Dean&Francis

ISSN 2959-6157

Analysis the Principle and Realization for Cosmic Dust Simulation

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Abstract:

Astrophysics simulations are becoming crucial to the understanding of how the universe came to be the way it is today. Cosmic dusts are quite important in these astrophysics' simulations, although they have only recently been introduced to the simulations. This study offers analysis on the different parts of current cosmic dust simulations. Astrophysics simulations and cosmic dusts' role in this simulation was first discussed. Simulation requirements on cosmic dusts were then evaluated, both in the software and the hardware. The realization of cosmic dusts simulations was then discussed, focusing on the creation, growth, and destruction of cosmic dusts and briefly discussing the algorithmic process of incorporating calculations and presenting data. At last, limitations on current cosmic dusts simulations and some future prospects were proposed. These results provide an organization of the different prospects of current progresses in cosmic dust simulations, which could be beneficial as an overview of the topic and a base for which directions for future researches could be suggested.

Keywords: Cosmic dusts; astrophysics simulations; grains; algorithm; radiation.

1. Introduction

Astrophysics simulations is a rather novel branch of astrophysics, but it had been crucial to the understanding of how the universe came to be the way it is today. The history of astrophysics simulations is largely relative to the development of computer technologies. The first stellar evolution codes were utilized as early as the 1950s, when computer technologies are still at their infancy [1]. The development of computer technologies and algorithm theories provided support to the development of new astrophysics simulation codes form then on. It was not until the 1970s when there was a burst of new astrophysics simulations. The first true cosmological simulation of structural formation was done in 1974 [2]. At the 1980s, the fields of astrophysics saw microcomputers coming into wide use over observations and simulations [1]. It was after that when astrophysics simulations saw an "explosion of activities" [2]. Dark matter, cosmological inflation, evolution of density fluctuations, Gaussian random fields, N-body algorithms, and other important topics that would be the core of astrophysics simulations entered the theater [2]. Indeed, dark matter has become an important topic in astrophysics simulation. Dark matter is an integral part of modern astrophysics, especially in cosmology and other studies of the cosmological structure, formation and evolution [3]. Thus, it would be no surprise that astrophysics simulations featuring dark matter as an important topic began to proliferate. In particular, simulations that involves simulating the cosmological structure, one essential topic in astrophysics simulations. In this perspective, there have been a burst of new codes for cosmological structure formation and evolution since the start of the 21st century, such as GADGET in 2001, RAMSES in 2002, ATHENA in 2008, ENZO in 2014, CHANGA in 2015, PHANTOM in 2018, etc. [4]. Newest astrophysics simulations are also incorporating factors such as radiation transfer and cosmic dusts into consideration, such as the codes AREPO-RT and RAMSES-RT, and the simulation suite THESAN [5-7].

The focus of this paper would be on the component of cosmic dust in these astrophysics' simulations. Thanks to the efforts and publication of astrophysics simulations containing the factor of dust, some results have been obtained. These results showcase the creation, accretion, clustering, and destruction of cosmic dust, along with their interactions with other subjects of astrophysics simulations such as radiation and the cosmological structure. Some simulations revealed some discoveries about certain principles, prescriptions, and assumptions of astrophysics. One example would be Aoyama et al., which revealed that dust-to-metal ratio is not fixed in certain cases, different from assumptions [8]. Other simulations revealed certain characteristics of dust as a whole interacting with other components of the galaxies, or as separate grain particles that interacts with each other. McKinnon et al. found a relationship between dust-to-stellar mass ratio and the stellar mass, along with other findings that helped explain the process of forming a dusty galaxy [9]. Mattsson and Hedvall, on the other hand, treated grain particles independently, obtaining results showing differences in grain movement properties relative to their inertia [10]. Besides these, cosmic dust are also important parts in the result of some new astrophysics simulations featuring them, such as its role in presenting the cosmological structure in simulations like THESAN [7].

Focusing on cosmic dusts in astrophysics simulation, this paper would be an overview of several parts of cosmic dust simulations. The next section would be an introduction into astrophysics simulations overall, along with a brief discussion on the role of dusts in these simulations. Then, the simulation requirements and the realization of cosmic dust simulation would be discussed. Lastly, some limitations and prospects of current cosmic dusts simulations would be brought out. Cosmic dust is a relatively new component to astrophysics simulation, which is a relatively new branch of astrophysics itself. The fact that this is a relatively new field would be one reason for writing this paper, aiming to explain some of the progresses relating to the topic. Another motivation would be to provide a relatively cohesive organization of the different prospects of cosmic dust simulations, which might be beneficial as a base to suggest future directions in researching relative topics.

