Low-variance deviational simulation Monte Carlo

Thomas M. M. Homolle

Aeronautics and Astronautics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Nicolas G. Hadjiconstantinou

Mechanical Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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We present and discuss a particle simulation method for solving the Boltzmann equation which incorporates the variance reduction ideas presented in L. L. Baker and N. G. Hadjiconstantinou [Physics of Fluids 17, 051703 (2005)]. The variance reduction, achieved by simulating only the deviation from equilibrium, results in a significant computational efficiency advantage for low speed flows compared to traditional particle methods such as the direct simulation Monte Carlo (DSMC). More specifically, the proposed method can efficiently simulate arbitrarily small deviations from equilibrium (e.g., low flow speed) at a computational cost that does not scale with the magnitude of the deviation from equilibrium, while maintaining the basic algorithmic structure of DSMC. © 2007 American Institute of Physics. [DOI: 10.1063/1.2717721]

In a previous Letter, 1 Baker and Hadjiconstantinou presented a general variance reduction formulation for solving the Boltzmann equation which addresses the serious limitation suffered by Monte Carlo approaches in the limit of small deviation from equilibrium, e.g., low Mach number flow. More specifically, they showed that by simulating only the deviation from equilibrium, it is possible to construct Monte Carlo simulation methods that can capture arbitrarily small deviations from equilibrium at a computational cost that is independent of the magnitude of this deviation. This is in sharp contrast to regular Monte Carlo methods, such as the prevalent method for solving the Boltzmann equation known as direct simulation Monte Carlo² (DSMC), whose computational cost (at constant signal to noise ratio) increases sharply³ as the deviation from equilibrium decreases, making noise-free simulation of low-speed, or more generally lowsignal, flows very expensive and in some cases intractable.

The benefits of variance reduction were demonstrated in the original Letter¹ where the concept was applied to a finite volume formulation. Here we present a new particle method which incorporates variance reduction while retaining the algorithmic structure and most basic features of DSMC. As discussed before, ¹ particle methods have a number of advantages which include simplicity, an intuitive formulation which naturally employs importance sampling, and low memory usage. Moreover, their natural treatment of the advection process means that they can easily handle and accurately capture traveling discontinuities in the distribution function.

We consider a hard-sphere⁴ gas of molecular mass m and hard-sphere diameter d, at a reference temperature T_0 and reference number density n_0 . The mean free path is given by $\lambda_0 = 1/(\sqrt{2}\pi n_0 d^2)$, the most probable molecular speed by $c_0 = \sqrt{2kT_0/m}$, and the molecular collision time by $\tau_0 = \sqrt{\pi}\lambda_0/(2c_0)$, respectively, where k is Boltzmann's constant. Let $f(\mathbf{r}, \mathbf{c}, t)$ be the velocity distribution function,⁴ where \mathbf{r}

=(x,y,z) is the position vector in physical space, $\mathbf{c} = (c_x,c_y,c_z)$ is the molecular velocity vector, and t is time. In the absence of external body forces, the Boltzmann equation can be written⁴ in the form

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} = \left[\frac{df}{dt} \right]_{\text{coll}} (\mathbf{r}, \mathbf{c}, t)$$

$$= \frac{1}{2} \int \int \int \left(\delta_2' + \delta_1' - \delta_2 - \delta_1 \right) f_1 f_2 g \sigma d^2 \Omega d^3 \mathbf{c}_1 d^3 \mathbf{c}_2,$$
(1)

where $\sigma = d^2/4$ is the differential collision cross section for hard spheres, $f_1 = f(\mathbf{r}, \mathbf{c}_1, t)$, $f_2 = f(\mathbf{r}, \mathbf{c}_2, t)$, $\delta_1 = \delta^3(\mathbf{c}_1 - \mathbf{c})$, $\delta_2 = \delta^3(\mathbf{c}_2 - \mathbf{c})$, $\delta_1' = \delta^3(\mathbf{c}_1' - \mathbf{c})$, and $\delta_2' = \delta^3(\mathbf{c}_2' - \mathbf{c})$. Here $\mathbf{c}_1, \mathbf{c}_2$ are the precollision velocities, $g = |\mathbf{c}_1 - \mathbf{c}_2|$ is the magnitude of the relative velocity vector, and $\mathbf{c}_1', \mathbf{c}_2'$ are the postcollision velocities, related to the precollision velocities through the scattering angle Ω . Here, and in the remainder of the paper, integration in velocity space extends from $-\infty$ to ∞ unless otherwise stated; similarly, the solid angle integration is over the surface of the unit sphere, unless otherwise stated.

