

# Heat Conduction Problem in a One-Dimensional Hard-Point Gas — Molecular Dynamics and Extended Thermodynamics —

S. Taniguchi<sup>a</sup>, M. Nakamura<sup>a</sup>, Masaharu Isobe<sup>a,\*</sup>, N. Zhao<sup>a,b</sup>, M. Sugiyama<sup>a</sup>

<sup>a</sup>Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan

<sup>b</sup>Department of Physics, Sichuan University, Chengdu 610064, China

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## Abstract

Stationary heat conduction in a one-dimensional hard point gas is studied numerically with molecular dynamics simulations and theoretically on the basis of extended thermodynamics. Temperature profile with jumps at the boundaries is analyzed consistently. Heat conductivity seems to converge as the system size tends to infinity.

*Key words:* one-dimensional hard point gas; heat conductivity; temperature profile; temperature jump; event-driven molecular dynamics; extended thermodynamics

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## 1. Introduction

Recently heat conduction phenomena in low dimensional systems have been intensively studied from the viewpoint of non-equilibrium statistical mechanics [1]. For stationary heat conduction in a one-dimensional hard point gas [2], the following interesting points are widely accepted: (A) Heat conductivity diverges as the system size tends to infinity (in a thermodynamic limit). (B) Temperature profile is, in general, an S-shaped curve. (C) There appear temperature jumps at the boundaries of the system.

In previous numerical studies [1], heat conductivity was estimated with the use of Fourier's law. However, as is well known, Fourier's law is one of the phenomenological linear relations in the thermodynamics of irreversible processes (TIP) with local equilibrium assumption [3]. The crucial point in its estimation from the numerical data is, therefore, to check the data whether these are really in the va-

lidity range of Fourier's law or not. As far as the authors know, there is no study of a hard point gas that takes this point into account seriously.

In this paper, stationary heat conduction in a one-dimensional hard point gas generated by event-driven molecular dynamics (MD) simulations is consistently studied on the basis of extended thermodynamics (ET) [4,5].

## 2. Model and Simulation Method

The model system is composed of two kinds of hard-point particles with different masses  $m_1$  and  $m_2$ , which are located alternately in a segment  $0 < x < L$  on the  $x$  axis. The system size  $L$  is changed such that the number density ( $N/L = 1$ ) is fixed ( $N$ ; total number of particles). Maxwell boundary conditions are adopted at the left and right sides of the system with the temperatures  $T_{WL}$  and  $T_{WR}$ , respectively.

There are three non-dimensional independent parameters in this model, which are  $N$ ,  $T_{WL}/T_{WR}$ , and  $r(=m_1/m_2)$  [2]. Efficient event-driven MD simulations [6] are performed systematically.

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\* Corresponding author.

*Email address:* isobe@nitech.ac.jp (Masaharu Isobe).

### 3. Extended Thermodynamics

ET is a thermodynamic theory which is valid beyond the local equilibrium assumption [4]. ET is wider than TIP. The basic equation for a hard point gas in ET can be obtained with the help of BGK equation with one relaxation time  $\tau$  as follows [5]:

$$G_3 = -\sqrt{\frac{3}{2}}P\tau \frac{d\theta}{dx} + 10G_3\tau^2 \frac{d^2\theta}{dx^2} \quad (1)$$

with  $G_3 = \text{const.}$  and  $P = \text{const.}$ , where  $G_3 = \sqrt{2/3}q$  ( $q$ ; heat flux),  $P$  is the pressure, and  $\theta = T/m$  ( $T$ ; kinetic temperature,  $m$ ; mass). The first term in the right hand side of eq. (1) is the leading term corresponding to Fourier's law, and the second term is its first-order correction. Note that heat conductivity  $\kappa$  is proportional to the relaxation time  $\tau$ .

Temperature jumps at the boundaries can be calculated explicitly from the conservation laws of mass and energy at the boundaries [7].

### 4. Results and Discussions

Figure 1 shows typical profiles of kinetic temperature obtained by MD simulations for several particle numbers  $N$ . These profiles are those for the subsystem composed of only light-mass particles. It is confirmed that the numerical results are consistent with the previous ones [2]. In Fig.1, theoretical curves derived from ET [7] are also depicted. To obtain theoretical curves and jumps, we need three values ( $\tau, G_3, P$ ). Here, the relaxation time  $\tau$  is assumed to have a suitable value, which is independent of  $N$ . Another two values ( $G_3, P$ ) are estimated by our simulation data. Gas temperatures at the boundaries obtained by MD simulations and ET are listed in Table 1.

$N$ ( $K_n$ )	1023 (0.0996)	2047 (0.0498)	4095 (0.0249)
$T_L$ (MD)	1.08971	1.09338	1.09570
$T_L$ (ET)	1.08643	1.09204	1.09568
$T_R$ (MD)	1.01192	1.00732	1.00438
$T_R$ (ET)	1.01278	1.00753	1.00410

Table 1

The comparison of gas temperatures at the boundaries between MD simulations and ET is shown. Knudsen number is defined as  $K_n = \tau\sqrt{T_{WR}/m_1}/L$ .

The agreement between the numerical results of the temperature profile including the temperature

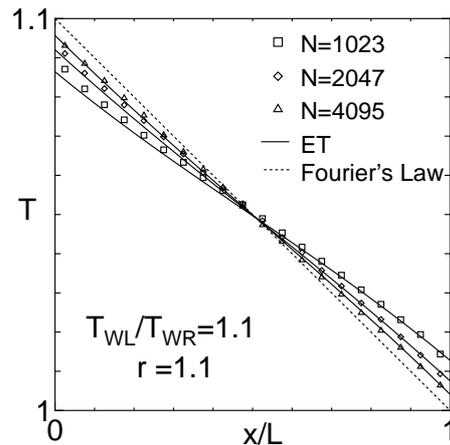


Fig. 1. Temperature profiles obtained by MD simulations for several  $N$ . Theoretical curves based on ET (solid lines) and Fourier's law (dashed line) are also shown.

jumps at the boundaries and the corresponding theoretical results is excellent. Therefore the assumptions adopted here may be acceptable. However, this means that heat conductivity seems to converge to a finite value in a thermodynamic limit. This is in sharp contrast to the widespread assertion (A).

In conclusion, the essentially new point in our analysis is that we can successfully divide heat flux into two parts; the part of Fourier's law and the part of its correction based on ET.

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