2012

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A Comparative Study of No-Time-Counter and Majorant Collision Frequency Numerical Schemes in DSMC

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Abstract. The direct simulation Monte Carlo (DSMC) method is a stochastic approach to solve the Boltzmann equation and is built on various numerical schemes for transport, collision and sampling. This work aims to compare and contrast two popular $O(N)$ DSMC collision schemes - no-time-counter (NTC) and majorant collision frequency (MCF) - with the goal of identifying the fundamental differences. MCF and NTC schemes are used in DSMC simulations of a spatially homogeneous equilibrium gas to study convergence with respect to various collision parameters. While the MCF scheme forces the reproduction of the exponential distribution of time between collisions, the NTC scheme requires larger number of simulators per cell to reproduce this Poisson process. The two collision schemes are also applied to the spatially homogeneous relaxation from an isotropic non-Maxwellian given by the Bobylev exact solution to the Boltzmann equation. While the two schemes produce identical results at large times, the initial relaxation shows some differences during the first few timesteps.

Keywords: non-equilibrium flows, direct simulation Monte Carlo, majorant collision frequency, Bobylev solution
PACS: 47.45.-n, 47.11.-j

INTRODUCTION

The direct simulation Monte Carlo (DSMC) [1] method is a stochastic approach to solve the Boltzmann equation. The DSMC algorithm often consists of a "move" step to represent the molecular free-flight and a "collide" step to simulate the binary molecular interactions though splitless algorithms [2] are also used. The DSMC method has constantly evolved with improvements in the "move" step largely driven by changes in computer architecture. Of the two different components of the collide step, the phenomenological models that determine the outcome of a collision have seen major improvements, whereas the collision schemes have seen few changes in the last two decades. Comparative studies involving various phenomenological models including models for elastic scattering, internal energy exchange and chemistry easily outnumber the studies performed comparing different collision schemes. This work attempts a comparative study of two popular collision schemes used in DSMC - the no-time-counter (NTC) and the majorant collision frequency (MCF).

While similar studies comparing the two collision schemes have been attempted in the past, these have been restricted to the comparison of macroscopic properties for one-dimensional problems. The studies have concluded that both collision schemes lead to results that agree extremely well with each other. However, minor differences between collision schemes are likely to be more significant in parameters such as convergence [3] in number of simulators, cell size and timestep than in macroscopic parameters such as density, temperature and velocity. Our objective, therefore, is to extend the comparison of collision schemes to more fundamental parameters. In essence, we attempt to dissect the two schemes in order to establish the exact, though minimal, differences between the schemes. In particular, the objectives of this work include the study of the influence of the collision scheme on DSMC simulations of a steady spatially homogeneous equilibrium gas and the spatially homogeneous relaxation process from an isotropic non-Maxwellian and compare with theory. The remainder of the paper is organized as follows. First, the various collision schemes used in DSMC as well as the Bobylev solution are outlined followed by the results and discussion with the final section reserved for the conclusions.

28th International Symposium on Rarefied Gas Dynamics 2012
AIP Conf. Proc. 1501, 489-495 (2012); doi: 10.1063/1.4769577

THEORY AND BACKGROUND

Here, we provide a brief overview of the various collision schemes used in the past in chronological order. The *time-counter* (TC) method [4] was one of the earliest collision schemes introduced by Bird in which a collision pair is chosen from among the simulators in a collision cell and the collision is accepted with the probability $((\sigma_T c_r)/(\sigma_T c_r)_{\max})$ using a standard acceptance-rejection scheme. Here, σ_T is the total collision cross section for the chosen pair and c_r is the relative speed of the collision pair. The time increment (Δt_c) for the collision is computed as

$$\Delta t_c = \frac{2\Delta V}{NNF_{\mathrm{NUM}}\sigma_T c_r}, \tag{1}$$

where ΔV is the cell volume, N is the number of simulators in the collision cell, $\bar{N}$ is its average and F_{NUM} is ratio of real molecules to simulators in the simulation. The post-collision velocities are computed if the collision is accepted but a new collision pair chosen if the collision is rejected. The steps are repeated until $\sum \Delta t_c \leq \Delta t$. The algorithm is computationally efficient with an $O(N)$ complexity, but the method does not reproduce the collision frequency under certain extreme non-equilibrium conditions.

