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Revaluation of the first-order upwind difference scheme to solve coarse-grained master equations

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Abstract

This study addresses the initial-boundary value problem of coarse-grained probability measure on the state space in which a differentiable vector field **v** is given and, as a consequence, the differenced continuity equation using the first-order upwind difference scheme (UDS) based on the finite volume method appears as the physical substance on the coarse-grained dynamics. At first, the UDS is theoretically shown to be equivalent to a class of coarse-grained master equations (CGME), brought by a principle that we cannot distinguish state points in the same partition with each other. The principle is based on the formulation of non-equilibrium statistical mechanics to resolve the macroscopic irreversibility. Moreover the entropy production evaluated by the UDS is also shown to be in accord with the average volume contraction rate in the steady state. This is essential for the non-equilibrium statistical dynamics and was numerically confirmed. Under the principle of coarse graining the UDS is very superior to the conventional Monte-Carlo method in computer time and storage and is very useful to solve the CGME.

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1. Introduction

The problem of the macroscopic and phenomenological irreversible change caused by the reversible microscopic dynamics has been the major problem in non-equilibrium statistical mechanics. In the Hamilton or volume-preserving system, the rate of increase of the conventional entropy, Gibbs entropy, without the coarse graining is the average volume expansion rate zero and, therefore, is not suitable for the explanation of the physical phenomena governed by the second law of thermodynamics. To my knowledge, there is no work to show that the entropy production on a Hamilton system is positive without coarse graining. Moreover

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the entropy cannot be defined on the sets of zero Lebesgue measure, such as fractal sets, and is not applicable to the non-equilibrium steady states of dissipative or thermostated systems [1]. Therefore, it is argued that the coarse graining should be performed.

In this study, as well as discussions on the entropy production, the term "coarse graining" is used within the meaning that a state space considered is divided into some partitions and that the points in the same partition cannot be distinguished with each other. Eventually, the system behavior is examined for the limit as the representative length scale of the partitions Δ goes to zero. The formulation has been widely accepted by the fact that the macroscopic or phenomenological entropy production can be explained thereby for various dynamical systems.

In the mesoscopic formulation the effects of the coarse graining are included in random force in the Langevin equation, and the resultant governing equation of probability density, Fokker–Planck equation, has a diffusion term with a strength parameter ε. The term does not vanish as ε tends to zero because the probability density has the singularity for the limit. It is shown that the term makes the mesoscopic entropy production based on the Gibbs entropy positive and that the production agrees with the average volume contraction rate in non-equilibrium steady state [2]. Except the case of quantum chaos [3–5] or the formulation based on Kolmogorov–Sinai entropy [6], most of the classical formulation based on the Gibbs entropy shows that multi-dimensional entropy production in the non-equilibrium steady state generally agrees with the negative sum of all Lyapunov exponents, i.e. average volume contraction rate [2,7–10].

In the microscopic formulation the coarse graining makes it possible to show that the entropy production is positive even in volume-preserving systems in terms of macroscopic dissipative structures caused by the boundary condition to bring non-equilibrium steady state [11] or of multifractal structures of invariant measure [12–14]. Though the explanation by the fractal underlying structures does not directly relate the average volume contraction rate with the entropy production, the production is shown to be in agreement with the phenomenological entropy production [12], corresponds to the above-mentioned mesoscopic entropy production, and the production is thereby related to the contraction rate. These discussions assert that the coarse-grained system with Δ tending to zero can explain the phenomena that cannot be explained by the formulation without the coarse graining, i.e. $\Delta = 0$.

In general, a coarse-grained system is governed by a master equation, hereafter referred to as coarse-grained master equation (CGME), and its numerical solver involves the evaluation of transition probabilities. For the purpose the Monte-Carlo method is widely utilized. In many cases to which the method is applied the "coarse-grained" partition scale Δ is sometimes held fixed and the limiting behavior as $\Delta \to 0$ is not paid attention. This is not the coarse graining of this study. Moreover, this study deal with the initial-boundary value problems of the coarse-grained probability measure on the (complete) state space and a differentiable vector field $\mathbf{v}$, by which state points evolves, is given in advance. Therefore, the fluctuation of a real state point ("realization" [15]) that corresponds to the change of the unsteady probability measure, or that of the probability density (measure) due to the uncertainty of the state stray from the main topic of this study; the fluctuation or noise raised by the Monte-Carlo simulations [16–20] are not involved in this study. In addition, if we apply the Monte-Carlo integration to evaluate the transition probability every time when needed for saving storage, the fluctuation of the computed probability is inevitable, and the "noise" essentially reduces the accuracy of lower probability measure and, therefore, they are not applicable to the evaluation of such a family of information $I^{(\beta)}$ on the invariant set [21] because the information of $\beta < 0$ extracts the characteristics of lower probability region. The methods to resolve the problem, e.g. more sample points, request more computer time or storage. In these situations the Monte-Carlo method is not necessarily useful.

In this study the numerical solution of the CGME considered is theoretically shown to be in agreement with that of the continuity equation discretized by the first-order upwind difference scheme (UDS) based on the (conservative) finite volume method. The scheme is very superior to the Monte-Carlo method in computer time and storage for solving the CGMEs and is effective even in multi-dimensional cases provided the partition size Δ is sufficiently small. Therefore, we authors has been numerically verified the agreement and used the UDS to evaluate the above-mentioned time-dependent information on invariant sets [21]. However the explanation for the agreement was entirely insufficient from the theoretical and computational viewpoints. Such an explanation is the main purpose of this study.

On the other hand, the behavior of the coarse-grained system within the meaning mentioned above is considered to be more physically essential for the second law of thermodynamics. In fact, this study shows that the UDS can be regarded as a Fokker–Planck equation with a diffusion term regulated by Δ, corresponding to the above-mentioned strength parameter ε. And the equation has the well-known important property in the non-equilibrium steady state, i.e. the average volume contraction rate is equal to the entropy production. The relation connects phase space dynamics with thermodynamics, and the above-mentioned macroscopic irreversible changes are explained thereby [11,22]. Therefore, this is also essential for the non-equilibrium dynamics [2], and the UDS is revealed and revalued to have genuinely physical, not numerical, substance on the coarse-grained system. It should be stressed that the second- or higher-order upwind schemes do not have the properties though the UDS itself is now being replaced with the schemes for many computations. We can show that the UDS is special among other schemes. To clarify the physical significance of the UDS is also the purpose of this study.

2. Coarse-grained master equation (CGME)

In this study the term "coarse graining" is used within the meaning that a state space considered is divided into some partitions and that the points in the same partition cannot be distinguished with each other and, therefore, the micro-structure of the probability measure in a partition is not paid attention. Whether or not the coarse graining of this study is appropriate is the major problem. Up to this time, however, it has been widely accepted because it leads to the phenomenological expression of the entropy production for various dynamical systems [12–14,23,24].

