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## Nonlocal thermal diffusion in one-dimensional periodical lattice

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#### 1 Abstract

2 Heat conduction in micro-structured rods can be simulated with unidimensional 3 periodical lattices. In this paper, scale effects in conduction problems, and more 4 generally in diffusion problems, are studied from a one-dimensional thermal lattice. 5 *The thermal lattice is governed by a mixed differential-difference equation, accounting* 6 for some spatial microstructure. Exact solutions of the linear time-dependent spatial 7 difference equation are derived for a thermal lattice under initial uniform temperature 8 field with some temperature perturbations at the boundary. This discrete heat equation 9 is approximated by a continuous nonlocal heat equation built by continualization of 10 the thermal lattice equations. It is shown that such a nonlocal heat equation may be 11 equivalently obtained from a nonlocal Fourier's law. Exact solutions of the thermal 12 lattice problem (discrete heat equation) are compared with the ones of the local and 13 nonlocal heat equation. An error analysis confirms the accurate calibration of the 14 length scale of the nonlocal diffusion law with respect to the lattice spacing. The 15 nonlocal heat equation may efficiently capture scale effect phenomena in periodical 16 thermal lattices. 17 18 Key words: Nonlocality, Diffusion equation, Gradient Fourier's law, Heat equation,

19 20

#### 21 **1. Introduction**

Lattice.

22

This paper explores the possibility to characterize the thermal behaviour of heterogeneous one-dimensional medium with a nonlocal approach, based on the introduction of some scale effects in the nonlocal diffusion model. A thermal lattice will be studied from a mixed differential-difference equation that will be analytically solved. The second part of the paper is devoted to the continuous approaches that may be valid to capture the scale effects inherent to the lattice properties. Scale effects may be predominant for engineering applications at different scales, from nanoscale 30 structures to macro-structures, where the size of unit cell may play some significant

31 roles.

32

33 The behaviour of a basic periodical thermal lattice with direct thermal interactions,

fully described in section 2.1, is explored. Such discrete media is based on a physical
thermal lattice ruled by a mixed difference differential equation, see [1]:

$$T_{i}^{\text{R}} = \alpha \frac{T_{i+1} - 2T_{i} + T_{i-1}}{a}$$
(1)

where  $T_i$  is the temperature at the node *i* and  $T_i^{\&}$  denotes its time derivative,  $\alpha$  is the 36 37 thermal diffusivity and *a* is the lattice spacing due to the discreteness of the discrete 38 thermal system.  $T_i(t)$  is discrete temperature field which is continuous in time at node *i*. 39 Such a lattice has been already considered, for instance with exact time-dependent 40 solutions for initial conditions defined as hat-function [2]. Eq. (1) is continuous in time 41 and discrete in space due to the lattice spacing. It can be also viewed as a discrete heat 42 equation in space. Zingales [3] studied the behaviour of an inhomogeneous thermal 43 lattice with spatial dependent thermal conductivity and specific heat coefficients.

44

The aim of the present paper is to investigate the capability of some nonlocal heat partial differential equations to capture the inherent scale effects into such periodical thermal lattice system. A nonlocal heat equation can be built from continualization of the thermal lattice system, using asymptotic expansion of the associated pseudodifferential operator. The nonlocal heat equation is augmented by some coupled spatial and time-dependent terms which are affected by the lattice parameters:

$$T^{\alpha} = \alpha T'' + l_c^2 T^{\alpha}$$
 with  $l_c^2 = a^2 / 12$  (2)

51 Eq. (2) is a nonlocal heat diffusion equation which can be also classified as a Guyer-52 Krumhansl equation [4] [5] (see for instance[2] [6] [7] or [8] for analytical solutions of 53 such an equation). As a simplification, we neglect in this study some additional 54 viscous terms specific of the Cattaneo-Vernotte model [9]. We show that the efficiency 55 of this continuous nonlocal heat model to capture the scale effects strongly depends on 56 the continualization of both the discrete field and the discrete initial conditions. It also 57 depends on the considered time during the evolution process as the continualization 58 process involves time and spatial coupling effects. Exact solutions will be derived for 59 both systems, the discrete one ruled by a discrete Fourier summation, and the nonlocal

60 continuous one governed by a continuous Fourier series formulation.

61

62 Since the energy balance equation may be written as:

$$\rho C T^{\mathcal{K}} = -\varphi' \tag{3}$$

63 where  $\varphi$  is the heat flux density,  $\rho$  is the density and *C* is the specific heat capacity of 64 the rod, the considered nonlocal heat equation given into Eq. (2) leads to a nonlocal 65 one-dimensional Fourier's law:

$$\varphi - l_c^2 \varphi'' = -\kappa T' \tag{4}$$

66 where,  $\kappa$  is thermal conductivity (with  $\kappa = \alpha \rho C$ ), and  $l_c$  is the characteristic length of 67 the nonlocal model containing the microstructure information due to its periodical 68 discreteness. It is worth to note that this differential nonlocal Fourier's law is 69 mathematically similar to the differential nonlocal model introduced by Eringen [10] 70 for nonlocal elasticity models, using a similar differential implicit law between the 71 stress and the strain.

72

Such nonlocal diffusion equation has been already considered for mass-transfer modeling by Barenblatt [11] applied to liquid flows in cracked rocks, and more recently in heat diffusion in the same periodically micro structured rod [2]. Exact solutions of this nonlocal heat equation have been derived for various initial and boundary conditions [2] [11] [12].

78

Nonlocal diffusion problems have been also studied by many authors, with an additional characteristic time making this equation both non local in time and space [13] [14] [15] [16] [17] [18] [19] [20] [21] [22]. The nonlocal Fourier's law is an evolution equation of Guyer-Krumhansl type which relates the heat flux with respect to the temperature field using an additional length scale for the flux. For the complete Guyer-Krumhansl type model, an additional relaxation time (as for Cattaneo's model) has to be considered in addition to the spatial nonlocal length scale, see [4] [5] [6] [23].

87 Thermal lattices have been already studied in the literature, from a thermal random 88 walk process connected with partial differential equations [24]. Weymann (1967) [25] 89 and Taitel (1972) [26] have characterized such discrete diffusion by a coupled spatial-90 time difference equation leading to higher-order gradient heat equation and have 91 looked for the possibility to treat this lattice difference equation from some extended 92 partial differential equations using higher-order gradient operators as an approximation 93 of the initial discrete problem. The expansion of the associated time and spatial 94 pseudodifferential operators using Taylor asymptotic expansion, gives higher-order 95 time and spatial derivatives in the heat equation. The same methodology has been 96 followed by Sobolev (1992, 2014) [27] [28] for the same thermal random walk 97 equation, see more recently [29]. The methodology presented in this paper is not so 98 far, even if the initial thermal lattice equation considered in this paper slightly differs 99 from the random walk equation, in the sense that the time evolution remains local for 100 the temperature variable (we only take into account spatial microstructures).

101

In this study, the exact resolution of the mixed differential-difference heat equation, valid for the thermal lattice (which may also cover other discrete diffusion processes) is presented. A nonlocal continuous approximation of this lattice model is thought, using a Padé approximant of the spatial pseudo-differential operator, thus avoiding higher-order spatial derivatives. The nonlocal heat equation finally uses coupled continuous spatial and time derivatives.

108

#### 109 2. Thermal discrete lattice.

#### 110 2.1. <u>Definition</u>

The physical discreteness of the material can be assumed at least at the atomic scale. Other heterogeneities at larger scales can also be considered. In this study, a periodic discrete lattice is assumed, consisting in *n* rigid elements with a constant length equal to a = L/n, as already studied by the authors [2] and, with additional heterogeneities by Zingales [3].



#### 118 119

#### Fig. 1 : Periodic thermal lattice of n elements-chain

120 The discrete-based (or lattice) approach is schematically presented in Fig. 1. Here, the 121 state parameters as masses, equal to  $a\rho_i$  or temperature  $T_i$  are located at each node. 122 Half common node masses are associated to both edge nodes so the total weight of the 123 whole chain is equal to  $\rho L$ , as for discrete chains already studied through mechanical 124 aspects and vibration problems [30]. Here, this consideration has no incidence on heat 125 diffusion, since the temperature is imposed at both edge nodes. The transfer parameters 126 as heat flux,  $q_{i+1/2}$ , and thermal conductivity  $\kappa_{i+1/2}$ , are defined at the interval between 127 nodes and considered as centered into the conductive elements. Based on the following 128 spatially discrete Fourier's law the associated energy balance gives:

$$\varphi_{i+1/2} = -\kappa_{i+1/2} \frac{T_{i+1} - T_i}{a} \text{ and } \rho C T_i^{\&} = -\frac{\varphi_{i+1/2} - \varphi_{i-1/2}}{a}$$
(5)

The discrete heat diffusion equation can then be formulated as Eq. (1). This mixed difference-differential equation slightly differs from the difference equation in space and in time studied by Taitel from a thermal random walk equation [26].