2. Astrophysics Simulations

2.1 The Components of Astrophysics Simulation

There are various different astrophysics simulations either finished or in session in this two decades. The principles of these astrophysics' simulations are, however, similar. Basically, astrophysics simulations comprised of the calculations over galaxy formation and the chosen identities (matter density, radiation, etc.) of different data points. These calculations would then be put into an algorithmic process, which might differ across different simulations, to operate the simulation. The last step would be processing the calculated data into visible images. The most important step in this process would be the algorithm of calculating and updating the various data that were the focus of the simulation. The components of this algorithm would then be the focus of this section. The description of the different components would be done using the example of the THESAN simulation. The reason for this is that THESAN is a comprehensive simulation in a way that it incorporates the galaxy formation model of IllustrisTNG, the radiation hydrodynamics solver AREPO-RT, dust models, etc. [7]. This made it capable to simulate not only the galactic structure of matter but also radiation, dust, and their interactions.

The components of astrophysics simulations could be induced from the way THESAN was constructed by IllustrisTNG and AREPO-RT. IllustrisTNG uses the AREPO moving-mesh code as the basic algorithm to calculate and simulate magnetic fields, hydrodynamics, galactic winds, etc. [11]. THESAN improved upon that by incorporating the new AREPO-RT code, which is a radiation hydrodynamic solver for the original AREPO code, and dust models [5]. In other words, THESAN simulation is made up of magnetic field calculations, hydrodynamics calculations, radiation calculations, dust calculations, and a code that incorporates all those into a complete algorithm.

Magnetic field calculations and hydrodynamics calculations were the core of a lot of astrophysics simulations from the beginning. These calculations would involve a wide range of equations and processes that would combine the two components into one: magneto-hydrodynamics (MHD). MHD is the study of electrically conducting fluid in the presence of a magnetic field [12]. The galaxy, according to this perspective, could be modeled as an electrically conducting fluid. This could be suitable, since stars fit this description well, and the void between stars could be viewed as a fluid with negligible density in most cases. Radiation calculations and dust calculations were also commonly combined together, given their intimate relationships, these relationships would be discussed in detail in Sec. 2.2.

The final component of astrophysics simulations would be the code that incorporates the magneto-hydrodynamic calculations and dust-radiation calculations together and presenting them. For AREPO and AREPO-RT mentioned previously in this section, a moving-mesh method was utilized. This method involved first tessellating the data presented in a plane, in this case the Voronoi tessellation, which would distribute cells in a way that the relative mesh-generating points would have equal distance with each other [4]. After this tessellation, each cells' various data would be calculated and updated for each time step, or a round of data updating. The interactions between each cell would be included in the process. The reason it is a "moving-mesh" is that the cells making up the span of data could move after each time step, depending on fluid velocity, local pressure induced accelerations, Lorenz force, gravity, etc. [4].

2.2 The Role of Dust in Astrophysics Simulations

The simulation of dust was not present in some early astrophysics' simulations. Nevertheless, it is being added into more newly done simulations because of its effects on the interactions between different components of astrophysics simulations. Particularly, for its role in the interactions of matter and radiation, and its use as an indicator and a representation of several physical properties of the environment. Cosmic dust has an important relationship with radiation present in the environment. This relationship is, in fact, quite crucial in understanding how radiation effects the properties of matter and how the galaxies formed. One important relationship in this case would be that dust acted as an important factor in calculating the effect of radiation on the temperature of the environment. Especially in the case of radiation-dust temperature coupling, it is crucial to put dust into the equation of radiation's effect onto the temperature of the environment [13]. This is mostly due to the fact that dust may be a source of opacity, altering the actual magnitude and effect of radiation [13]. There could be other interactions between dust and radiation due to this opacity and other factors, which are prevalent in simulations containing the factor of dust.

Besides the essential relationship between cosmic dust and cosmic radiation, dusts could also be important as an indicator and representation of various physical properties of the environment they are in. The composition, crystallographic structure, and morphology of these cosmic dusts could record some important information of the environments in which they formed (e.g., temperature, pressure, materials available, and heating and cooling rate) [14]. Moreover, dusts are relatively more tangible than a lot of other data, being actual physical matter. For these reasons, dusts could be suitable representations for various data obtained in astrophysics simulations. A suitable representation of data would be crucial to the presenting step of astrophysics simulations, thus this shows one important role of dust in these simulations.