In this partitioning the Markov partition [7,23] is often used. For more complicated dynamical system, e.g. modified Lorentz equation of this study, however, it's not practical to divide the state space into the Markov partition and the state space is forced to be divided into the super cube (super cuboid). In this case, however, the limiting behavior of $\Delta \to 0$ is expected to be the same as that of Markov partition for wide class of dynamical systems. That is to say, both of the singularity due to the fractal structure described in Section 1 and the convenient partition which is independent of the vector field give the reason why the limiting behavior is focussed on. The indistinctness of the present coarse-graining in the same partition creates randomness. However this causes no problem when the limit as $\Delta \to 0$ is considered and, as above described, the difference in behaviors between $\Delta = 0$ and the limit as $\Delta \to 0$ explains the second law of thermodynamics.

The definition completely determines the coarse-grained dynamics. In this section we derive a governing equation of coarse-grained probability measure, and then the equation is theoretically shown to be in agreement with a difference scheme.

2.1. CGME and transition probability

It is well known that the equation for the probability density ρ of an D-dimensional ordinary differential equation system $\mathrm{d}\mathbf{x}/\mathrm{d}t = \mathbf{v}$ with a differentiable vector field $\mathbf{v} = (v_1, v_2, \ldots, v_D)$ is expressed as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0. \tag{1}$$

The equation is often referred to as "continuity equation" [1] and the equation has the physical meaning as the master equation without coarse graining (see Appendix A.1). The density ρ has the form to be

$$\rho(\mathbf{x}, t) = \mathrm{e}^{K(\mathbf{x},t)}\rho(T^{-t}\mathbf{x}, 0), \tag{2}$$

where

$$K(\mathbf{x}, t) = -\int_0^t (\nabla \cdot \mathbf{v})(T^{-s}\mathbf{x})\,\mathrm{d}s,$$

and T^t is the time-evolution operator that moves a point to its t-evolved one along the trajectory. $(\nabla \cdot \mathbf{v})(\mathbf{x})$ is the value of $\nabla \cdot \mathbf{v}$ at $\mathbf{x}$. In this study $\mathbf{v}$ is assumed to be independent of t, i.e. $\mathbf{v} = \mathbf{v}(\mathbf{x})$. However the discussion below can be easily generalized for $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$.

Now we perform the coarse graining over the state space considered. At first, we divide the state space into N partitions $V_i\,(i = 1, 2, \ldots, N)$ so that they do not overlap with each other, and introduce the probability measure P_i on V_i, defined by

$$P_i \equiv \int_{V_i} \rho(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}. \tag{3}$$

Next, assuming the initial probability density on each partition is uniform or the variation of probability measure in each partition cannot be captured, we have the following difference between P_i's at $t = a$ and $t = b$ by integrating the continuity equation (1) with t over the surface S_i of V_i:

$$P_i(b) - P_i(a) = \sum_j \widehat{W}_{ij}^{(b-a)} P_j(a), \tag{4a}$$

where

$$\begin{aligned} \widehat{W}_{ij}^{(T)} &\equiv -\int_0^T \mathrm{d}t \int_{S_{ij}(t)} \mathrm{d}S \mathrm{e}^{K(\mathbf{x},t)} (\mathbf{v}\cdot\mathbf{n})/\Delta V_j, \\ S_{ij}(t) &= \left\{\mathbf{x} \in S_i : T^{-t}\mathbf{x} \in V_j\right\}, \end{aligned} \tag{4b}$$

and $\mathbf{n}$ and ΔV_j is the outward-pointing normal vector on S_i and the volume of the jth partition V_j, respectively.

The transition probability from jth to ith partition $W_{ij}^{(T)}$ for time span T is defined as the probability measure $P_i(T)$ when $P_j(0) = 1$. Therefore from Eq. (4a) we obtain

$$W_{ij}^{(T)} \equiv \begin{cases} \widehat{W}_{ij}^{(T)} : i \neq j, \\ 1 + \widehat{W}_{ii}^{(T)} : i = j. \end{cases} \tag{4b′}$$

We can easily ascertain that $\sum_i W_{ij}^{(T)} = 1$. Using the $W_{ij}^{(T)}$ we have an another expression of Eq. (4a):

$$\text{(ICGME)} \quad P_i(b) = \sum_j W_{ij}^{(b-a)} P_j(a). \tag{4a′}$$

Moreover, substituting from $a + \Delta t$ in b of Eq. (4a) and taking the limit as Δt approaches to zero, we obtain

$$\text{(CGME)} \quad \mathrm{d}P_i/\mathrm{d}t = \sum_j w_{ij} P_j - \sum_j w_{ji} P_i, \tag{5a}$$

where

$$w_{ij} \equiv \lim_{\Delta t \to 0} \widehat{W}_{ij}^{(\Delta t)}/\Delta t. \tag{5b}$$

It should be noted that (5) is satisfied when the probability density is uniform on all of the partitions at an instant. Therefore the continuous dynamical system governed by (5) expresses the coarse-grained dynamics of this study. Eq. (5a) is well known as one of master equations (abstract master equation [25]). For the reasons mentioned above Eq. (5a) is hereafter referred to as a coarse-grained master equation (CGME). If we observe the probability measure non-uniformized in a partition as time passes, this is due to the fact that state points in the partition are distinguishable, inconsistent with the postulate of the coarse graining of this study. Therefore, it is worthwhile noting that the evolved probability measure, forced to continually fulfill the CGME, corresponds to the measure with the postulate continually fulfilled.

Eq. (4a′), the time-integrated equation of Eq. (5a), is similarly referred to as an integrated CGME (ICGME) in this study. Their corresponding transition probabilities are given by Eqs. (4b′) and (5b). The convergence problem of Eq. (4a′) with respect to the representative partition size Δ has been resolved for natural invariant (steady) measures (SRB measure) of invertible maps including multifractal cases [26–28], and it is reasonable to assert that the CGME and ICGME can be used to evaluate the time-dependent probability measure that does not have an absolute continuous density even if they are derived from Eq. (1) with the definition (3).

2.2. CGME and first-order upwind difference scheme (UDS)

In the following we divide state space into N (super) rectangular solids with the same side widths Δ_i ($i = 1, \ldots, D$), parallel to the ith axis. From Eq. (4b) the transition probability (5b) can be expressed as

$$w_{ij} = \lim_{\Delta t \to 0} \widehat{W}_{ij}^{(\Delta t)}/\Delta t = -\lim_{\Delta t \to 0} \int_0^{\Delta t} \mathrm{d}t \int_{S_{ij}(t)} \mathrm{d}S\, \mathrm{e}^{K(\mathbf{x},t)}(\mathbf{v}\cdot\mathbf{n})/(\Delta V_j \Delta t), \tag{5b′}$$

where $\Delta V_j = \Delta V \equiv \Delta_1 \times \ldots \times \Delta_D$. The ith and jth partitions should adjoin to satisfy $w_{ij} \neq 0$, i.e. they should share $D-1$ dimensional region through which they contact with each other. Because if jth partition is apart from ith one $S_{ij}(t) = 0\left(\widehat{W}_{ij}^{(\Delta t)} = 0\right)$ when Δt is sufficiently small and, therefore, the probability is zero. And if they share a $D-2$ or smaller dimensional region on S_i, $S_{ij}(t)$ is $\mathrm{O}(\Delta t^a)$ ($a > 0$) and, therefore, $\widehat{W}_{ij}^{(\Delta t)}$ is $\mathrm{O}(\Delta t^b)$ ($b > 1$). Consequently w_{ij} goes to zero as Δt approaches to zero. Hereafter we focus on the discussion of w_{ij} for the adjoining partition sets (i,j).