DSMC solves⁵ the Boltzmann equation by simulating molecular motion as a series of collisionless advection and collision time steps of length Δt . During the collision step, binary collisions are processed between collision partners chosen at random within the same computational cell.² During the advection step, the positions of all particles are updated according to their velocities, while the velocities remain constant.²

As shown before, ¹ a variance-reduced formulation is obtained by considering the deviation $f^d \equiv f - f^{MB}$ from an *arbitrary* Maxwell-Boltzmann distribution (MBD),

$$f^{\text{MB}} = \frac{n_{\text{MB}}}{\pi^{3/2} c_{\text{MB}}^3} \exp \left[-\frac{(\mathbf{c} - \mathbf{u}_{\text{MB}})^2}{c_{\text{MB}}^2} \right].$$
 (2)

In the work that follows this distribution will be identified with the local equilibrium distribution and thus $c_{\rm MB} = \sqrt{2kT_{\rm MB}/m}$ is the most probable speed based on the local equilibrium temperature $T_{\rm MB}$, $\mathbf{u}_{\rm MB}$ is the local equilibrium flow velocity, and $n_{\rm MB}$ is the local equilibrium density. Upon substitution into Eq. (1), we obtain

$$\left[\frac{df^{d}}{dt}\right]_{\text{coll}}(\mathbf{r},\mathbf{c},t) = \left[\frac{df}{dt}\right]_{\text{coll}}(\mathbf{r},\mathbf{c},t) = \int \int \int (\delta'_{1} + \delta'_{2} - \delta_{1}) d^{3}\mathbf{c}_{1} d^{3}\mathbf{c}_{2} + \frac{1}{2} \int \int \int \int (\delta'_{1} + \delta'_{2} - \delta_{1} - \delta_{2}) f_{1}^{\text{MB}} f_{2}^{d} g \sigma d^{2} \Omega d^{3}\mathbf{c}_{1} d^{3}\mathbf{c}_{2} + \frac{1}{2} \int \int \int \int (\delta'_{1} + \delta'_{2} - \delta_{1} - \delta_{2}) f_{1}^{d} f_{2}^{d} g \sigma d^{2} \Omega d^{3}\mathbf{c}_{1} d^{3}\mathbf{c}_{2}$$

$$= \mathcal{L}(f^{d}) + \mathcal{J}(f^{d}, f^{d}) \tag{3}$$

since the integral involving $f_1^{\rm MB}f_2^{\rm MB}$ is identically zero. The last equality shows that the collision integral can be written as the sum of a linear $[\mathcal{L}(f^d)]$ and a quadratic $[\mathcal{J}(f^d, f^d)]$ term. We thus seek to develop a particle formulation in which particles simulate the deviation from equilibrium. Collision rules for the deviational particles are to be rigorously derived from the "new," variance-reduced collision integral [Eq. (3)]. Particles may be positive or negative, depending on the sign of the deviation from equilibrium at the location in phase space where the particle resides. As in DSMC, each computational deviational particle represents an effective number of physical deviational particles, denoted by $N_{\rm eff}$. In the present implementation, the effective number is common for all particles. Given $N_{\rm eff}$, the initial number of deviational particles is determined similarly to DSMC; the only difference is that its value is such that the simulation particles represent, at each value of the molecular velocity, the excess or deficit of particles (e.g., per unit volume) from the underlying MBD.

Based on our choice for the underlying equilibrium distribution, $f^{\rm MB}$, the advection step may be different^{6,7} from DSMC. We will discuss the advection step last, when our choice for $f^{\rm MB}$ has been explained.

