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## A new model of the heat transfer in materials: the surfacic potential algorithm

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**Abstract:** This paper proposes a new simulation method of thermal transfers based on the concepts of Brownian motion via the theory of potential and the characteristics of materials. In our simulation the particles take their origins on the surface and we propose an algorithm called ‘Surfacic Potential Algorithm’ that allows to determine the cartography of the temperatures. This algorithm has a better convergence than the one resulting from the potential theory and allows to treat adiabatic surfaces. It also includes the thermal heterogeneity of material. Its relevance is verified on thermal problems whose analytical solution is known.

**Keywords:** thermal problems; conductivity; simulation; Monte Carlo; potential theory; Brownian motion; phonons.

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## 1 Introduction

Since in reality all engineering surfaces are rough to some degree, the modelling of the contact between these rough surfaces is very important. Modelling the contact between rough surfaces leads to an improved understanding of the friction, wear, thermal and electrical conductance between surfaces (Sellgren et al., 2003). A proper numerical treatment of the important physical phenomena that occur in a contact zone requires detailed discretisation of the actual topography and a thorough material model. For instance, to obtain a good estimate of the forces that are transferred through the contact zone, a reasonable portion of the actual assembly of bodies must also be represented in the numerical model (Batrouni, 2002). The need to make the model as simple as possible embodies the contradictory requirement to restrict the problem to a manageable size. Whenever there is steady heat transfer across a joint formed by two rough surfaces under relatively light contact pressures, a large temperature drop is observed at that joint. It is demonstrated that rms roughness and mean absolute slope are both needed for evaluating contact heat transfer (Xu and Xu, 2005). Thermoelastic deformations can have a significant effect on the contact between elastic bodies, particularly in cases where the thermal boundary conditions at the interface are influenced by the contact pressure (Barber, 1999). The main problems occur in the case of fractal surfaces when using the Finite Element Method (FEM) (Ciavarella et al., 2003; Hyun et al., 2004) that can lead to ill-posed steady-state problems. Contact problems for thermoelastic bodies can exhibit instability associated with thermomechanical

coupling at the contact interface (Liu et al., 2006). In this paper, we analyse a different way to treat thermal mechanism on surfaces because conventional physical computation based on roughness datum mesh may be time consuming. This approach is based on Monte Carlo procedure used to solve Laplace's equation (Reynolds, 1965; Sadiku and Garcia, 1993) without the need to solve the boundary-value problem in the whole domain and so is an alternative to model physics phenomena on fractal interface. We propose an alternative methodology that consists to model the interface rather than the bulk. Briefly speaking, our methodology that extends Monte-Carlo EDP solver is an analogy on the problem between Boundary Element Method (BEM) and FEM. We focus on a classical problem related to heat transfer and analyse the efficiency of the new proposed algorithm.

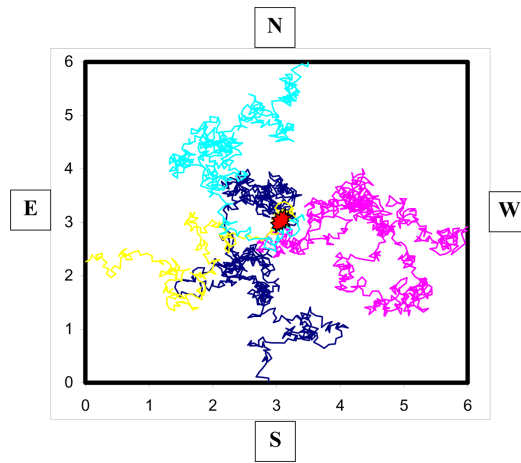
Many problems arise to the thermician concerning the validity of the Fourier law. The latter is commonly accepted by the heat transfer community for large values of time and space. However, the alternative model involves many problems with respect to the theories of statistical thermodynamics. Great controversies appear and nothing nowadays is allowed (Guillemet and Bardon, 2000). In spite of many efforts to 'hyperbolise' the Fourier's law, no model gives full satisfaction. The introduction of a hyperbolic term into the differential equation introduces conceptual artefacts which can be solved only by wave-particle duality of the phonons and free electrons. Which is the unknown origin of these dilemmas? We postulate that the origin of these controversies is due to the fact that at the distance and time where singularities appear, time and space cannot be considered any more independent as it is the case in the differential formulation. Indeed, it is not acceptable to consider the space-time as derivable. If the time scale (classical  $dt$  of the differential formalism) is such that the motion of the particles of heat transfer (phonons or Fermi electrons) is seen like a non-differentiable motion, it appears dangerous to postulate a differential law. Moreover, unless considering a purely wave theory (via Schrodinger wave equation), it becomes unreasonable to explain the physical origin of the hyperbolic corrective term introduced into the heat transfer equation. It is thus necessary to use a non-differential formalism of the heat transfer, and the Monte Carlo methods constitute an alternative. Unfortunately, these methods are rarely applied in thermal science for mesoscopic modelling. Admittedly, some publications preach the recourse to these methods to solve the heat equation. The principle consists in discretising space by a square grid and uses finite differences scheme of the heat equations. It involves that interface is almost everywhere derivable (and excludes any fractal surface). Then, the temperature is estimated at a point by taking into account the adjacent points of the grid. This methodology can be seen as equivalent to a simplex algorithm where jump probabilities in a direction are given by the adjacent temperatures themselves after an appropriate normalisation. However, in more complex problems of heat transfer, this normalisation is far from being easy due to negative jump probabilities (Kowsary and Arabi, 1999)