If the surface S through which the partitions adjoin is normal to the mth direction, the outward-pointing component of vector $\mathbf{v}$ on S around its center for the ith partition can be expressed as follows:

$$(\mathbf{v}\cdot\mathbf{n})(\mathbf{x}) \equiv v_n(\mathbf{x}) = v_{n\mathrm{c}} + \left(\frac{\partial v_n}{\partial x_{k(\neq m)}}\right)_{\mathrm{c}} (x_k - x_{\mathrm{c}k}) + \frac{1}{2}\left(\frac{\partial^2 v_n}{\partial x_{k(\neq m)}\partial x_{l(\neq m)}}\right)_{\mathrm{c}} (x_k - x_{\mathrm{c}k})(x_l - x_{\mathrm{c}l}) + \mathrm{O}(\Delta^3), \tag{6}$$

where subscript c denotes the quantity at the center of the surface S and $\Delta \equiv \Delta V^{1/D}$ is the representative partition size. In this equation the possible summation with $k, l(\neq m)$ direction should be performed. Also we can obtain

$$\int_0^{\Delta t} \mathrm{e}^{K(\mathbf{x},t)}\mathrm{d}t = \Delta t - \frac{\Delta t^2}{2}(\nabla\cdot v)(\mathbf{x}) + \mathrm{O}(\Delta t^3). \tag{7}$$

Substituting from Eqs. (6) and (7) in Eq. (5b′) we obtain the transition probability w_{ij} as follows:

$$w_{ij} = -\frac{\alpha_1 S v_{n\mathrm{c}}}{\Delta V} - \frac{\alpha_2^{(k)}}{24}\left(\frac{\partial^2 v_n}{\partial x_{k(\neq m)}^2}\right)_{\mathrm{c}} \frac{\Delta_k^2 S}{\Delta V} - \beta_1^{(k)}\left(\frac{\partial v_n}{\partial x_{k(\neq m)}}\right)_{\mathrm{c}} \frac{\Delta_k S}{\Delta V} - \frac{\beta_2^{(k,l)}}{2}\left(\frac{\partial^2 v_n}{\partial x_{k(\neq m)}\partial x_{l(\neq m)}}\right)_{\mathrm{c}} \frac{\Delta_k \Delta_l S}{\Delta V} + \mathrm{O}(\Delta^2), \tag{8}$$

where $S(=\Delta V/\Delta_m)$ is the area of the surface S and

$$\alpha_1 \equiv \int_S I_{ij}\,\mathrm{d}S/S,$$
$$\alpha_2^{(k)} \equiv 12\int_S I_{ij}(x_k - x_{\mathrm{c}k})^2\,\mathrm{d}S/\Delta_k^2 S,$$
$$\beta_1^{(k)} \equiv \int_S I_{ij}(x_k - x_{\mathrm{c}k})\mathrm{d}S/\Delta_k S,$$
$$\beta_2^{(k,l)} \equiv \int_S I_{ij}(x_k - x_{\mathrm{c}k})(x_l - x_{\mathrm{c}l})(1-\delta_{kl})\mathrm{d}S/\Delta_k\Delta_l S.$$

Herein

$$I_{ij}(\mathbf{x}) \equiv \begin{cases} 1: & v_n(\mathbf{x}) < 0, \\ 0: & \text{otherwise.} \end{cases}$$

When Δ is sufficiently small, I_{ij} is uniform on S for almost entire set of (i, j). It follows that $\beta_1 = \beta_2^{(k)} = 0$ and

$$\alpha_1 = \alpha_2^{(k)} = \begin{cases} 1: & v_{n\mathrm{c}} < 0, \\ 0: & \text{otherwise.} \end{cases}$$

Therefore for almost all adjoining partition sets (i,j) we have

$$w_{ij} = \frac{1}{\Delta_m}\max(v_{j\to i,\mathrm{c}}, 0) + \frac{\mathrm{sgn}(v_{j\to i,\mathrm{c}}) + 1}{48}\left(\frac{\partial^2 v_{j\to i}}{\partial x_{k(\neq m)}^2}\right)_{\mathrm{c}} \frac{\Delta_k^2}{\Delta_m} + \mathrm{O}(\Delta^2) \equiv w'_{ij} + \mathrm{O}(\Delta), \tag{9}$$

where $v_{j\to i} \equiv -v_{nc}$ is the velocity component of $\mathbf{v}$ in the direction from the jth partition to the ith one. For another partition sets, as described above, the probability is zero. So we can omit the summation in Eq. (5a) for the sets.

On the other hand, if we regard the entire state space divided by the partitions as a grid, we can discretize the convection term of the continuity equation (1) on the space by the first-order upwind difference scheme based on the finite volume method. Fig. 1 shows the definition of physical quantities in the j direction around the basic ith cell when we use the staggered grid. Then we obtain the following discretized equation (UDS):

$$\begin{aligned}(\text{UDS})\quad \frac{\mathrm{d}\rho_i}{\mathrm{d}t} &\equiv -\sum_j \frac{J^+_{j,i} - J^-_{j,i}}{\Delta_j} \\ &= -\sum_j \left[\left(\max(v^+_{j,i},0)\rho_i - \max(-v^+_{j,i},0)\rho^+_{j,i}\right)/\Delta_j - \left(\max(v^-_{j,i},0)\rho^-_{j,i} - \max(-v^-_{j,i},0)\rho_i\right)/\Delta_j\right] \\ &= \sum_j \left[\max\left(v_{j^+\to i},0\right)\rho^+_{j,i} + \max\left(v_{j^-\to i},0\right)\rho^-_{j,i}\right]/\Delta_j - \sum_j \left[\max\left(v_{i\to j^+},0\right) + \max\left(v_{i\to j^-},0\right)\right]\rho_i/\Delta_j \\ &= \sum_{j,\mathrm{sign}} w'_{ij^{\mathrm{sign}}}\rho^{\mathrm{sign}}_{j,i} - \sum_{j,\mathrm{sign}} w'_{j^{\mathrm{sign}}i}\rho_i. \end{aligned} \tag{10}$$

Herein $v_{j^\pm\to i}$ denote the velocity component of $\mathbf{v}$ in the direction from the adjoining $j^\pm$th cell to its basic ith one, and "j, sign" expresses the summation with respect to possible cells adjoining the ith cell for all directions and sides. From Eqs. (5a), (9) and (10) the numerical solution of the continuity equation (1) discretized by the first-order upwind difference scheme (UDS) based on the (conservative) finite volume method agrees well with the numerical solution of CGME (5a) when Δ is sufficiently small and the initial and boundary conditions of P_i and ρ_i are identical. Thus, the UDS acquires physical substance on the coarse-grained system.

This fact does not assert that the time-dependent measure obtained by solving Eq. (5a) can be expressed by the probability density for small Δ, i.e. the measure has an absolute continuous density. It is clear that such a relation cannot be found when the continuity equation (1) is discretized by higher-order upwind difference schemes. Hence it should be emphasized that this coincidence is only numerical and has been verified by authors [21] (see also Appendix A).

