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3D fluid-structure simulation of innovative composites for the design and thermal management of electronic devices

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Abstract

Thermal management of electronic devices remains a challenging issue, especially the cooling of electronic components. Current methods mostly involve noisy, cumbersome and underperforming fans. It has recently been shown that phase change materials (PCMs) can perform better and offer more efficient damping of temperature variations in electronic components. Here, we present three novel contributions. First, we consider a triply-periodic minimal surface, called a gyroid, as a porous architected structure containing the PCM. Such a topology mathematically maximizes the exchange surface between the copper structure and the PCM. Heat transfer and thus the performance of such a composite are therefore optimized. Second, we set up a complete 3D coupled fluid-structure model of the composite. This model simulates the heat transfer (conduction and convection) inside both the PCM and the porous structure, as well as the mechanical stresses induced on the container by thermal expansion of the PCM. The 3D coupled theoretical model is based on open-source software codes, OpenFOAM, CalculiX and preCICE. With this novel model, deformation of the structure and mechanical stresses are now predictable. It is therefore possible to anticipate whether a configuration will be prone to leakage due to mechanical failure. Thermal contact resistance is also computed, giving information on heat transfer quality at the interface between the composite and the electronic component. Third, the application of this model to the innovative composite shows that reducing the initial filling level of PCM is a better solution than strengthening the container to maximize thermal management.

Keywords: Electronic component; Gyroid; Phase change materials and conductive matrix composite; Fluid-structure interaction; Conjugate heat transfer; CFD

43

44 List of symbols

c_p	Specific heat at constant pressure ($J.kg^{-1}.K^{-1}$)
d	Structure displacement (m)
D	Thermal diffusivity ($m^2.s$)
E	Young's modulus (Pa)
g	Gravitational acceleration ($m.s^{-2}$)
L	Characteristic length (m)
m	Mass (kg)
p	Pressure (Pa)
R_{th}	Thermal resistance ($K.m^2.W^{-1}$)
s	Phase change interface position (m)
T	Temperature (K)
u	Velocity ($m.s^{-1}$)
V	Volume (m^3)

45

46 Greek symbols

α	Solid fraction
β	Coefficient of thermal expansion (K^{-1})
δ	Peak to valley (m)
Δh_f	Heat of fusion ($J.kg^{-1}$)
ε	Temperature range where melting occurs (K)
$\boldsymbol{\varepsilon}$	Infinitesimal strain tensor
ζ	Square root of the liquid thermal diffusivity over the solid one
η	Poisson's ratio
κ	Penalization parameter ($10^{20} kg.m^{-3}.s^{-1}$)
λ	Thermal conductivity ($W.m^{-1}.K^{-1}$)
μ	Dynamic viscosity ($Pa.s$)
ν	Cinematic viscosity ($m^2.s^{-1}$)
ξ	Filling level of PCM
ρ	Density ($kg.m^{-3}$)
$\boldsymbol{\sigma}$	Stress tensor (Pa)
τ	Characteristic time (s)
χ_T	Adiabatic compressibility (Pa^{-1})

47

48 Subscripts

0	Reference configuration
air	Air properties
conv	Convection
diff	Diffusion
l	Liquid properties
m	Melting
s	Solid properties

49

50 Acronyms

CFD	Computational Fluid Dynamics
-----	------------------------------

CHT Conjugate Heat Transfer
FSI Fluid-Structure Interaction
OF OpenFOAM
PCM Phase Change Material

51

52 **1. Introduction**

53 Phase change materials (PCMs) are taking an increasingly prominent place in many fields
54 relating to energy management. With current and future energy issues, applications of these
55 materials are emerging or improving. Thermal energy storage is of great interest for
56 renewable energies [1]. Solangi et al. [2] have proposed to use MXene PCMs to store solar
57 energy. Palomba et al. [3] assessed the performance of a prototype based on PCMs for
58 renewable energy purposes. More broadly, many studies have been conducted on thermal
59 storage using PCMs over the years [4], [5]. PCMs are also widely used in buildings to
60 improve their insulation [6], [7]. The impact of such materials on electricity consumption has
61 been studied by Qureshi et al. [8], among others.

62

63 Thermal management with PCMs is also of great interest in electronics [9], [10], with cooling
64 of electronic components being a key issue in this area. Currently, most of these components
65 are used in combination with fin heat exchangers that dissipate heat by natural or forced
66 convection and radiation. The coolers are mainly composed of noisy moving parts such as
67 fans, which have many disadvantages in terms of performance, ergonomics and safety. Sahoo
68 et al [11] have shown that use of PCMs is particularly suitable for cooling electronic
69 components with intermittent operation. These observations have been confirmed by
70 numerous studies that have shown these technologies to be useful [12], [13], [14]. PCMs
71 considerably delay the onset of overheating and limit the energy requirements inherent in
72 moving parts [11], [15], [16]. In this regard, Gharbi et al. [17] compared the thermal
73 performances of several PCMs, while a cascade configuration of PCMs to cool devices was
74 studied experimentally and numerically by Huang et al. [18]. The cooling performance of
75 carbon nanotubes associated with paraffin was also investigated experimentally [19]. Ho et al.
76 tried to optimize geometries to improve thermal management [20].

77

78 Most studies in this field are experimental because theoretical predictions are made difficult
79 by the complexity of the physical phenomena involved. However, experimentation can
80 become expensive and some configurations may be out of reach. Nowadays, thanks to
81 improved computational performance, Computational Fluid Dynamics (CFD) is increasingly
82 helpful as a complement to experimentation. In particular, simulation can predict the physical
83 behavior of thermal management based on PCMs. Many authors manage heat transfer in
84 PCMs considering only conduction, without convection [21], [22]. Other works take
85 convection into account, which modifies the temperature field and thus thermal performance
86 [23], [24]. These numerical studies were carried out with commercial codes. To reduce the
87 cost of simulations, open-source software should be used. There are a few investigations with
88 free codes such as OpenFOAM [25], since the set of governing equations cannot be solved
89 directly but must be implemented personally. 2D numerical simulations of PCMs have been
90 conducted with OpenFOAM [26], [27].

91

92 Although the technology is promising, containers can suffer from leakage due to the high
93 mechanical stresses induced by thermal expansion [28], [29]. Such issues are not theoretically
94 predictable at present, however, and there are no studies focusing on this limiting problem. To
95 address it, a fully coupled model should set up between a PCM, which is either solid or liquid,

96 and solid structures containing the PCM. This model should consider conjugate heat transfers
97 (CHT) and fluid-structure interactions (FSI). There are two ways of solving such a complex
98 problem. First, the monolithic approach [30] considers one set of equations involving every
99 physical phenomenon (fluid and solid). This method is numerically stable but very time-
100 consuming, and is therefore very scarcely used by authors. Second, the partitioned approach
101 [31] considers several sets of equations, which are solved one at a time, often by different
102 software. This method requires an interface coupling between the codes that are used. For
103 configurations involving a fluid and a solid, there is often one code handling the fluid, a
104 second one managing the solid, and a third one coupling them. Numerical stability issues can
105 occur, but this approach is often preferred in the literature since it is less time-consuming.

106
107 Critical temperatures and power losses depend on the electronic components. Based on the
108 requirements specified for the component, a PCM and a conductive porous matrix must be
109 selected. The investigation of a composite and the modeling of its thermal behavior could
110 make it possible to optimize thermal performance by selecting the porous matrix topology that
111 maximizes heat transfers. The objective of this paper is therefore to propose and model the
112 thermal and mechanical behavior of new composite materials (architected conductive
113 porous matrix containing phase change materials) that meet precise specifications, such as the
114 highest possible energy density, adapted phase change temperatures, limited volume
115 expansion, properties allowing the intensification of transfers, and the lowest possible thermal
116 resistance between the electronic constituents of the composite materials. Some technical and
117 technological obstacles could be overcome thanks to a better fundamental understanding of
118 the phase transition and transfer phenomena involved in these new heterogeneous materials.
119 Development of innovative solutions for the thermal management of electronic components
120 therefore necessarily requires particular attention to the material scale.

