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Nonlocal thermal diffusion in one-dimensional periodical lattice

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Abstract

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

Lattice.

1. Introduction

23 This paper explores the possibility to characterize the thermal behaviour of 24 heterogeneous one-dimensional medium with a nonlocal approach, based on the 25 introduction of some scale effects in the nonlocal diffusion model. A thermal lattice 26 will be studied from a mixed differential-difference equation that will be analytically 27 solved. The second part of the paper is devoted to the continuous approaches that may 28 be valid to capture the scale effects inherent to the lattice properties. Scale effects may 29 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,

34 fully described in section 2.1, is explored. Such discrete media is based on a physical 35 thermal lattice ruled by a mixed difference differential equation, see [1]:

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

36 where T_i is the temperature at the node *i* and $T_i^{\mathcal{R}}$ denotes its time derivative, α is the 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

45 The aim of the present paper is to investigate the capability of some nonlocal heat 46 partial differential equations to capture the inherent scale effects into such periodical 47 thermal lattice system. A nonlocal heat equation can be built from continualization of 48 the thermal lattice system, using asymptotic expansion of the associated pseudo-49 differential operator. The nonlocal heat equation is augmented by some coupled spatial 50 and time-dependent terms which are affected by the lattice parameters:

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

$$
\rho C \mathcal{P}^{\mathcal{L}} = -\varphi' \tag{3}
$$

63 where φ is the heat flux density, ρ 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, *κ* 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

73 Such nonlocal diffusion equation has been already considered for mass-transfer 74 modeling by Barenblatt [11] applied to liquid flows in cracked rocks, and more 75 recently in heat diffusion in the same periodically micro structured rod [2]. Exact 76 solutions of this nonlocal heat equation have been derived for various initial and 77 boundary conditions [2] [11] [12].

78

79 Nonlocal diffusion problems have been also studied by many authors, with an 80 additional characteristic time making this equation both non local in time and space 81 [13] [14] [15] [16] [17] [18] [19] [20] [21] [22]. The nonlocal Fourier's law is an 82 evolution equation of Guyer-Krumhansl type which relates the heat flux with respect 83 to the temperature field using an additional length scale for the flux. For the complete 84 Guyer-Krumhansl type model, an additional relaxation time (as for Cattaneo's model) 85 has to be considered in addition to the spatial nonlocal length scale, see [4] [5] [6] [23]. 86

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

102 In this study, the exact resolution of the mixed differential-difference heat equation, 103 valid for the thermal lattice (which may also cover other discrete diffusion processes) 104 is presented. A nonlocal continuous approximation of this lattice model is thought, 105 using a Padé approximant of the spatial pseudo-differential operator, thus avoiding 106 higher-order spatial derivatives. The nonlocal heat equation finally uses coupled 107 continuous spatial and time derivatives.

108

109 **2. Thermal discrete lattice.**

110 *2.1. Definition*

111 The physical discreteness of the material can be assumed at least at the atomic scale. 112 Other heterogeneities at larger scales can also be considered. In this study, a periodic 113 discrete lattice is assumed, consisting in *n* rigid elements with a constant length equal 114 to $a = L/n$, as already studied by the authors [2] and, with additional heterogeneities by 115 Zingales [3].

119

118 *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 $a\hat{\rho}_i$ 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 ρL , 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:

$$
\varphi_{i+1/2} = -\kappa_{i+1/2} \frac{T_{i+1} - T_i}{a} \text{ and } \rho C T_i^{\mathcal{R}} = -\frac{\varphi_{i+1/2} - \varphi_{i-1/2}}{a} \tag{5}
$$

129 The discrete heat diffusion equation can then be formulated as Eq. (1).This mixed 130 difference-differential equation slightly differs from the difference equation in space 131 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

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

138 The following dimensionless parameters, normalized with respect to the physical 139 characteristics of the rod, *L* and α 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 $\bar{\varphi}$ such as:

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

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

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

142

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

$$
\overline{\mathcal{I}_i^{\mathcal{K}}} = n^2 \left(\overline{T}_{i+1} - 2\overline{T}_i + \overline{T}_{i-1} \right)
$$
 (8)

145

146 The local difference equation of the thermal lattice system (with $l_c = 0$) has been 147 widely studied through numerical treatments using time and spatial discretization, for 148 instance in [31] [32], [33] and more recently in [34]. In this paper, it should be noted 149 that local difference equation of the thermal lattice exactly matches the finite-150 difference formulation of the one-dimensional heat diffusion equation with a 151 continuous time parameter.