The above form of the collision integral suggests that two types of collisions must be considered: those involving a deviational particle and the underlying MBD $(f_1^{\text{MB}}f_2^d)$, and those between two deviational particles $(f_1^lf_2^d)$. Let us consider the first type of collision briefly: from (3) we see that particle 1 drawn from f^{MB} collides with particle 2 drawn from f^d and leads to the creation of four particles: $\text{sgn}(f_2^d)\delta_1', \text{sgn}(f_2^d)\delta_2', -\text{sgn}(f_2^d)\delta_1, -\text{sgn}(f_2^d)\delta_2$. The existing particle 2 $[\text{sgn}(f_2^d)\delta_2]$ is cancelled by the new $-\text{sgn}(f_2^d)\delta_2$ particle, thus leading to a net creation of three particles. The $f_1^df_2^d$ term can be interpreted and implemented analogously. (Note that if $f^{\text{MB}} = 0$, $f^d > 0$, we recover DSMC, where the newly created particles $-\delta_1, -\delta_2$ cancel the colliding particles and thus the algorithm simply proceeds by updating particles $\delta_1, \delta_2 \rightarrow \delta_1', \delta_2'$.)

The deviational scheme just described has already been developed⁶ and extensively tested. It has been found⁶ to be very efficient for $Kn=\lambda_0/L \gtrsim 1$, where L is the flow charac-

teristic length scale; in this regime, the rate of particle-wall collision (which leads to significant particle cancellation) is sufficiently high for the number of deviational particles to stabilize. Unfortunately, for Kn < 1 the high rate of intermolecular collisions compared to collisions with the system walls leads to a high net rate of particle creation that results in a divergence in the number of particles, unless a particle cancellation scheme is introduced. Such a scheme was introduced and shown to be capable of stabilizing the calculation; unfortunately, particle cancellation schemes effectively introduce a velocity space discretization (with associated numerical error—particularly obvious in the higher moments of the distribution and storage requirements); this is a major disadvantage compared to DSMC, which does not require discretization of the velocity space.

The purpose of the present Letter is to describe an alternative, *rigorous* method for treating the collision step which removes the necessity for a cancellation step. In essence, the proposed technique *rigorously* avoids creating a large fraction of the deviational particles generated by the collision process by "consolidating" their net effect (after all possible cancellation has taken place) into a change in the local MBD.

In the interest of simplicity and because the major contribution of the present work is the treatment of the linear term $[\mathcal{L}(f^d)]$, we will focus on the linearized version of the Boltzmann equation. This choice is not restrictive since the present method has been developed for, and holds an advantage over DSMC, in cases where the deviation from equilibrium is small; this coincides with the regime where the contribution of the quadratic term is negligible. If desired, the proposed method may be extended to include the nonlinear part of the collision operator.

Particle cancellation at each time step is achieved by absorbing as large a fraction of the action of the collision operator over one time step as possible into a change of the underlying local MBD, and generating deviational particles to represent *only the remaining part* (that cannot be expressed as a change of the local MBD). The rationale for this choice is that the action of the collision operator is to drive the system towards local equilibrium, namely, a MBD. In other words, in a homogeneous calculation starting from a distribution away from equilibrium (and thus some arbitrary distribution of deviational particles) the action of the collision operator should be such that the final state is that of a local MBD—at the (conserved) system mass, momentum and energy—and zero deviational particles. To this end, we write

$$\mathcal{L}(f^d)\Delta t = \Delta f^{\text{MB}} + \Delta f^d, \tag{4}$$

where

$$\Delta f^{\text{MB}} = \left[\frac{1}{n_{\text{MB}}} \Delta n_{\text{MB}} + 2 \frac{\mathbf{c} - \mathbf{u}_{\text{MB}}}{c_{\text{MB}}^2} \cdot \Delta \mathbf{u}_{\text{MB}} + \frac{1}{c_{\text{MB}}} \left(2 \frac{(\mathbf{c} - \mathbf{u}_{\text{MB}})^2}{c_{\text{MB}}^2} - 3 \right) \Delta c_{\text{MB}} \right] f^{\text{MB}}.$$
 (5)

In other words, by changing the number density, mean velocity, and temperature of the local MBD, we absorb part of the action of the collision integral and, as will be seen later,

reduce the number of deviational particles generated drastically. A number of possibilities exist for choosing the amounts $\Delta n_{\rm MB}$, $\Delta {\bf u}_{\rm MB}$, $\Delta c_{\rm MB}$; the particular choice made in this work is explained below.