121
122 Here, we present coupled simulations of a PCM inside gyroid structures [32]. Gyroids are
123 triply-periodic minimal surfaces, which maximizes the heat exchange surface between PCMs
124 and the surrounding structure. The simulations were managed by a fully open-source software
125 suite composed of OpenFOAM [25], CalculiX [33] and preCICE [34]. For the first time,
126 coupled fluid-solid simulations of PCMs are performed. 3D conjugate heat transfer is
127 considered first between the solid container and melting PCM. Convection of the liquid PCM
128 is taken into account. Then, 3D fluid-structure simulations of the global system are
129 performed. In particular, the fluid pressure caused by thermal expansion and then the induced
130 stresses in the structure are calculated. This global simulation allows us to predict potential
131 failures and leakage, which is a major step forward. In addition, with the simulated solid
132 deformation, contact thermal resistance can be calculated. This theoretical advance allows the
133 assessment of heat transfer losses due to imperfect contact between PCM systems and
134 electronic components, for instance. While most studies focus on the development of new
135 materials increasing heat transfers and exchanges [35], [36], [37], [38], [39], contact thermal
136 resistance plays a significant role in the thermal management of components and is the first
137 obstacle to be overcome for good thermal management. The fluid-structure coupling will thus
138 allow us to design the porous structure correctly to maintain the same contact between the
139 component and the innovative composite throughout the different thermal cycles undergone
140 by the component. The present study therefore challenges the following points:

- 141 • creating a 3D open-source coupled FSI and CHT modeling of PCMs and porous
142 architected structures
- 143 • computing stresses in porous architected structures induced by thermal expansion of
144 PCMs to settle mechanical failures
- 145 • computing structure displacements to assess the contact thermal resistance

- 146 • applying the modeling to gyroid structures which mathematically maximize the
147 exchange surface
- 148 • assessing the influence of the initial filling level of PCM and the thickness of the
149 gyroid branches on the structure displacements and mechanical stresses

150

151 In the paper, we begin by describing the theoretical modeling of both a PCM and a conductive
152 gyroid solid structure in section 2. The CHT and FSI couplings are described more
153 particularly. The PCM model was implemented in OpenFOAM and must thus be validated.
154 Section 3 focuses on the comparison between our PCM model and the analytical solution of
155 the Stefan problem, as well as experimental data from a specific configuration. Section 4
156 presents the numerical configuration of the simulations. In particular, a parameter study is
157 performed on the geometry and filling level of the PCM. Section 5 concerns the results of
158 these simulations. Temperatures, velocities, mechanical stresses and structure displacements
159 are studied specifically. The last section discusses the most suitable geometry given the
160 simulated mechanical stresses and displacements.

161

162

163 2. Numerical methods

164 The paper focuses on 3D numerical simulation of the fusion of a Newtonian PCM within a
165 porous architected structure. First, we present the equations governing the PCM, then those
166 describing the thermo-mechanical behavior of the structure, and finally the interface coupling
167 between both solvers.

168

169 2.1 PCM modeling

170 2.1.1 Equations

171 After melting, the liquid PCM is Newtonian and the incompressible Navier-Stokes equations
172 (1) thus govern its behavior reliably. The variation in density with temperature is considered
173 by the Boussinesq approximation. The influence of this assumption will be addressed in
174 section 3.2. To avoid any velocity in the remaining solid material, a penalization term is
175 added into the momentum equation. The energy equation is based on the equivalent enthalpy
176 approach, where the melting process is considered through an additional source term.

177

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho_0} + (1 - \beta(T - T_0))\mathbf{g} + \nu \Delta \mathbf{u} - \frac{\kappa \alpha}{\rho_0} \mathbf{u} \\ (\rho c_p)_{eq} \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (\lambda_{eq} \nabla T) - \rho_s \Delta h_f \frac{d\alpha}{dt} \end{cases} \quad (1)$$

178

179 In equations (1), \mathbf{u} is the velocity ($\text{m}\cdot\text{s}^{-1}$), p is the pressure (Pa), T is the temperature (K), T_0 is
180 a reference temperature (K), ρ_0 is the density at the reference temperature ($\text{kg}\cdot\text{m}^{-3}$), β is the
181 coefficient of thermal expansion (K^{-1}), \mathbf{g} is the gravitational acceleration ($\text{m}\cdot\text{s}^{-2}$), ν is the
182 kinematic viscosity ($\text{m}^2\cdot\text{s}^{-1}$), α is the solid fraction, κ is a huge penalization parameter
183 ($10^{20} \text{ kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$) aiming to avoid velocity in the solid domain, ρ is the density which
184 depends on temperature ($\text{kg}\cdot\text{m}^{-3}$), c_p is the specific heat capacity ($\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$), λ is the thermal
185 conductivity ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$), ρ_s is the solid density at melting temperature ($\text{kg}\cdot\text{m}^{-3}$) and Δh_f is
186 the heat of fusion ($\text{J}\cdot\text{kg}^{-1}$). The index *eq* in the energy equation refers to equivalent properties
187 giving

$$(\rho c_p)_{eq} = (1 - \alpha)\rho_l c_{p,l} + \alpha\rho_s c_{p,s} \quad (2)$$

$$\lambda_{eq} = (1 - \alpha)\lambda_l + \alpha\lambda_s \quad (3)$$

188 where the l and s indices refer to liquid and solid respectively.

189 Due to the temporal derivative of the solid fraction in the energy equation, a C^1 function is
 190 required for α and must be equal to 0 for temperatures greater than the melting temperature,
 191 and equal to 1 for lower temperatures, with as sharp a transition as possible around the
 192 melting temperature. Equation (4) presents the chosen function, already used in other models
 193 [40], [41]:

$$\alpha = \frac{1}{2} \left(\tanh\left(\frac{T_m - T}{\varepsilon}\right) + 1 \right) \quad (4)$$

195 where T_m is the melting temperature of the solid PCM (K) and ε (K) a small parameter
 196 controlling the sharpness of the transition. Here we chose $\varepsilon = 10^{-2}K$, which is a common
 197 choice to avoid numerical issues while maintaining a sharp transition [40], [41]. The
 198 derivative of the solid fraction in the energy equation becomes:
 199

$$\frac{d\alpha}{dt} = -\frac{1}{2\varepsilon} \left(1 - \tanh^2\left(\frac{T_m - T}{\varepsilon}\right) \right) \frac{dT}{dt} \quad (5)$$

201 To be efficient, the penalization term to avoid velocity inside solid parts must be treated
 202 implicitly in the linear resolution, in order to get a huge value on the diagonal of the matrix
 203 and thus avoid velocity. The sign of this term also has an impact on numerical stability. In
 204 order for the matrix to be strictly diagonally dominant, it is better to add a positive
 205 penalization term to the matrix diagonal.
 206

207 Turbulence is not considered in the resolution. The greatest velocities encountered are about 1
 208 cm.s^{-1} (section 5) while the structure is also of the order of 1 cm. This leads to a Reynolds
 209 number approximately equal to $Re = \frac{uL}{\nu} \sim \frac{10^{-2} \times 10^{-2}}{10^{-6}} \sim 100$, which allows us to assume
 210 laminar flows.
 211