## **2 Potential theory**

The potential theory is used to formulate heat transfer in an isotropic and homogeneous media in two dimensions. The retained classical algorithm is called the Volumic Potential Algorithm (VPA) (Sadiku, 2001). Principle of simulation (Figure 1):

- Make a square grid, which represents part  $\theta(i, j)$ , to represent the temperature as in point  $(i, j)$ .
- Take a random point  $(x_0, y_0)$  in the part that belongs to the grid. Simulate a random walk of length  $< L$ .
- As the particle reaches the frontier, prescribed temperature of the boundary found is noted. By reproducing this simulation a great number of times, the average temperature of all boundary temperature corresponds to an estimate of the temperature at point  $(x_0, y_0)$ .

**Figure 1** Simulation by VPA method of the calculation of the temperature located in the centre of the part (see online version for colours)



### 3 2D analysis on a square mesh

#### 3.1 Analytical solution

The solution of the heat transfer in a plate height  $H$  and width  $L$  in stationary regime if three faces would be at null temperature and the last ( $y = H$ ) at temperature  $\theta_0$  is given by:

$$\frac{\theta(x, y)}{\theta_0} = 2 \sum_{n=1,3,5,\dots}^{\infty} \frac{2}{n\pi} \left( \frac{\sinh \frac{n\pi y}{L}}{\sinh \frac{n\pi H}{L}} \right) \sin \frac{n\pi x}{L}. \quad (1)$$

#### 3.2 Density of probability of the temperature in a point of the grid

Let us now analyse at first the Probability Density Function (PDF) of the temperature distribution at a given point of the grid. We note  $\theta_i(i, j)$  the temperature obtained at point  $(i, j)$  of the grid after  $n$  random walks and  $\theta_N$ ,  $\theta_S$ ,  $\theta_E$  and  $\theta_W$  the temperature respective on the borders north, south, east and west of the rectangular part and  $n_x(i, j, n)$

the number of particles which touch border  $X$  after  $n$  departures at point  $(i, j)$  of the grid with relation:

$$n = n_N(i, j, n) + n_S(i, j, n) + n_E(i, j, n) + n_W(i, j, n). \quad (2)$$

An estimate of the temperature at the point  $(i, j)$  is thus given by:

$$\theta_n(i, j) = (n_N(i, j, n)\theta_N + n_S(i, j, n)\theta_S + n_E(i, j, n)\theta_E + n_W(i, j, n)\theta_W) / n. \quad (3)$$

By noting  $p_X(i, j, n)$  the probability that a particle reaches border  $X$ , one gets:

$$\theta_n(i, j) = p_N(i, j, n)\theta_N + p_S(i, j, n)\theta_S + p_E(i, j, n)\theta_E + p_W(i, j, n)\theta_W. \quad (4)$$

