

# Lattice Monte Carlo Analyses of Thermal Diffusion in Laminar Flow

Thomas Fiedler, Irina V. Belova, and Graeme E. Murch

**Abstract**—Lattice Monte Carlo methods are an excellent choice for the simulation of non-linear thermal diffusion problems. In this paper, and for the first time, Lattice Monte Carlo analysis is performed on thermal diffusion combined with convective heat transfer. Laminar flow of water modeled as an incompressible fluid inside a copper pipe with a constant surface temperature is considered. For the simulation of thermal conduction, the temperature dependence of the thermal conductivity of the water is accounted for. Using the novel Lattice Monte Carlo approach, temperature distributions and energy fluxes are obtained.

**Keywords**—Coupled Analysis, Laminar Flow, Lattice Monte Carlo, Thermal Diffusion

## I. INTRODUCTION

THE Monte Carlo method was first developed at Los Alamos during the WWII Manhattan Project for the purposes of modeling neutron trajectories during fission. Since that time, the Monte Carlo method has undergone enormous developments and has enjoyed numerous applications in virtually every area of science and engineering. Intrinsically a computationally very demanding method, the Monte Carlo method has naturally become far more popular as computers have become faster, less expensive and more accessible. The Monte Carlo method has been a popular method to address both mass and thermal diffusion problems in materials. For mass diffusion, the Monte Carlo method has been used for many years for addressing atomistic problems in crystalline solids (in such problems it is now usually called the Kinetic Monte Carlo (KMC) method; see [1] for an early review and [2] for a typical recent KMC calculation. Recently, a wholly different type of Monte Carlo method has been developed for addressing multi-scale phenomenological diffusion problems (where it is called the Lattice Monte Carlo (LMC) method [3,4]). In the LMC method, the phenomenological diffusion problem is mapped onto a simple cubic (usually) lattice which is then explored by virtual particles. Depending on the physics of the problem considered, the virtual particles correspond to fixed amounts of matter (mass diffusion analysis), thermal energy (thermal diffusion analysis) or even elastic deformation energy (elastic analysis) [5].

Thomas Fiedler is with the University of Newcastle, Australia.  
e-mail Thomas.Fiedler@newcastle.edu.au

From another perspective, the LMC method is basically a finite-difference method that is embedded in a quasi-simulation of the physical process. The LMC method has shown itself to be very capable for solving complex phenomenological mass and thermal diffusion problems. For example, it has been used to calculate effective mass diffusivities in inhomogeneous materials where the diffusivity may depend on position [6] and to calculate concentration profiles where the diffusivity depends on position [3]. It has also been used to address steady state and transient thermal problems in multi-phase materials. Analogous to effective mass diffusivities, effective thermal conductivities can be obtained for composites [7,8] using LMC steady-state simulation. Furthermore, transient thermal behaviour can be addressed where thermal conductivities are functions of position [9] and temperature [10]. In a recent publication, the LMC method was also used to address diffusion coupled with chemical reaction [11].

The numerical LMC is an alternative to the well established finite difference and finite element methods and therefore must be able to compete with them. A major advantage of the LMC method is excellent memory efficiency that allows calculations with large models, e.g. based on computed tomography analysis. In addition, the LMC method is numerically very stable and thus is an excellent choice for highly non-linear (i.e. temperature dependent material properties) analysis.

In this paper, and for the first time, the Lattice Monte Carlo method is used in the analysis of combined thermal conduction and convection. In the compass of this preliminary research, the convection term is based on a velocity field obtained by an analytical solution. However, future development aims towards a fully coupled thermal and fluid dynamic analysis.

## II. LATTICE MONTE CARLO METHOD

In the LMC method, geometries are discretized as lattice models. In principle, any topology of lattice nodes can be chosen, for reasons of simplicity normally a primitive cubic arrangement is selected. In this study, only two-dimensional models are addressed, however, the transition to the three-dimensional case can be easily achieved by adding an additional jump direction and layers of nodes. Each lattice node is assigned a nodal volume  $s^3$  where  $s$  is the minimum distance between two nodes. For thermal simulations, nodes are assigned material properties (i.e. thermal conductivity  $\lambda$ ,

specific heat  $C$  and density  $\rho$ ), a thermal energy content  $E_N$  and a velocity vector  $v$ .