212 2.1.2 Numerical schemes

213 The PCM equations are solved with OpenFOAM where they have been implemented. The
 214 discretization of the equations is based on the finite volume method. Resolution of the
 215 velocity-pressure coupling relies on the classical PISO (Pressure Implicit with Splitting of
 216 Operator) algorithm. The temporal term is discretized with a blend between the Euler and
 217 Crank-Nicolson schemes. In the simulations, the weight associated with the Crank-Nicolson
 218 scheme is 0.9, which ensures an almost second-order time discretization with enough
 219 numerical diffusion to avoid divergence. The advection term in the momentum equation (1) is
 220 discretized with the second-order upwind scheme. In the energy equation, the advection term
 221 is discretized with a TVD (Total Variation Diminishing) scheme switching between first
 222 (upwind) to second order (centered) depending on the velocity gradient. The central
 223 difference discretization is applied to the diffusion term. The mesh discretization and the
 224 boundary conditions are discussed in section 4.
 225

226 2.2 Porous architected structure modeling

227 The structure is governed by the linear elastic thermo-mechanical equations (6). The first
 228 equation computes heat conduction while the second describes mechanics.
 229

230

$$\begin{cases} \frac{\partial T}{\partial t} = D_s \Delta T \\ \rho_s \frac{\partial^2 \mathbf{d}}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma} \end{cases} \quad (6)$$

231

232 $D_s = \frac{\lambda_s}{\rho_s c_{p,s}}$ is the thermal diffusivity of the solid, which is assumed to remain constant, \mathbf{d} is
 233 the structure displacement and $\boldsymbol{\sigma}$ is the stress tensor based on Hooke's law and an additional
 234 thermal term $\boldsymbol{\sigma} = \frac{E}{1+\eta} \boldsymbol{\varepsilon} + \frac{E\eta}{(1+\eta)(1-2\eta)} \text{tr}(\boldsymbol{\varepsilon})\mathbf{I} - \frac{E\beta}{1-2\eta} (T - T_0)\mathbf{I}$. E is Young's modulus of the
 235 structure, η is Poisson's ratio, \mathbf{I} is the second rank unity tensor and $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla^T \mathbf{d} + \nabla \mathbf{d})$.

236

237 These equations were solved with CalculiX, which is based on the finite element method. The
 238 temporal terms are discretized with the second-order backward Euler scheme. Section 4
 239 presents a mesh convergence on the structure.

240

241 2.3 Coupling

242 2.3.1 Physical considerations

243

244 In order to optimize the calculation time, we first conduct a dimensional analysis to predict
 245 which phenomena can be neglected in the simulations. Section 4 presents the properties of the
 246 materials involved in the simulations in section 5. We use these properties in the following
 247 preliminary calculations. The results presented in section 5 show that the velocity is about 1
 248 cm.s⁻¹. The convection time is $\tau_{conv} = \frac{L}{u} \sim \frac{10^{-2}}{10^{-2}} \sim 1$ s, the thermal diffusion characteristic time

249 is $\tau_{diff,s} = \frac{L^2}{D} \sim \frac{10^{-4}}{10^{-4}} \sim 1$ s in the porous architected structure and $\tau_{diff,s} =$

250 $\frac{L^2 \rho c_p}{\lambda} \sim \frac{10^{-4} \times 10^3 \times 10^3}{10^{-1}} \sim 10^3$ s in the PCM, and the mechanical characteristic time is $\tau_{mech} =$

251 $\frac{L}{\sqrt{\frac{E}{\rho}}} \sim \frac{10^{-2}}{\sqrt{10^{11} \times 10^{-3}}} \sim 10^{-6}$ s. The deformation velocity of the porous architected structure is

252 thus far higher than the other phenomena velocities in the problem. Then, we can consider
 253 quasi-static calculations for the mechanical equations.

254

255 Now, let us estimate the impact of mechanical deformations on liquid convection. The
 256 calculated liquid pressures in the simulations discussed in section 5 are of the order of 100 Pa.

257 The ratio of the dynamic pressure over the pressure is $\Pi = \frac{\frac{1}{2}\rho u^2}{p} \sim \frac{10^3 \times 10^{-4}}{10^2} \sim 10^{-3}$. The

258 pressure variations are thus weakly related with the velocity field, and rather linked with
 259 density variations due to the increase in temperature. The simulated structure displacements in
 260 section 5 are smaller than 10^{-4} m. This weak value can globally impact neither heat transfer
 261 nor convection in the melted PCM.

262

263 Therefore, the impact of solid deformations is negligible on the PCM melting process. The
 264 calculations can thus be divided into two simulations and the mechanical and thermal
 265 equations can be uncoupled. First, a transient Conjugate Heat Transfer (CHT) simulation is
 266 carried out, without solving the mechanical equations. Second, steady Fluid-Structure
 267 Interaction (FSI) simulations are performed.

268

269 2.3.2 Conjugate heat transfer coupling

270 In the CHT coupling, mesh deformation is neglected. This allows us to perform the simulation
 271 in an explicit way, whereas considering mesh motion would have required implicit coupling
 272 with several sub-iterations. The boundary conditions at the interface for both software codes
 273 (OpenFOAM and CalculiX) are based on a Robin-Robin coupling. This means that the
 274 temperatures and heat fluxes at the interface are exchanged between the PCM and the
 275 structure. Then, a Robin boundary condition is applied to the interface in both codes. This part
 276 of the process was handled with preCICE.

277

278 2.3.3 Fluid-structure interaction coupling

279 The volume of the solid PCM is smaller than that of the liquid PCM after melting. In addition,
 280 as temperature increases, the liquid PCM expands. If the container volume is smaller than the
 281 liquid volume, then pressure can surge. The paper aims to compute the mechanical impact of
 282 the thermal expansion of the PCM on the surrounding porous architected structure.
 283 However, the impact of the expansion of the volume of the liquid on pressure is not calculated
 284 in the model described in the prior sections since an incompressible fluid has been considered.
 285 Density is therefore assumed to be independent of pressure, but does depend on the
 286 temperature thanks to the Boussinesq approximation. This assumption is sufficient for the
 287 previous CHT simulation, but not for the FSI one. The compressibility of the melted PCM
 288 must be considered to estimate the pressure variation induced by the fluid thermal expansion.
 289 Solving the compressible Navier-Stokes equations requires an equation of state and there is no
 290 such a relation in the literature.

291

292 We will thus not be able to compute the liquid pressure during the melting process. However,
 293 we are interested in the maximum mechanical stresses in the porous architected structure.
 294 This happens at the end of the simulation, when all the PCM has melted and involves the
 295 maximum liquid expansion. When the porous architected structure is only filled with a
 296 liquid at a similar temperature thanks to convection, the pressure can be assumed
 297 homogeneous. As noticed previously, the pressure gradients induced by the liquid velocity are
 298 indeed very weak, and the temperature heterogeneities in the liquid PCM are very low at the
 299 end of the melting process.