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

153 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 155 the dimensionless temperature at node *i*, leads to:

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

156

The time dependent term, $\tau(t^*)$, can be first easily integrated: $\tau = P_1 \exp(-\gamma t^*)$ 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

159 remains. The homogeneous linear second-order difference with constant coefficients 160 may be solved if a power law function is introduced [35], i.e. $\xi_i = \xi \lambda^i$, see for instance 161 [36], giving the auxiliary equation according to λ :

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

162

163 Eq. (10) is symmetrical with respect to interchanging λ and 1/ λ . This equation admits 164 the two complex solutions λ_1 and λ_2 for $0 \le \gamma n^2 \le 4$, i.e. if $\left|1 - \gamma/2n^2\right| < 1$.

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

165

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

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

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)

These conditions leads to: $A_k = (2/n) \sum_{p=1}^{n-1} \sin(k\pi p/n)$ 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:

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

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. Boundary conditions of equivalent continuous media*

186 The key point is the consideration of a disturbance of the discrete temperature field at 187 both ends of the finite discrete rod. In this study, we will explore the capability of 188 continuous nonlocal heat equation to capture some scale effects of such discrete 189 thermal lattices. For the continuous approach, the full definition of the temperature 190 field is needed within all the bar. Many continualized initial temperature fields built 191 from a homogeneous initial discrete temperature can be assumed from homogeneous 192 initial discrete temperature.

193

194 We will consider four basic assumptions about initial continuous field of temperature, 195 according to $x^* = x/L$, in the continualized nonlocal chain. These assumptions on the 196 discrete case are transposed from a finite continuous rod, initially at stable and 197 constant temperature T_0 and disturbed at $t = 0$ with the same temperature imposed at 198 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,
\n
$$
\forall x^* \in [1/n;1-1/n], \overline{T}(x^*,0) = 1
$$
in other cases
\nif $t \ge 0$, $\overline{T}_0(0,t^*) = \overline{T}_n(1,t^*) = 0$ (16)

199

200 In the continuous case, the initial temperature (at $t = 0$) corresponds to a step function 201 located at both ends, made of a combination of Heaviside functions, discontinuous in 202 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 206 elements. This transposition of the discontinuous Heaviside distribution of temperature 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

218 In order to avoid discontinuity in time evolution of temperature, the initial distribution 219 of temperature, at $t = 0$, has to make the edge nodes temperatures already equal to T_{imp} . 220 To approximate as much as possible the classical Heaviside distribution, the next node 221 temperature, inward the chain, has to be equal to T_0 . The remaining question is about 222 initial distribution of temperature into the edge elements, i.e. between the nodes 0 and 223 1, and the nodes $n-1$ and n , see Fig. 2.

224

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

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

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

228

229 – The second assumption assumes an initial distribution of temperature with a constant 230 gradient, ∆*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 dimensionless part function of $\overline{T}(x^*,0)$ in this case is defined by $f_{edge,p}(x^*)$ 240 *dimensionless part function of* $T(x^*,0)$ *in this case is defined by* $f_{edge,p}(x^*)$ *according* 241 to *p* as:

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

242

243 The "trapezoidal" case corresponds to the case $p = 1$, while the "heavisisde" case 244 corresponds to $p \rightarrow \infty$, see Fig. 3. It should be note that in introduced "polynomial" 245 functions, the spatial gradient of $T(x^*,0)$ is discontinuous at the boundaries, in $x^* = 0$ 246 and $x^* = 1$.