132

133 The aim of this study is to focus on time evolution of temperature into this finite 134 discrete rod, initially at stable and constant temperature  $T_{ini}$  and disturbed at t = 0 with 135 the same imposed temperature at both ends  $T_{imp}$ , with  $T_{imp} \neq T_{ini}$ , remaining constant 136 for t > 0. Thereafter, the normalized dimensionless temperature,  $\overline{T}$ , is considered

$$\overline{T} = 1 - \frac{T_{imp} - T}{T_{imp} - T_{ini}} = \frac{T - T_{ini}}{\Delta T} \text{ with } \Delta T = T_{imp} - T_{ini} \neq 0$$
(6)

138 The following dimensionless parameters, normalized with respect to the physical 139 characteristics of the rod, L and  $\alpha$  are introduced. They correspond to longitudinal 140 coordinate,  $x^*$ , and the elapsed time after the imposed change in temperature at 141 boundaries,  $t^*$ , and the normalized heat flux density  $\overline{\varphi}$  such as:

$$x^{*} = \frac{x}{L} \text{ or } x_{i}^{*} = \frac{i}{n} \text{ in case of discrete lattice;}$$

$$t^{*} = \frac{\alpha t}{L^{2}} \text{ with } \alpha = \frac{\kappa}{\rho C} \text{ such as } \vec{T}^{*} = \frac{\partial \overline{T}}{\partial t^{*}} = \frac{1}{\Delta T} \frac{\partial T}{\partial t^{*}} = \frac{L^{2}}{\alpha \Delta T} \frac{\partial T}{\partial t} \text{ and}$$

$$\vec{\varphi} = \frac{L}{\Delta T} \frac{\varphi}{\kappa} \text{ such as Eq.(1) gives } \vec{\varphi}' = \frac{L^{2}}{\Delta T} \frac{\varphi'}{\kappa} = \frac{L^{2}}{\alpha \Delta T} \frac{\varphi'}{\rho C} = -\frac{\partial \overline{T}}{\partial t^{*}} = -\dot{\overline{T}}$$
(7)

142

143 The dimensionless discrete heat diffusion equation of the thermal lattice can then be 144 reformulated from Eq. (1), as:

$$\vec{T}_{i} = n^{2} \left( \vec{T}_{i+1} - 2\vec{T}_{i} + \vec{T}_{i-1} \right)$$
(8)

145

The local difference equation of the thermal lattice system (with  $l_c = 0$ ) has been widely studied through numerical treatments using time and spatial discretization, for instance in [31] [32], [33] and more recently in [34]. In this paper, it should be noted that local difference equation of the thermal lattice exactly matches the finitedifference formulation of the one-dimensional heat diffusion equation with a continuous time parameter.

#### 152 2.2. Exact solution of the thermal lattice difference equation

As for the classical resolution of the local heat equation, the method of separation of continuous time and discrete space variables, based on  $\overline{T}_i(t^*) = \xi_i \tau(t^*)$ , where  $\overline{T}_i$  is the dimensionless temperature at node *i*, leads to:

$$\frac{\mathbf{t}}{\tau} = n^2 \frac{\xi_{i+1} - 2\xi_i + \xi_{i-1}}{\xi_i} \text{ with } \mathbf{t} = \frac{d\tau}{dt^*}$$
(9)

156

157 The time dependent term,  $\tau(t^*)$ , can be first easily integrated:  $\tau = P_1 \exp(-\gamma t^*)$  where 158  $P_1$  is a constant parameter. Then, a linear second-order difference equation in space remains. The homogeneous linear second-order difference with constant coefficients may be solved if a power law function is introduced [35], i.e.  $\xi_i = \xi \lambda^i$ , see for instance [36], giving the auxiliary equation according to  $\lambda$ :

$$\xi_{i+1} + \left(\frac{\gamma}{n^2} - 2\right)\xi_i + \xi_{i-1} = 0 \text{ leads to } \lambda + \frac{1}{\lambda} = 2 - \frac{\gamma}{n^2}$$
(10)

162

163 Eq. (10) is symmetrical with respect to interchanging  $\lambda$  and 1/ $\lambda$ . This equation admits 164 the two complex solutions  $\lambda_1$  and  $\lambda_2$  for  $0 < \gamma/n^2 < 4$ , i.e. if  $|1 - \gamma/2n^2| < 1$ :

$$\lambda_{1,2} = \cos(\phi) \pm j\sin(\phi) \quad \text{with } \phi = \arccos\left(1 - \gamma/2n^2\right) \text{ and } j = \sqrt{-1} \tag{11}$$

165

166 In real basis, the solution of the finite difference equation can be written as: 167  $\xi_i = P_2 \sin(\phi_i) + P_3 \cos(\phi_i)$  where  $P_2$  and  $P_3$  are constant parameters. From the boundary 168 conditions:  $\overline{T}_0(t^*) = \overline{T}_n(t^*) = 0$  which are equivalent to  $\xi_0 = \xi_n = 0$ , the solution of  $\xi_i$ 169 can be written as:

$$\xi_i = P_2 \sin\left(\frac{k\pi i}{n}\right) = P_2 \sin\left(k\pi x_i^*\right) \tag{12}$$

170 where k is a positive integer. Introducing  $\phi = m\pi/n$  into  $\phi = \arccos(1 - \gamma/2n^2)$  leads to 171  $\gamma = 4n^2 \sin^2(m\pi/2n)$ . The exact solution of temperature evolution at nodes is then 172 defined as a discrete Fourier summation:

$$\overline{T}_{i,exact}\left(x_{i}^{*},t^{*}\right) = \sum_{k=1}^{n-1} A_{k} \sin\left(k\pi \frac{i}{n}\right) \exp\left[-4n^{2} \sin^{2}\left(k\pi/2n\right)t^{*}\right]$$
(13)

173

174 where  $A_k$  are the discrete Fourier summation coefficients depending on the initial 175 conditions, inspired from the classical Heaviside initial temperature distribution:

if 
$$t = 0$$
,  $T_i(0) = T_{ini} = T_{imp} + \Delta T$ , i.e.  $\forall i \in [0,n], \ \overline{T_i} = 1$  and  
if  $t \ge 0$ ,  $T_0(t) = T_n(t) = T_{imp}$ , i.e.  $\overline{T_0}(t^*) = \overline{T_n}(t^*) = 0$  (14)

176 These conditions leads to:  $A_k = (2/n) \sum_{p=1}^{n-1} \sin(k\pi p/n)$  [37]. The double summation 177 obtained from injection of  $A_k$  into Eq. (13) can be also turned into a single finite 178 summation, see Appendix A, for a faster and accurate computation:

$$\overline{T}_{i,exact}\left(x_{i}^{*},t^{*}\right) = \frac{1}{n} \sum_{k=1}^{n-1} \frac{1 - (-1)^{k}}{\tan\left(k\pi/2n\right)} \sin\left(k\pi \frac{i}{n}\right) \exp\left[-4n^{2} \sin^{2}\left(k\pi/2n\right)t^{*}\right]$$
(15)

180 Hereafter, this solution is used as a reference at node 1 or (n-1) and the mid node (n/2)181 to compare the results obtained from continualized model.

182

#### 183 **3.** Nonlocal continuous heat equation

184

#### 185 3.1. <u>Boundary conditions of equivalent continuous media</u>

The key point is the consideration of a disturbance of the discrete temperature field at both ends of the finite discrete rod. In this study, we will explore the capability of continuous nonlocal heat equation to capture some scale effects of such discrete thermal lattices. For the continuous approach, the full definition of the temperature field is needed within all the bar. Many continualized initial temperature fields built from a homogeneous initial discrete temperature can be assumed from homogeneous initial discrete temperature.

193

We will consider four basic assumptions about initial continuous field of temperature, according to  $x^* = x/L$ , in the continualized nonlocal chain. These assumptions on the discrete case are transposed from a finite continuous rod, initially at stable and constant temperature  $T_0$  and disturbed at t = 0 with the same temperature imposed at both ends. The initial and boundary conditions of equivalent continuous media are:

if 
$$t = 0$$
,  $\forall x^* \in ]0;1[, \overline{T}(x^*, 0) = 1$  in "Heaviside" case,  
 $\forall x^* \in [1/n; 1-1/n], \overline{T}(x^*, 0) = 1$  in other cases
(16)  
if  $t \ge 0, \overline{T}_0(0, t^*) = \overline{T}_n(1, t^*) = 0$ 

199

In the continuous case, the initial temperature (at t = 0) corresponds to a step function located at both ends, made of a combination of Heaviside functions, discontinuous in time and space.