3. Simulation Requirements for Cosmic Dust Simulations

Cosmic dust simulations would require several elements. The simulation of cosmic dust is highly relevant to the simulation of other components in an astrophysics simulation, especially with the cosmic radiation. Besides requirements for other components in astrophysics simulations, some requirements that exists in simulations without featuring cosmic dusts would be considered as well. One especially important component in astrophysics simulations that has deep connections to the simulation of dust is radiation. As discussed in Sec. 2.2, cosmic dust has an important relationship with radiation, due to the opacity of cosmic dusts and other reasons. Radiation can have radiation pressure on the population of grains of dusts, dusts could absorb some photons in return and effect the effects of radiation on other identities of the cell [13]. Radiation with multiple frequencies could all interact with cosmic dusts in some ways via multifrequency radiation-dust coupling [13]. Ultraviolet (UV) radiation and optical radiation could go through the dusts and be reprocessed, which would contribute to the infrared (IR) radiation sector [13]. The IR radiation would be a more complicated sector in terms of interactions with cosmic dust grains. By IR-dust temperature coupling, IR radiation could interact with cosmic dusts to affect the thermal identities of the cell. This could be a complex matter as sometimes dust grains, especially small ones, could be affected significantly by "stochastic heating and temperature fluctuations", along with other complications [13]. Some simulations involving cosmic dusts would simplify the situation by neglecting these small fluctuations, and solely investigate IR-dust temperature coupling by calculations of their energy density [13]. Therefore, in the case of radiation as a simulation requirement for cosmic dusts, the true requirement lies in the energy density of IR radiation, with UV and optical radiation being supplements and other factors sometimes neglected. Other interactions between dusts and other components of astrophysics simulations also exists, although not effecting the simulation of dusts to a significant degree. These interactions are mostly about the effect of dusts on the other components of astrophysics simulations, such as the change of total mass in the cell by change in the total mass of dust.

There are also some requirements that apply to most astrophysics' simulations, with or without the presence of cosmic dusts. One such requirement is the initial conditions for the simulation. Any kinds of simulation would require something to begin with, which is the initial conditions on which simulations of change would be operated. These initial conditions would be about what are the required identities for the cell to begin simulation and what kinds of limit could exist for these required identities. The required identities would differ quite a lot across simulations done for different purposes. Regardless, in the case of astrophysics simulations involving dusts, some basic parameters would usually always be included. This would include some kind of model that would divide a space by cells, such as a space processed by Voronoi tessellation; matter and energy density with some kind of algorithm that would fill these identities into the space simulated; the time period and basic cosmological parameters associated with the period, etc. [4, 13, 15]. One of the most important requirements for dusts simulations in particular are the choices of the characteristic growth time-scale (τg or τa) and the characteristic destruction time-scale (τd), which could be different for each cell and needs to be determined at the beginning of the simulation [15, 16]. The limitations on the initial identities for the simulation would also differ according to the purpose of the simulation. For example, the universe model that would be used could be different for different simulations. For simulations involving the evolution of the early eras of the universe, such as THESAN, the universe model would involve several cosmological parameters specific to the universe, such as the values in the Friedmann equation [7]. For some simulations, a special universe model could be chosen for some reasons, such as the Einstein-de Sitter universe and the ΛCDM model [15, 17]. Some dust simulations did not put an emphasis on the choice of universe model because they were done on a local scale [18]. The parameters of τg and τd would be more complicated, as they are related to the individual cells, this would be discussed in Sec. 4.

Besides these requirements in “software”, there could also be requirements to the hardware. It is true that astrophysics simulations have once been done on some computers that might not be considered as supercomputers today [1, 2]. However, the scope and scale of astrophysics simulations have long evolved since then. Nowadays, most astrophysics simulations that would generate new insights into fields of astrophysics would require a sufficient set of hardware. The reason for this would be that the number of calculations for conducting astrophysics simulations would be quite demanding for the hardware, among other reasons. For some simulations like the THESAN, the minimum requirement for the number of computing cores required for holding simulation memory is 57600 cores, and the 28 million core hours spent is also quite a large number [7]. Although THESAN is a comprehensive simulation that could require more calculation than some other astrophysics simulations involving cosmic dusts, these numbers still provide insights into the high demand for computation powers for the hardware. Nonetheless, the demand for computation powers may somehow be mitigated by suitable measures. With measures like double precision on the algorithm side, and improved storage and parallel-calculation technologies in computer science, the requirement for hardware could be alleviated to a lower degree [7]. The scale and scope of astrophysics simulations involving cosmic dusts could be expanded with innovations in computation, though; hence, hardware might remain an important requirement for such simulations in the future.