249 – The fourth assumption, names as "Sinusoidal" is finally introduced in order to ensure 250 the continuity of the temperature and of its first spatial derivative over the whole 251 • length of the chain. $\overline{T}(x^*,0)$ and $\frac{\partial \overline{T}(x^*,0)}{\partial x^*}$ are then continuous at both nodes of 252 edges elements, i.e. at the nodes $0,1$, $n-1$ and n , see Fig. 3. The dimensionless part 253 function of $\overline{T}(x^*,0)$ in this case is defined as:

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

255

256 *Fig. 3 : Initial temperature distribution into edge elements*

257

258 *3.2. Analytical solution of the nonlocal model*

259 Following the classical method using the separation of variables, already exposed in 260 section 2.2, based on $\overline{T}(x, t^*) = \xi(x^*) \tau(t^*)$, the nonlocal heat diffusion equation, see 261 Eq. (2) can be written in dimensionless form as:

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

262 For a given continuous abscissa x^* , the first term $\frac{dx}{x}$ remains constant. Assuming 263 *c* $\oint_C \tau = -\gamma$, the following equality is obtained: $\frac{\xi''}{\xi} = \gamma / (\gamma_c^2 - 1)$ with $l_c^* \leq 1/\gamma$. This 264 last condition about l_c will be discussed later and justified by Eq. (23). The solution of 265 $\tau(t^*)$ and $\xi(x^*)$ can then be written:

248

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

266 where P_4 , P_5 and P_6 are constant parameters to be determined according the initial 267 boundary conditions, given into Eq. (16) and equivalent to $\xi(0) = \xi(1) = 0$. As a 268 consequence, the constant parameter P_6 in Eq. (21) is null and $\xi(x^*)$ reduces to:

$$
\xi(x^*) = P_5 \sin(m\pi x^*)
$$
\n(22)

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

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

270 This equation assumes a positive value of χ and in accordance with the inequality 271 previously assumed to set the Eq. (21), it can be checked that $0 < \gamma < 1/l_c^{2}$ whatever 272 the value of *m*.

273

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

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

275

276 where A_m are the continuous Fourier series coefficients defined according the initial 277 continuous conditions given into Eq. (17) i.e. according to $f_{edge}(x^*)$ the Fourier series 278 coefficients are all presented in Appendix A.

279

280 It should be noted that the nonlocal solution in Eq. (24) leads to the classical well-281 known local solution if the characteristic length, l_c , is null i.e., when $n \to \infty$. This 282 solution is also compared to compared to numerical ones based on the resolution of the 283 local and nonlocal heat differential equation according to the characteristic length, *lc*. 284 The semi-implicit resolution method used and relative details are given in Appendix B. 285

286 As already observed for A_k in section 2.2, the coefficient A_m are always null for even 287 values of *m*. Hence, the Fourier series can be expressed and computed more efficiently

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

289 *3.3. Extrapolation of the lattice exact solution*

290 The discrete solution at the nodes of the lattice given into Eq. (13) can also be 291 extended as a continuous solution using the same integration over the whole length of 292 the chain to determine the A_m coefficients of Fourier series:

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

293

294 The extended exact solutions computed from this equation are plotted through the 295 continuous abscissa x^* between the nodes in Fig. 4 *a*) and *b*). Whatever the continuous 296 initial distribution of temperature, the node temperatures converge rapidly toward the 297 same solution given by Eq. (13), matching exactly the lattice temperature at the node 298 abscissa, i.e. for $x^* = x_i^* = i/n$. These analytical results are checked with numerical 299 ones. The numerical finite difference scheme used and more details are presented in 300 Appendix B.

301

302 As a consequence, all the results obtained from Eq. (25) with the various Fourier 303 coefficients A_m , (see Appendix A) give surprisingly the same exact results at node 304 abscissa, while initial shape of temperature distribution into the edge element 305 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 313 increases. For instance, with computation of $10⁶$ harmonics, this phenomena is so 314 concentrated that it cannot appear on the presented plots in Fig. 4.