Let us note  $p_X(i, j)$  the true probability, i.e., when the number of departures aims towards the infinity. Which is the form of the density of discrete probability (PDFD)? Which are the parameters likely to modify this PDFD? The probability  $p_X(i, j)$  is as high as the starting point of the particle that approaches border  $X$ . Moreover, this probability is higher if the Euclidean distance of this point to the other surfaces is large. Then it becomes obvious that the highest probability is located at the closer point of the middle of the border where  $p_X$  is calculated on four considered borders,  $p_X(N/2, N-1)$  and also  $p_X(1, N/2)$  are the same probability for a grid square at the point. The estimation of  $p_X(1, N/2)$  is not easy in dimension 2 because it requires to calculations on the Markovian processes. We now give a numerical estimate of these probabilities (Table 1). For that, a grid size  $N = 7$ , ( $i = 0.7, j = 0.7$ ) is taken and 1000,000 departures are carried out on each interior point of the grid with jump with maximal length of  $1/10$ . Applied to our example 1, we obtain relation  $\theta_n(i, j) = (n_N(i, j, n) \times 100) / n = p_N(i, j, n)$  where  $p_N(i, j, n)$  represents an estimate of the probability that a particle at the point  $(i, j)$  reaches the northern border at  $100^\circ\text{C}$ . We note  $p_N(i, j)$  the true probability, i.e., when the number of departures tends to infinity. This probability will be as high as the starting point of the particle approaches the ‘heating’ border, i.e., when  $i = 1$ . Once again, this probability is as high as the Euclidean distance from this point on the surface of null temperature is high. Then it becomes obvious that the highest probability is located at the point  $p_N(N-1, N/2)$ . Now, we focus on the density of probability of the temperatures  $\theta_n(i, j)$  obtained at the time of simulation.

**Table 1** Probability that a random walk reaches one of the four frontier ( $W, N, E, S$ ) by taking origin from a  $(i, j)$  coordinate of the mesh

| $ij$ |   | 1     | 2     | 3     | 4     | 5     |
|------|---|-------|-------|-------|-------|-------|
| 1    | W | 0.469 | 0.242 | 0.092 | 0.071 | 0.031 |
|      | E | 0.031 | 0.071 | 0.092 | 0.242 | 0.469 |
|      | N | 0.469 | 0.632 | 0.034 | 0.632 | 0.469 |
|      | S | 0.031 | 0.055 | 0.782 | 0.055 | 0.031 |
| 2    | W | 0.632 | 0.380 | 0.203 | 0.120 | 0.055 |
|      | E | 0.055 | 0.120 | 0.203 | 0.380 | 0.632 |
|      | N | 0.242 | 0.380 | 0.489 | 0.380 | 0.242 |
|      | S | 0.071 | 0.120 | 0.105 | 0.120 | 0.071 |

**Table 1** Probability that a random walk reaches one of the four frontier ( $W, N, E, S$ ) by taking origin from a  $(i, j)$  coordinate of the mesh (continued)

| $l/j$ |   | 1     | 2     | 3     | 4     | 5     |
|-------|---|-------|-------|-------|-------|-------|
| 3     | W | 0.782 | 0.489 | 0.250 | 0.105 | 0.034 |
|       | E | 0.034 | 0.105 | 0.250 | 0.489 | 0.782 |
|       | N | 0.092 | 0.203 | 0.250 | 0.203 | 0.092 |
|       | S | 0.092 | 0.203 | 0.250 | 0.203 | 0.092 |
| 4     | W | 0.632 | 0.380 | 0.203 | 0.120 | 0.055 |
|       | E | 0.055 | 0.120 | 0.203 | 0.380 | 0.632 |
|       | N | 0.071 | 0.120 | 0.105 | 0.120 | 0.071 |
|       | S | 0.242 | 0.380 | 0.489 | 0.380 | 0.242 |
| 5     | W | 0.469 | 0.071 | 0.092 | 0.071 | 0.031 |
|       | E | 0.031 | 0.242 | 0.092 | 0.242 | 0.469 |
|       | N | 0.031 | 0.055 | 0.034 | 0.055 | 0.031 |
|       | S | 0.469 | 0.632 | 0.782 | 0.632 | 0.469 |

Equation (3) is the average temperature value (expectation) and does not include the statistical variations which depend on  $n$ . Each probability can thus be described in terms of binomial random variable. If we suppose the probability of the jumps known, then the variance of the temperatures can be expressed by:

$$E[\text{var}[\theta_n(i, j)]] = \frac{(\theta_N - \bar{\theta})^2 p_N(i, j, n) + (\theta_S - \bar{\theta})^2 p_S(i, j, n) + (\theta_W - \bar{\theta})^2 p_W(i, j, n) + (\theta_E - \bar{\theta})^2 p_E(i, j, n)}{n}. \quad (5)$$