300

301 The liquid pressure can then be calculated with the following analytical approach. Let us note
 302 $\chi_T = -\frac{1}{V} \frac{\partial V}{\partial p}_T$ the adiabatic compressibility (Pa^{-1}). Under the assumption that this property
 303 remains constant during compression,
 304

$$p - p_0 = \frac{1}{\chi_T} \ln \frac{V_0}{V} \quad (7)$$

305

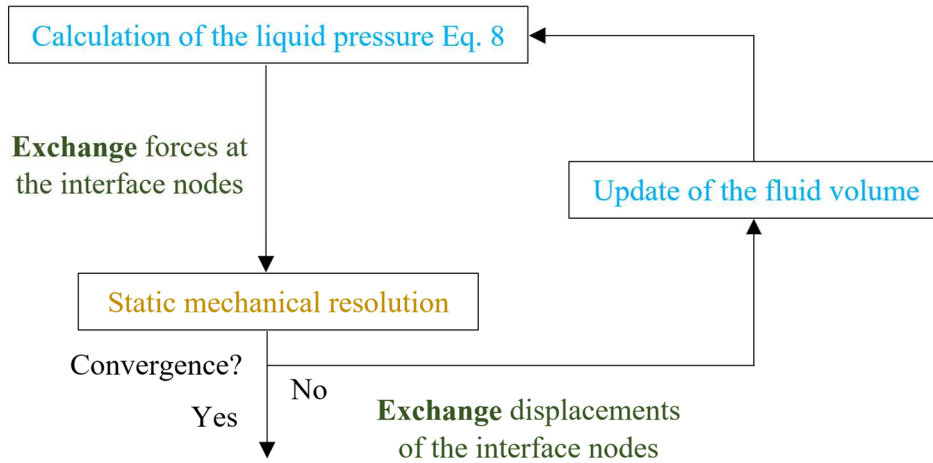
306 where V_0 is the volume of the liquid phase under pressure p_0 . With $p_0 = 0 Pa$, V_0 would be
 307 the volume of the melted PCM without constraint. We assume that the encapsulating structure
 308 is initially partially filled with the PCM at the melting temperature such that $m = \xi_0 \rho_l(T_m) V_p$
 309 where V_p is the volume of the encapsulating structure, $\rho_l(T_m)$ is the liquid PCM density at the
 310 melting temperature and ξ_0 is the initial filling level of liquid PCM. Due to thermal
 311 expansion, the volume at temperature T becomes $V' = \frac{m}{\rho_l(T)} = \xi_0 \frac{\rho_l(T_m)}{\rho_l(T)} V_p$. This corresponds
 312 to the volume of the melted PCM without compression. So $V' = V_0$. The pressure is therefore
 313 given by
 314

$$p = \frac{1}{\chi_T} \ln \xi \frac{\rho_l(T_m) V_p}{\rho_l(T) V} \quad (8)$$

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The pressure on the structure walls will expand the initial liquid volume, while the stresses induced in the elastic porous architected structure will tend to avoid such a displacement. To calculate the mechanical balance between pressure and solid stresses, an implicit FSI coupling is necessary.

A static simulation based on the temperatures at the final CHT time step is considered. The pressure in the liquid is first calculated with equation 8 based on OpenFOAM. The forces undergone by the solid are exchanged and a mechanical computation is performed by CalculiX. Note that the thermal expansion of the solid structure is also considered in the simulation. The displacement of the solid PCM structure interface is sent to OpenFOAM, which first deforms the mesh and then computes the new pressure value based on the new liquid volume. The process iterates until convergence. This procedure is summarized in Fig. 1.



330
331
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333

Fig. 1. Resolution procedure of the fluid-structure interaction simulation. The interface corresponds to the surface between the PCM and the porous architecture structure. Blue refers to OpenFOAM, ochre to CalculiX and green to preCICE.

334
335
336
337
338

The implicit coupling is based on the IQN-ILS method (Quasi-Newton Inverse Least Squares) to accelerate the convergence [42].

339
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343

3. Validation of the PCM model

The theoretical model described in section 2.1 was implemented in version 7 of OpenFOAM. Here, we present two test cases to validate this implementation, both analytically and experimentally.

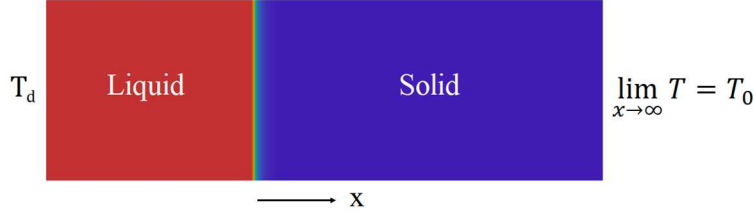
344

3.1 Stefan problem

345
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We first compare the model with the analytical solution of the Stefan problem. This consists in a semi-infinite one-dimensional geometry, which is initially considered as solid at temperature T_0 . On the left boundary, a Dirichlet temperature boundary condition T_d is enforced in order to melt the material. When x tends to infinity, the temperature is supposed to be equal to the initial temperature T_0 . Fig. 2 displays this configuration.

350



351

352 **Fig. 2.** Stefan problem corresponding to a 1D semi-infinite material initially solid at the
 353 temperature T_0 . The left side is then heated, which makes the material melt.

354 The phase change interface position s and the temperature field T are known analytically
 355 according to the two following relations [43]:

356

$$T(x, t) = \begin{cases} T_d + (T_m - T_d) \frac{\operatorname{erf}\left(\frac{x}{2\sqrt{D_l t}}\right)}{\operatorname{erf}(\psi)} & \text{if } x < s(t) \\ T_0 + (T_m - T_0) \frac{\operatorname{erfc}\left(\frac{x}{2\sqrt{D_s t}}\right)}{\operatorname{erfc}(\psi\zeta)} & \text{otherwise} \end{cases} \quad (9)$$

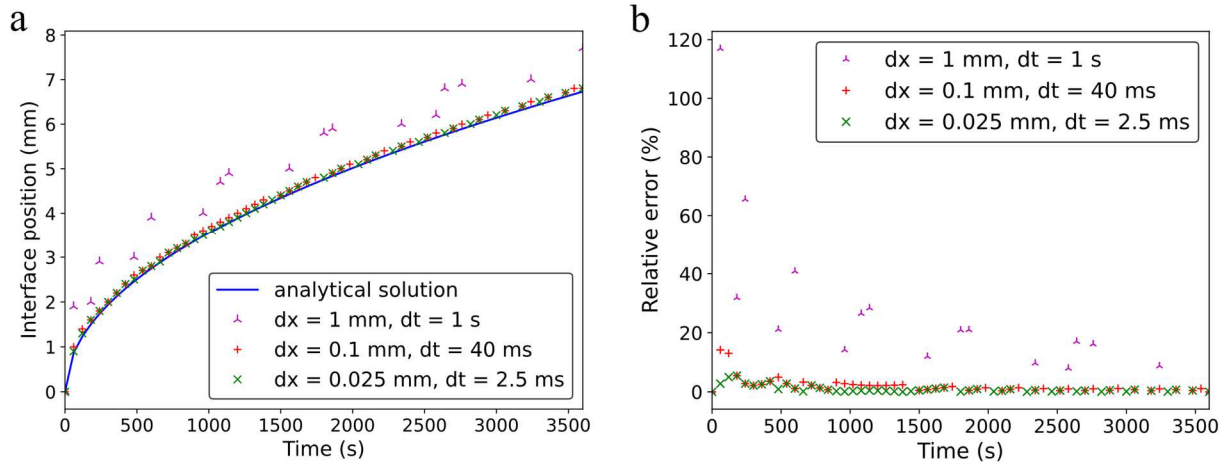
$$s(t) = 2\psi\sqrt{D_l t} \quad (10)$$

357 where $\zeta = \sqrt{D_l/D_s}$ and ψ is the solution of the transcendental equation

$$\frac{\lambda_s}{\lambda_l} \zeta (T_m - T_0) \frac{e^{-\psi^2 \zeta^2}}{\operatorname{erfc}(\psi\zeta)} + (T_m - T_d) \frac{e^{-\psi^2}}{\operatorname{erf}(\psi)} + \psi \Delta h_f \sqrt{\pi} \rho_s \frac{D_l}{\lambda_l} = 0 \quad (12)$$

358 Let us consider the following properties and parameters of water: $\rho_l = 1000 \text{ kg} \cdot \text{m}^{-3}$, $\rho_s =$
 359 $920 \text{ kg} \cdot \text{m}^{-3}$, $\lambda_l = 0.5 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, $\lambda_s = 1.3 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, $c_{p,l} = 4.2 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$, $c_{p,s} =$
 360 $2 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$, $\Delta h_f = 333.4 \text{ kJ} \cdot \text{kg}^{-1}$, $T_m = 0^\circ\text{C}$, $T_0 = -5^\circ\text{C}$ and $T_d = 5^\circ\text{C}$.