4. Realization of Cosmic Dust Simulations

The realization of cosmic dust simulation could be divided into several parts, much alike the process of astrophysics simulations overall described in the former sections. The first part would be about the calculations about cosmic dusts and their interactions with other components of astrophysics simulations. The next part would be an algorithm that put these calculations into a logical process of updating and progressing. The last part would be to present the results visually, or through other ways of exhibiting the data. For the first part, calculations would be done on both cosmic dusts alone and cosmic dusts’ interactions with other subjects of astrophysics simulations. The latter part, which is the interactions, has been discussed in section 3. Therefore, only the calculations involved in cosmic dust simulations relative to the dusts’ own properties would be discussed in this section. These calculations would mainly include the creation of dusts, the growth of dusts in the interstellar medium, and the destruction of dusts by several means. McKinnon et al. provided a detailed description of the calculations for these processes, which would be showcased in this section [16]. It was known that cosmic dust particles come from two main sources: Asymptotic Giant Branch (AGB) stars and Supernovae [16]. AGB stars are stars with one to eight solar masses on their last phase of stellar evolution [19]. During this phase, all the helium in the core has been depleted, leaving a carbon-oxygen core, the variable ratio between these carbon and oxygen would be important when determining cosmic dust generated during this period [19]. In fact, for AGB stars with cores composed with carbon as majority, only compounds of carbon would be released as cosmic dusts, with the formula $\delta(\Delta M_C - 0.75\Delta M_O)$, where δ is the carbon condensation efficiency for the star, and the latter part is the weighted difference in the mass change of carbon and mass change of oxygen [16]. Whereas, for ones with cores composed with oxygen as majority, compounds of oxygen and other elements would be released, but not carbon [16]. The formulae for calculating oxygen dusts are provided below:

$$oxygendusts = 10 \sum_{j=Mg,Si,Fe} \delta \Delta \mathrm{M}_j / \mu_j \tag{1}$$

where μ is the mass in atomic mass units [16]. Besides the special cases of AGB stars with more carbon at the core, cosmic dusts of elements other than oxygen, whether from supernovae or AGB stars, could be calculated by $\delta\Delta\mathrm{M}_i$, where i is the specie of the dust (e.g., Carbon, Oxygen) [16].

After cosmic dusts were generated, they could experience growth and destruction in the interstellar medium. Gas-phase elements might collide with cosmic dusts and form more cosmic dusts [16]. The formula of this growth of cosmic dusts in the interstellar medium would be:

$$\left(\frac{dM_{i,dust}}{dt}\right)_g = (1-\frac{M_{i,dust}}{M_{i,metal}})\left(\frac{M_{i,dust}}{\tau_g}\right) \tag{2}$$

In which the masses involved are the totality in a certain cell, and the τ_g, mentioned in Sec. 3, is the characteristic growth time-scale [16]; τg could be determined in each cell by:

$$\tau_g = \tau_g^{ref}\left(\frac{\rho^{ref}}{\rho}\right)\left(\frac{\mathrm{T}^{ref}}{\mathrm{T}}\right)^{1/2} \tag{3}$$

Here, ρ and T are the density and the temperature of the cell, respectively; all terms with the superscript “ *ref* ” refers to the fixed values for molecular clouds [16]. The τ_g^{ref}, though, has to be chosen carefully, because it is “an overall normalization” influenced by numerous factors [16]. This is why the choice of τg has to be considered from the beginning, as mentioned earlier.