204 - The first assumption considers a direct transposition of the continuous case, i.e. the 205 same initial temperature distribution in the discrete system, even into the edge elements. This transposition of the discontinuous Heaviside distribution of temperature 206 207 to the discrete one assumes a discontinuous time evolution of temperature at both edge 208 nodes. This assumption on the discrete system, named as "Heaviside" boundary 209 condition, will be used as a reference thereafter, since it is usually considered to 210 numerically solve the basic heat equation. However, if a non-null mass is located in 211 both edge nodes as assumed in discrete system, it is not physically consistent. With 212 lower values of n, this lead to a paradox at both tip nodes, that have to be set at a 213 different temperature of the rest of edge (first and last) elements of the chain. 214 Preliminary studies [38] have shown that such strong discontinuity induces a bias into 215 the resolution of difference equations and Fourier series as in the continualization 216 process exposed in the next part.

217

In order to avoid discontinuity in time evolution of temperature, the initial distribution of temperature, at t = 0, has to make the edge nodes temperatures already equal to  $T_{imp}$ . To approximate as much as possible the classical Heaviside distribution, the next node temperature, inward the chain, has to be equal to  $T_0$ . The remaining question is about initial distribution of temperature into the edge elements, i.e. between the nodes 0 and 1, and the nodes n-1 and n, see Fig. 2.



224

Fig. 2 : Initial distribution of temperature into equivalent continuous media

Here after, dimensionless part functions of  $\overline{T}(x^*, 0)$  are considered, such as:

$$\overline{T}(x^{*},0) = f_{edge}(x^{*}) \leq 1 \qquad \text{for } x^{*} \in [0;1/n]$$

$$\overline{T}(x^{*},0) = 1 \qquad \text{for } x^{*} \in [1/n;1-1/n] \qquad (17)$$

$$\overline{T}(x^{*},0) = f_{edge}(1-x^{*}) \leq 1 \qquad \text{for } x^{*} \in [1-1/n;1]$$

228

229 – The second assumption assumes an initial distribution of temperature with a constant 230 gradient,  $\Delta T/a$  into both edge elements. Due to the shape of the temperature 231 distribution according to the longitudinal coordinate, it is name as "trapezoidal". 232 However this initial distribution lead to a discontinuous spatial derivative of 233 temperature at nodes 0 and 1, as well as at nodes n-1 and n, that may still induced 234 bias into nonlocal models.

235

236 – The third assumption, names as "polynomial" assumes an initial distribution of 237 temperature with a polynomial function of degree p (with p > 1) into the edge elements 238 such as spatial gradient of  $T(x^*,0)$  is null and continuous at the nodes closed the 239 boundaries, i.e. at the nodes 1 and n-1 or at abscissa  $x^* = 1/n$  and  $x^* = 1-1/n$ . The 240 dimensionless part function of  $\overline{T}(x^*,0)$  in this case is defined by  $f_{edge,p}(x^*)$  according 241 to p as:

$$f_{edge,p}\left(x^{*}\right) = 1 - \left(1 - nx^{*}\right)^{p}$$
(18)

242

The "trapezoidal" case corresponds to the case p = 1, while the "heavisisde" case corresponds to  $p \rightarrow \infty$ , see Fig. 3. It should be note that in introduced "polynomial" functions, the spatial gradient of  $T(x^*, 0)$  is discontinuous at the boundaries, in  $x^* = 0$ and  $x^* = 1$ . - The fourth assumption, names as "Sinusoidal" is finally introduced in order to ensure the continuity of the temperature and of its first spatial derivative over the whole length of the chain.  $\overline{T}(x^*, 0)$  and  $\partial \overline{T}(x^*, 0)/\partial x^*$  are then continuous at both nodes of edges elements, i.e. at the nodes 0,1, n-1 and n, see Fig. 3. The dimensionless part function of  $\overline{T}(x^*, 0)$  in this case is defined as:

$$f_{edge}\left(x^{*}\right) = \frac{1}{2} \left[1 - \cos\left(n\pi x^{*}\right)\right]$$
(19)



255 256

Fig. 3 : Initial temperature distribution into edge elements

257

#### 258 3.2. <u>Analytical solution of the nonlocal model</u>

Following the classical method using the separation of variables, already exposed in section 2.2, based on  $\overline{T}(x,t^*) = \xi(x^*)\tau(t^*)$ , the nonlocal heat diffusion equation, see Eq. (2) can be written in dimensionless form as:

$$\frac{\mathbf{x}}{\tau} = \frac{\xi''}{\xi} + l_c^{*2} \frac{\xi''}{\xi} \frac{\mathbf{x}}{\tau} \text{ with } \mathbf{x} = \frac{d\tau}{dt^*}$$
(20)

For a given continuous abscissa  $x^*$ , the first term  $t \not < \tau$  remains constant. Assuming  $t \not < \tau = -\gamma$ , the following equality is obtained:  $\xi'' / \xi = \gamma / (\gamma l_c^{*2} - 1)$  with  $l_c^{*2} < 1/\gamma$ . This last condition about  $l_c$  will be discussed later and justified by Eq. (23). The solution of  $\tau(t^*)$  and  $\xi(x^*)$  can then be written:

$$\tau = P_4 \exp\left(-\gamma t^*\right) \text{ and } \xi = P_5 \sin\left(m\pi x^*\right) + P_6 \cos\left(m\pi x^*\right)$$
(21)

where  $P_4$ ,  $P_5$  and  $P_6$  are constant parameters to be determined according the initial boundary conditions, given into Eq. (16) and equivalent to  $\xi(0) = \xi(1) = 0$ . As a consequence, the constant parameter  $P_6$  in Eq. (21) is null and  $\xi(x^*)$  reduces to:

$$\xi(x^*) = P_5 \sin(m\pi x^*) \tag{22}$$

269 where *m* is a positive integer. Substitution of  $\xi''/\xi$  by  $(m\pi)^2$  gives:

$$\gamma = \frac{(m\pi)^2}{1 + l_c^{*2} (m\pi)^2}$$
(23)

This equation assumes a positive value of  $\gamma$ , and in accordance with the inequality previously assumed to set the Eq. (21), it can be checked that  $0 < \gamma < 1/l_c^{*2}$  whatever the value of *m*.

273

274 The solution is obtained through Fourier series for a continuous abscissa  $x^*$ :

$$\overline{T}(x^*,t^*) = \sum_{m=1}^{\infty} A_m \sin(m\pi x^*) \exp\left(\frac{-m^2\pi^2 t^*}{1+m^2\pi^2 l_c^{*2}}\right)$$
(24)

275

where  $A_m$  are the continuous Fourier series coefficients defined according the initial continuous conditions given into Eq. (17) i.e. according to  $f_{edge}(x^*)$ . the Fourier series coefficients are all presented in Appendix A.

279

It should be noted that the nonlocal solution in Eq. (24) leads to the classical wellknown local solution if the characteristic length,  $l_c$ , is null i.e., when  $n \rightarrow \infty$ . This solution is also compared to compared to numerical ones based on the resolution of the local and nonlocal heat differential equation according to the characteristic length,  $l_c$ . The semi-implicit resolution method used and relative details are given in Appendix B.

As already observed for  $A_k$  in section 2.2, the coefficient  $A_m$  are always null for even values of *m*. Hence, the Fourier series can be expressed and computed more efficiently

with summation of odd values only of harmonics, *m*.

#### 289 3.3. Extrapolation of the lattice exact solution

The discrete solution at the nodes of the lattice given into Eq. (13) can also be extended as a continuous solution using the same integration over the whole length of the chain to determine the  $A_m$  coefficients of Fourier series:

$$\overline{T}_{exact}(x^*,t^*) = \sum_{m=1}^{\infty} A_{2m-1} \sin\left[(2m-1)\pi x^*\right] \exp\left[-4n^2 \sin^2\left(\frac{(2m-1)\pi}{2n}\right)t^*\right]$$
(25)

293

The extended exact solutions computed from this equation are plotted through the continuous abscissa  $x^*$  between the nodes in Fig. 4 *a*) and *b*). Whatever the continuous initial distribution of temperature, the node temperatures converge rapidly toward the same solution given by Eq. (13), matching exactly the lattice temperature at the node abscissa, i.e. for  $x^* = x_i^* = i/n$ . These analytical results are checked with numerical ones. The numerical finite difference scheme used and more details are presented in Appendix B.

301

As a consequence, all the results obtained from Eq. (25) with the various Fourier coefficients  $A_m$ , (see Appendix A) give surprisingly the same exact results at node abscissa, while initial shape of temperature distribution into the edge element propagates to the others as shown in Fig. 4 *a*) and *b*).

306

307 In case of Heaviside distribution of temperature, due to the initial jump discontinuity at 308 boundaries, the discontinuities propagates between nodes with time evolution. A well-309 known Gibbs phenomenon occurs at the transitions to/from the vertical sections, i.e. an 310 overshoot of the Fourrier sums, limited to 18% of the jump value [39], that rapidly 311 converges toward the midpoint of the jump equal to the values of the horizontal 312 section, especially when the number of harmonics, m, used for numerical computation increases. For instance, with computation of  $10^6$  harmonics, this phenomena is so 313 314 concentrated that it cannot appear on the presented plots in Fig. 4.