### A. Thermal Diffusion

In the Lattice Monte Carlo method, thermal energy transport by conduction is considered as a diffusion problem. As an example frequently found experimentally, we will focus on the situation where the temperature at the surface or source is held constant at  $T_S$ . The number of virtual thermal particles in the source plane is  $N_S$ . The amount of thermal energy  $E_p$  corresponding to a virtual thermal energy particle is then given by the relation:

$$E_p = T_s \cdot s^3 \cdot \rho \cdot C \cdot \frac{1}{N_s}, \quad (1)$$

where  $s$  is the distance between two neighbouring lattice sites,  $C$  the specific heat capacity and  $\rho$  the density of the material.

We organize the random walks of the particles in such a way that they are now directed by two parameters: the jump probability  $p_j$  (the scaled thermal conductivity) and the selection probability  $p_s$  (the scaled inverse product  $\rho_i \cdot C_i$ ). We treat the selection probability as an ‘amount of thermal inertia’ assigned to a virtual thermal energy particle in the particular phase: i.e. the higher the specific heat in the phase the slower the virtual thermal particle. Both jump and selection probabilities depend on the material parameters of the phase  $i$ . The jump and selection probabilities  $p_j$  and  $p_s$  are defined to have values between zero (the event never occurs) and unity (the event always occurs). Then the jump probability in a phase must be scaled with respect to the highest thermal conductivity so that:

$$p_{j,i} = \lambda_i / \lambda_{\max} \quad (2)$$

and the selection probability  $p_{s,i}$  is scaled with respect to the lowest value of the product  $\rho_i \cdot C_i$ :

$$p_{s,i} = \frac{(\rho_j C_j)_{\min}}{\rho_i C_i}. \quad (3)$$

According to Eq. (3), materials with a high specific heat and density possess a low selection probability. Different selection probabilities between sites from different material regions results in the modified Eq. (1) definition of the energy  $E_p$  corresponding now to a virtual thermal particle:

$$E_p = T_c \cdot s^3 \cdot (\rho \cdot C_p)_{\min} \cdot \frac{1}{N_n}. \quad (4)$$

Let us assume a multi-phase material where phase 1 has a lower selection probability than phase 2 i.e.:  $p_{s,1} < p_{s,2}$ . The overall probability of a jump of a probing thermal particle in phase 1 is then equal to  $p_{s,1} \cdot p_{j,1}$  and similarly for a particle in phase 2. (This value is, in fact, a scaled thermal diffusivity.) The increased number of unsuccessful jump attempts in phase 1 simulates an accumulation of virtual thermal particles in that phase. It should be mentioned here that the selection of  $p_s$  and jump probabilities  $p_j$  of virtual thermal particles inside the source plane ( $x = 0$ ) are equal to unity.

At the beginning of each time-step  $\Delta t$ , a particle is

randomly selected. Next, a random number between 0 and 1 is generated and compared to the selection probability corresponding to the material parameters at that lattice site. If this random number is higher than the selection probability, the attempt is unsuccessful; the LMC time is increased and another particle is randomly chosen. Otherwise, a jump direction for the particle is randomly chosen and, depending on the phase(s) of the starting and target lattice sites, the jump probability  $p_j$  is now determined. In the case that the jump attempt is successful, the coordinates of the particle are updated before the LMC time is increased and a new particle is selected. The incremental increase to the Monte Carlo time  $t_{MC}$  depends on the total number  $N_{tot}$  of virtual thermal particles in the system. At specified times  $t_{MC}$  the positions of all of the particles are recorded to derive temperature profiles. In order to obtain temperature profiles, the thermal particles are translated into site temperatures  $T$  according to:

$$T = \frac{n \cdot E_p}{s^3 \cdot (\rho_i \cdot C_{p,i})_{\min}}, \quad (5)$$

where  $n$  is the number of virtual thermal particles currently located at the site.