We proceed by writing

$$\mathcal{L}^{0}(f^{d}) = \int \left[K_{1}(\mathbf{c}, \mathbf{c}_{1}) - K_{2}(\mathbf{c}, \mathbf{c}_{1}) \right] f^{d}(\mathbf{c}_{1}) d^{3}\mathbf{c}_{1} - \nu(\mathbf{c}) f^{d}(\mathbf{c}), \quad (6)$$

where $K_1(\mathbf{c}, \mathbf{c}_1)$, $K_2(\mathbf{c}, \mathbf{c}_1)$, and $\nu(\mathbf{c})$ are given in a slightly different form by Cercignani⁴

$$K_{1}(\mathbf{c}, \mathbf{c}_{1}) = \sqrt{\frac{2}{\pi^{3}}} \frac{1}{\lambda_{0} c_{0}^{2}} \frac{1}{|\hat{\mathbf{c}} - \hat{\mathbf{c}}_{1}|} \exp \left[-\hat{\mathbf{c}}^{2} + \frac{(\hat{\mathbf{c}} \times \hat{\mathbf{c}}_{1})^{2}}{|\hat{\mathbf{c}} - \hat{\mathbf{c}}_{1}|^{2}} \right]$$

$$= \sqrt{\frac{2}{\pi^{3}}} \frac{1}{\lambda_{0} c_{0}^{2}} \frac{1}{|\hat{\mathbf{c}} - \hat{\mathbf{c}}_{1}|} \exp \left[-\frac{[\hat{\mathbf{c}} \cdot (\hat{\mathbf{c}} - \hat{\mathbf{c}}_{1})]^{2}}{|\hat{\mathbf{c}} - \hat{\mathbf{c}}_{1}|^{2}} \right],$$

$$K_{2}(\mathbf{c}, \mathbf{c}_{1}) = \sqrt{\frac{1}{2\pi^{3}}} \frac{1}{\lambda_{0} c_{0}^{2}} |\hat{\mathbf{c}} - \hat{\mathbf{c}}_{1}| \exp[-\hat{\mathbf{c}}^{2}], \qquad (7)$$

$$\nu(\mathbf{c}) = \sqrt{\frac{1}{2\pi}} \frac{c_{0}}{\lambda_{0}} \left[\exp[-\hat{\mathbf{c}}^{2}] + \left(2|\hat{\mathbf{c}}| + \frac{1}{|\hat{\mathbf{c}}|} \right) \times \int_{0}^{|\hat{\mathbf{c}}|} \exp[-\xi^{2}] d\xi \right]$$

and $\hat{\mathbf{c}} = \mathbf{c}/c_0$. The superscript/subscript 0 denotes that the collision integral has been linearized about the global equilibrium $f^0(\mathbf{c}) = n_0 (\pi c_0^2)^{-3/2} \exp[-\hat{\mathbf{c}}^2]$. The last term can be directly implemented as a particle sink (deletion). We thus focus on implementing the first two terms in Eq. (6) as a combined particle generation and local MBD change. This change is chosen such that it absorbs the mass, momentum, and energy change due to the action of the first two terms in Eq. (6); in other words,

$$\int \Delta f^{\text{MB}}\{1, \mathbf{c}, |\mathbf{c}|^2\} d^3 \mathbf{c} = \Delta t \int \int \left[K_1(\mathbf{c}, \mathbf{c}_1) - K_2(\mathbf{c}, \mathbf{c}_1) \right] f^d(\mathbf{c}_1)$$

$$\times \{1, \mathbf{c}, |\mathbf{c}|^2\} d^3 \mathbf{c}_1 d^3 \mathbf{c}. \tag{8}$$

Using the fact that collisions conserve mass, momentum, and energy, the following solution is obtained:

$$\Delta n_{\rm MB} = \Delta t \int \nu(\mathbf{c}) f^d(\mathbf{c}) d^3 \mathbf{c}, \quad \Delta \mathbf{u}_{\rm MB} = \frac{\Delta t}{n_{\rm MB}} \int \mathbf{c} \nu(\mathbf{c}) f^d(\mathbf{c}) d^3 \mathbf{c},$$

$$\Delta c_{\rm MB} = \frac{\Delta t}{3n_{\rm MB}c_{\rm MB}} \int \left[\mathbf{c}^2 - \frac{3}{2} c_{\rm MB}^2 \right] \nu(\mathbf{c}) f^d(\mathbf{c}) d^3 \mathbf{c}.$$
(9)

Although other choices for Δf^{MB} are possible, the one adopted here is both convenient (in terms of allowing the above closed form solution) and appears to work very well.