316Fig. 4 : Extended exact temperatures of the discrete system in a half part of a 6317elements system at dimensionless time: -a)  $t^* = 0.016; -b$ )  $t^* = 0.064$ 

319 In case of semi-infinite system,  $L \to \infty$  and  $t^* \to 0$  according to Eq. (7) while  $n \to \infty$  as 320 well. This particular case cannot be directly compared with the considered discrete 321 system but with the continuous one.

322

Semi-infinite system with an imposed temperature at the border,  $T_0$ , are classically studied. As in the finite system, for an infinite elapsed time, temperatures tends asymptotically towards  $T_0$ , when  $t \rightarrow \infty$ , while the temperature decreases instantaneously in the whole chain for t > 0. Since  $n \rightarrow \infty$ , the difference equation given into Eq. (1) is the same as the differential equation of the continuous case. It finds the well-known solution of local parabolic Fourrier equation, based on error function,  $\operatorname{erf}(x)$ , in case of the semi-infinite continuous medium:

$$\overline{T}_{\infty}\left(x^{*},t^{*}\right) = \operatorname{erf}\left(\frac{x^{*}}{2\sqrt{t^{*}}}\right)$$
(26)

330

331 Thereafter, this solution is used to compare the results from local and nonlocal models332 with the exact temperature at some node abscissas, see Fig. 7.

#### **4.** Comparison between the lattice and the nonlocal solution

334

#### 335 4.1. <u>Continualization procedure</u>

Based on a Taylor expansion of the spatial difference operator in Eq. (8), the continualization procedure considers that for a sufficiently smooth temperature distribution of temperature  $\overline{T_i} = \overline{T} (x = ia)$  and

$$\overline{T}(x+a,t) = \sum_{k=0}^{\infty} \frac{a^k \partial_x^k}{k!} \overline{T}(x+a,t) = e^{a\partial_x} \overline{T}(x,t)$$
(27)

where  $\partial_x = \partial/\partial x$  is the spatial differentiation and  $e^{a\partial x}$  is a pseudo differential operator as introduced for instance in [40] [41] and widely used for mechanical problems [42] [43] [44] [45] [46].

342 By expanding the finite difference operator using Eq. (24), Eq. (8) can be 343 continualized as:

$$\overline{T}_{i+1} - 2\overline{T}_{i} + \overline{T}_{i-1} = \left(e^{a\partial_{x}} - 2 + e^{-a\partial_{x}}\right)\overline{T}\left(x,t\right) = 4\sinh^{2}\left(\frac{a}{2}\partial_{x}\right)\overline{T}\left(x,t\right)$$
(28)

344 The pseudo-differential operator can be approximated by the following Taylor 345 expansion, if the considered hold sufficiently smooth variation:

$$\frac{4}{a^2}\sinh^2\left(\frac{a}{2}\partial_x\right) = \partial_x^2 + \frac{a^2}{12}\partial_x^4 + O(a^4)$$
(29)

which leads to a gradient-type temperature diffusion problem with the square of characteristic length,  $l_c^2$ , equal to  $a^2/12$  [2].

348 A numerical solution could be directly computed from the second-order continualized 349 equation, which may be expressed as a gradient heat equation with higher-order 350 temperature gradient terms. A similar methodology of expanding difference operators 351 for lattice diffusion processes has been used by Weymann (1967) [25], Taitel (1972) 352 [26] and more recently by Sobolev (1992, 2014) [27] [28]. Theses authors considered a 353 lattice ruled by a linear random walk equation (another kind of lattice), which is a discrete system both in space and in time, as opposed to the thermal lattice considered 354 355 in this paper which is only discrete in space. The pseudodifferential operator can also 356 be efficiently approximated by Padé's approximant to avoid higher-order gradient 357 terms and additional difficulties related to higher-order boundary conditions. Such 358 rational expansion of the pseudodifferential operator has been successively applied to

mechanical problems such as vibration of axial lattices [44] [45] [40] [41].

360

A numerical solution could be directly computed from the second-order continualized equation, however, the pseudo-differential operator can also be efficiently approximated by Padé's approximant to compute dynamic responses [44] [45] [40] [41], or recently in cases of of linear elastic lattice [47], even inelastic lattice such as damage mechanics [48] or elastoplastic problems [49].

366

To avoid the difficulties associated with higher-order boundary conditions needed in
the resolution of such continualized schemes [50], Padé's approximation of the finite
difference Laplacian is introduced:

$$\frac{4}{a^2}\sinh^2\left(\frac{a}{2}\partial_x\right) = \frac{\partial_x^2}{1 - \frac{a^2}{12}\partial_x^2} + \dots$$
(30)

to turn the Eq. (28) into analytical formulation:

$$\vec{T} = \vec{T}'' + l_c^{*2} \vec{T}^{*}$$
 with  $l_c^{*2} = \frac{a^2}{12L^2} = \frac{1}{12n^2}$  (31)

This nonlocal diffusion law is physically supported by the cell length, *a*, of the periodical lattice heat model.

373

374 With this length scale calibration, analytical results are checked with numerical ones 375 (see Appendix B) and compared with the exact solutions at the node of the discrete 376 system, used as references. With a limited number, n, of cell elements, the scale effect 377 departing continuous and discrete system are magnified. All plotted results are 378 hereafter obtained with n = 6. Due to the symmetry of the problem, the first half part of 379 the rod is only presented, allowing a better focus on the evolution of temperature 380 distribution at the edge. Local and nonlocal heat profiles are plotted at various 381 dimensionless time in Fig. 5.



Fig. 5 : Temperature profiles of the left half part of a n=6 elements system for some dimensionless times ranging from 4.10<sup>-3</sup> to 128.10<sup>-3</sup> with initial temperature distribution into the edge elements corresponding to:
-a) Heaviside case; -b) Trapezoidal, P<sup>1</sup>; -c) Polynomial P<sup>12</sup>; -d) Sinusoidal.

As observed in Fig. 5 a), in case of Heaviside initial temperature distribution, the nonlocal model highlights an unexpected temperature discontinuity at the boundary for the shortest evolution times. A focus on this discontinuity phenomenon for shorter evolution time with the same n = 6 elements system is presented in Fig. 6.

395



396

400

Fig. 6 : Focus on discontinuities of temperature at the boundaries of a n=6 elements
system in case of Heaviside initial temperature distribution at beginning of evolution,
for dimensionless times ranging from 0.125.10<sup>-3</sup> to 4.10<sup>-3</sup>.

401 Barenblatt et. al [11] obtained a similar nonlocal diffusion equation as presented in 402 Eq. (2). They demonstrate that first boundary value problem dealing with the theory of 403 non-steady-state seepage in fissured rock induces a jump in state parameter due to the 404 discontinuity of the initial conditions, at the rod extremities in Heaviside case.

405 Here, the difference between temperature T(0+,t)-T(0-,t) and T(L-,t)-T(L+,t),

406 can be analytically identified on both sides of discontinuity, as shown by Barenblatt et.

407 al [11]. A short demonstration is presented in Appendix C. Hence, the temperature408 evolution at the inside borders can be expressed a dimensionless form:

$$\overline{T}\left(0+,t^{*}\right) = \exp\left(-\frac{t^{*}}{l_{c}^{2^{*}}}\right) = \overline{T}\left(1-,t^{*}\right)$$
(32)

409 As a consequence, the initial discontinuity propagates with a decreasing range in time 410 according to Eq. (32). This relationship match perfectly the analytical results of the 411 nonlocal model calibrated with  $l_c^2 = a^2/12$  or  $l_c^{*2} = 1/12n^2$ , plotted in Fig. 6.

#### 412 *4.3.* Efficiency of the nonlocal diffusion model to predict the nodes temperature

The nonlocal model does not predict always the node temperature with a better accuracy than the local one. As shown in Fig. 5, for a given node, the efficiency of the nonlocal model depends on the node abscissa and evolution time. The difference between the exact node temperature and predictions according to the local and nonlocal models of a n = 6 elements system are plotted versus time evolution at the first nodes beyond the boundary (i.e. i = 1 or i = n - 1) in Fig. 7 a) and c) at the mid node (i.e. i = n/2) in Fig. 7 b) and d).

420

421 It can be checked that all models predict normalized temperature below than the semi-422 infinite continuous system at the mid node, see Eq. (26). However, at the first node, 423 close to the imposed gap of temperature, only local models remain below the local 424 semi-infinite predictions, see Fig. 7 c). The exact temperature at the first node of 6-425 elements system is actually slightly higher than the semi-infinite continuous system at the same abscissa when  $t^*$  is close to 2.10<sup>-2</sup>. In case of Heaviside boundary condition, 426 427 the nonlocal model integrates such size effect on temperature at the first node, as 428 shown in Fig. 5, but this increase in temperature is largely magnified, especially at 429 earlier evolution time.