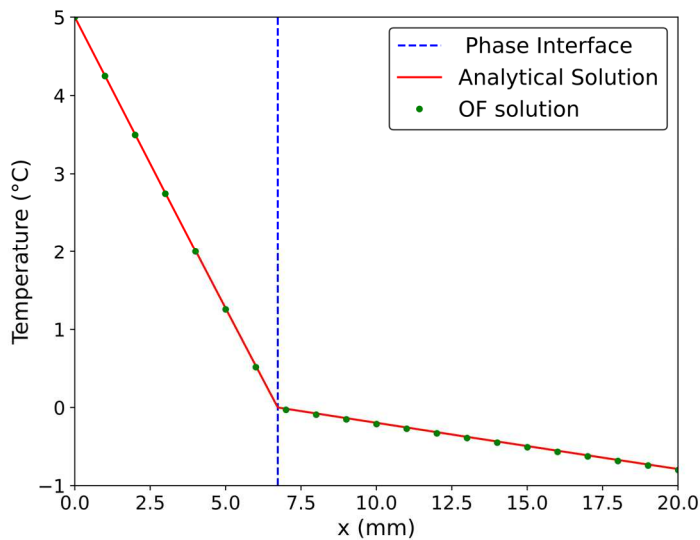
361 Fig. 3.a displays the phase change interface position against time, while Fig. 3.b shows the
 362 relative error with the analytical solution. The analytical solution is compared with the results
 363 from the corresponding simulation with OpenFOAM. In the figure, dx refers to the spatial
 364 step and dt to the temporal step in the simulation. The two most refined simulations lead to
 365 similar accurate results.



367
368 **Fig. 3.** a) Comparison of the phase change interface position displacement calculated
369 analytically and with three OpenFOAM simulations. b) Relative error of the phase change
370 interface position.

371 Fig. 4 presents the temperature field one hour after the start of heating. The theoretical
372 interface position is also presented. The OpenFOAM (OF) solution corresponds to the
373 intermediate refinement level in Fig. 3. The simulated temperature is almost equal to the
374 analytical solution, all along the 1D geometry. The energy equation in the set of equations (1)
375 thus gives consistent results.

376



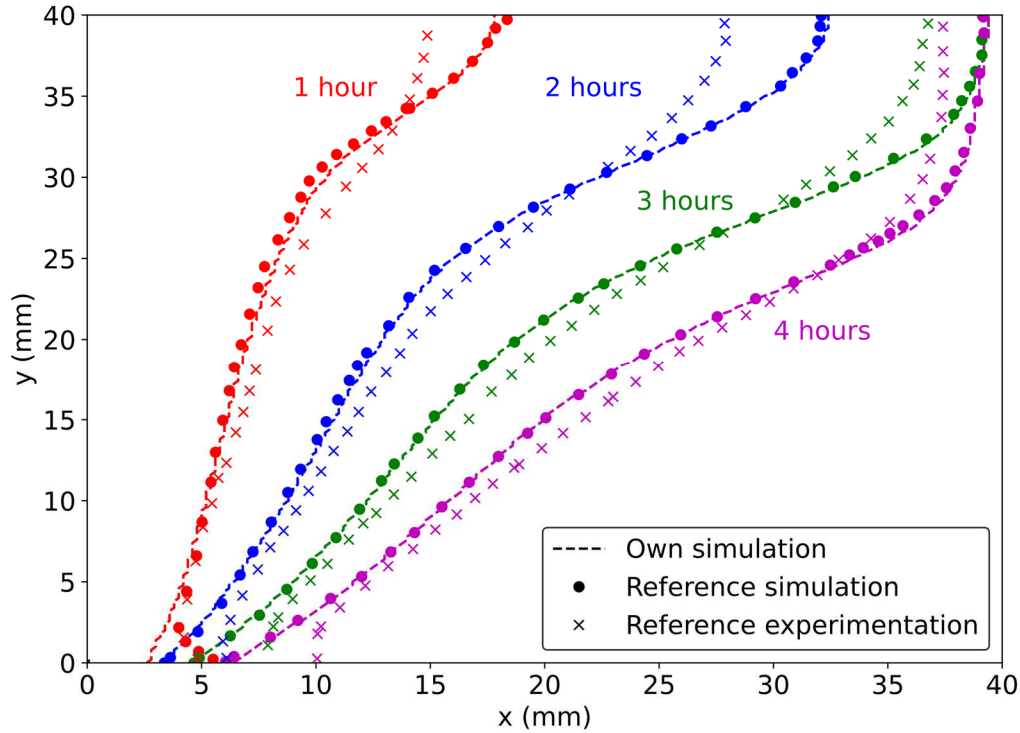
377
378 **Fig. 4.** Comparison of the analytical and the simulated temperature field, after one hour.

379

380 3.2 2D validation with experimental and numerical results

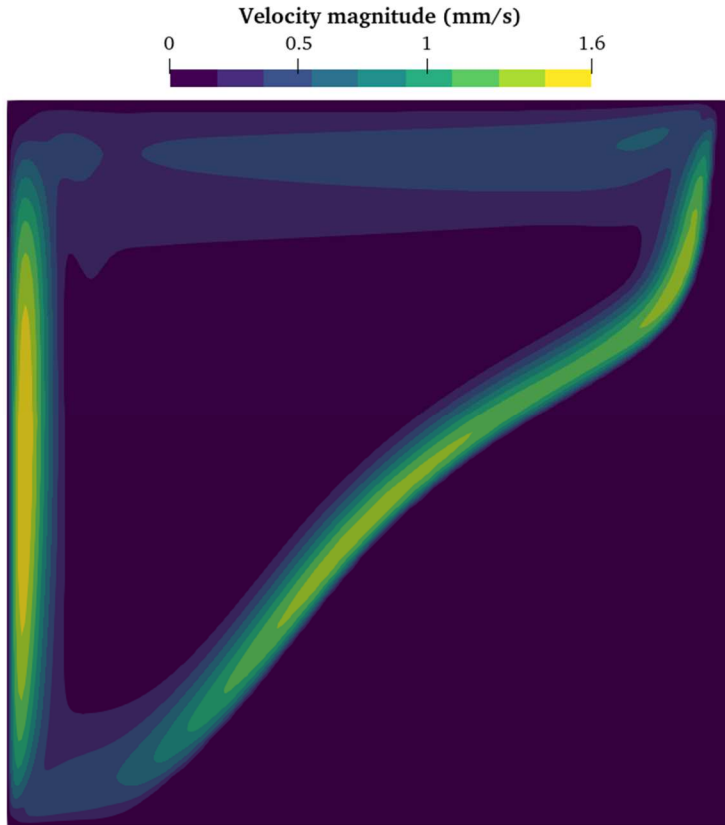
381 This section concerns the validation of the model, which can be 3D, based on the 2D
382 numerical results presented in [26], which have been successfully compared with the
383 corresponding experiment carried out by the same authors [44]. The test case consists in
384 melting a PCM within a square which is heated on the left side at 308.15 K and maintained at
385 298.15 K , the initial temperature, on the right side. The bottom and top edges are considered
386 to be adiabatic in the simulation discussed in [26], whereas they actually result from

387 conduction in thin plates in the experiment. In our simulation, adiabatic walls are considered.
 388 The same PCM properties given in [26] are considered in the present simulation. Note that
 389 there is a small opening at the upper left corner in the experimentation to drain the excess
 390 amount of fluid resulting from the volume expansion during melting. Fig. 5 compares the
 391 phase change interface at different times from our simulation with the simulation and the
 392 experimentation achieved by Faden et al. [26] The mesh is composed of 40,000 cells; the
 393 same mesh is used in the reference simulation.