2.3. Coarse-grained entropy

In this study an entropy on the coarse-grained system, defined by

$$S \equiv \sum_j P^*_j \ln(P_j/\Delta V), \tag{11}$$

is introduced, where P^*_j is the invariant measure on the jth partition. The entropy differs from the conventional one in that P_j is partially replaced with P^*_j and is not multiplied by -1. The entropy corresponds to a member

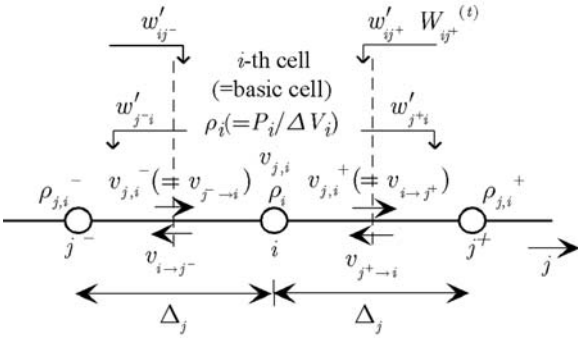

Fig. 1. Definition of physical quantities in the j direction around the basic ith cell on the staggered grid.

of a family of information for the coarse-grained system proposed by authors [21], generalized from an entropy functional on the invariant set proposed by Goldstein et al. [1]. The entropy does not involve the identification of the repelling area in the computational domain and is easy to compute its time variations. Moreover it provides the time-dependent measure on the most probable region that affects the behavior of macroscopic observables [21]. In the (non-equilibrium) steady state the entropy agrees with the conventional coarse-grained entropy times -1 [7,12]. Using the entropy the numerical solutions of UDS (CGME) will be shown to have the physical property that the conventional entropy production corresponds with the average volume contraction rate in the state.

2.3.1. Coarse-grained entropy and its increasing rate

When we evaluate the probability measure P_j on the jth partition by solving UDS (10) and denote the (coarse-grained) probability density $P_j/\Delta V$ by ρ_j its increasing rate is expressed as

$$\frac{\mathrm{d}\rho_j}{\mathrm{d}t} = -\frac{1}{\Delta_k}\left(\frac{\rho^+_{k,j}+\rho_j}{2}v^+_{k,j} - \frac{\rho_j+\rho^-_{k,j}}{2}v^-_{k,j}\right) + \frac{\widehat{J}^+_{k,j}-\widehat{J}^-_{k,j}}{\Delta_k} \equiv C_j + D_j, \tag{12}$$

where

$$\widehat{J}^{\pm}_{k,j} \equiv \pm\frac{|v^{\pm}_{k,j}|\Delta_k}{2}\frac{\rho^{\pm}_{k,j}-\rho_j}{\Delta_k}.$$

In Eq. (12) the possible summation with k-direction should be performed. Therefore, the increasing rate of the entropy S becomes

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_j \frac{P^*_j}{\rho_j}(C_j + D_j) \equiv K_0 + K_1. \tag{13}$$

The term K_1 in Eq. (13) can be divided into two parts as follows:

$$K_1 = \sum_j \frac{P^*_j}{\rho_j}\left(D_{1_j} + D_{2j}\right) \equiv K_{11} + K_{12}, \tag{14}$$

where

$$D_{1j} \equiv \frac{\rho_j}{\Delta_k}\left[\frac{2}{\rho^+_{k,j}+\rho_j}\widehat{J}^+_{k,j} - \frac{2}{\rho_j+\rho^-_{k,j}}\widehat{J}^-_{k,j}\right],$$

$$D_{2j} \equiv \frac{1}{2}\left[\frac{|v^+_{k,j}|\Delta_k}{2}\frac{2}{\rho^+_{k,j}+\rho_j}\left(\frac{\rho^+_{k,j}-\rho_j}{\Delta_k}\right)^2 + \frac{|v^-_{k,j}|\Delta_k}{2}\frac{2}{\rho_j+\rho^-_{k,j}}\left(\frac{\rho_j-\rho^-_{k,j}}{\Delta_k}\right)^2\right].$$

Herein K's formally coincide with the discretized form of the following:

$$K_0 \sim \int_{V^*} -\frac{\rho^*}{\rho}\nabla\cdot(\rho\mathbf{v})\,\mathrm{d}V,$$

$$K_1 \sim \int_{V^*} \frac{\rho^*}{\rho}\frac{\partial}{\partial x_j}\left(\frac{|v_j|\Delta_j}{2}\frac{\partial\rho}{\partial x_j}\right)\mathrm{d}V,$$

$$K_{11} \sim \int_{V^*} \rho^*\frac{\partial}{\partial x_j}\left(\frac{|v_j|\Delta_j}{2}\frac{1}{\rho}\frac{\partial\rho}{\partial x_j}\right)\mathrm{d}V,$$

$$K_{12} \sim \int_{V^*} \frac{|v_j|\Delta_j}{2}\frac{\rho^*}{\rho^2}\left(\frac{\partial\rho}{\partial x_j}\right)^2\mathrm{d}V,$$

where V^* and ρ^* denote the invariant set and invariant (steady) probability density. Note that they are formal expressions because the probability density is not necessarily absolutely continuous as t goes to infinity as mentioned above. K_{11} and K_{12} correspond to the rate of increase by the entropy flow and the entropy production, respectively.

2.3.2. Entropy production in non-equilibrium steady state

In non-equilibrium steady state the coarse-grained entropy production is known to be equal to the average volume contraction rate [2]. As mentioned in Section 1 the relation is very essential for non-equilibrium statistical mechanics and the UDS is verified to be suitable for the coarse-grained dynamics provided the UDS fulfills the relation. In this section we will confirm that the coarse-grained steady entropy production K_{12}^* fully agrees with the corresponding average volume contraction rate based on the formulation of UDS (CGME).

From Eqs. (12)–(14) K_0^* and K_1^* satisfies $K_0^* + K_1^* = 0$ in the steady state, where the superscript * indicates quantities in the state. And we can easily obtain

$$K_{11}^* = \langle \nabla \cdot \mathbf{v} \rangle_c^* + K_0^* + K_1^* + I_1^* + I_2^* + I_3^* + I_4^*, \tag{15a}$$

where

$$\langle \nabla \cdot \mathbf{v} \rangle_c^* \equiv \sum_j \Delta V \rho_j \frac{v_{k,j}^+ - v_{k,j}^-}{\Delta_k}, \tag{15b}$$

$$I_1^* \equiv -\sum_j \frac{\Delta V}{\Delta_k} \left(D_{k,j}^+ \frac{\phi(\rho_{k,j}^+) + \phi(\rho_j)}{2} \frac{\rho_{k,j}^+ - \rho_j}{\Delta_k} - D_{k,j}^- \frac{\phi(\rho_j) + \phi(\rho_{k,j}^-)}{2} \frac{\rho_j - \rho_{k,j}^-}{\Delta_k} \right), \tag{15c}$$

$$I_2^* \equiv \sum_j \frac{\Delta V}{\Delta_k} \left(\frac{\phi(\rho_{k,j}^+) + \phi(\rho_j)}{2} \frac{\rho_{k,j}^+ + \rho_j}{2} v_{k,j}^+ - \frac{\phi(\rho_j) + \phi(\rho_{k,j}^-)}{2} \frac{\rho_j + \rho_{k,j}^-}{2} v_{k,j}^- \right), \tag{15d}$$

$$I_3^* \equiv \sum_j \frac{\Delta V}{\Delta_k} \left(r_{k,j}^+ D_{k,j}^+ \frac{\rho_{k,j}^+ - \rho_j}{\Delta_k} - r_{k,j}^- D_{k,j}^- \frac{\rho_j - \rho_{k,j}^-}{\Delta_k} \right), \tag{15e}$$

$$I_4^* \equiv -\sum_j \frac{\Delta V}{\Delta_k} \left(r_{k,j}^+ \frac{\rho_{k,j}^+ + \rho_j}{2} v_{k,j}^+ - r_{k,j}^- \frac{\rho_j + \rho_{k,j}^-}{2} v_{k,j}^- \right). \tag{15f}$$