Koura introduced the *collision frequency* (CF) scheme [5], which is an exact Monte Carlo scheme in which the collision frequency (ν) is computed as the average value of $\sigma_T c_r$ over all collision pairs in the cell as

$$\nu = \frac{nN}{2}\int\int f(v)f(v_1)\sigma_T c_r dv dv_1 \approx \frac{F_{\mathrm{NUM}}}{\Delta V}\sum_{i=1}^{N}\sum_{\substack{j=1 \\ i\neq j}}^{N}(\sigma_T c_r)_{i,j}. \tag{2}$$

Once ν is computed, the time increment for the next collision is sampled from an exponential distribution given by

$$f(\delta t) = \nu \exp(-\nu \delta t), \tag{3}$$

which models the collision as a Poisson process. In a Monte Carlo simulation, this is sampled as $\delta t = -\ln(R)/\nu$ where R is a uniform random number between 0 and 1. The post-collision velocities of the chosen collision pair are computed and the steps repeated until $\sum \delta t < \Delta t$. Though this is an exact scheme to describe the collision process, the inefficient $O(N^2)$ algorithm is a disadvantage.

In the *no-time-counter* (NTC) scheme, introduced by Bird in 1989 [6], the number of potential collision pairs (N_{coll}) during any given timestep is obtained as

$$N_{\mathrm{coll}} = \frac{1}{2}\frac{N(N-1)F_{\mathrm{NUM}}(\sigma_T c_r)_{\max}\Delta t}{\Delta V}. \tag{4}$$

The scheme then chooses N_{coll} random pairs and accepts the collision between a given pair with a probability $(\sigma_T c_r)/(\sigma_T c_r)_{\max}$.

The *majorant collision frequency* (MCF) scheme [7, 8, 9] computes the majorant frequency $(\nu_{\max})$ as

$$\nu_{\max} = \frac{1}{2}\frac{N(N-1)F_{\mathrm{NUM}}(\sigma_T c_r)_{\max}}{\Delta V}, \tag{5}$$

where the parameters are the same as those used to compute N_{coll}. Here, it is worth mentioning that σ_T is a function of c_r depending on the molecular model. For example, for a variable hard sphere (VHS) model [1],

$$\sigma_T = \pi d_{\mathrm{ref}}^2 \frac{1}{\Gamma(5/2-\omega)}\left(\frac{2kT_{\mathrm{ref}}}{m_r c_r^2}\right)^{\omega-1/2}, \tag{6}$$

where ω is the viscosity-temperature exponent. For a hard sphere gase, $\omega = 0.5$ and for a Maxwell gas used in this work, $\omega = 1$. For the Lennard-Jones gas,

$$\sigma_T = \pi B_{\max}^2, \tag{7}$$

where, assuming a cut-off scattering angle of 0.1 radians, $B_{\max}$ is given by [10, 11]

$$B_{\max} = \sigma_{\mathrm{LJ}}\max\left[\left(\frac{0.4\pi\varepsilon_{\mathrm{LJ}}}{m_r c_r^2/2}\right)^{1/6}, \left(\frac{0.6\pi\varepsilon_{\mathrm{LJ}}}{m_r c_r^2/2}\right)^{1/12}\right]. \tag{8}$$

Once the majorant frequency is computed, a local timestep δt is sampled from an exponential distribution as

$$\delta t = -\frac{\ln R}{\nu_{\max}}, \tag{9}$$

where R is a random number uniformly distributed between 0 and 1. A collision pair is chosen at random and the collision is accepted with the probability $(\sigma_T c_r)/(\sigma_T c_r)_{\max}$. Since the value of $(\sigma_T c_r)_{\max}$ could have changed due to the chosen collision pair, $\nu_{\max}$ is re-computed and δt is sampled once again from the exponential distribution (Eq. (9)) with the process repeated until $\sum \delta t \leq \Delta t$. The *null collision* (NC) technique introduced by Koura [12] is very similar to the MCF scheme.