Note that using the linearized form about global equilibrium [i.e., using $\mathcal{L}^0(f^d)$ instead of $\mathcal{L}(f^d)$] is consistent with using the deviation about a *local* MBD because $\mathcal{L}^0(f^d) = \mathcal{L}^0(f-f^{\text{MB}}) = \mathcal{L}^0(f-f^0) - \mathcal{L}^0(f^{\text{MB}}-f^0)$ and the last term is of second order since $\mathcal{L}^0(f^{\text{MB}}-f^0) + \mathcal{J}(f^{\text{MB}}-f^0,f^{\text{MB}}-f^0) = 0$.

The collision step can thus be written as

$$\mathcal{L}^{0}(f^{d})\Delta t = \left\{ \Delta t \int \left[K_{1}(\mathbf{c}, \mathbf{c}_{1}) - K_{2}(\mathbf{c}, \mathbf{c}_{1}) \right] f^{d}(\mathbf{c}_{1}) d^{3} \mathbf{c}_{1} - \Delta f^{\text{MB}} \right\} + \Delta f^{\text{MB}} - \nu(\mathbf{c}) f^{d}(\mathbf{c}) \Delta t$$
(10)

and the algorithm is summarized as follows:

- Delete deviational particles of velocity \mathbf{c} with probability proportional to $\nu(\mathbf{c})\Delta t$;
- Change the underlying MBD by the amount given in Eq. (9). The integrals in (9) are calculated by sampling a subset of the deviational particles in the cell;
- Generate deviational particles according to the distribution

$$\left\{\Delta t \int \left[K_1(\mathbf{c}, \mathbf{c}_1) - K_2(\mathbf{c}, \mathbf{c}_1)\right] f^d(\mathbf{c}_1) d^3 \mathbf{c}_1 - \Delta f^{\text{MB}}\right\}(\mathbf{c}).$$

Because the functional form of the above expression is not known *a priori*, the particles are generated through an acceptance-rejection technique⁷ in which $N_1 = N_{\text{eff}}^{-1} \int g(\mathbf{c}) d^3 \mathbf{c}$ candidate particles are drawn from a distribution $g(\mathbf{c})$; the latter is chosen such that it bounds $|\Delta t[\int [K_1(\mathbf{c}, \mathbf{c}_1) - K_2(\mathbf{c}, \mathbf{c}_1)] f^d(\mathbf{c}_1) d^3 \mathbf{c}_1] - \Delta f^{\text{MB}}|$. Candidate particles of velocity \mathbf{c} and sign $\text{sgn}[\Delta t[\int [K_1(\mathbf{c}, \mathbf{c}_1) - K_2(\mathbf{c}, \mathbf{c}_1)] f^d(\mathbf{c}_1) d^3 \mathbf{c}_1] - \Delta f^{\text{MB}}|$ are generated if $|\Delta t[\int [K_1(\mathbf{c}, \mathbf{c}_1) - K_2(\mathbf{c}, \mathbf{c}_1)] f^d(\mathbf{c}_1) d^3 \mathbf{c}_1] - \Delta f^{\text{MB}}|(\mathbf{c}) \geq \mathcal{R}g(\mathbf{c});$ here \mathcal{R} is a random number in [0, 1].

More details will be presented in a future publication.

We now discuss the advection step. It is easy to show^{6,7} that if f^{MB} is independent of space and time, the advection step for deviational particles is identical to that of physical (DSMC) particles. Here, however, we allow f^{MB} to vary between cells, leading to discontinuities of this function at the boundaries between cells. To ensure molecular flux conservation, the advection step is supplemented by generation of deviational particles at the cell interfaces. Let us illustrate that by considering cells j and j-1 in the x direction; conservation of molecular flux requires⁷ that deviational particles drawn from the distribution $c_x(f_{j-1}^{MB} - f_j^{MB})$ be generated at the cell boundary and advected as other particles. Generating particles according to this distribution is accomplished by using an acceptance-rejection scheme, although under certain conditions (e.g., isothermal flow with no flow normal to cell interface) direct generation of particles from this distribution is possible.