316 *Fig. 4 : Extended exact temperatures of the discrete system in a half part of a 6* 317 *elements system at dimensionless time: – a)* $t^* = 0.016$; – b) $t^* = 0.064$

19 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

323 Semi-infinite system with an imposed temperature at the border, T_0 , are classically 324 studied. As in the finite system, for an infinite elapsed time, temperatures tends 325 asymptotically towards T_0 , when $t \rightarrow \infty$, while the temperature decreases 326 instantaneously in the whole chain for $t > 0$. Since $n \to \infty$, the difference equation 327 given into Eq. (1) is the same as the differential equation of the continuous case. It 328 finds the well-known solution of local parabolic Fourrier equation, based on error 329 function, $erf(x)$, in case of the semi-infinite continuous medium:

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

330

331 Thereafter, this solution is used to compare the results from local and nonlocal models 332 with the exact temperature at some node abscissas, see Fig. 7.

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

334

335 *4.1. Continualization procedure*

336 Based on a Taylor expansion of the spatial difference operator in Eq. (8), the 337 continualization procedure considers that for a sufficiently smooth temperature 338 distribution of temperature $\overline{T}_i = \overline{T}(x = ia)$ and

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

339 where $\partial_x = \partial/\partial x$ is the spatial differentiation and $e^{a\partial_x}$ is a pseudo differential operator 340 as introduced for instance in [40] [41] and widely used for mechanical problems [42] 341 [43] [44] [45] [46].

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

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

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

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

346 which leads to a gradient-type temperature diffusion problem with the square of 347 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 354 discrete system both in space and in time, as opposed to the thermal lattice considered 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

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

360

361 A numerical solution could be directly computed from the second-order continualized 362 equation, however, the pseudo-differential operator can also be efficiently 363 approximated by Padé's approximant to compute dynamic responses [44] [45] [40] 364 [41], or recently in cases of of linear elastic lattice [47], even inelastic lattice such as 365 damage mechanics [48] or elastoplastic problems [49].

366

367 To avoid the difficulties associated with higher-order boundary conditions needed in 368 the resolution of such continualized schemes [50], Padé's approximation of the finite 369 difference Laplacian is introduced:

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

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

$$
\vec{T}^{\!\mathcal{K}} = \vec{T}'' + l_c^{*2} \vec{T}^{\!\mathcal{K}} \text{ with } l_c^{*2} = \frac{a^2}{12L^2} = \frac{1}{12n^2} \tag{31}
$$

371 This nonlocal diffusion law is physically supported by the cell length, *a*, of the 372 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 4.10-3 to 128.10-3 with initial temperature distribution into the edge elements corresponding to: 387 $- a)$ *Heaviside case;* $-b)$ *Trapezoidal,* P^1 *;* $-c)$ *Polynomial* P^{12} *;* $-d)$ *Sinusoidal.*

391 As observed in Fig. 5 a), in case of Heaviside initial temperature distribution, the 392 nonlocal model highlights an unexpected temperature discontinuity at the boundary for 393 the shortest evolution times. A focus on this discontinuity phenomenon for shorter 394 evolution time with the same $n = 6$ elements system is presented in Fig. 6.

395

396

400

397 *Fig. 6 : Focus on discontinuities of temperature at the boundaries of a n=6 elements* 398 *system in case of Heaviside initial temperature distribution at beginning of evolution, for dimensionless times ranging from* $0.125.10^{3}$ *to* 4.10^{3} *.*

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 temperature 408 evolution at the inside borders can be expressed a dimensionless form:

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

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*

413 The nonlocal model does not predict always the node temperature with a better 414 accuracy than the local one. As shown in Fig. 5, for a given node, the efficiency of the 415 nonlocal model depends on the node abscissa and evolution time. The difference 416 between the exact node temperature and predictions according to the local and 417 nonlocal models of a $n = 6$ elements system are plotted versus time evolution at the 418 first nodes beyond the boundary (i.e. $i = 1$ or $i = n - 1$) in Fig. 7 a) and c) at the mid 419 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 426 the same abscissa when t^* is close to 2.10⁻². In case of Heaviside boundary condition, 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

431 As shown in Fig. 7, whatever the boundary condition, the magnitude of the difference 432 with the exact temperature is always higher with local models than with the nonlocal 433 ones, meaning a better accuracy of the enriched model based on nonlocal 434 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 trigonometric 442 continualization process.

Fig. 7 : Evolution of differences between normalized temperature of the models (local and nonlocal) and the exact ones for a n = 6 elements system: – c) at node 1 or (n–1) with Heaviside, Trapezoidal and Sinusoidal boundary conditions – a) at the mid length (i.e. node n/2) with Heaviside, Trapezoidal and Sinusoidal boundary conditions 450 $-d$) 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 455 nonlocal model for given condition and node could change drastically with time 456 evolution, the efficiency of models is globally compared for all node temperatures 457 introducing a time dependent error function, $Err(t^*)$, based on the residual sum of 458 squares, i.e. $\sum (\overline{T}_i - \overline{T}_{i, exact})^2$. Both term of temperature are theoretically null at the 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 :

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

461

452

462 It should be noted here, that edge node temperature is actually not null for Heaviside 463 initial assumption, see Eq. (32). If the whole nodes are considered, The *Err* function of 464 the nonlocal model in the Heaviside case would be higher in the first instants of the 465 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 470 local one. The Fig. 8 b) confirms that Polynomial P^2 initial temperature distribution 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 $t^* = 10^{-2}$ 474 with *Err* function computed from the $n-1$ centered nodes. Whatever initial 475 conditions, the nonlocal model gives significantly less residual values at nodes on the 476 whole studied time evolution, i.e. with $10^{-5} < t^* < 1$.

477 *Fig. 8 : Time evolution of the residual sum of squares at node abscissa of the models* 478 *(local and nonlocal), Err, for a n = 6 elements system:* 479 *– a) with Heaviside, Trapezoidal and Sinusoidal boundary conditions* 480 $- b$) with Heaviside, Polynomial, P^2 , P^4 , and P^{12} . 481

482 *4.4. Length scale calibration*

183 In order to calibrate the length scale, the optimal characteristic length $l_{c, opt}^2$, associated 484 to the nonlocal model is introduced. The Eq. (31) can be written according a second 485 variable, β , such as $l_{c, opt}^2 = a^2/\beta$, equivalent to $l_{c, opt}^{*2} = 1/\beta n^2$. The minimum of 486 *Err* (t^*, β) provides the β value, i.e. the optimal characteristic length $l_{c, opt}^2$. The value 487 of β can be computed according t^* by solving $\frac{\partial Err}{\partial \beta} = 0$, that can be numerically 488 computed as follow :

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

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

497 In accordance with the previous observations about the prediction accuracy according 498 to initial temperature distributions, the Polynomial P^2 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
$$
\beta = (n^2 l_{c,opt}^{*2})^{-1}
$$

\n502 – a) as a function of time (t^*) with the considered initial conditions
\n503 – b) as a function of time (t^*) according to various values of n

505 *4.5. Prediction of heat flow at boundaries*

506 The outlet heat flow density at boundaries in a dimensionless and normalized form is 507 introduced: $\overline{\varphi}_0$, at $x^* = 0$ or $\overline{\varphi}_1$, at $x^* = 1$. Eq. (3) and Eq. (7) lead to: $(x^* = 0)$ $^{1/2}$ \mathcal{B}_{1} * $\overline{\varphi}_0 = -\overline{\varphi}_{(x^*=0)} = \int_0^{1/2} \overline{f}^3 \overline{\varphi}_{\overline{\chi}}^* \text{ or } \overline{\varphi}_{(x^*=1)} = -\int_{1/2}^1 \overline{f}^3 \overline{\varphi}_{\overline{\chi}}^*$ 508 $\overline{\varphi}_0 = -\overline{\varphi}_{(x^*=0)} = \int_0^{1/2} \overline{f} dx^*$ or $\overline{\varphi}_{(x^*=1)} = -\int_{1/2}^1 \overline{f} dx^*$. Due to symmetrical conditions it can be 509 easily checked that $\overline{\varphi}_0 = \overline{\varphi}_1$.