Bobylev Solution to the Unsteady Boltzmann Equation

One of the problems considered in this work is the unsteady relaxation from an initial non-Maxwellian distribution which is one of the exact solutions to the Boltzmann equation presented by Bobylev [13]. The initial condition for the Bobylev solution is an isotropic velocity distribution function slightly perturbed from the equilibrium Maxwellian distribution and given by

$$f(\mathbf{v},0) = F(\mathbf{v};\beta_0) = \left(\frac{m(1+\beta_0)}{2\pi kT}\right)^{3/2} \left(1+\beta_0\left[\frac{m(1+\beta_0)}{2kT}v^2 - \frac{3}{2}\right]\right) \exp\left(-\frac{m(1+\beta_0)}{2kT}v^2\right), \tag{10}$$

where β_0 is the initial value of the non-equilibrium parameter β ($0 \leq \beta \leq 2/3$), which decreases to zero at equilibrium. The Bobylev solution for the velocity distribution function is given by

$$f(\mathbf{v},t) = F(\mathbf{v};\beta(t)), \tag{11}$$

where the time dependence of β is given by

$$\beta(t) = \frac{\beta_0 \exp(-\lambda_B t)}{1+\beta_0[1-\exp(-\lambda_B t)]}. \tag{12}$$

The value of λ depends on the molecular model and operating conditions and is given by

$$\lambda = \int_0^\pi \sigma c_r \sin^3\chi d\chi, \tag{13}$$

where χ is the scattering angle and σc_r is the product of the differential cross section and the relative velocity. For Maxwell molecules with a potential given by κ/r^4, the above expression can be simplified to (following Bird's convention)

$$\lambda_B = \left(\frac{2\kappa}{m}\right)^{1/2} \int_0^\infty W_0 dW_0 \sin^2\chi = 0.436\left(\frac{2\kappa}{m}\right)^{1/2} \tag{14}$$

Comparing with the expression for viscosity for Maxwell molecules given by

$$\mu = \frac{2}{3\pi}\left(\frac{m}{2\kappa}\right)^{1/2} \frac{kT}{A_2(5)}, \tag{15}$$

we get

$$\lambda_B = \frac{p}{3\mu}, \tag{16}$$

which gives the Bobylev distribution function's approach to the Maxwellian distribution function, which is equivalent to β_0 approaching 0. In order to compare distribution functions obtained from simulations with theory, the x-velocity distribution given by

$$f(c_x) = \left(\frac{m(1+\beta)}{2\pi kT}\right)^{1/2} \exp\left(-\frac{m(1+\beta)}{2kT}c_x^2\right)\left[1+\beta\left(\frac{m(1+\beta)}{2kT}c_x^2 - \frac{1}{2}\right)\right] \tag{17}$$

is obtained. Also, the fourth moment of the x-velocity distribution is obtained as

$$< c_x^4 >= 3\left(\frac{kT}{m}\right)^2 \frac{1+2\beta}{\beta^2} \tag{18}$$

and used as a parameter to quantify the differences between theory and DSMC simulations. It should be mentioned that the second moment, which is the temperature, is a constant during the Bobylev relaxation and hence is not used for comparison.

RESULTS AND DISCUSSION

0-D Steady Case

The first problem considered is a spatially homogenous problem of an equilibrium monatomic gas. The gas comprises of Maxwell molecules with a reference diameter of 0.4 *nm* at a reference temperature of 273 *K*. The molecular mass of the gas was assumed to be 5×10^{-26} *kg*. The zero-dimensional code by Bird was modified to include the MCF collision scheme and was used to perform simulations using both NTC and MCF schemes with the goal of studying the collision quantities obtained. The number density of the gas was taken as $1.4 \times 10^{20}\ 1/m^3$ and the temperature was fixed at 273 *K*. One of the quantities of interest was the pdf of time between collisions which has a theoretical expression given by

$$f(t) = \frac{1}{\tau}\exp\left(\frac{-t}{\tau}\right), \tag{19}$$

where τ is the mean collision time. For the number density, temperature and molecular model parameters specified above, τ can be obtained as 32.115 μs. The time between successive collisions was monitored for all particles, and a pdf was constructed for DSMC simulations using both collision schemes for $2 \leq N_c \leq 100$. It should be mentioned that, the values of Δx, Δt and total number of particles were fixed for all simulations in order to isolate the error due to varying number of simulators/cell. The cell size was chosen as $\Delta x = 1$ *mm* which is about $1/10^{th}$ the mean free path corresponding to the operating conditions. The timestep was chosen as $\Delta t = 1\ \mu s$ which is about $1/30^{th}$ the mean collision time. The total number of simulators in the computational domain was fixed at 10000. The number of simulators/cell was varied by changing the extent of the domain, ratio of real molecules to simulators and the number of cells. For example, to obtain 2 simulators/cell with a total of 10000 simulators, the number of cells was fixed as 5000. For $\Delta x = 1$ *mm* this corresponds to a domain size of 5.0 *m*. On the other hand, to obtain 20 simulators/cell, the number of cells was changed to 500 which corresponds to a domain size of 0.5 *m*.