The boundary treatment requires consideration of both deviational particles and the flux of particles due to the underlying $f^{\rm MB}$. In this work we consider diffuse boundary conditions, although the method is in no way limited to these. The algorithm used here is an adaptation of the one already presented in detail before. ^{6,7}

We performed a number of tests to validate the new method which we will refer to as LVDSMC; all tests yielded excellent agreement with DSMC solutions. Below we present a representative sample of our validation results.

To isolate the effects of collisions and thus validate the new treatment of the collision integral, we study the homogeneous relaxation of the gas from an initial condition of $f^i = 0.5(f^0(c_x - \alpha, c_y, c_z) + f^0(c_x + \alpha, c_y, c_z))$. We monitor the relaxation by plotting the evolution of $\langle c_x^4 \rangle$ as a function of

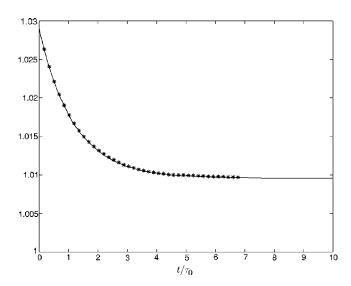


FIG. 1. Comparison between DSMC (stars) and LVDSMC (solid line) results for a homogeneous relaxation problem. Relaxation of moment $\langle c_x^4 \rangle/c_0^4$ from initial distribution f^i .

time (due to mass, momentum, and energy conservation as well as symmetry considerations, lower moments provide less interesting variations). This test highlights the basic principle on which LVDSMC is based: starting from an initial $f^{\rm MB}=f^0$ and a number of deviational particles representing f^i-f^0 , the simulation proceeds to a final equilibrium state characterized by a MBD at the final temperature, given by $T_f=T_0+m\alpha^2/(3k)$, and zero deviational particles. A comparison between LVDSMC and DSMC results for $m\alpha^2/(3kT_0)=0.0048$ is shown in Fig. 1. The agreement is excellent.

We also performed a number of validation tests for spatially dependent problems. Here we show the results for an impulsively started shear flow, in which at time t=0 the two (diffuse) walls bounding the system start moving in opposite directions in their plane with velocities $\pm U$. The distance between the two walls (L) is one mean free path, making this a problem where both advection and collisions are important. The same spatial and time discretization as well as the same number of simulation particles was used in the two methods. The agreement between the results is excellent (see Fig. 2). Similar levels of agreement have been achieved for L = $10\lambda_0$ (representing the collision dominated case) and L = $0.1\lambda_0$ (representing the advection dominated case). Those results are not shown here due to space constraints.

In summary, we have developed a new particle method for solving the Boltzmann equation. This method can capture arbitrarily small deviations from equilibrium at constant computational cost; this is achieved by simulating only the deviation from equilibrium. The method is closely related to DSMC and deviates only in ways necessary to consider the deviation from equilibrium. The most important feature of this method compared to other variance reduction approaches—one that also makes DSMC very powerful—is that it requires no discretization of the velocity space (e.g., for particle cancellation). In LVDSMC it is achieved by writing the action of the collision integral in the form of a change

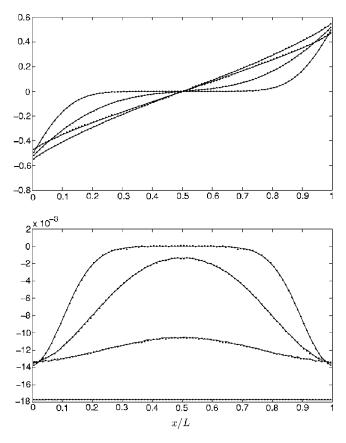


FIG. 2. Comparison between DSMC (stars) and LVDSMC (solid line) results for an impulsively started shear flow with $L=\lambda_0$. Top: normalized velocity u/U. Bottom: normalized shear stress $\tau_{xy}/(mn_0c_0^2)$. Snapshots at 0.17, 0.34, 0.68 collision times and steady state.

in the local equilibrium distribution function (representing the net effect of cancellation of a number of deviational particles) and an "irreducible" set of deviational particles (the remaining particles that cannot be cancelled).

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