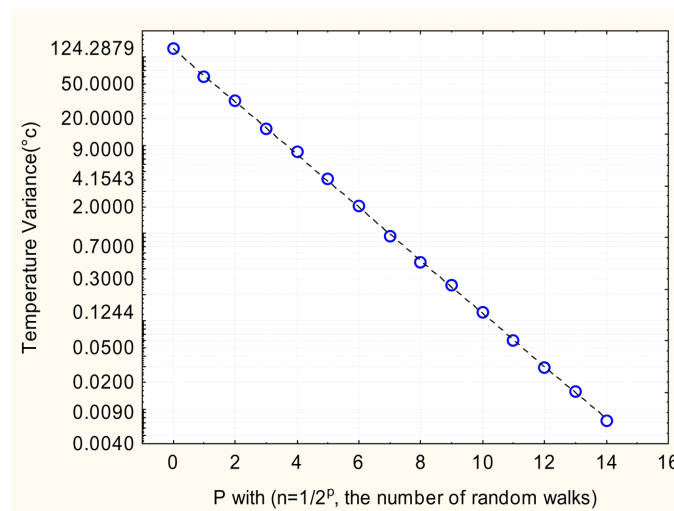
At  $(N/2, N/2)$  point,  $\bar{\theta} = (\theta_N + \theta_S + \theta_E + \theta_W)/4$  and  $p_X = 1/4$ , by taking  $\theta_0 = 20$ , one obtains:

$$E[\text{var}[\theta_n(N/2, N/2)]] = \frac{1/4}{n} [(\theta_N - \bar{\theta})^2 + (\theta_S - \bar{\theta})^2 + (\theta_E - \bar{\theta})^2 + (\theta_W - \bar{\theta})^2] = 125/n. \quad (6)$$

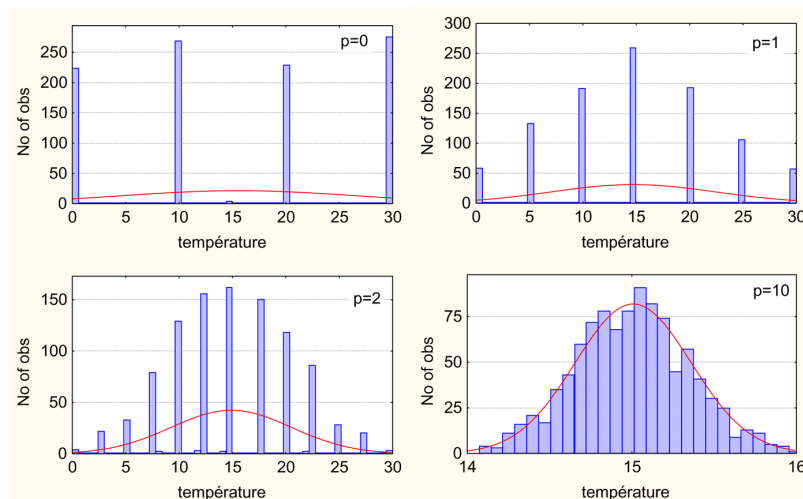
These equations show that the variance is quadratic with respect to the temperature variations compared with the average temperature of the borders. Comparison between simulated and equation (6) is perfect (see Figure 2). This shows the relevance of our approach. Uncertainty on the determination of the temperature is then directly connected to the differences in temperature on the borders. When the number of jump  $n$  tends to the infinity, the variance tends to zero and thus the estimate of the temperature is carried out without noise. However, the PDF of the temperature is still unknown. According to the central limit theorem, as  $n$  tends to infinity,  $\theta_n(i, j)$  converges to a Gaussian law with a mean given by the equation (4) and the standard deviation by equation (5). However, this theorem does not concern the speed of convergence. By taking back the demonstration of Lindenberg and Levy, the more the statistical moments of  $\theta_n(i, j)$  of order greater than two are (Skewness, Kurtosis ...), the less the rate of convergence is. Consequently, the strong skewness of the PDFD  $p_X(i, j)$  let predict for grid points with a weak convergence. To quantify this convergence, random walks are proceeded at each point of the grid with a jump of  $1/6$  and the empirical PDF can be built.