In these equations the superscript $*$ is omitted for the probability density ρ. Herein $D_{k,j}^\pm$ and $r_{k,j}^\pm$ are defined by

$$D_{k,j}^\pm \equiv \frac{|v_{k,j}^\pm| \Delta_k}{2},$$

$$r_{k,j}^\pm \equiv \pm \frac{\phi(\rho_{k,j}^\pm) - \phi(\rho_j)}{2} \pm \frac{\rho_j - \rho_{k,j}^\pm}{\rho_j + \rho_{k,j}^\pm},$$

and $\phi = \phi(x)$ is an arbitrary function of x, evaluated on each partition, such that the following condition is satisfied:

$$\lim_{x \to 0} x\phi(x) = 0.$$

In Eq. (15a) the average volume expansion rate, defined in Eq. (15b), appears.

For a sufficiently large space the density and its gradient can be regarded as zero on the boundary. From Eqs. (13) and (15c)–(15f), K_0^*, K_1^* and $I_1^* \sim I_4^*$ can reduce to the surface integral (summation) on the boundary and, therefore, equal zero. Consequently the entropy production term K_{12}^* satisfies

$$K_{12}^* = K_1^* - K_{11}^* = -K_{11}^* = -\langle \nabla \cdot \mathbf{v} \rangle_c^*. \tag{16}$$

From Eqs. (15) and (16) the term fully agrees with the discretized average volume contraction rate. Therefore, the entropy production evaluated by the UDS agrees with the average volume contraction rate. It should be noted that the agreement is independent of the partition scale Δ. This property is essential for the coarse-grained dynamics.

If the boundary condition of probability measure is periodic the condition for ϕ is needless to hold Eq. (16) and ϕ is genuine arbitrary. Such degrees of freedom of ϕ is surprising because we can easily ascertain that $\phi(x) = \ln(x)$ for the continuous dynamics from the formal continuous expression of K_{11} (K_{12}) mentioned above.

Eq. (16) is numerically confirmed in Fig. 2. The model equation and computational method are based on those proposed by authors [21]: the equation is a modified Lorentz model, defined by

$$dx/dt = \sigma z(y - x), \quad dy/dt = x(R - z) - y, \quad dz/dt = xy - bz,$$

where $\sigma = 0.1465$, $R = 45.92$, $b = 4.0$. Unlike the original Lorentz model, it does not have uniform volume expansion rate, i.e. the rate is a function of $\mathbf{x}$, and is suitable for the discussion on Eq. (16). The computational domain was taken to be $-60 \leqslant x \leqslant 60$, $-90 \leqslant y \leqslant 90$, $-25 \leqslant z \leqslant 155$ so that the high probability region is included and that the density gradient on the boundary is sufficiently small. The boundary condition of the probability measure is zero and the initial distribution of the measure, generated by random numbers [29], is not uniform. The partitions are the super cubes of the same side width $\Delta_i = 1.5$ ($i = 1, 2, 3$). The time integration was performed by the first-order explicit method and time increment $\Delta t = 5.0 \times 10^{-5}$. It should be noted that the computational domain has a repelling area and the total probability on the domain is not preserved. That is why the probability measure was normalized by the total probability in the steady state. The normalization corresponds to make the initial probability measure in the repelling area set to zero. Note that the operation does not affect the evaluation of the entropy (11). It is one of the merits to compute the time-variation of the entropy. The determination of the steady state was based on a global indicator:

$$I_{\mathrm{gc}} \equiv \sum_{j(P_j \neq 0)} (\mathrm{d}P_j/\mathrm{d}t)^2 / P_j,$$

and the exponential escape rate λ of probability from the computational domain. In the present computation the state that $I_{\mathrm{gc}} < 5.0 \times 10^{-5}$ and $\lambda < 5.0 \times 10^{-5}$ was determined to be the 'de facto' steady state.

Fig. 2 shows the time variation of K's (Eqs. (13) and (14)), in addition to the average volume contraction rate in the steady state. For $t < 0.1$ the figure shows K_0 approaches to the average volume contraction rate owing to the entropy production K_1 (K_{12}). As described in Ishida and Kimoto [21] this is a part of the phenomena caused by the uniformization of probability density on the invariant set. The uniformization is expected to explain the mechanism that makes the mesoscopic level difference of initial distribution lose and realizes the same macroscopic unsteady state if its macroscopic initial state is identical as irreversible processes go [21]. For $t > 1$ the K's take on the constant value: the terms K_0 and K_1 go to zero and the entropy production K_{12} goes to the average volume contraction rate. The former ensures that UDS goes to the continuity equation (1) as Δ decreases, and the latter makes satisfy the condition (16) in the non-equilibrium steady state. Thus, the UDS combines the discretization scheme of the continuity equation (1) with the coarse-grained master equation (5a).

3. Discussion – applicability of UDS

3.1. Merits and demerits of UDS

This study addresses the initial-boundary value problems of the probability measure on the state space when the partition size Δ is small, based on the above-described coarse graining, and differentiable vector field $\mathbf{v}$ is given. Under the restrictions this study revealed that the method is superior to the numerical evaluation of transition probabilities by Monte-Carlo (MC) integration because these conditions diminish advantages to perform MC simulations.

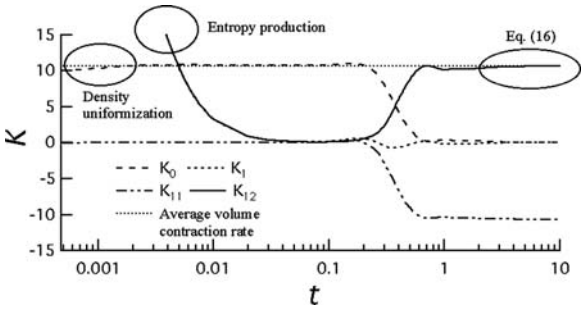

Fig. 2. Time variation of the terms that constitute the rate of increase of entropy.

As precisely shown in Section 2.2, the transition probability in the CGME vanishes for non-adjoining partition pairs, and the proposed UDS method just evaluates the remaining probabilities by the component of vector $\mathbf{v}$ normal to partition boundaries. Therefore, the method is effective even in multi-dimensional cases. On the other hand, the MC integration to evaluate the probabilities needs positive Δt and, therefore, the increase of the number of partitions to which sample points move from a partition for the interval Δt requires additional memory to store the transition probabilities. The MC integration evaluating the probabilities at every time step can save such memories. But the method takes enormous time and the resultant meaningless fluctuation of the probabilities makes it impossible to evaluate the lower probability measure accurately.