Next, the Monte Carlo time  $t_{MC}$  needs to be converted into real time  $t$ . To do this, we will use a standard parametric analysis approach. Consider the Heat Equation in its dimensionless form:

$$\frac{dT}{dt'} = \frac{\kappa t^*}{(x^*)^2} \operatorname{div}(\nabla T), \quad (6)$$

where  $x^*$  is a characteristic length for which we will use the jump distance  $s$ :  $x^* = s$ ,  $t^*$  is a characteristic time that is most naturally a jump attempt per virtual thermal particle and  $t^*$  should be determined in real time units;  $t'$  and  $x'$  are the dimensionless time and space coordinates.  $\kappa t^*/(x^*)^2$  is the dimensionless parameter of the thermal diffusion processes. It is obvious that the value of this parameter used in LMC simulations should be equal to its value in real units.

For the case of multiphase material, it is clear that we need to consider this correspondence only in one phase, provided that the other phases are modelled correctly. Let us choose phase  $i$  where the thermal conductivity is the highest  $\lambda_{\max}$ . Then the LMC value of the thermal diffusion parameter is:

$$\left( \frac{\kappa t^*}{(x^*)^2} \right)^{MC} = \frac{1}{6} \frac{(\rho C)_{\min}}{\rho_i C_i} \frac{1}{t'^2}. \quad (7)$$

Equating this value to the thermal diffusion parameter in the real units we have that:

$$\frac{\lambda_{\max} t^*}{\rho_i C_i s^2} = \frac{\kappa t^*}{(x^*)^2} = \left( \frac{\kappa t^*}{(x^*)^2} \right)^{MC} = \frac{1}{6} \frac{(\rho C)_{\min}}{\rho_i C_i}. \quad (8)$$

Solving the equation between the leftmost term and the rightmost term we soon arrive at:

$$t^* = \frac{1}{6} \cdot \frac{s^2 (\rho C)_{\min}}{\lambda_{\max}}. \quad (9)$$

Therefore, for the total time in real units we have the following connection to the LMC simulation time as follows:

$$t = t^* t_{\text{MC}} = \frac{t_{\text{MC}}}{6} \cdot \frac{s^2 (\rho C)_{\min}}{\lambda_{\max}}. \quad (10)$$

### B. Bulk Motion

The velocity field of the laminar flow is obtained using the Hagen-Poiseuille equation [12]. This equation is valid for laminar flow of a viscous and incompressible fluid passing through a cylindrical pipe where the inner diameter  $R$  is small in comparison the length  $L$  of the pipe. The velocity field is then given according to:

$$v = -\frac{1}{4\mu} \frac{\Delta P}{x} (R^2 - r^2), \quad (11)$$

where  $\mu$  is the kinematic viscosity,  $x$  is the distance in flow direction and  $r$  is the distance from the center of the pipe. The pressure drop  $\Delta P$  can be calculated using the volumetric flow rate  $Q$ :

$$\Delta P = \frac{8\mu \cdot x \cdot Q}{\pi \cdot r^4} \quad (12)$$

Combining Eqs. (11) and (12) we obtain the velocity field as a function of the volumetric flow rate and the geometric dimensions of the pipe:

$$v = -\frac{2Q}{\pi \cdot r^4} (R^2 - r^2). \quad (13)$$

For a known velocity field, bulk motion can be readily implemented in the LMC simulation: after each time step  $\Delta t$  (i.e. a jump attempt in the thermal diffusion simulation) the displaced volume  $\Delta V$  is evaluated for all nodal volumes:

$$\Delta V = v \cdot s^2 \cdot \Delta t. \quad (14)$$

If we assume that the thermal energy  $E_N$  is distributed homogeneously inside the nodal volumes, the transferred energy  $\Delta E_{\text{bulk}}$  can be calculated:

$$\Delta E_{\text{bulk}} = E_n \cdot \frac{\Delta V}{s^3} = E_n \cdot v(x, r) \cdot \frac{\Delta t}{s} \quad (15)$$

Based on the direction of the velocity vector, the target node is identified and the nodal energies are updated.