For the middle point, Figure 3 represents the density of probability of the temperatures according to the number of jumps. Variance are calculated to test the adequacy with the gaussian model. As the probability for this particular point of reaching each border is equally likely, this PDF will be always symmetrical (Skewness nul). With  $n = 1/2^p$  the number of random walks, in the case corresponding to  $p = 0$  (only one departure), we have a density of discrete uniform probability. For the case corresponding to  $p = 1$ , the probability density function converges to a discrete triangular law (sum of two uniform discrete probability density functions). Then as  $p$  increases, the distribution converges towards Gaussian and consequently towards a continuous law (Figure 3).

**Figure 2** Comparison of the variance of the mean temperature between simulation (dot) and model given by equation (6) (dashed lines) (see online version for colours)



**Figure 3** Probability Density Function of temperatures for the centre point of the part according to the number of jump  $2^p$  (see online version for colours)





### 3.3 Size influence of the yardstick

The size of the yardstick of the random walks is a difficult task in the Monte-Carlo simulation. In fact, the size must be small enough to conserve the fractal structure of the random walk. However, the larger the yardstick is, the longer the time simulation is. An issue must be emphasised: in the floating random walks, what means to reach the frontier? The probability the coordinates of the walk to be exactly those of the frontier is null. As a consequence, the value of temperature can only be incremented if the wall passes the frontier. If the temperature of the frontier is uniform, no problems occur but the temperature on the boundary presents a singularity, the temperature increment is ill-posed. For example, on the corner, the coordinates of the walk can pass over the vertical and the horizontal frontier. In this case, the mean of the temperature of the two frontiers will be retained. To test the efficiency of our approach, three origins are taken:

$X = 1, Y = 1$ : Border with geometry singularity and temperature singularity.

$X = 3, Y = 3$ : The lower probability to reach a corner.

$X = 5, Y = 5$ : Border with geometrical singularity but homogeneous temperature ( $\theta = 0$ ).

By taking the yardstick size equal to  $1/s$  (mesh size is equal to unity) 100,000 random walks are simulated. First time, the number of walks is computed such that errors are less than  $0.1^\circ$  in 95% confidence interval. Under the gaussian hypothesis of the temperature distribution, one gets that  $n > 16\alpha/E^2$  with

$$\alpha = (\theta_N - \bar{\theta})^2 p_N(i, j, n) + (\theta_S - \bar{\theta})^2 p_S(i, j, n) + (\theta_W - \bar{\theta})^2 p_W(i, j, n) + (\theta_E - \bar{\theta})^2 p_E(i, j, n) \quad (7)$$

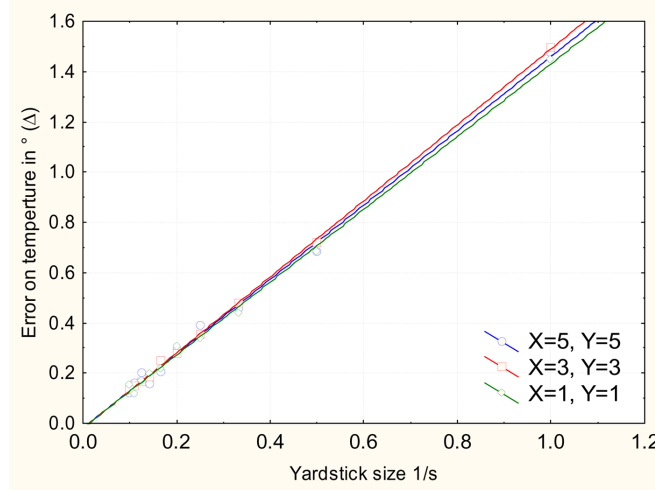
and  $E$  the wanted precision. For the three cases, one gets:

$$E[\text{var}[\theta_n(1,1)]] = 780/n, \quad E[\text{var}[\theta_n(3,3)]] = 487/n \text{ et } E[\text{var}[\theta_n(5,5)]] = 2970/n. \quad (8)$$