This study does not discuss on the fluctuation or noise [16–20] originated from the uncertainty of state on an incomplete state space, e.g. chemical master equation (CME), because this study deal with the time-evolution of the probability measure on the (complete) state space. Such a fluctuation generally requires observations on the level of noise as the partition size or time step changes [16]. But they are needless in this study. The UDS's superiority to the MC is not affected by the time step if only the partition size Δ is sufficiently small.

In addition, the UDS has the desirable properties based on the coarse graining of this study, e.g. the entropy production agrees with the average volume contraction rate in non-equilibrium steady state. We can confirm the physical necessity of the UDS to appear in coarse-grained dynamics, discussed in Appendix A.2.

Above-described merits and demerits of the UDS are summarized as follows:

3.1.1. Merits

(1) The transition probability can be evaluated immediately even in multi-dimensional cases when a differentiable vector field $\mathbf{v}$ is given and Δ is sufficiently small.
(2) The storage to save the probabilities becomes minimum.
(3) The fundamental properties based on the coarse graining of this study are retained.
(4) The method has advantages in solving the initial-boundary value problems of coarse-grained probability measure on the state space.
(5) The evaluation of transition probabilities causes no fluctuations. This is essential for the time-evolution of the lower probability measure.

3.1.2. Demerits

(1) In general it is impractical to handle state spaces. Because they are higher dimensional. The method is not directly applicable to the master equation on incomplete state spaces, on which the probability measure can fluctuate.
(2) There are many cases in which Δ cannot be sufficiently small. In this situation the Monte-Carlo integration is substantially superior.

Even if the vector field $\mathbf{v}$ is discontinuous, the method of UDS is effective if such a field is piecewise differentiable. However the method is not applicable if the field is not differentiable in any open region. In this case Monte-Carlo integration is useful. The condition of "differentiable" vector field may be relaxed to "continuous" one. But it remains the issue of future works.

3.2. Applicability of UDS to various cases

In this study we propose a method to solve the governing equation of the coarse grained probability measure CGME by replacing the equation with the UDS. The method is very effective on the state space as this study addresses. Conversely the method is not directly applicable when there is the fluctuation or noise of the probability measure caused by the uncertainty of the state, such as a chemical master equation (CME). In this

case, however, the method can be also effective when we are to obtain the evolved probability measure with an appropriate partition scale Δ and time step Δt.

If the given (ensemble-averaged) dynamics is chaotic and dissipative on a space, the probability density cannot be generally defined on the space, but the probability measure can be defined. In order to obtain the measure numerically the space should be divided into some partitions, represented by the scale Δ, and the measure on each partition should be evaluated. In this case we cannot capture the inner structure of the probability measure in a partition, but the scale Δ can be taken to be sufficiently small if needed. The situation corresponds to the coarse graining of this study.

Then the UDS is widely applicable provided we can specify the appropriate value of Δ and Δt so that the master equation can be approximated by the UDS: (1) the partition is super-cuboid and its scale Δ is sufficiently small, and (2) vector field $\mathbf{v}$ is spatially differentiable. It is the distinctive merit of the UDS that it simply requests v_n, the component of vector $\mathbf{v}$ normal to a partition boundary positioned at its center, to evaluate transition probabilities (w'_{ij}). Even for the case of CME, not defined on a state space, every method to obtain a realization, e.g. τ-leap method [15], can be utilized to evaluate the vector $\mathbf{v}$ and v_n from the change of position $\Delta\mathbf{x}$ divided by the time step Δt at the center of a partition and, as a consequence, the transition probabilities are obtained. The total amount of Monte-Carlo operations to simply evaluate the normal component of the vector $\mathbf{v}$ from realizations at a specific position would be smaller than those to evaluate the transition probability between an adjoining set of partitions, i.e. Monte-Carlo integration. Thus the effective method to obtain an evolved probability measure on any space can be developed by the UDS in conjunction with the every method to obtain a realization.

The remaining problem is how the partition size Δ and the time step Δt are determined for such a case of CME. The size Δ is desirable to be large enough both to confine the total amount of computation and to regard the vector field $\mathbf{v}$, evaluated by $\Delta\mathbf{x}/\Delta t$, as continuous and differentiable on the scale of Δ. At the same time Δ should be small enough to satisfy the condition for the UDS. Similarly, Δt needs to be large enough to regard the vector field $\mathbf{v}$ as spatially differentiable. Such a field $\mathbf{v}$ is a ensemble-averaged or lowpass-filtered quantity, and the τ-leap-based methods [15,18–20] are suitable for the evaluation of the change in the state $\Delta\mathbf{x}$ for a relatively large time interval Δt. Conversely, if Δt is taken to be too large, such a simulation cannot reproduce the original fluctuation (noise) of the probability measure. The problem of how Δ and Δt should be taken and of whether or not the UDS is effective in various cases remains the issue to be addressed in the future.

4. Concluding remarks

This study addresses the initial-boundary value problem of coarse-grained probability measure on the state space in which the differentiable vector field $\mathbf{v}$ is given. The coarse graining of this study is based on a principle that we cannot distinguish state points in the same partition with each other. This is based on the formulation of the non-equilibrium statistical mechanics to resolve the macroscopic irreversibility. The definition determines the mathematical form of the coarse-grained master equations (CGME), and the equation is theoretically shown to be equivalent to the differenced continuity equation using the first-order upwind difference scheme (UDS) based on the finite volume method. The difference is the order of partition size Δ and is negligible when Δ is sufficiently small. Moreover the entropy production evaluated by the UDS is also shown to be in accord with the average volume contraction rate in the steady state. This is essential for the non-equilibrium statistical dynamics, and was confirmed numerically in this study. As a result, the UDS is shown to have physical substance in the coarse-grained dynamics. Under the coarse graining the UDS is very superior to the conventional Monte-Carlo method in computer time and storage and is very useful to solve the CGME.

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Appendix A. UDS and other expressions

A.1. UDS, ICGME and Fokker–Planck equation

In the conventional method the transition probability is evaluated by the Monte-Carlo method [26]. In this case ICGME (4a′) is more useful than CGME (5a). Because the transition probability $W_{ij}^{(T)}$ in Eq. (4a′) can be easily evaluated by the ratio of the number of particles in the ith partition after time T to that of initial particles positioned randomly in the jth partition, where each point is evolved by $\mathrm{d}\mathbf{x}/\mathrm{d}t = \mathbf{v}$. However it is worthwhile noting that the (analytical) solution of the ICGME differs from that of the CGME (UDS) because $W_{ij}^{(T)}$ generally differs from $w_{ij}T$ when $T > 0$. The present computational method based on the UDS has been verified through the comparison with the ICGME whose transition probability is evaluated by the conventional Monte-Carlo method [21]. Therefore the difference in these methods needs to be discussed here.