The destruction of cosmic dusts, on the other hand, would be more complicated, given the various ways dusts could be destructed. Supernovae, which produce some cosmic dusts, could also destroy existing dusts by SN shocks [16]. Dusts could also be destructed by sputtering and grain-grain collisions [16]. A formula for the overall destruction rate could be expressed as:

$$\left(\frac{dM_{i,dust}}{dt}\right)_d = -\frac{M_{i,dust}}{\tau_d} \tag{4}$$

where the masses involved are the totality in a certain cell, and the “ τ_d ”, mentioned in section 3, is the characteristic destruction time-scale [16]; τd could be determined in each cell by:

$$\tau_d = \frac{M_g}{\in \gamma \mathrm{M}_s(100)} \tag{5}$$

where g” refers to gas, “ $\in$ ” is the the destruction efficiency by SN shocks, “ γ” is the local Type II SN rate, and “ $\mathrm{M}_s(100)$ ” refers to the mass of gas shocked to at least 100km/s [16]. Out of the terms in the formula, most would require a determination at the start of the simulation. This would be a reason why, similar to τg, τd would require a careful choice at the beginning of the simulation, as mentioned in Sec. 3. These calculations would then be put into an algorithmic process that would update data according to calculation, time step by time step. The procedure would often require a specific order of calculating and updating each value of the identities of the cell. For the dust creation, growth, and destruction, etc. in McKinnon et al. 2016, a specific procedure has been provided: for each time step, the net growth rate would first be calculated, then the net increase would be evaluated, the local dust mass is thus updated [16]. The net growth rate would be the difference between the local growth rate and the local destruction rate, and the net increase would be the local dusts generated minus reductions when star particles are created [16]. These procedures are the core of the algorithm of calculating and updating identities of cosmic dusts in the cell. Some other algorithmic process would need to be operated to suit the calculations to different usages, such as incorporating into more comprehensive simulations such as THESAN [7]. To exhibit the results of the simulations, a lot of different approaches could be taken. One commonly taken approach would be the visualization of data into a graphical evolution map. An example of a set of simulation results by this approach, the evolution of certain properties of the early universe in the THESAN simulation, is provided in Fig. 1. Data could also be presented as simple graphs, such as an example, also from THESAN, as illustrated in Fig. 2.

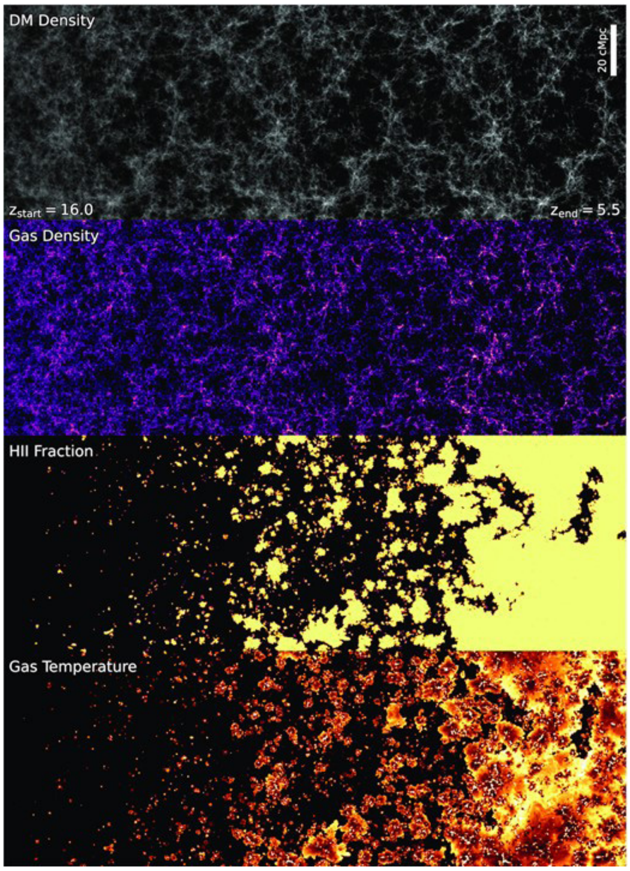

Fig. 1 Evolution of certain properties of the early universe in the THESAN simulation [7].