### C. Numerical Model

A two-dimensional model of a short section of a cylindrical pipe is considered (cf. Fig. 1). The inner radius of the pipe is  $R = 0.25$  cm, the thickness is  $t = 0.1$  cm and the length of the investigated section is  $L = 2$  cm. The temperature at the outer pipe surface is constant  $T_s = 550$  K. The initial temperature of fluid and copper as well as the constant temperature of fluid entering the system is 300 K. The effective thermal conductivity, density and specific heat of the copper (UNS C10100) pipe are  $\lambda_p = 385.8$  W/(m K),  $\rho_p = 8936.8$  kg/m<sup>3</sup> [13] and  $C_p = 383.6$  J/(kg K) [14], respectively. The corresponding material parameters of the fluid (water) are  $\lambda_f = 0.562 - 0.001967 \cdot T \cdot (1 + 0.00338 \cdot T)$  W/(m K),  $\rho_f = 1005$  kg/m<sup>3</sup> [15] and  $C_f = 4181.9$  J/(kg K) [16]. A fully developed velocity field according to Eq. (13) is presumed.

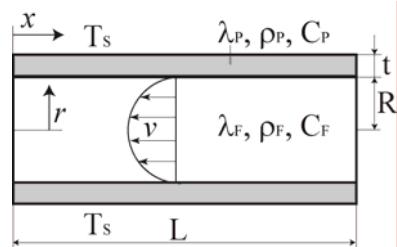


Fig. 1 Numerical model

### III. RESULTS OF THE NUMERICAL SIMULATION

Figure 2 shows temperature profiles obtained by the numerical simulation at the times  $t = 1$  s, 3 s and 7.5 s for the volumetric flow rate  $Q = 5 \cdot 10^{-8}$  m<sup>3</sup> s<sup>-1</sup>. Water at  $T = 300$  K enters the system at the right opening of the pipe. Due to its high thermal conductivity, the copper pipe, initially also at 300 K, heats rapidly to its constant surface temperature  $T_s = 550$  K and thermal energy is then transferred into the passing liquid. At  $t = 7.5$  s, a constant temperature profile (steady state) is reached.

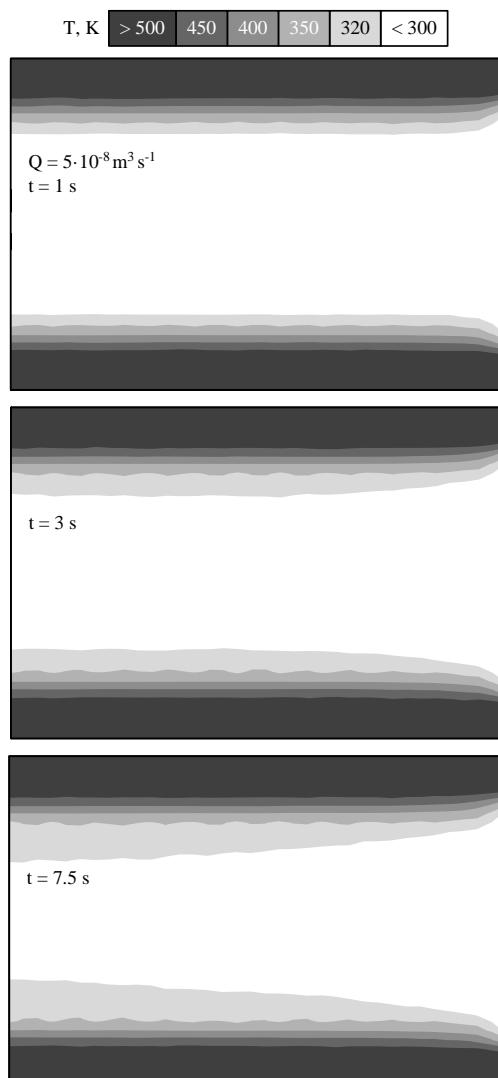


Fig. 2 Temperature distributions

Thermodynamic analysis of the numerical model reveals energy transfers at three locations of the system boundary: (i) energy transfer by heat  $\dot{E}$  to maintain the constant temperature boundary condition  $T_s$  at the pipe surface, (ii) energy transfer accompanying mass transfer  $\dot{m}_i$  of fluid entering the pipe section and (iii) energy transfer accompanying mass transfer  $\dot{m}_e$  of fluid leaving the pipe section. For an incompressible substance and a one-inlet one-exit system the mass rate balance simplifies to:

$$\dot{m}_i = \dot{m}_e = \dot{m} \quad (16)$$

Accordingly, the energy rate balance of the system can be written as:

$$\frac{dU}{dt} = \dot{E} + \dot{m} \cdot (u_i - u_e), \quad (17)$$

where  $U$  is the internal system energy,  $u_i$  the average specific internal energy of the fluid at the inlet and  $u_e$  the average specific internal energy of the fluid at the exit. Steady state of the coupled conduction - convection problem is reached when all system properties become constant. Figure 3 shows the energy  $U$  contained inside the system plotted versus time. It can be seen that the criterion is only met for the highest volumetric flow rate  $Q = 5 \cdot 10^{-8} \text{ m}^3 \text{ s}^{-1}$  and  $t > 7.5 \text{ s}$ .

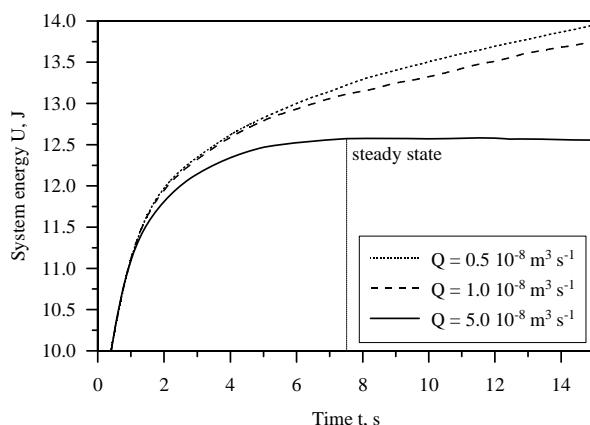


Fig. 3 System energy plotted versus time

Next to temperature profiles, energy fluxes at the system boundaries are of special interest. Figure 4 shows the total amount of energy  $E = \int \dot{E} dt$  conducted to the surface of the copper pipe from the surroundings and the energy increase of the water leaving the pipe given by  $\int \dot{m} \cdot (u_i - u_e) \cdot dt$ . It can be observed that both values increase for higher volumetric flow rates. It should be mentioned here that the difference between the two integrals is equal to the system energy  $U$  shown in Fig. 3.

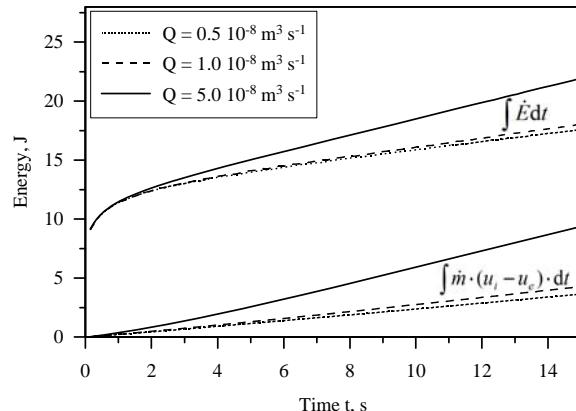


Fig. 4 Transferred energies plotted versus time

#### IV. CONCLUSIONS AND OUTLOOK

In this paper, and for the first time, Lattice Monte Carlo analysis was used towards the combined analysis of thermal conduction and convection. Laminar flow inside a copper tube was simulated and temperature distributions as well as energy fluxes were obtained. In the compass of the present preliminary research, the velocity field was obtained by an analytical solution and prescribed as a boundary condition. A more realistic simulation is obtained by accounting for the dependence of the velocity field on local temperature, pressure and density (in the case of a compressible fluid) variations. To this end, a suitable numerical method will be identified in the future and included in the current LMC analysis. The velocity field can then be calculated and updated after each time increment resulting in a highly accurate numerical simulation technique.