Applying similar formulation in Sections 2.2 and 2.3 to the ICGME (4a′) with $a = t$ and $b = t + \Delta t$, we can obtain the following (formally) equivalent partial differential equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho v_j) = \frac{\partial}{\partial x_j}\left[\left(1 - \frac{\Delta t}{2}\nabla \cdot \mathbf{v}\right)\frac{|v_j|\Delta_j}{2}\frac{\partial \rho}{\partial x_j} - \frac{v_j v_k \Delta t}{2}\frac{\partial \rho}{\partial x_k}\right] + \mathrm{O}(\Delta t^2, \Delta^2). \tag{17}$$

In this equation ρ_i is defined by $P_i/\Delta V_i$. Similarly, from Eq. (12) the UDS (10) can be expressed as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho v_j) = \frac{\partial}{\partial x_j}\left[\frac{|v_j|\Delta_j}{2}\frac{\partial \rho}{\partial x_j}\right] + \mathrm{O}(\Delta^2). \tag{18}$$

From Eqs. (17) and (18) we can find that Δt should be sufficiently smaller than Δ to ensure that both of the numerical solutions agree well, i.e. $\Delta t/\Delta$ should goes to zero as Δ goes to zero. Needless to say that the condition is stricter than that of the stability condition of the UDS, e.g. $\Delta t/\Delta < a$ for the first-order explicit method. For the case of the Lorentz model the agreement has been ascertained for $\Delta = 1.5$ and $\Delta t = 1.0 \times 10^{-3}$.

As mentioned above, the ICGME and CGME (UDS) are applicable to evaluate the probability measure that does not have continuous density, e.g. the measure on a fractal support. Therefore Eqs. (17) and (18) are merely formal expressions. From Eq. (18), however, we can find that the UDS corresponds to the Fokker–Planck equation [25,30]. Because a half of the second moment of the transition probability in the jth direction on the ith partition $\Gamma_{j,i}$ satisfies

$$\begin{aligned} 2\Gamma_{j,i} &= \lim_{\Delta t \to 0} \langle \Delta x_j^2 \rangle / \Delta t = \lim_{\Delta t \to 0} \left[\Delta_j^2 (W_{j^+ i}^{(\Delta t)} + W_{j^- i}^{(\Delta t)}) + 0^2 W_{ii}\right] / \Delta t \\ &= \lim_{\Delta t \to 0} \Delta_j \Delta t \left(\max\left(v_{j,i}^+, 0\right) + \max\left(-v_{j,i}^-, 0\right)\right) / \Delta t, \end{aligned} \tag{19}$$

and, therefore, $\Gamma_{j,i} = |v_{j,i}|\ \Delta_j/2$ when Δ is sufficiently small. The evaluation (19) is based on the principle of the coarse graining of this study. That is to say, the variation of the moving distance of a reference particle in the jth direction Δx_j is ignored when the particle is in the same partition, and Δx_j^2 is Δ_j^2 if and only if the particle moves from a partition to a neighboring one in the jth direction. And we are again convinced that the first-order upwind difference scheme has the physical meaning on the coarse-grained dynamics. Without the coarse graining $\Delta x_j^2 = |v_{j,i}|^2 \Delta t^2$, and the second (or higher) moment goes to zero. In this case the derived equation (master equation) becomes to be the continuity equation (1).

A.2. UDS and other first-order approximated difference schemes

The expression of the UDS, the approximated equation of the CGME, is not a mere approximation of the continuity equation, i.e. the governing equation of probability density without coarse graining. Such an approximated equation should (1) retain the original meaning of the coarse graining and (2) has the desirable limiting property as $\Delta \to 0$. The expression of the UDS happens to be an approximated continuity equation discretized by the first-order upwind difference scheme based on the finite volume method (FVM), and to have a false diffusion term to explain the entropy production. Therefore, it is worthwhile clarifying here that only the UDS in the first-order approximated equations based on the FVM satisfy the above conditions.

A.2.1. General expression of the flux $\rho\mathbf{v}$ in continuity equation

Now we are to derive the general expression of the approximated continuity equation. If the flux **J** is defined as $\mathbf{J} \equiv \rho\mathbf{v}$, its j direction component J_j at the center of the partition boundary which separates two partitions adjoining in the j direction should be expressed as $J_j = f(v_j, \Delta_j, \rho^+, \rho^-)$. The quantities are defined in Fig. 3, focussed on around the j direction boundary shown in Fig. 1. This is because **J** is related to the probability flow and the transition probability w_{ij} is zero except the adjoining partition sets (i,j). If J_j is a function of density ρ in addition to ρ^+ and ρ^-, the transition probabilities between the possible combinations of the partitions to which the three densities attribute are not zero. One of them, at least, is the transition probability between a non-adjoining partition set, inconsistent with the property of w_{ij}.

From the definition of the flux **J** it is natural that J_j satisfies the following condition:

$$aJ_j + bC(v_j, \Delta_j) = J_j(v_j, \Delta_j, a\rho^+ + b, a\rho^- + b). \tag{20}$$

Differentiation of Eq. (20) with respect to a or b, and substitution of $a = 1$ and $b = 0$ leads to

$$J_j = \frac{\partial J_j}{\partial \rho^-}\rho^- + \frac{\partial J_j}{\partial \rho^+}\rho^+, \tag{21a}$$

$$\frac{\partial J_j}{\partial \rho^-} + \frac{\partial J_j}{\partial \rho^+} = C(v_j, \Delta_j). \tag{21b}$$

The differential of Eqs. (21a) and (21b) with respect to $\rho^\pm$ reduces to:

$$\frac{\partial^2 J_j}{\partial \rho^{-2}} = \frac{\partial^2 J_j}{\partial \rho^- \partial \rho^+} = \frac{\partial^2 J_j}{\partial \rho^{+2}} = 0. \tag{22}$$

From Eq. (22) we obtain

$$\frac{\partial J_j}{\partial \rho^-} = C^-(v_j, \Delta_j), \tag{23a}$$

$$\frac{\partial J_j}{\partial \rho^+} = C^+(v_j, \Delta_j). \tag{23b}$$

Substituting from Eq. (23) in Eq. (21a) we have

$$J_j = C^-(v_j, \Delta_j)\rho^- + C^+(v_j, \Delta_j)\rho^+ = C^-(|v_j|, \Delta_j, s)\rho^- + C^+(|v_j|, \Delta_j, s)\rho^+, \tag{24}$$

where s (+1 or −1) is the sign of v_j. When we rewrite Eq. (24) as

$$J_j/|v_j| = \chi^-(|v_j|, \Delta_j, s)\rho^- + \chi^+(|v_j|, \Delta_j, s)\rho^+, \tag{24′}$$

the coefficient $\chi^\pm$ is dimensionless from the definition of J_j. If we take $|v_j|$ and Δ_j as primary quantities, the dimensionless coefficient is a function of only the sign s from Buckingham's Π theorem. Referring to the discussion of Patankar [31], the condition that $J_j = \rho v_j$ for the case of $\rho = \rho^+ = \rho^-$ and the consistency for the coordinate inversion, we obtain $\chi^\pm = \mp\alpha + s/2$ with an arbitrary real number α. As a consequence, we have the following general expression:

$$J_j = \left(\alpha|v_j| + \frac{v_j}{2}\right)\rho^- - \left(\alpha|v_j| - \frac{v_j}{2}\right)\rho^+. \tag{25}$$

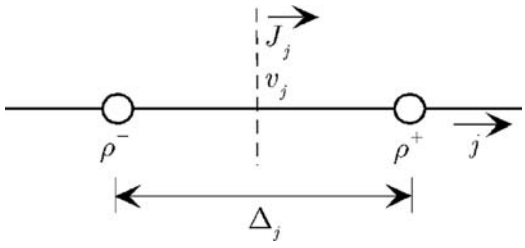

Fig. 3. Definition of physical quantities around two partition boundary.