430

As shown in Fig. 7, whatever the boundary condition, the magnitude of the difference
with the exact temperature is always higher with local models than with the nonlocal
ones, meaning a better accuracy of the enriched model based on nonlocal
considerations.

435 At the mid node as well as the first node, the Polynomial  $P^2$  boundary condition leads 436 to the better fit of the exact values, while the Heaviside and the Trapezoidal conditions 437 lead to a less efficient prediction. As the Polynomial degree increases, the initial 438 temperature distribution tends toward the Heaviside one and the discrepancy of the 439 results increases. Finally, the Sinusoidal initial condition lead to similar but smaller 440 differences than those obtained with Trapezoidal condition, probably due to the



441 continuity of the spatial derivative of temperature included with the trigonometric442 continualization process.

444 Fig. 7 : Evolution of differences between normalized temperature of the models (local and nonlocal) and the exact ones for a n = 6 elements system:
446 - c) at node 1 or (n-1) with Heaviside, Trapezoidal and Sinusoidal boundary conditions
448 - a) at the mid length (i.e. node n/2) with Heaviside, Trapezoidal and Sinusoidal boundary conditions
449 boundary conditions
450 d) at node 1 or (n-1) with Heaviside, Bahmamial P<sup>2</sup> P<sup>4</sup> and P<sup>12</sup>

- -d) at node 1 or (n-1) with Heaviside, Polynomial,  $P^2$ ,  $P^4$ , and  $P^{12}$
- -b) at the mid length (i.e. node n/2) with Heaviside, Polynomial,  $P^2$ ,  $P^4$ , and  $P^{12}$

453 The efficiency of the models according initial conditions depends on both node 454 abscissa and time evolution. As the result of the comparison between local and nonlocal model for given condition and node could change drastically with time 455 456 evolution, the efficiency of models is globally compared for all node temperatures introducing a time dependent error function,  $Err(t^*)$ , based on the residual sum of 457 squares, i.e.  $\sum (\overline{T_i} - \overline{T_{i,exact}})^2$ . Both term of temperature are theoretically null at the 458 459 edge nodes. The mean squared error at the other nodes can be computed from Eq. (25) 460 and Eq. (24), through the Err function :

$$Err(t^{*}) = \frac{1}{n-1} \sum_{i=1}^{n-1} \sum_{m=1}^{\infty} \left[ A_{m} \sin\left(\frac{m\pi i}{n}\right) \right]^{2} \left[ \exp\left(\frac{-m^{2}\pi^{2}t^{*}}{1+m^{2}\pi^{2}l_{c}^{*2}}\right) - \exp\left(-4n^{2}\sin^{2}\left(\frac{m\pi}{2n}\right)t^{*}\right) \right]^{2}$$
(33)

461

452

It should be noted here, that edge node temperature is actually not null for Heaviside initial assumption, see Eq. (32). If the whole nodes are considered, The *Err* function of the nonlocal model in the Heaviside case would be higher in the first instants of the evolution.

466 For small *n* values, the difference between nonlocal and local model is magnified, i.e. 467 in presence of strong scale effect induced by the microstructure. Fig. 8 shows the 468 global efficiency of the nonlocal model for a n = 6 system. For a given initial 469 temperature distribution,  $Err(t^*)$  is always lower for the nonlocal model than for the local one. The Fig. 8 b) confirms that Polynomial  $P^2$  initial temperature distribution 470 471 associated with the considered nonlocal model gives the most efficient prediction, 472 while the Heaviside condition lead the greater value of  $Err(t^*)$ . Moreover, the nonlocal 473 and local model tends rapidly toward the same highest residual value, beyond  $t^* = 10^{-2}$ with Err function computed from the n-1 centered nodes. Whatever initial 474 475 conditions, the nonlocal model gives significantly less residual values at nodes on the whole studied time evolution, i.e. with  $10^{-5} < t^* < 1$ . 476



477Fig. 8 : Time evolution of the residual sum of squares at node abscissa of the models478(local and nonlocal), Err, for a n = 6 elements system:479-a) with Heaviside, Trapezoidal and Sinusoidal boundary conditions480-b) with Heaviside, Polynomial,  $P^2$ ,  $P^4$ , and  $P^{12}$ .481

#### 482 4.4. Length scale calibration

In order to calibrate the length scale, the optimal characteristic length  $l_{c,opt}^2$ , associated to the nonlocal model is introduced. The Eq. (31) can be written according a second variable,  $\beta$ , such as  $l_{c,opt}^2 = a^2/\beta$ , equivalent to  $l_{c,opt}^{*2} = 1/\beta n^2$ . The minimum of  $Err(t^*,\beta)$  provides the  $\beta$  value, i.e. the optimal characteristic length  $l_{c,opt}^2$ . The value of  $\beta$  can be computed according  $t^*$  by solving  $\partial Err/\partial \beta = 0$ , that can be numerically computed as follow :

$$(n-1)\frac{\partial Err}{\partial \beta}(t^*,\beta) = \sum_{i=1}^{n-1} \sum_{m=1}^{\infty} \left[ A_m \sin\left(\frac{m\pi i}{n}\right) \right]^2 \left\{ 2t^* \left(\frac{n}{\beta(n/m\pi)^2 + 1}\right)^2 \exp\left(\frac{-\beta n^2 t^*}{\beta(n/m\pi)^2 + 1}\right) \right\} = 0$$
(34)
$$\left[ \exp\left(-4n^2 \sin^2\left(\frac{m\pi}{2n}\right)t^*\right) - \exp\left(\frac{-\beta n^2 t^*}{\beta(n/m\pi)^2 + 1}\right) \right] \right\}$$

 $\partial Err/\partial \beta$  is a monotonic increasing function of  $\beta$ , and the numerical resolution of 489 Eq. (34) gives only one solution, straightly assessed through numerical resolution. Fig. 490 9 shows that  $\beta$  tends rapidly toward 12, i.e.  $l_{c,opt} \rightarrow l_c$ , especially beyond  $t^* = 10^{-2}$  for a 491 n = 6 elements system, and before this dimensionless time when n increases. The 492 493 asymptotic value of  $\beta$  for higher values of  $t^*$  is also closest to 12 when *n* increases. As 494 already observed with such nonlocal diffusion law [2], the time independent length scale,  $l_c^2 = a^2/12$ , is reached after a transitory time, inversely proportional to the 495 number of lattice element, *n*, see Fig. 9 b). 496

497 In accordance with the previous observations about the prediction accuracy according 498 to initial temperature distributions, the Polynomial P<sup>2</sup> and Trapezoidal conditions give 499 the closest values of  $l_c^2$  at the beginning of evolution, while the Heaviside one gives 500 the farthest.



501 Fig. 9 : Numerical evaluation of 
$$\beta = (n^2 l_{c,opt}^{*2})^{-1}$$
  
502  $-a$ ) as a function of time  $(t^*)$  with the considered initial conditions  
503  $-b$ ) as a function of time  $(t^*)$  according to various values of n

#### 505 4.5. <u>Prediction of heat flow at boundaries</u>

The outlet heat flow density at boundaries in a dimensionless and normalized form is introduced:  $\overline{\varphi}_0$ , at  $x^* = 0$  or  $\overline{\varphi}_1$ , at  $x^* = 1$ . Eq. (3) and Eq. (7) lead to:  $\overline{\varphi}_0 = -\overline{\varphi}_{(x^*=0)} = \int_0^{1/2} \vec{T} dx^*$  or  $\overline{\varphi}_{(x^*=1)} = -\int_{1/2}^1 \vec{T} dx^*$ . Due to symmetrical conditions it can be easily checked that  $\overline{\varphi}_0 = \overline{\varphi}_1$ .

510 Time derivation and space integration of Eq. (24) give the solution of  $\overline{\varphi}_0$  for both local 511  $(l_c^* = 0)$  and nonlocal models as follow:

$$\overline{\varphi}_{0} = \pi \sum_{m=1}^{\infty} \frac{mA_{m}}{1 + m^{2} \pi^{2} l_{c}^{*2}} \exp\left(\frac{-m^{2} \pi^{2} t^{*}}{1 + m^{2} \pi^{2} l_{c}^{*2}}\right)$$
(35)

512 where  $A_m$  is the series coefficient defined according to the initial conditions, see 513 Eq. (18), and Appendix A.