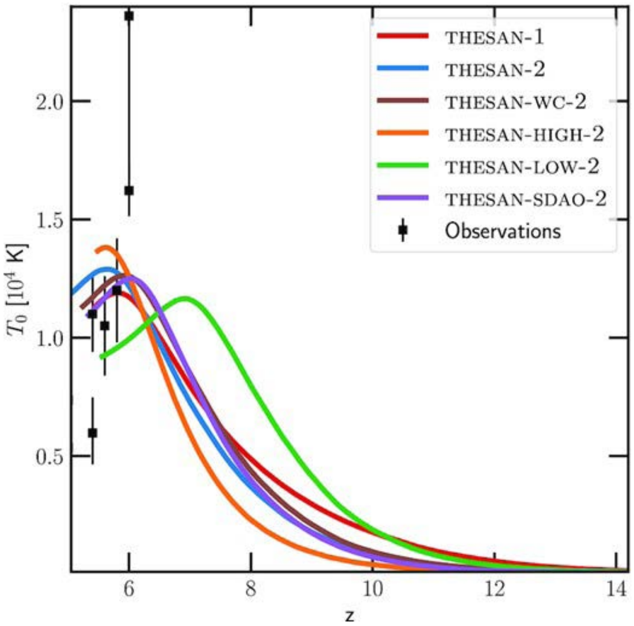

Fig. 2 Evolution of the intergalactic medium temperature at mean density for several THESAN simulations [7].

The process of achieving the presentation of these kinds of visualization could vary greatly across different simulations. One noteworthy component in a lot of these processes is the Flexible Image Transport System (FITS) [20]. This is a widely used data processing system and storage format in astrophysics, able to convert images into data and vice versa [20]. Astrophysics simulations could utilize an algorithm similar to FITS, and often producing FITS files [20]. Some publicly available astrophysics results, such as the Cosmic Microwave Background map from the Planck missions, were produced in “.fits” files. Since the images are stored as data in this perspective, FITS files could be compatible to most computers, and easily convertible to images, making it a suitable part of presenting the results of astrophysics simulations.

5. Limitations and Prospects

Various limitations still exist on current simulations involving cosmic dusts. Some of these limitations are over the scope of the simulations, others could be on the scale. Some of these limitations would be proposed or exhibited in this section, along with some future prospects into improving upon these limitations and expanding the subject.

There are a lot of limitations on the scope of cosmic dusts simulations. There are limitations on the time scope, on the universe model scope, and on the scope of properties, among other scopes. The time scope, or the era of the universe that was simulated, could be quite limited; this could be due to a lack of understanding of some of the properties of the universe in its earliest stages, such as the abundances of high-redshift dusty galaxies [9]. The scope of universe model could also be limited, but this would not be the crucial issue compared to other limitations, as most studies aim to investigate properties of the universe, for which the prominent universe models focused on. The scope of properties of cosmic dusts involved in simulations is also quite limited, as some topics such as interstellar dusts’ chemistry have been experiencing difficulties [21]. Future researches could aim to expand the time scope of astrophysics simulations, given new insights into the first minutes of the universe; investigate conditions in different universe models; and expand upon the properties investigated about cosmic dusts in astrophysics simulations, given new advancements in other fields of science related to cosmic dusts.

There are also some limitations on the scale of some astrophysics simulations involving cosmic dusts, both on the scale of each simulation and the number of simulations in a given period. This could be due to the high hardware demand of these simulations, as mentioned in Sec. 3. With a hard demand and pressure on the hardware, current computer technologies could not really support astrophysics simulations with extremely large scale. Although current simulations could already reach hundreds of megaparsecs in their scale, this would not be enough to determine the cosmological structure on a much larger scale. In addition, since there are a limited amount of supercomputers in the world available to do these simulations, and even a smaller amount of these supercomputers that would be vacant from other tasks, the number of simulations in a given period of time would be quite limited. With new advancements in parallel computing (and even quantum computing), the scale of astrophysics simulations could be enlarged significantly in the future. Future cosmic dusts simulations could therefore expand their scale, moreover, more of these simulations could be done in a fixed period of time.

6. Conclusion

To sum up, this paper provided a brief overview of the parts of current cosmic dusts simulations. Cosmic dusts, although introduced late into astrophysics simulations, played quite an important role in these simulations, namely for its interactions with radiation, and its use as an indicator and a representation of several physical properties of the environment. To simulate cosmic dusts, several requirements need to be met, such as the inclusion of other components of astrophysics simulations (notably radiation), inclusion and choice of some initial conditions, and some hardware requirements. When all the requirements are met, cosmic dusts simulations could be realized by calculations of their creation, their growth, and their destruction, along with an algorithm that incorporates these calculations together and displays the results. Some limitations nevertheless existed in current astrophysics simulations involving cosmic dusts, both in the scope and the scale of these simulation. Cosmic dusts were introduced into astrophysics simulations only recently, which would be why an organization of this topic is needed. This paper provided such an organization in a brief way, which would be beneficial in suggesting future directions for researches about relative topics.

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