394
 395 **Fig. 5.** Phase change interface 1, 2, 3 and 4 hours after the start of heating. The dot points and
 396 the crosses stem from [26].

397 Fig. 6 also displays the velocity field in the physical domain after four hours. The same figure
 398 is proposed in [26] and is very similar. It is worth noting that our results are close to the
 399 numerical simulation managed by Faden et al. [26], and they are also consistent with the
 400 experimental results [26], [44].



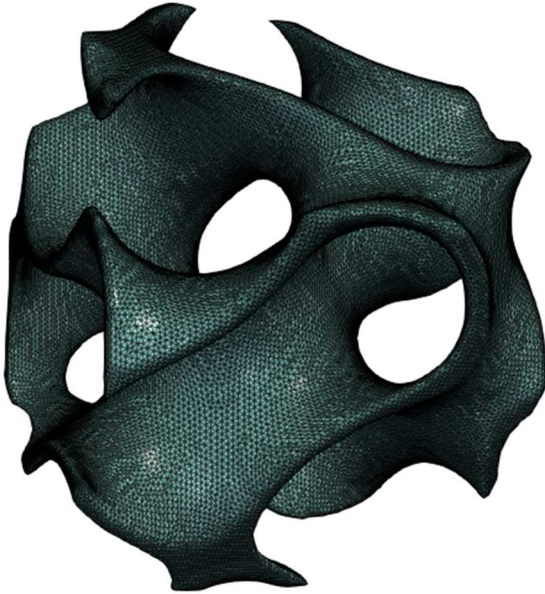
402 **Fig. 6.** Velocity magnitude in the geometry four hours after the start of heating. The OF
 403 simulation is based on a mesh composed of 40,000 cells. The left side is heated to 10 K
 404 warmer than the initial temperature.
 405

406
 407 The reference simulation is based on the compressible Navier-Stokes equations, while ours is
 408 based on the Boussinesq approximation. The prior results clearly show that the Boussinesq
 409 approximation is reliable for this range of temperature variation and is satisfactory in
 410 comparison with compressible equations, which are more time-consuming to solve.
 411

412 **4. Numerical setup**

413 **4.1 Configuration**

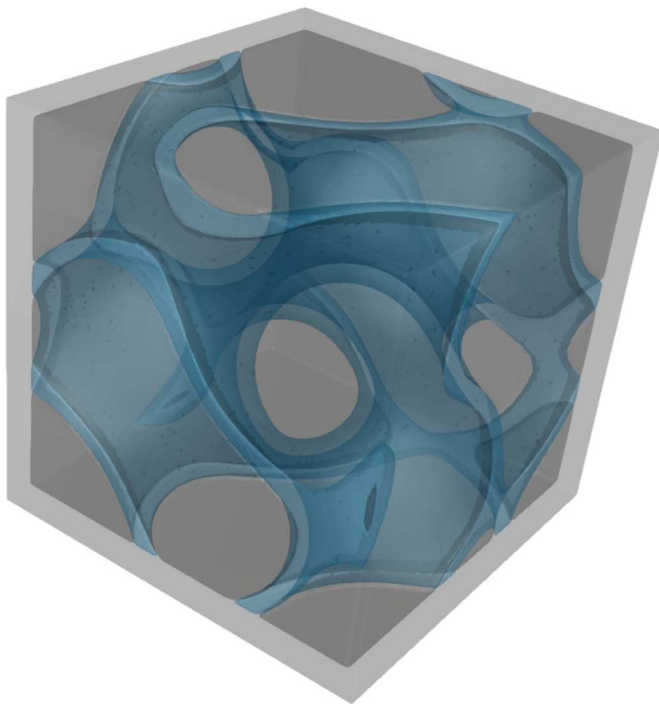
414 The geometry of the encapsulating structure is based on triply-periodic minimal surfaces,
 415 which optimize the heat transfer exchange surface [32]. Here, we consider a gyroid surface,
 416 given by the implicit equation $\cos(x) \sin(y) + \cos(y) \sin(z) + \cos(z) \sin(x) = 0.15$.
 417 Giving a thickness to this surface leads to the geometry in Fig. 7. This geometry contains two
 418 isolated volumes.



420
421 **Fig. 7.** Thick gyroid volume where the thickness of branches is equal to 2% of the bounding
422 box side length.

423 Based on this idea, we propose to build a porous architected structure containing a volume
424 like in Fig. 7 enclosed by a cube with the same thickness as the thick faces of the gyroid
425 branches. This geometry is then filled with PCM. Fig. 8 displays the general geometry that is
426 investigated in the remaining part of the paper. The side length of the surrounding box is
427 equal to 5 cm.

428



429
430 **Fig. 8.** Geometry investigated in the paper. The blue parts and the surrounding box are solid,
431 while the remaining part is liquid.

432 The porous architected structure will be made of copper, while the PCM will be palmitic
433 acid. The melting temperature of palmitic acid is slightly below the usual critical temperature

434 of electronic components. Copper allows a fast thermal conduction process which makes heat
 435 transfer efficient. Tab. 1 itemizes the considered properties for both materials. The palmitic
 436 acid properties mainly stem from [45], except for thermal conductivities [46]. The
 437 gravitational acceleration is assumed to be equal to $g = 9.81 \text{ m.s}^{-2}$ in the simulations.
 438

Properties	Solid palmitic acid	Liquid palmitic acid	Copper
$T_m \text{ (K)}$	335.35	-	-
$\Delta h_f \text{ (kj.kg}^{-1}\text{)}$	211.85	-	-
$\rho \text{ (kg.m}^{-3}\text{)}$	989.6	$-0.7349(T - 273.15) + 907.54$	8950
$c_p \text{ (J.g}^{-1}\text{.K}^{-1}\text{)}$	Fig. 3 [45]	2.39	380
$\lambda \text{ (W.m}^{-1}\text{.K}^{-1}\text{)}$	0.22	0.16	401
$\mu \text{ (Pa.s)}$	-	$4.381 \times 10^{-6} e^{2488.8/T}$	
$\beta \text{ (K}^{-1}\text{)}$	-	0.11	1.7×10^{-6}
$E \text{ (GPa)}$	-	-	130
η	-	-	0.33

439 **Tab. 1.** Properties of the materials involved in the simulations. The blank cells are not
 440 considered or have no physical meaning.
 441

442 In sections 5 & 6, several thicknesses for the gyroid volume will be tested to compare the
 443 mechanical stresses. The thicknesses will vary from 2 to 10% of the box side length. The
 444 filling level of the structure ξ_0 will also vary between 98.5% and 100%. Below these values,
 445 we can check that the thermal expansion of the liquid does not involve compression under
 446 85°C (equation 8), which will not be exceeded in this paper. Higher temperatures damage
 447 electronic components, so there is no interest in exceeding this temperature.

448 In section 5, the bottom face of the box will be heated with a constant power equal to 30 W
 449 which is a common power experienced by electronic components. Even if this power involves
 450 temperatures greater than 85°C , the simulations will be stopped at this temperature. The other
 451 external faces of the box will undergo a convective heat transfer with a coefficient $h =$
 452 $5 \text{ W.m}^{-2}\text{.K}^{-1}$ and an outside temperature of 22°C (which is also the initial temperature).
 453 The faces will be free to move.