514 In a same way, the exact solution  $\varphi_{0,exact}^*$  used as a reference is obtained by time 515 derivation and space integration of Eq. (13).

$$\overline{\varphi}_{0,exact} = \frac{4n^2}{\pi} \sum_{m=1}^{\infty} \frac{A_m}{m} \sin^2\left(\frac{m\pi}{2n}\right) \exp\left[-4n^2 \sin^2\left(\frac{m\pi}{2n}\right)t^*\right]$$
(36)

516 Only derivation of the time dependent departs from models. Time evolution of  $\phi_0^*$  for 517 the initial conditions giving the greater differences are plotted in Fig. 10 a) and b). 518





Fig. 10 : Time evolution of the normalized outgoing heat flow density at boundaries,
 - a) for Heaviside and Sinusoidal initial conditions
 - b) for Polynomial P<sup>12</sup> and Trapezoidal initial conditions

524  $\overline{\varphi}_{0,exact}(t^*)$  is the same for Sinusoidal and Trapezoidal cases. This means that for a 525 same initial continuous amount of heat,  $\overline{\varphi}_{0,exact}(t^*)$  does not depend on its initial 526 distribution. The increasing degree of polynomial initial temperature distribution 527 induces a continuous evolution from trapezoidal (P<sup>1</sup>) toward Heaviside (to P<sup>12</sup>). To 528 analyze the efficiency of the models about outgoing heat flow density, the relative 529 differences  $(\overline{\varphi}_{0,exact} - \overline{\varphi}_0)/\overline{\varphi}_{0,exact}$  are plotted in Fig. 11.



a)

531 *Fig.* 11 : *Relative difference between the exact,*  $\overline{\varphi}_{0 exact}$ *, and local and nonlocal* 532 outgoing heat flow density at boundaries,  $\overline{\varphi}_0$ , versus dimensionless time evolution  $t^*$ . 533 -a) for Heaviside, Sinusoidal and Trapezoidal initial conditions (-b) for Heaviside and Polynomial  $P^{12}$ ,  $P^4$  and  $P^2$  initial conditions 534

536 Along the studied evolution time, numerous curves intersections occur from same 537 initial condition, and analysis may not be trivial. However, the main global tendencies 538 are :

539 - At the earliest time of evolution the nonlocal as the local model largely overestimate the values  $\overline{\varphi}_0$  in comparison of  $\overline{\varphi}_{0,exact}$  and nonlocal model is far to be efficient until 540  $t^* = 8.10^{-3}$  in the case of n = 6 elements system. 541

542 - After a transitory step, the superiority of the nonlocal model as compared to the local 543 model appears. Depending on the number n of element, this step occurs approximately 544 when  $t^* = 8.10^{-3}$  for n = 6 i.e. when the decrease in mid node normalized temperature 545 reaches 0.5%. If the value of *n* increases, this step occurs earlier as the beginning of 546 the convergence time of  $\beta$  toward 12 does, see Fig. 9 b). Beyond this transitory time, 547 the nonlocal model gives better results than the local one, except for Polynomial  $P^2$ 548 initial case where the local model could be still punctually better.

#### 550 4.6. <u>Prediction of the global amount of heat</u>

551 The amount of heat Q (in joule), or for instance the internal energy of the rod with a 552 cross section area equal to S, can be deduced from:

$$Q(t) = \rho CS \int_{0}^{L} T(x,t) dx \text{ equivalent to}$$

$$\overline{Q}(t^{*}) = \int_{0}^{1} \overline{T}(x^{*},t^{*}) dx^{*} = \overline{Q}(0) - 2\int_{0}^{t^{*}} \phi_{0}^{*} dt^{*} \text{ with } \overline{Q} = \frac{Q}{\rho SLC\Delta T} - \frac{T_{0}}{\Delta T}$$

$$(37)$$

where  $\overline{Q}(t^*)$  is the normalized amount of heat equal to the average temperature along the finite continualized rod. Based on Eq. (24) or on Eq. (35),  $\overline{Q}(t^*)$  from local  $(l_c^*=0)$ and nonlocal models, according to the considered system, is computed as follow:

$$\overline{Q}(t^*) = \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{A_m}{m} \exp\left(\frac{-m^2 \pi^2 t^*}{1 + m^2 \pi^2 l_c^{*2}}\right)$$
(38)

556 The same spatial dependent term is found in Eq. (24) and Eq. (25) defining 557  $\overline{T}_{exact}(x_i^*, t^*)$ . Only the time dependent term departs and integration of  $\overline{T}_{exact}$  gives the 558 mean values of the exact temperature over the whole continualized system as stated in 559 Eq. (37). The exact solution  $\overline{Q}(t^*)_{exact}$  used as reference is then computed for each 560 initial temperature distribution from Eq. (25) as:

$$\overline{Q}(t^*)_{exact} = \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{A_m}{m} \exp\left[-4n^2 \sin^2\left(\frac{m\pi}{2n}\right)t^*\right]$$
(39)

It should be noted that according to the initial distribution  $\overline{T}(x^*, 0)$  defined in section 561 2.2,  $\overline{Q}_{(t^*=0)} = 1$  in Heaviside case,  $\overline{Q}_{(t^*=0)} = 1 - 2/n(p+1)$  in Polynomial case with a 562 degree equal to p, and  $\overline{Q}_{\binom{n}{t}=0} = 1-1/n$  in Trapezoidal and Sinusoidal cases, see Fig. 12 563 with n = 6. Moreover, as shown in section 2.2, the exact temperature at the node 564  $\overline{T}_{i,exact}(t^*)$  does not depend on initial distribution of temperature since all the Fourier 565 566 series coefficients used in Eq. (25) produce the same results at nodes. The shape of the 567 initial temperature distribution into the edge element propagates into all elements during evolution, see Fig. 4 and integration of Eq. (25) over the whole length removes 568 the space dependent term. As a consequence, the ratio  $\bar{Q}_{exact}(t^*)/\bar{Q}_{exact}(t^*=0)$  remains 569 the same whatever the initial condition considered (i.e. whatever the selected  $A_m$ 570

571 coefficient). For instance,  $\overline{Q}_{exact}(t^*)$  is the same for Sinusoidal and Trapezoidal case, 572 as it can be already observed with  $\overline{\varphi}_0$  in Fig. 11.



574 Fig. 12 : Time evolution of the normalized amount of heat into the system
575 - a) for Heaviside and Sinusoidal initial conditions
576 - b) for Polynomial P<sup>12</sup> and Trapezoidal initial conditions

577

Evolution of  $\overline{Q}$ , plotted in Fig. 12, shows that both local and nonlocal models underestimate the remaining amount of heat into the system during the evolution in Heaviside and similar boundary condition as polynomial P<sup>12</sup> while the curves are very closed without clear tendency in sinusoidal or Trapezoidal case. The differences with the exact case are detailed in Fig. 13 for each initial case.

583

Results show that the nonlocal model give better prediction than the local one, from the beginning of the evolution, to predict the amount of heat, in particular with Heaviside and Polynomial, Trapezoidal included, initial conditions, see Fig. 13 *b*). In these cases, local model leads to a significant underestimation in comparison of the nonlocal model, especially at the beginning of the evolution, until  $t^* = 8.10^{-3}$  with n = 6, when the scale effect results in a delayed diffusion.



591Fig. 13 : Relative difference between amount of heat deduced from exact formulation592 $\overline{Q}_{exact}$  and from local and nonlocal model  $\overline{Q}$  versus dimensionless time evolution  $t^*$ .593-a) for Heaviside, Sinusoidal and Trapezoidal initial conditions594-b) for Heaviside and Polynomial  $P^{12}$ ,  $P^4$  and  $P^2$  initial conditions595

596 For Trapezoidal as for sinusoidal initial condition, the curves intersect at many times 597 the exact results, see Fig. 13 *a*). Except for lower values of  $t^*$ , in case of trapezoidal 598 initial conditions, the nonlocal model is significantly better, very closed to the exact 599 solution,  $\overline{Q}_{exact}$ , with alternation of slight over and underestimation of the amount of 600 heat, compared to the exact solution.

601 Globally, beyond a transitory time, for instance after  $t^* = 8.10^{-3}$  with n = 6 elements. 602 the nonlocal model gives a better prediction of the remaining total of heat amount  $\overline{Q}$ 603 in comparison of the local one, whatever the initial temperature distribution into the 604 edges elements. This transitory step becomes shorter when *n* tends to be larger. 605 Increasing value of *n* induces a lower relative error of the models but tends to magnify 606 the relatives differences induced by the initial condition.

#### 608 5. Conclusion

Thermal diffusion in a one-dimensional periodically microstructured lattice can be
described within a quasi-continuum approach governed by a nonlocal Fourier's law,
similar to the differential model of Eringen [10] initially devoted to material elasticity.
This nonlocal Fourier law can be also cast into a more general Guyer-Krumhansl type
model [5].

614

Using a continualization procedure, the characteristic length scale of the nonlocal heat model is calibrated from the lattice spacing, *a*. This calibration appears also to be optimal, since minimization of the sum of squares of residuals node temperature makes the square of this length scale, with time evolution and/or increasing number of element *n*, rapidly converge toward  $l_c^2 = a^2/12$ .

620

621 Despite strong discontinuity of the initial temperature profile, like in the case of 622 uniform initial temperature introduced from Heaviside operator, the continualized 623 nonlocal heat model based on a Padé asymptotic expansion of the spatial difference 624 operator (of the associated lattice problem) is able to capture scale effect. The nonlocal 625 model produces a better global prediction of the node temperatures than local model 626 (without any length scale), as compared to the exact thermal lattice solution. The 627 nonlocal model also predicts more efficiently the remaining amount of heat into the 628 discrete systems.