#### REFERENCES

- [1] G. E. Murch, "Simulation of Diffusion Kinetics with the Monte Carlo Method" in *Diffusion in Crystalline Solids*, G. E. Murch, A.S. Nowick, Eds, Orlando: Academic Press, 1984, pp. 379 - 427.
- [2] Y. Mishin, I. V. Belova, and G. E. Murch, "Atomistic Modelling of Diffusion in the TiAl Compound" *Defect Diffus. Forum*, vol. 237-240, pp. 271 - 276, 2005.
- [3] I. V. Belova and G. E. Murch, "Bridging Different Length and Time Scales in Diffusion Problems Using a Lattice Monte Carlo Methods" *Sol. St. Phen.*, vol. 129, pp. 1 - 10, 2007.
- [4] I. V. Belova, G. E. Murch, N. Muthubandara, and A. Öchsner, "Analysis of Oxygen Segregation at Metal-Oxide Interfaces Using a New Lattice Monte Carlo Method" *Sol. St. Phen.*, vol. 129, pp. 111 - 118, 2007.
- [5] I. V. Belova, G. E. Murch, T. Fiedler, and A. Öchsner, "Lattice-based walks and the Monte Carlo method for addressing mass, thermal and elasticity problems" *Defect Diffus. Forum*, vol. 283-286, pp. 13 - 23, 2009.
- [6] I. V. Belova, G. E. Murch, T. Fiedler, and A. Öchsner, *Diffusion Fundamentals*, vol. 4, pp. 15.1-15.23, 2007. On-line.
- [7] T. Fiedler, A. Öchsner, N. Muthubandara, I. V. Belova, G. E. Murch, "Calculation of the Effective Thermal Conductivity in Composites Using Finite Element and Monte Carlo Methods" *Mater. Sci. Forum*, vol. 553, pp. 51 - 56, 2007.
- [8] T. Fiedler, A. Öchsner, I. V. Belova, and G. E. Murch, "Calculations of the effective thermal conductivity in a model of syntactic metallic hollow sphere structures using a Lattice Monte Carlo method" *Defect Diffus. Forum*, vol. 273-276, pp. 216 - 221, 2008.
- [9] I. V. Belova and G. E. Murch, "Thermal Properties of Composite materials and Porous Media: Lattice-Based Monte Carlo Approaches" in *Cellular and Porous Materials. Thermal Properties, Simulation and*

- Prediction, A. Öchsner, G. E. Murch, J. S. de Lemos, Eds Weinheim: Wiley VCH, 2008, pp. 73 - 95.
- [10] T. Fiedler, I. V. Belova, A. Öchsner, and G. E. Murch, "Non-linear calculations of transient thermal conduction in composite materials" Comp. Mater. Sci., vol. 45, pp. 434 - 438, 2009.
  - [11] T. Fiedler, I. V. Belova, G. E. Murch, "A Lattice Monte Carlo analysis on coupled reaction and mass diffusion" Comp. Mater. Sci., accepted for publication.
  - [12] C. O. Bennett and J. E. Myers, Momentum, Heat, and Mass Transfer, New York: McGraw-Hill Book Company, 1982.
  - [13] C. Y. Ho, R. W. Powell, and P. E. Liley, "Thermal Conductivity of the Elements" J. Phys. Chem. Ref. Data, vol. 1, pp. 279-442, 1972.
  - [14] G. K. White and S.J. Collocott, "Heat Capacity of Reference Materials" J. Phys. Chem. Ref. Data, vol. 13, no 4, pp. 1251-1257, 1984.
  - [15] F. L. Levy, "The thermal conductivity of commercial brines and seawater in the freezing range", Int. J. Refrig., vol. 5, pp. 155-159, 1982.
  - [16] D. R. Lide, CRC Handbook of Chemistry and Physics. Boca Raton: CRC Press, 1998.