The variance of the temperature increases with the frontier geometrical complexity and temperature singularities. One must have 1300,000, 5000,000 and 800,000 to obtain the precision of 0.1, respectively. However, the value of the variance does not mean that no bias can occur in the simulation, i.e., the simulated temperature is not equal to the analytical solution. To quantify this bias, the following indicator  $\Delta = |\theta_M - \theta_T|$ , where  $\theta_M$  is the modelled temperature and  $\theta_T$  the true one, is proposed and estimated with different size values. Figure 4 represents this bias value vs. the inverse yardstick size. A bias occurs with an amplitude that does not depend on the temperature singularities. As a consequence, bias is only due to geometrical complexity of the frontier. This bias diminishes with the yardstick size. This is of major importance for Monte Carlo simulation: in the classical algorithm of the potential theory, the size of the yardstick plays a major influence. Let's now model this bias: under Gauss-Markov hypothesis (that are not rejected in our analyses), one gets a null intercept and finally the following equations are found:

$$\Delta(X = 1, Y = 1) = 1.41/s, \quad \Delta(X = 3, Y = 3) = 1.47/s, \quad \Delta(X = 5, Y = 5) = 1.44/s. \quad (9)$$

**Figure 4** Error on the temperature determination vs. the yardstick size of the random walk on three points of the mesh ( $X=5, Y=5$ ;  $X=3, Y=3$ ;  $X=1, Y=1$ ) (see online version for colours)



Roughly, one could admit that  $\Delta = 1.5/s$ . Of course,  $\lim_{s \rightarrow \infty} \Delta = 0$  but the slow convergence involves a high number of simulation to reach the true value with a high accuracy. For example, to have a bias lower than 0.2,  $s = 7.5$  is needed. However, a surprising result is that the error does not depend on the location of the beginning of the walk: boundary geometrical singularity plays the same role near the surface and far from the interface on the temperature bias evaluation. However, intuitively, the bias takes its origin near the frontier: the yardstick must be small enough with regard to the geometrical singularity. It can be possible to increase the yardstick size when the origin of random walk becomes far from the interface (distance  $L$ ) and, according to the macroscopic diffusion equation, can be weighted by a  $\sqrt{L}$  factor. However, we will propose in the next section an original algorithm that avoids this major discrepancy.

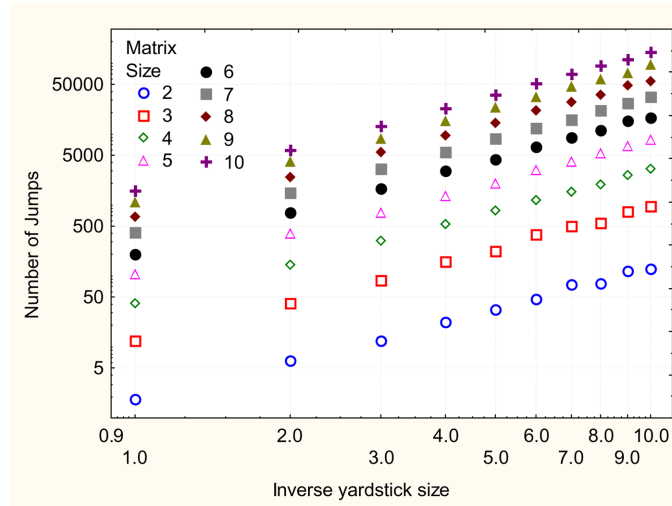
### 3.4 The number of jump

The number of jumps of the random walk is now analysed by taking into account both the yardstick length and the matrix size. 1,000,000 random walks are generated from the gravity centre of the piece. Then, the number of jumps who reach the surfaces is recorded. Relation 10 is found (see Figure 5):

$$n_s = 0.140_{\pm 0.006} s^{1.96 \pm 0.01} t^{4.04 \pm 0.02}. \quad (10)$$

This equation is compatible with diffusion equation: diffusion front increases with respect to the square root of time. So, if the yardstick size is half reduced then the time to reach the same points must be then increased by a four factor and this is confirmed by the coefficient of 1.96 close to the two value. The same reasoning can be applied to the coefficient 4.04 of the mesh. Normalisation of the number of jump in each point of the mesh (one has to divide  $n_s$  by  $t^2$ ) leads to the factor 2 again.