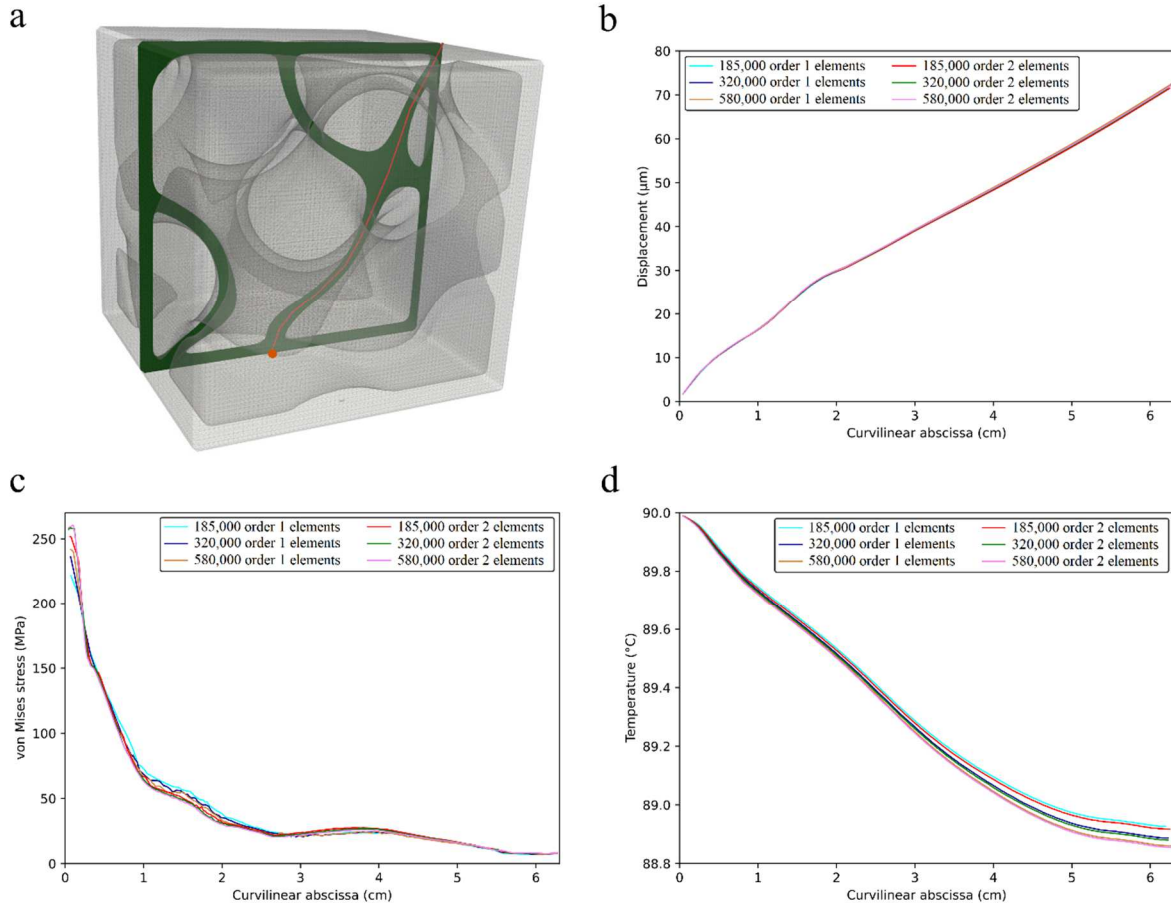
454 A few studies focus mainly on the measurement of the adiabatic compressibility of palmitic
 455 acid. Due to uncertainties on its value, two FSI simulations will be performed for each
 456 configuration. They will rely on $\chi_T = 4 \times 10^{-10} \text{ Pa}^{-1}$ and $\chi_T = 10^{-9} \text{ Pa}^{-1}$ [47], [48], [49],
 457 [50].
 458

459 4.2 Mesh convergence

460 4.2.1 Porous architected structure

461 Mesh convergence is achieved on the solid part of the geometry (Fig. 8). Only for mesh
 462 convergence, the bottom face is fixed and heated to 90°C . The same boundary conditions as
 463 in section 4.1 are considered elsewhere. The properties of the copper are summed up in Tab.1.
 464 The static results relying on six meshes are compared in Fig. 9. The meshes consist of 185,
 465 320 and 580 thousand first or second order elements respectively. The element sizes are
 466 respectively equal to 1 mm, 0.8 mm and 0.65 mm. The comparison is made along a
 467 curvilinear line in red located in the middle plane in green in Fig. 9.a. The displacement, von
 468 Mises stress and temperature along this curve are presented in Fig. 9. There is almost no
 469 difference on the displacement (Fig. 9.b). The von Mises stress also varies weakly with the
 470 meshes (Fig. 9.c). The greatest deviations appear close to the bottom face, where the stress is
 471 most significant. The simulated temperatures are grouped according to the number of
 472 elements rather than the order of the elements (Fig. 9.d). The order does influence the results

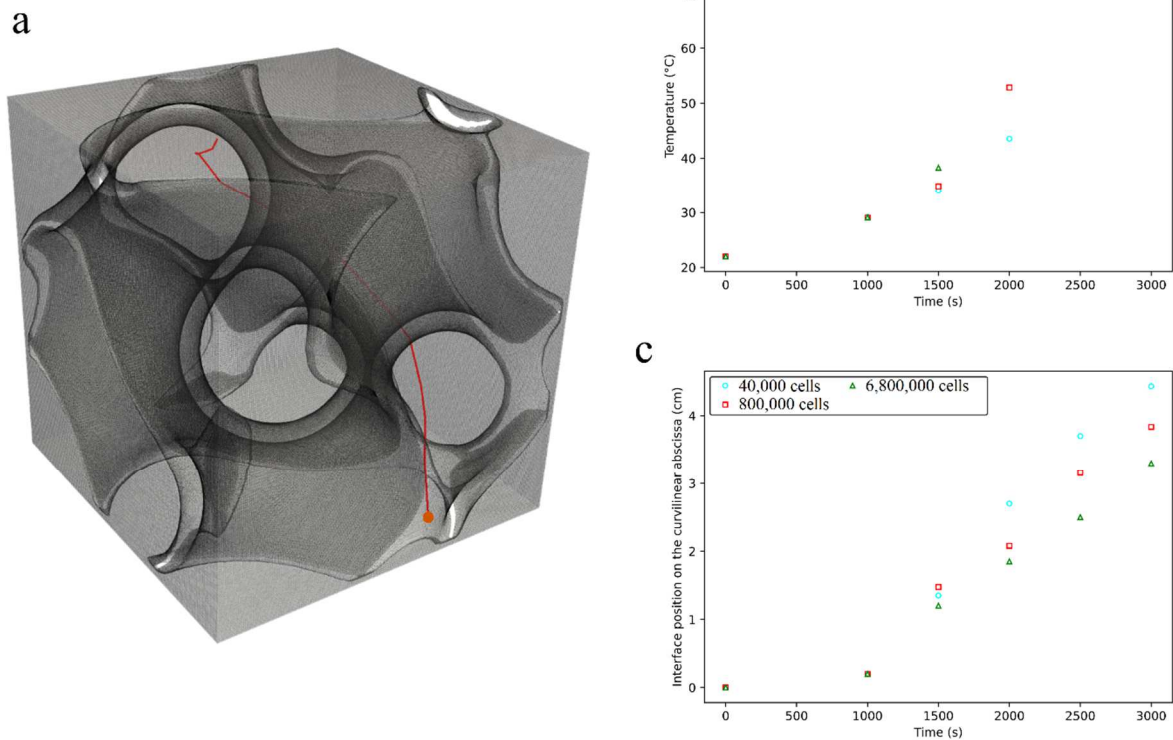
473 considerably for the three variables. The number of elements also has a weak impact. Since it
 474 does not lead to a prohibitive calculation time, we have chosen the second mesh with 320,000
 475 order 1 elements rather than the coarsest one, where there are only 2 tetrahedra in the
 476 thickness of the surrounding box, which decreases the stress values close to the bottom face.
 477