The pdf of time between collisions was constructed using data from 10 million collision pairs, and therefore the sample size was 20 million since 2 simulators participate in each collision. Figure 1 shows a comparison of the ratio of the pdf of time between collisions obtained from DSMC to the theoretical value for both NTC and MCF schemes. Clearly, since the MCF scheme has been designed to reproduce the pdf of time between collisions, it shows good agreement with the theoretical pdf even for $N_c = 20$. The NTC method, on the other hand, shows good agreement with theory only for $N_c = 100$. Here, it should be mentioned that the NTC scheme forces the reproduction of only the mean collision time but still reproduces the Poisson process by reproducing the pdf of time between collisions when sufficiently large number of simulators/cell are used. In order to quantify the agreement with theory for the two schemes, the first five moments of the pdf of time between collisions are compared for both NTC and MCF schemes, as shown in Fig. 2. It can be seen that while the error for 2 simulators/cell is similar for both cases, the MCF converges to the theoretical solution faster than the NTC scheme.

0-D Unsteady Relaxation: Bobylev Solution

In this subsection, we consider the spatially homogeneous relaxation to equilibrium and compare the DSMC solutions obtained using NTC and MCF schemes with the theoretical solution. The gas considered here consists of Maxwell molecules with a d_{ref} of 0.417 *nm* at $T_{\text{ref}} = 273$ *K* with a molecular mass of 6.64×10^{-26} *kg*. The temperature of the gas was fixed at 273 *K* and the number density was chosen as $1 \times 10^{20}\ 1/m^3$ resulting in Bobylev parameter $\lambda_B = 5931.98\ 1/s$. The initial value of β was chosen as 0.65. Simulators in the DSMC simulation were initialized by sampling from the Bobylev distribution corresponding to $\beta = 0.65$ using the acceptance-rejectance method.

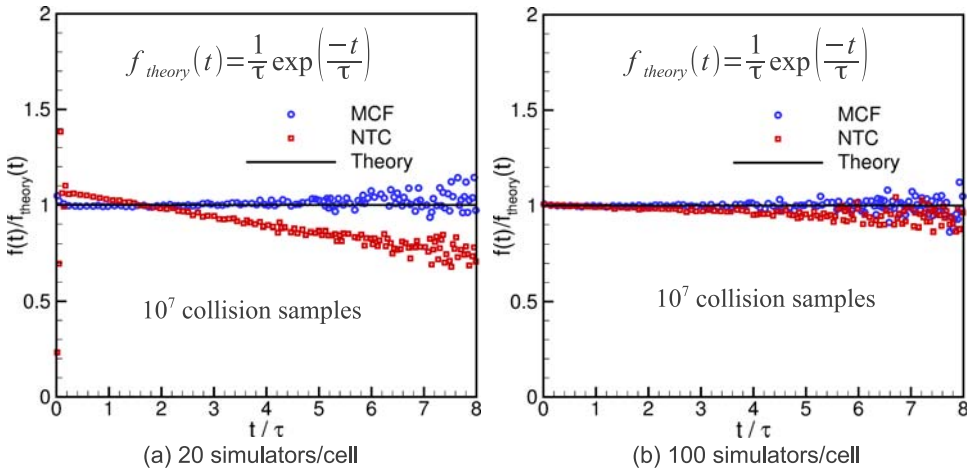


FIGURE 1. Comparison of probability distribution function of time between collisions in an equilibrium gas using both NTC and MCF collision schemes.