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

$$
\overline{\varphi}_0 = \pi \sum_{m=1}^{\infty} \frac{m A_m}{1 + m^2 \pi^2 l_c^{*2}} \exp\left(\frac{-m^2 \pi^2 t^*}{1 + m^2 \pi^2 l_c^{*2}}\right)
$$
(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 ϕ_0^* for 517 the initial conditions giving the greater differences are plotted in Fig. 10 a) and b). 518

520 *Fig. 10 : Time evolution of the normalized outgoing heat flow density at boundaries,* 521 *– a) for Heaviside and Sinusoidal initial conditions – b) for Polynomial P¹²* 522 *and Trapezoidal initial conditions*

524 $\bar{\varphi}_{0,exact}(t^*)$ 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 $(P¹)$ toward Heaviside (to $P¹²$). 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.

Fig. 11 : Relative difference between the exact, $\overline{\varphi}_{0, \text{exact}}$, and local and nonlocal 532 *...* outgoing heat flow density at boundaries, $\bar{\varphi}_0$, versus dimensionless time evolution t^* . 533 *– a) for Heaviside, Sinusoidal and Trapezoidal initial conditions – b) for Heaviside and Polynomial P¹², P⁴ and P²* 534 *initial conditions*

535

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 540 the values $\bar{\varphi}_0$ in comparison of $\bar{\varphi}_{0,exact}$ and nonlocal model is far to be efficient until 541 $t^* = 8.10^{-3}$ in the case of $n = 6$ elements system.

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 β toward 12 does, see Fig. 9 b). Beyond this transitory time, the nonlocal model gives better results than the local one, except for Polynomial P^2 547 548 initial case where the local model could be still punctually better.

550 *4.6. Prediction of the global amount of heat*

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:

$$
Q(t) = \rho CS \int_0^L T(x, t) dx
$$
 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)

553 where $\overline{Q}(t^*)$ is the normalized amount of heat equal to the average temperature along 554 the finite continualized rod. Based on Eq. (24) or on Eq. (35), $\overline{Q}(t^*)$ from local $(l_c^* = 0)$ 555 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 Eq. (37). The exact solution $\overline{Q}(t^*)$ 559 Eq. (37). The exact solution $Q(t^*)_{\text{exact}}$ used as reference is then computed for each 560 initial temperature distribution from Eq. (25) as:

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

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

571 coefficient). For instance, $\overline{Q}_{exact}(t^*)$ is the same for Sinusoidal and Trapezoidal case, 572 as it can be already observed with $\bar{\varphi}_0$ 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 – b) for Polynomial P¹²* 576 *and Trapezoidal initial conditions*

578 Evolution of \overline{Q} , plotted in Fig. 12, shows that both local and nonlocal models 579 underestimate the remaining amount of heat into the system during the evolution in 580 Heaviside and similar boundary condition as polynomial $P¹²$ while the curves are very 581 closed without clear tendency in sinusoidal or Trapezoidal case. The differences with 582 the exact case are detailed in Fig. 13 for each initial case.

583

577

584 Results show that the nonlocal model give better prediction than the local one, from 585 the beginning of the evolution, to predict the amount of heat, in particular with 586 Heaviside and Polynomial, Trapezoidal included, initial conditions, see Fig. 13 *b)*. In 587 these cases, local model leads to a significant underestimation in comparison of the 588 nonlocal model, especially at the beginning of the evolution, until $t^* = 8.10^{-3}$ with 589 $n = 6$, when the scale effect results in a delayed diffusion.