629

630 It is shown that the efficiency of the continualized nonlocal model to predict the 631 accurate temperature field of the lattice problem is sensitive to the continualized initial 632 conditions, especially at the border of the microstructured rod. A difficult question 633 consists in extending the discrete nodal temperature outside the lattice nodes, for the 634 computation of the continualized nonlocal problem. The continualized nonlocal model 635 gives better results for smoothed continualized initial conditions, in particular for a 636 parabolic temperature distribution (named here as  $P^2$ ) into the edge elements. 637 However, the sinusoidal initial condition does not make the nonlocal model produce 638 better results than the trapezoidal condition. The presented nonlocal model, initially 639 based on sufficiently smooth variation of temperature is not affected by the initial 640 gradient continuity, while it is able to remain relevant for temperature discontinuity in 641 case of imposed jump at boundaries. But in this last case, the asymptotic solution at the

642 inner boundary differs from the imposed value at the extremities.

643

The present spatially nonlocal model, is able to predict delayed diffusion phenomena in thermal lattices ruled by mixed differential-difference equations. It is probably possible to extend such nonlocal model for discrete problems with both space and time discreteness, leading to generalized nonlocal continuous diffusion problems, both in space and in time.

649

#### 650 **Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal

relationships that could have appeared to influence the work reported in this paper.

653

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### 659 Nomenclature

	Parameters	Dimension	Relative dimensionless parameters
а	Element length	[L]	$a^* = a/L = 1/n$
$A_{k,m}$	Fourier coefficients	_	
С	Specific heat capacity	$[L^2.T^{-2}.\theta^{-1}]$	
k	Harmonic of discrete Fourier summation	-	
$l_c$	Characteristic length of the Nonlocal model	[L]	$l_c^* = l_c/L$
L	Length of the beam	[L]	
т	Harmonic of continuous Fourier series	—	
п	Number of elements	—	
р	Degree of the polynomial function	—	
Q	Amount of heat	$[M.L^2.T^{-2}]$	$\overline{Q} = Q / (\rho SLC\Delta T) - T_0 / \Delta T$
S	Rod section	$[L^2]$	
t	Elapsed time from initial state	[T]	$t^* = \alpha t/L^2$
Т	Temperature	[θ]	$\overline{T} = (T_0 - T) / \Delta T$
x	Longitudinal coordinate	[L]	$x^* = x/L$
α	Thermal diffusivity: $\alpha = \kappa / \rho C$	$[L^2.T^{-1}]$	
β	Variable associated to the optimal characteristic length $l_{c,opt}^2$	_	$\beta = a^2 / l_{c,opt}^2$
γ	Eigenvalue for time differential operators	_	
δ	Element partition for implicit finite difference computation	_	
λ	Eigenvalues for space differential operators		
$\Delta T$	Imposed maximum gap of temperature at time $t = 0$	[θ]	
K	Thermal conductivity	$[M.L.T^{-3}.\theta^{-1}]$	
ξ	Space-temperature eigenfunction	_	
τ	Time-temperature eigenfunction	-	
ρ	Rod density	$[M.L^{-3}]$	
φ	Heat flux density	[M.T <sup>-3</sup> ]	$\overline{\varphi} = L \varphi / (\kappa \Delta T)$

#### 662 Appendix A: Fourier series

#### 663 *Fourier summation coefficients for discrete system*

664 The resolution at the node of the discrete system only needs finite Fourier series using 665 coefficients  $A_k = (2/n) \sum_{p=1}^{n-1} \sin(k\pi p/n)$  that can be expressed as a single analytical 666 expression:

$$A_{k} = \sum_{p=1}^{n-1} \sin\left(k\pi \frac{p}{n}\right) = \operatorname{Im}\left(\sum_{k=1}^{n-1} e^{jk\pi \frac{p}{n}}\right) = \operatorname{Im}\left(\frac{e^{jk\frac{\pi}{n}} - e^{jk\pi}}{1 - e^{jk\frac{\pi}{n}}}\right) = \frac{\sin^{2}\left(\frac{k\pi}{2}\right)}{\tan\left(\frac{k\pi}{2n}\right)} = \frac{1 - (-1)^{k}}{2\tan\left(\frac{k\pi}{2n}\right)} \quad (40)$$

667

668 This relation allows to reduce computation of exact node solution to the single finite 669 summation of odd values of k given into Eq. (15).

#### 670 *Fourier series coefficients for continualized system*

671 To satisfy the initial state solution of the continuous one-dimensional media, 672 continuous functions  $\overline{T}_{ini}(x^*) = \overline{T}(x^*, 0)$  are defined for  $x^* \in [0;1]$ . The Fourier series 673 coefficient,  $A_m$ , are then defined as:

$$A_{m} = 2 \begin{bmatrix} \int_{(n-1)/n}^{1} f_{edge} \left(1 - x^{*}\right) \sin\left(m\pi x^{*}\right) dx^{*} \\ + \int_{1/n}^{(n-1)/n} \sin\left(m\pi x^{*}\right) dx^{*} \\ + \int_{0}^{1/n} f_{edge} \left(x^{*}\right) \sin\left(m\pi x^{*}\right) dx^{*} \end{bmatrix}$$
(41)

674

675 Where  $f_{edge}(x^*)$  is the initial distribution of temperature into the edge element, 676 defining the whole initial distribution of temperature  $\overline{T}(x^*,0)$  in the rod, see Eq. (17). 677 In order to verify  $\overline{T}(x^*,0) = \sum_{m=1}^{\infty} A_m \sin(m\pi x^*)$  according to Eq. (13) or Eq. (24), the 678 Fourier series coefficients with the various  $f_{edge}(x^*)$  introduced into section 2.2 give : 679 — with an Heaviside initial distribution of temperature  $\overline{T}(x^*, 0)$ ;

$$A_{m}^{H} = \frac{2}{m\pi} \Big[ 1 - (-1)^{m} \Big]$$
(42)

680

681 — with a "Trapezoidal"  $\overline{T}(x^*, 0)$ , or polynomial with p = 1, see Eq. (18);

$$A_m^{P_1} = \frac{2n}{\left(m\pi\right)^2} \left[1 - \left(-1\right)^m\right] \sin\left(\frac{m\pi}{n}\right)$$
(43)

682

683 - with a "Polynomial" 
$$\overline{T}(x^*, 0)$$
, with  $p = 2$ , see Eq. (18);

$$A_{m}^{P2} = \frac{2}{m\pi} \left[ 1 - (-1)^{m} \right] \left( 1 - \cos \frac{m\pi}{n} \right)$$
(44)

684

685 - with a "Polynomial"  $\overline{T}(x^*, 0)$ , with an even value degree p = 2q (where q is a 686 positive integer greater than 1), see Eq. (18);

$$A_{m}^{P2q} = \frac{2\left[1 - (-1)^{m}\right]}{m\pi} \begin{cases} (-1)^{q+1} (2q)! \left(\frac{n}{m\pi}\right)^{2q} \left[1 - \cos\left(\frac{m\pi}{n}\right)\right] \\ + \sum_{j=1}^{q-1} \frac{(-1)^{(j+1)} (2q)!}{(2(q-j))!} \left(\frac{n}{m\pi}\right)^{2j} \end{cases}$$
(45)

687

688 – with a "Sinusoidal"  $\overline{T}(x^*, 0)$ , see Eq. (19);

$$A_{m}^{s} = \frac{\left[1 - \left(-1\right)^{m}\right]}{m\pi} \left(\frac{n^{2}}{n^{2} - m^{2}}\right) \left(1 + \cos\frac{\pi m}{n}\right)$$
(46)

689

690 In case of an infinite number of elements into the chain of length *L*, the initial 691 trapezoidal distribution of temperature become steeper and tends toward an Heaviside 692 function, i.e., toward an uniform one along the whole chain. Hence, when  $n \to \infty$ , it 693 can be checked that the Fourier series coefficients tends toward  $A_m^H$ .

694 It should be noted that due to initial conditions, all Fourrier coefficients are null for 695 even values of m.

#### Appendix B: Numerical resolution

699 Semi-implicit finite difference method is applied to compute numerically the evolution of temperature along the chain discretized according to  $n\delta$  elements, with  $\delta$  the 700 701 additional partition of each element giving the length discretization  $\Delta x = L/n\delta$ . Presented computations, done to checked theoretical solutions, are made with  $\delta = 500$ . 702 703 To observe the large part of the diffusion process and be accurate at the beginning of the heat diffusion. With  $300 \times n$  computation times, time steps  $\Delta t^*$  are logarithmically 704 spaced into a range from  $10^{-5}$  to 1, in order to get more accuracy at the beginning of 705 706 the evolution.