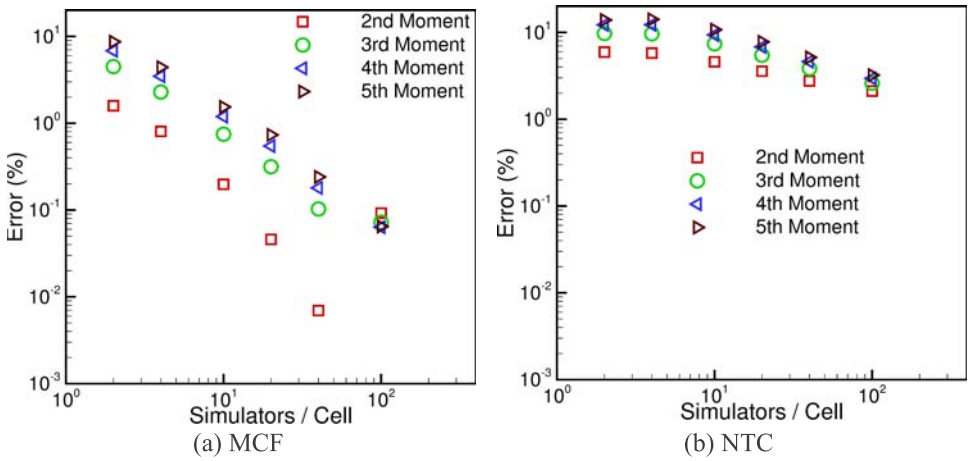


FIGURE 2. Comparison of second to fifth moments of the pdf of time between collisions in an equilibrium gas for various values of N_c using both MCF and NTC schemes

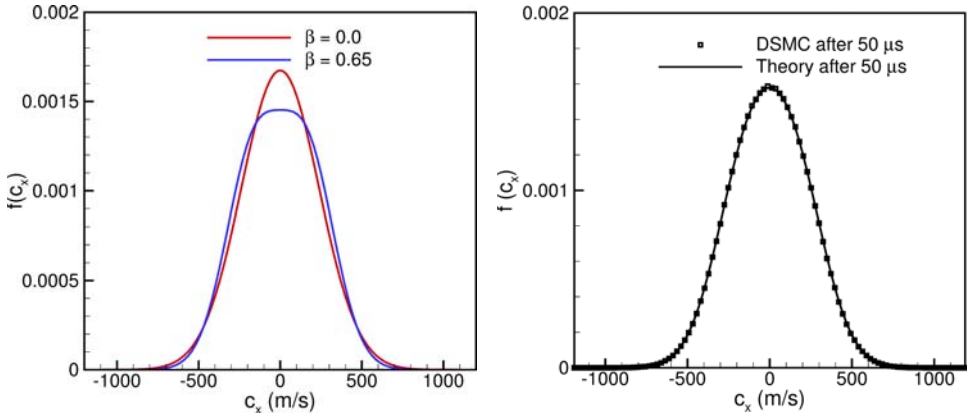
The DSMC simulations were performed using a total of 4 million simulators with $\Delta x = 10\ mm$ and $\Delta t = 25\ \mu s$. The cell size is less than the mean free path of 12 *mm* and the timestep is less than the mean collision time of about 38 μs. It was also ensured that the timestep is less than the mean residence time of the simulators in a given cell. It should be mentioned that there is a finite statistical error while sampling from the initial Bobylev distribution. However, for the case of 4 million total simulators, this error is not significant. Specifically, the initial value of the fourth moment of the x-velocity distribution function is 8.1276×10^9 which differs by only about 0.3 % from the theoretical value of 8.1588×10^9.

The Bobylev solution is a case of relaxation from weak non-equilibrium as can be seen in Fig. 3. Figure 3 also shows a comparison of the theoretical and DSMC solution for the x-velocity distribution function after 50 μs, and the agreement is very good. In order to enable a more rigorous comparison between theory and DSMC solutions, the fourth moment of the x-velocity distribution function obtained using MCF and NTC schemes is compared with the theoretical solution in Fig. 4 for 8 simulators/cell and 40 simulators/cell.

The solution obtained with 8 simulators/cell using both MCF and NTC schemes agrees reasonably well with the theoretical evolution in time. Though there appears to be a significant discrepancy between the DSMC and theoretical solutions, the actual difference is quite small and is about 0.9 % after 450 μs. The theoretical solution is about 9.6504×10^9 in comparison to 9.5601×10^9 and 9.5523×10^9 obtained using the MCF and NTC schemes respectively.