In Eq. (25) $\alpha = 1/2$ and 0 correspond to the first-order upwind difference scheme and central difference scheme, respectively.

From Eq. (25) and the definition in Fig. 1 the approximated continuity equation based on the FVM, a general form of the governing equation of the coarse-grained density ρ_i (12), can be expressed as

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\frac{1}{\Delta_j}\left(\frac{\rho^+_{j,i}+\rho_i}{2}v^+_{j,i} - \frac{\rho_i+\rho^-_{j,i}}{2}v^-_{j,i}\right) + \frac{\varphi^+_{j,i}-\varphi^-_{j,i}}{\Delta_j}, \tag{26}$$

where

$$\varphi^{\pm}_{j,i} \equiv \pm\alpha|v^{\pm}_{j,i}|\Delta_j\frac{\rho^{\pm}_{j,i}-\rho_i}{\Delta_j}.$$

Eq. (26) has a (false) diffusion term and, therefore, any first-order approximated continuity equation apparently explains the entropy production term K_{12}. However the discussion is wrong.

A.2.2. Significance of UDS among other schemes as an approximated equation of the CGME

As described above, the physically significant equation for the probability measure is not the continuity equation but the CGME. The UDS is the approximated equation of not the continuity equation but the CGME. We can show that the UDS is the only difference scheme to approximate the CGME as follows.

From the general expression (26) we have the following generalized CGME, corresponding to the CGME (5a):

$$\mathrm{d}P_i/\mathrm{d}t = \sum_j w''_{ij}P_j - \sum_j w''_{ji}P_i, \tag{27}$$

where

$$w''_{ij} = \frac{1}{\Delta_m}\left[\max(v_{j\to i,c},0) + \left(\alpha-\frac{1}{2}\right)|v_{j\to i,c}|\right], \tag{28}$$

and the quantities in Eq. (28) is based on those used in Eq. (9).

On the other hand, Eq. (28) should take the form of Eq. (9) for Eq. (27) to be an approximated equation of the CGME (5a). The second term of the right hand side of Eq. (28) has the same order of the first one. Therefore, the condition leads to $\alpha = 1/2$. That is to say, the generalized CGME must be the UDS. This is the physical necessity of the UDS: this is the only difference scheme to retain the original meaning of the coarse-graining and to approximate its resultant governing equation CGME.

In Section 2.3.2 we show the UDS has the desirable property that the entropy production equals the average volume contraction rate. Moreover, the property for the fixed point in the state space as $\Delta \to 0$ also clarify the physical necessity of the UDS.

Now we assume that there is a stable sink, fixed point at which all of the trajectories near the point gather. We perform the coarse graining and set Δ to be sufficiently small. Providing the fixed point is centered by the ith partition and $P_j = \delta_{ij}$, Eq. (27) leads to

$$\frac{\mathrm{d}P_i}{\mathrm{d}t} = (2\alpha-1)\frac{v^+_{j,i}-v^-_{j,i}}{2\Delta_j}P_i. \tag{29}$$

Herein the relation that $v^+_{j,i} < 0$ and $v^-_{j,i} > 0$ is used. In this situation P_i should be held fixed at one because the invariant probability density approaches to Dirac's delta function as $\Delta \to 0$. In order to fulfill the condition, α should be 1/2 again, i.e. the difference scheme should be the UDS. If $\alpha < 1/2$ the right hand side of Eq. (29) positive and P_i exponentially diverges. The diverse causes minus probability measure around the ith partition, inconsistent with the physical law. Conversely, if $\alpha > 1/2$ P_i exponentially decreases and the change is dissipative.

The expressions (12) and (18) makes the diffusion term appeared and are useful to understand the diffusion effects in the CGME. However, it should be noted that the understanding owes to the expression of the UDS because we cannot obtain any more from the expression of CGME (5a). As mentioned above, we must note

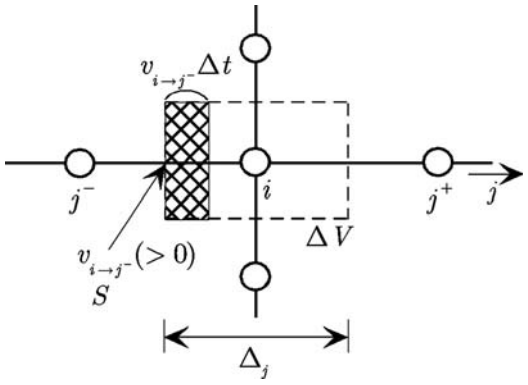

Fig. 4. Definition of quantities on a grid divided by imaginary partitions.

that its "diffusion" term does not simply play a role in diffusion: it's directive and can contribute to the concentration. This is also the significant property of the CGME and also clarify the physical necessity of the UDS.

A.3. UDS and master equation defined on grid

The derivation of CGME (5a) cannot be comparative with another ones. However its approximated equation UDS (10) can be derived along the line of the derivation of the master equation from a difference equation, e.g. [32], and the equation can be interpreted as a master equation defined on a D dimensional grid, shown in Fig. 4. It may be useful to understand the expression of the UDS.

At first, we set an imaginary partition boundary so as to evaluate transition probability w_{ij}. The boundary is expressed by the dotted line in Fig. 4, and its enclosed volume is ΔV. If the representative velocity from ith to j^-th point $v_{i\to j-}$, defined on the boundary center, is positive, the state points in the shaded region moves to the adjoining partition centered by j^-th point for the interval Δt. Provided the state points in the same partition is indistinguishable, the transition probability for Δt, denoted by $W^{(\Delta t)}_{j^-i}$, can be evaluated as the ratio of the region to the partition volume. Conversely, if $v_{i\to j-}$ is less than or equal to zero, the transition probability should be zero. Consequently, we have

$$W^{(\Delta t)}_{j^-i} = \max\left(Sv_{i\to j^-}\Delta t/\Delta V, 0\right) = \frac{\Delta t}{\Delta_j}\max\left(v_{i\to j^-}, 0\right), \tag{30}$$

where S is the area of the boundary adjoining imaginary two partitions centered by the points i and j^-. From Eq. (30) we obtain the following transition probability per unit time

$$w_{j^-i} \equiv \lim_{\Delta t\to 0} W^{(\Delta t)}_{j^-i}/\Delta t = w'_{j^-i}, \tag{30'}$$

and the probability flow per unit time from i to j^-th point (partition) can be expressed as $w'_{j^-i}P_i$. The rate of increase of the probability measure P_i, defined on the ith point, is the summation of all of the probability flows to the point subtracted by those from the point. As a result, we recover the expression of the UDS (10) for the coarse-grained probability density $\rho_j \equiv P_j/\Delta V$.

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