591 *Fig. 13 : Relative difference between amount of heat deduced from exact formulation* 592 $\overline{Q}_{\text{exact}}$ and from local and nonlocal model \overline{Q} versus dimensionless time evolution t^* . 593 *– a) for Heaviside, Sinusoidal and Trapezoidal initial conditions – b) for Heaviside and Polynomial P¹², P⁴ and P²* 594 *initial conditions* 595

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**

609 Thermal diffusion in a one-dimensional periodically microstructured lattice can be 610 described within a quasi-continuum approach governed by a nonlocal Fourier's law, 611 similar to the differential model of Eringen [10] initially devoted to material elasticity. 612 This nonlocal Fourier law can be also cast into a more general Guyer-Krumhansl type 613 model [5].

614

615 Using a continualization procedure, the characteristic length scale of the nonlocal heat 616 model is calibrated from the lattice spacing, *a*. This calibration appears also to be 617 optimal, since minimization of the sum of squares of residuals node temperature makes 618 the square of this length scale, with time evolution and/or increasing number of 619 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

644 The present spatially nonlocal model, is able to predict delayed diffusion phenomena 645 in thermal lattices ruled by mixed differential-difference equations. It is probably 646 possible to extend such nonlocal model for discrete problems with both space and time 647 discreteness, leading to generalized nonlocal continuous diffusion problems, both in 648 space and in time.

649

650 **Declaration of competing interest**

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

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

653

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659 **Nomenclature**

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 coefficients $A_k = (2/n) \sum_{p=1}^{n-1} \sin(k\pi p/n)$ 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:

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

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, *Am*, are then defined as:

$$
A_{m} = 2\begin{bmatrix} \int_{(n-1)/n}^{1} f_{edge}(1-x^{*})\sin\left(m\pi x^{*}\right)dx^{*} \\ + \int_{1/n}^{(n-1)/n} \sin\left(m\pi x^{*}\right)dx^{*} \\ + \int_{0}^{1/n} f_{edge}\left(x^{*}\right)\sin\left(m\pi x^{*}\right)dx^{*} \end{bmatrix}
$$
(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). In order to verify $\overline{T}(x^*,0) = \sum_{m=1}^{8} A_m \sin(m\pi x^*)$ $(0,0) = \sum A_m \sin m$ *m* $T(x^*,0) = \sum A_m \sin(m\pi x)$ ∞ = 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 $\overline{T}(x^*,0)$;

$$
A_m^H = \frac{2}{m\pi} \left[1 - \left(-1 \right)^m \right] \tag{42}
$$

680

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

$$
A_m^{P1} = \frac{2n}{\left(m\pi\right)^2} \left[1 - \left(-1\right)^m\right] \sin\left(\frac{m\pi}{n}\right) \tag{43}
$$

682

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

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

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);

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

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 coeficients are null for 695 even values of *m*.

697 **Appendix B: Numerical resolution**

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

707

708 Symmetrical boundary conditions allows to compute only a half rod with $n\delta/2+1$ nodes 709 to optimize the solving process, leading to the following specific boundary conditions: 710 $\overline{T}_0^j = 0$ and adiabatic wall in the middle corresponding to $\overline{T}_{n\delta/2-1}^j = \overline{T}_{n\delta/2+1}^j$ while the 711 initial condition leads to $\overline{T}_1^0 = 0$ and $\overline{T}_i^0 = 1$ for $i > 1$ in the Heaviside case, or 712 $\overline{T}_i^0 = f_{edge}(\delta)$ for $i \leq p$ and $\overline{T}_i^0 = 1$ for $i > p$ in all other cases.

