CCN activation and entrainment/mixing that significantly affect particle spectra. Consequently, for application of the Lagrangian particle-based approach in such models, one should consider simplified methods to simulate cloud droplet formation [e.g., activation parameterization as in Grabowski et al. (2018)], and to represent physically subgrid-scale turbulence affecting particle motion and growth (e.g., Grabowski and Abade 2017; Abade et al. 2018). These developments should eventually allow a truly multiscale simulation of different cloud systems, advance our understanding of cloud–aerosol interactions, and improve our understanding of the role of clouds in weather and climate. We are excited for the potential of these advances and anticipate the community moving forward in this effort.

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