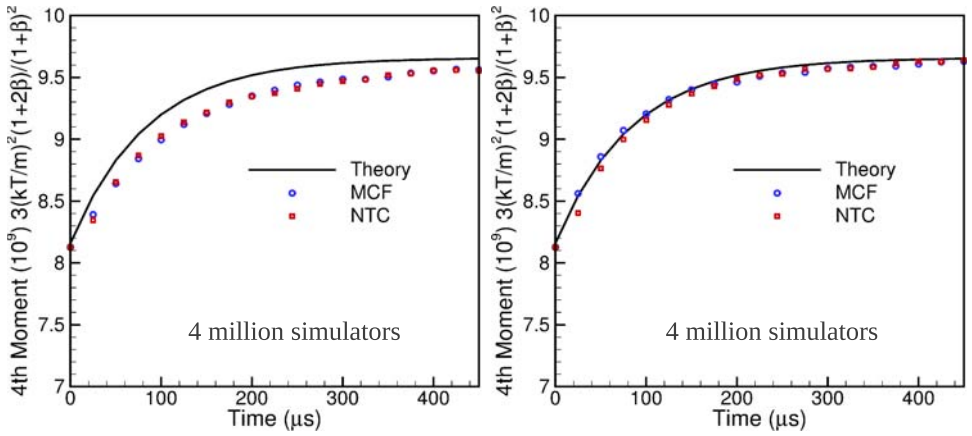
It should be mentioned that this error has contributions from both the initial statistical error of about 0.3 % due to a finite number of simulators as well as the evolution error due to using only 8 simulators/cell. Using only 8 simulators/cell could result in small but finite errors in the collision frequency even in an equilibrium gas as pointed out in Bird [1] which is the cause of the slightly larger difference even at large times. On the other hand, when the number of simulators/cell is increased to 40, the error after 450 μs decreases to about 0.3 % which is same as the initial statistical error.

Though there is good overall agreement between the two collision schemes, the MCF scheme agrees better with the theoretical solution when sufficient number of simulators/cell are used particularly during the initial timesteps. This difference can be largely attributed to the fact that the NTC scheme requires a few timesteps to establish the right collision frequency whereas the MCF scheme due to the use of local timesteps within a global timestep leads to the right collision frequency right at the first timestep. Apart from the minor differences, the MCF and NTC solutions both show very good agreement at large times using both 8 simulators/cell and 40 simulators/cell indicating that the difference due to different pdf of time between collisions is not significant for relaxation from a Bobylev distribution.



(a) Theory for β = 0 and β = 0.65 (b) Theory vs DSMC

FIGURE 3. Comparison of theoretical and DSMC solutions of the Bobylev 0-D relaxation after 50 μs ($\approx 1.32\tau$) from an initial value of $\beta = 0.65$. The figure on the left shows the Bobylev distribution corresponding to $\beta = 0.65$ and $\beta = 0$



(a) 8 simulators/cell (a) 40 simulators/cell

FIGURE 4. Comparison of time history of fourth moment of the x-velocity distribution function of the Bobylev solution using both NTC and MCF collision schemes.

CONCLUSIONS

A comparative study of two popular DSMC collision schemes - NTC and MCF - was performed with the goal of identifying the fundamental differences. DSMC simulations using the MCF and NTC schemes were used to study various collision parameters in a spatially homogeneous equilibrium gas. While the MCF scheme is designed to reproduce the exponential distribution function for the time between collisions, the NTC requires larger number of simulators/cell to reproduce the Poisson process. As a result, the MCF scheme displays faster convergence to the theoretical value for the higher moments of the pdf of time between collisions. The two collision schemes were also used to study the 0-D relaxation given by Bobylev's exact solution to the Boltzmann equation for Maxwell molecules. While the two schemes produced identical results at longer times, the initial relaxation process showed minor differences. The differences can be attributed to the fact that the NTC scheme requires a few timesteps to establish the right collision frequency which could be important in unsteady problems. A rigorous convergence study for both collision schemes should be performed for various benchmark problems in 0-D and 1-D.

ACKNOWLEDGMENTS

This work has been supported by NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems at Purdue University under contract number DE-FC52-08NA28617.
A part of this work was performed at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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