713

714 The dimensionless discrete local diffusion in Eq. (8) matches exactly the finite-715 difference formulation. The continuous local heat equation can be numerically 716 computed according a Crank-Nicolson scheme, combining the stability of an implicit 717 method with the accuracy of a second order method in both space and time:

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

718

719 Here both the left- and right-hand sides are centered at time step *j*+1/2, so the method 720 is second-order accurate in time, while a fully implicit method is only first-order 721 accurate in time [51].

722 The following system of $n\delta/2$ dimensionless equations allow to solve the node 723 temperatures of next time step \overline{T}^{j+1} according to the boundary conditions mentioned 724 above:

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

726 The dimensionless discrete nonlocal diffusion equation, see Eq. (8) is reformulated 727 according to the same Crank-Nicolson finite difference scheme as:

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

728

129 leading to solve the node temperatures of next time step \overline{T}_i^{j+1} with the following 730 system of $n\delta/2$ 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

732 The maximum relative differences of the numerical results with analytical ones are 733 obtained with Heavisde and trapezoidal initial conditions. As shown in Fig. 14, the 734 relative differences does not exceed 10^{-3} , and are around 10^{-6} or lower the this value 735 for the main diffusion period, i.e. from $t^*=10^{-4}$ to $t^*=7.10^{-1}$. These numerical results, in 736 very good accordance with the analytical ones, allow to validate the presented 737 analytical formulations.

739 *Fig. 14 : Relative differences in temperature between numerical and analytical results* 740 *of the lattice model used as reference (named as "exact") and local or nonlocal* 741 *continualized model* 742 *– a) at node 1 or n–1* 743 *– b) at the mid length, i.e. at node n/2.* 744

746 **Appendix C: Discontinuity of nonlocal diffusion model at the boundaries** 747

748 Integration of the nonlocal diffusion equation defined in Eq. (2) over the region Ω , close to the boundary, at the first extremity located at $x = 0$ such as $(-h \le x^* \le +h)$, for 750 $0 \le t \le \Gamma$), leads to:

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

751 When *h*→0, the first integral tends toward 0 and as consequence:

$$
\int_{0}^{1} \mathbf{F}' + l_c^2 \mathbf{F}' \frac{\partial \mathbf{F}'}{\partial \theta} dt = 0
$$
\n(52)

752 where the double bracket sign \hat{S} 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 Γ, the first condition at the boundary is 755 obtained:

$$
\mathcal{L}_{\alpha}^{\mathcal{D}} \overline{\mathcal{A}}^{\mathcal{T}} + l_c^2 \overline{\mathcal{B}}^{\mathcal{L}} \overline{\mathcal{D}} = \alpha \mathcal{L}^{\mathcal{T}} \mathcal{B} + l_c^2 \mathcal{L}^{\mathcal{L}} \overline{\mathcal{D}} = 0 \tag{53}
$$

756 Unfortunately, \overline{T}' is unknown, and a second condition based on \overline{T} has to be defined. Integration over the region Ω of the nonlocal diffusion equation multiplied by x^* gives:

$$
\int_{-h}^{+h} \left[\overline{T}\left(x^*,\Gamma\right) - \overline{T}\left(x^*,0\right) \right] x^* dx^* - \int_{0}^{h} \sqrt{\omega} \overline{C} \overline{T}' + x l_c^2 \overline{T}' \sqrt{\omega} dt + \int_{0}^{h} \sqrt{\omega} \overline{T} + l_c^2 \overline{T}' \sqrt{\omega} dt = 0 \tag{54}
$$

758 When *h*→0, the first and second integral tend toward 0. Hence, the condition at the 759 boundary is obtained:

$$
\frac{dQ}{dt} \partial \overline{T} + l_c^2 \overline{T} + \frac{dQ}{dt} \overline{T} + l_c^2 \overline{Q} + l_c^2 \overline{T} + l_c^2 \overline{T}
$$

760 It should be noted that due to the symmetry of the diffusion problem, the same 761 demonstration can be made at the opposite boundary, at the second extremity located 762 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:

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

766 This solution fulfills as well the first condition at the boundary previously established 767 in Eq. (53).

- 768
- 769

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