707

Symmetrical boundary conditions allows to compute only a half rod with  $n\delta^2 + 1$  nodes to optimize the solving process, leading to the following specific boundary conditions:  $\overline{T}_0^{\ j} = 0$  and adiabatic wall in the middle corresponding to  $\overline{T}_{n\delta/2-1}^{\ j} = \overline{T}_{n\delta/2+1}^{\ j}$  while the initial condition leads to  $\overline{T}_1^0 = 0$  and  $\overline{T}_i^0 = 1$  for i > 1 in the Heaviside case, or  $\overline{T}_i^0 = f_{edge}(\delta)$  for  $i \le p$  and  $\overline{T}_i^0 = 1$  for i > p in all other cases.

713

The dimensionless discrete local diffusion in Eq. (8) matches exactly the finitedifference formulation. The continuous local heat equation can be numerically computed according a Crank-Nicolson scheme, combining the stability of an implicit method with the accuracy of a second order method in both space and time:

$$\frac{1}{\Delta t^{*}} \left( \overline{T}_{i}^{j+1} - \overline{T}_{i}^{j} \right) = \frac{1}{2 \left( \Delta x^{*} \right)^{2}} \left( \overline{T}_{i+1}^{j+1} - 2\overline{T}_{i}^{j+1} + \overline{T}_{i-1}^{j+1} + \overline{T}_{i+1}^{j} - 2\overline{T}_{i}^{j} + \overline{T}_{i-1}^{j} \right)$$
(47)

718

Here both the left- and right-hand sides are centered at time step j+1/2, so the method is second-order accurate in time, while a fully implicit method is only first-order accurate in time [51].

The following system of  $n\delta/2$  dimensionless equations allow to solve the node temperatures of next time step  $\overline{T_i}^{j+1}$  according to the boundary conditions mentioned above:

$$-\frac{(n\delta)^{2}}{2}\overline{T}_{i-1}^{j+1} + \left(\frac{1}{\Delta t^{*}} + (n\delta)^{2}\right)\overline{T}_{i}^{j+1} - \frac{(n\delta)^{2}}{2}\overline{T}_{i+1}^{j+1} = \frac{(n\delta)^{2}}{2}\overline{T}_{i-1}^{j} + \left(\frac{1}{\Delta t^{*}} - (n\delta)^{2}\right)\overline{T}_{i}^{j+1} + \frac{(n\delta)^{2}}{2}\overline{T}_{i+1}^{j+1}$$
(48)

The dimensionless discrete nonlocal diffusion equation, see Eq. (8) is reformulatedaccording to the same Crank-Nicolson finite difference scheme as:

$$\frac{1}{\Delta t^{*}} \left( \overline{T}_{i}^{j+1} - \overline{T}_{i}^{j} \right) = \frac{1}{2 \left( \Delta x^{*} \right)^{2}} \left( \overline{T}_{i+1}^{j+1} - 2\overline{T}_{i}^{j+1} + \overline{T}_{i-1}^{j+1} + \overline{T}_{i+1}^{j} - 2\overline{T}_{i}^{j} + \overline{T}_{i-1}^{j} \right) 
+ \frac{l_{c}^{*2}}{\Delta t^{*} \Delta x^{*2}} \left( \overline{T}_{i+1}^{j+1} - 2\overline{T}_{i}^{j+1} + \overline{T}_{i-1}^{j+1} - \overline{T}_{i+1}^{j} + 2\overline{T}_{i}^{j} - \overline{T}_{i-1}^{j} \right)$$
(49)

728

129 leading to solve the node temperatures of next time step  $\overline{T}_i^{j+1}$  with the following 130 system of  $n\partial 2$  equations.

$$-(n\delta)^{2} \left(\frac{1}{2} + \frac{l_{c}^{*2}}{\Delta t^{*}}\right) \overline{T}_{i-1}^{j+1} + \left[\frac{1}{\Delta t^{*}} + 2\left(\frac{1}{2} + \frac{l_{c}^{*2}}{\Delta t^{*}}\right)(n\delta)^{2}\right] \overline{T}_{i}^{j+1} - (n\delta)^{2} \left[\frac{1}{2} + \frac{l_{c}^{*2}}{\Delta t^{*}}\right] \overline{T}_{i+1}^{j+1} \\ = (n\delta)^{2} \left(\frac{1}{2} - \frac{l_{c}^{*2}}{\Delta t^{*}}\right) \overline{T}_{i-1}^{j} + \left[\frac{1}{\Delta t^{*}} - 2\left(\frac{1}{2} - \frac{l_{c}^{*2}}{\Delta t^{*}}\right)(n\delta)^{2}\right] \overline{T}_{i}^{j} + (n\delta)^{2} \left(\frac{1}{2} - \frac{l_{c}^{*2}}{\Delta t^{*}}\right) \overline{T}_{i+1}^{j}$$
(50)

731

The maximum relative differences of the numerical results with analytical ones are obtained with Heavisde and trapezoidal initial conditions. As shown in Fig. 14, the relative differences does not exceed  $10^{-3}$ , and are around  $10^{-6}$  or lower the this value for the main diffusion period, i.e. from  $t^*=10^{-4}$  to  $t^*=7.10^{-1}$ . These numerical results, in very good accordance with the analytical ones, allow to validate the presented analytical formulations.



Fig. 14 : Relative differences in temperature between numerical and analytical results of the lattice model used as reference (named as "exact") and local or nonlocal continualized model
continualized model
-a) at node 1 or n-1
-b) at the mid length, i.e. at node n/2.

# 746 Appendix C: Discontinuity of nonlocal diffusion model at the boundaries747

Integration of the nonlocal diffusion equation defined in Eq. (2) over the region  $\Omega$ , close to the boundary, at the first extremity located at x = 0 such as  $(-h \le x^* \le +h)$ , for  $0 \le t \le \Gamma$ , leads to:

$$\int_{-h}^{+h} \left[ \overline{T} \left( x^*, \Gamma \right) - \overline{T} \left( x^*, 0 \right) \right] dx - \int_{0}^{\Gamma} \left[ \left( \alpha \overline{T}' + l_c^2 \overline{T}^{\mathbf{x}} \right) \right]_{-h}^{h} dt = 0$$
(51)

751 When 
$$h \rightarrow 0$$
, the first integral tends toward 0 and as consequence:

$$\int_{0}^{\Gamma} \sqrt{T}' + l_c^2 \vec{T} \sqrt{T} dt = 0$$
(52)

where the double bracket sign §" designates the difference in value on both side of the discontinuity, i.e. at  $x = 0^-$  and  $x = 0^+$ . Since the expression under the integral sign is a 754 continuous function of dimensionless time until  $\Gamma$ , the first condition at the boundary is 755 obtained:

$$\bigvee_{\ll}^{\mathbb{D}} \alpha \overline{T}' + l_c^2 \overline{T}' \stackrel{\mathbb{D}}{\mathbb{R}} - \alpha \overset{\mathbb{D}}{\ll} \overline{T}' \stackrel{\mathbb{D}}{\mathbb{R}} + l_c^2 \overset{\mathbb{D}}{\ll} \stackrel{\mathbb{D}}{\mathbb{R}} = 0$$
(53)

756 Unfortunately,  $\overline{T}'$  is unknown, and a second condition based on  $\overline{T}$  has to be defined.

757 Integration over the region  $\Omega$  of the nonlocal diffusion equation multiplied by  $x^*$  gives:

$$\int_{-h}^{+h} \left[ \overline{T} \left( x^*, \Gamma \right) - \overline{T} \left( x^*, 0 \right) \right] x^* dx^* - \int_{0}^{\Gamma} \int_{0}^{\infty} x \alpha \overline{T}' + x l_c^2 \overline{T}_{\overline{C}} dt + \int_{0}^{\Gamma} \partial \alpha \overline{T} + l_c^2 \overline{T}' \partial t = 0$$
(54)

When  $h \rightarrow 0$ , the first and second integral tend toward 0. Hence, the condition at the boundary is obtained:

$$\sqrt[2]{\alpha}\overline{T} + l_c^2 \overline{T} \stackrel{r}{\otimes} \alpha \otimes \overline{T} \stackrel{r}{\otimes} l_c^2 \otimes \overline{T} \stackrel{r}{\otimes} 0$$

$$(55)$$

It should be noted that due to the symmetry of the diffusion problem, the same demonstration can be made at the opposite boundary, at the second extremity located at x = L or  $x^* = 1$  in Heaviside case.

763 Solving this first order differential equation, according to the initial conditions at both

764 boundaries, i.e.  $\overline{T}(0^+,0) - \overline{T}(0^-,0) = 1 = \overline{T}(L^-,0) - \overline{T}(L^+,0)$  according to Eq. (6),

765 gives the temperature immediately to the inside boundary:

$$\overline{T}\left(0^{+},t\right) = \exp\left(-\frac{\alpha t}{l_{c}^{2}}\right) = \overline{T}\left(L^{-},t\right)$$
(56)

This solution fulfills as well the first condition at the boundary previously establishedin Eq. (53).

768

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