**Figure 5** Number of jumps needed to reach the surface from the origin located in the centre of the piece vs. the yardstick size for different mesh sizes (see online version for colours)



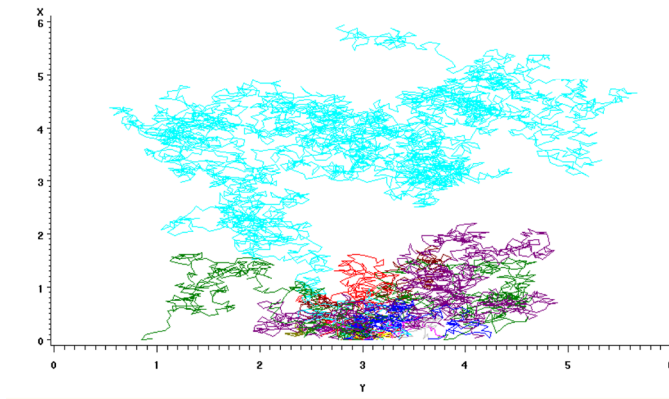
#### 4 Surface Potential Algorithm (SPA)

The principle of the algorithm is as follows:

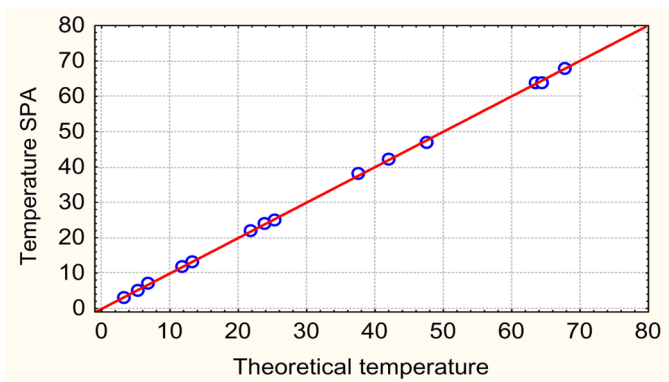
- 1 like VPA theory, volume as well as surface is discretised in a finished number of points
- 2 in each point of surface, similar random walks of particles described in the VPA by noting the temperature are performed
- 3 for each passage of the particle in a cell centred at a grid point other than surface, two counters are implemented receptively of an unit and the temperature
- 4 as soon as the particle reaches a surface (except in the case of adiabatic surface), this one disappears and another departure is performed
- 5 Steps 2–4 are reproduced a high number of times on each point of surface and, by carrying out the average temperature in each cell of the volume, the temperatures cartography is obtained.

This algorithm postulates the existence of a flow in space that is in fact the resultant of two flows of opposite directions (Figure 6(a)). SPA converges towards the solution given by equation (1) (Figure 6(b)). The best algorithm (SPA or VPA) is the one that will give for a same number of jumps the best estimation of all temperatures (lower variance of the estimate in each point). For the SPA Method, an initial number of jumps is fixed and is the same for the VPA one. To quantify the accuracy, the standard deviation of the temperatures is computed and one finds  $\sigma_{VPA} = 1.75\sigma_{SPA}$ . This proves the efficiency of our algorithm (Figure 4(c)).

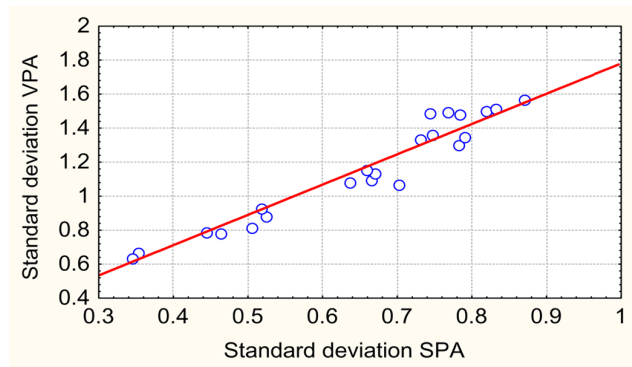
**Figure 6** SPA simulations (a), SPA Result for the problem given by equation (1) (b), comparison of the standard deviation of the temperatures obtained from the two methods SPA and VPA (c) (see online version for colours)



(a)



(b)



(c)

## 5 Conclusion

A new stochastic method of calculation of the heat transfer was proposed and gives results less dispersed than the classical method of the floating random walk. A major advantage of this method is to consider that frontier is at the origin of the random walk and then no problem occurs to determine the temperature at the interface as in the classical algorithm (intersection random walk with frontiers). This property is of major interest in the case of fractal surfaces. In the future, this method will be applied on linear elasticity to model contact on fractal surfaces.

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