478 **Fig. 9.** a) Comparison of the results from six different meshes along the red curve in the green plane.
 479 The origin of the curve is on the bottom face (red point). b) Evolution of the structure displacement
 480 along the red curve. c) Evolution of the von Mises stress along the red curve. d) Change in the
 481 temperature along the red curve (1 k = 1000).
 482

483 4.2.2 PCM

484 Here, only the volume associated with the PCM is studied. The material properties in the
 485 simulations are gathered in Tab. 1. Like in section 4.2.1, the bottom face is heated to 90°C
 486 while zero Neumann boundary conditions are imposed on the other faces. The PCM is
 487 initially solid at 22°C. The phase change interface position is plotted along the red line in
 488 Fig. 10.a. It should be noted that it was not possible to choose a planar curve considering the
 489 winding PCM geometry. Three meshes were compared with 40 thousand, 800 thousand and
 490 6.8 million cells, corresponding to cell sizes of 1 mm, 0.5 mm and 0.25 mm respectively.
 491 There are expected differences in the temperature field during the melting process, 33 minutes
 492 after the start of heating (Fig. 10.b). Except at this moment, the gaps remain small.
 493 Concerning the change phase interface position, the deviations increase with time (Fig. 10.c).
 494 They are linked with the observation of the temperature around the delay on the melting
 495 process. Since the computation time of the finest mesh is very long (4 days with 192
 496 processors), we consider that the accuracy given by this mesh is not sufficient. In addition,
 497 coupled CHT-FSI simulations will be explored, which increases calculation time even more.
 498 We thus chose the medium mesh.



500

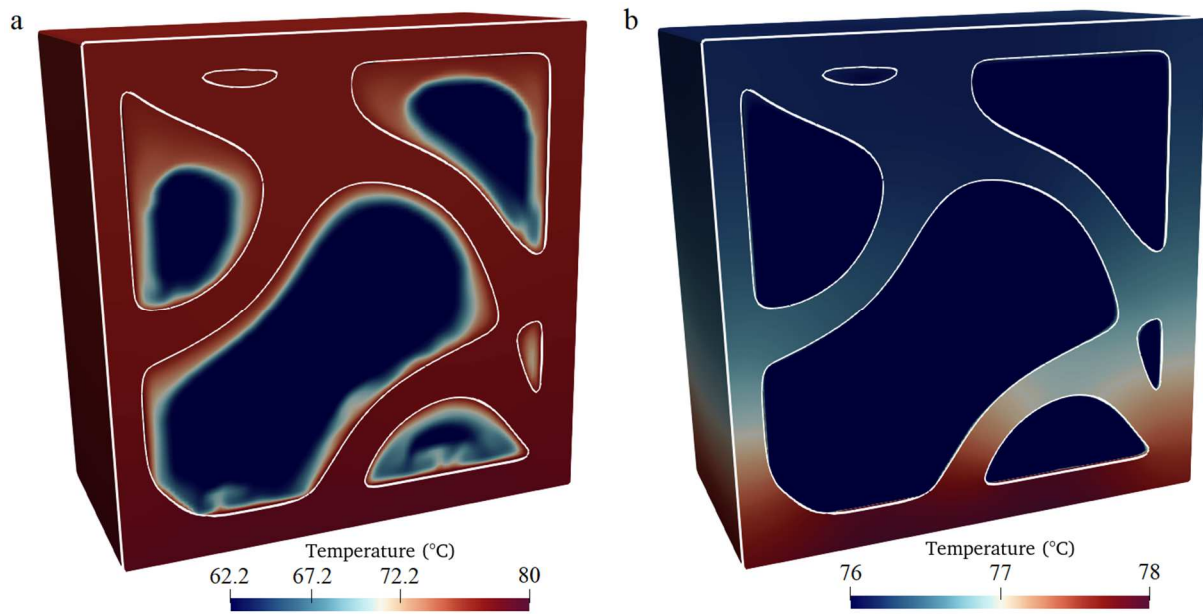
501 **Fig. 10.** a) PCM geometry. The phase change interface position is plotted along the red line
 502 inside the geometry. The origin of the curve is on the bottom face (red point). b) Temperature
 503 according to time at point (0.02, 0.005, 0.02). This point was chosen close to the bottom face,
 504 where the heating process begins early. c) Phase change interface position according to time.

505

506 5. Results

507 5.1 Conjugate Heat Transfer simulations

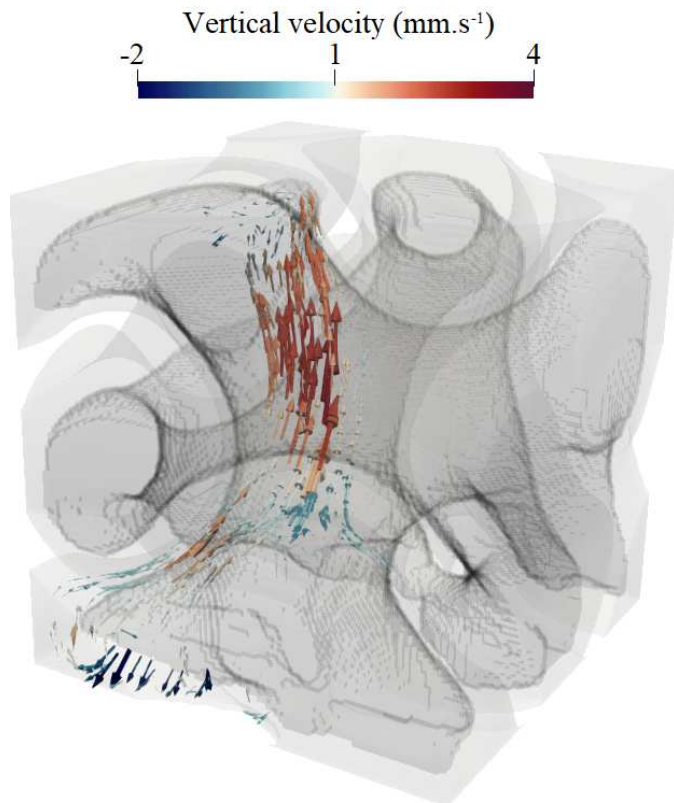
508 This section focuses on the thermal coupling exclusively, i.e., on the heat transfer and the
 509 melting process of the palmitic acid in the porous architected conductive structure. Five
 510 simulations with different gyroid thicknesses (from 2 to 10% of the box side length) are
 511 performed. The general behavior of the coupled phenomena is described in specific
 512 configurations. Fig. 11 displays the temperature in the middle cross-section of the gyroid box
 513 (8% thickness), 17 minutes after the start of heating. The copper temperature, between 76 and
 514 78°C, is far greater than that of the PCM. This stems from the thermal conductivity of copper
 515 which is 2,000 times higher than for the PCM (Tab. 1). Therefore, even if only the bottom
 516 face is heated, the PCM is actually heated mainly by the whole interface with the copper
 517 gyroid. Since the PCM melts at 62.2°C, a significant part of the palmitic acid is still solid as it
 518 is quite far from edges.



520

521 **Fig. 11.** Temperature field both in the PCM and copper, 17 minutes after the start of heating,
 522 in the middle cross-section of the porous architected structure. The configuration
 523 corresponds to a gyroid thickness of 8%. The white contour corresponds to the limit between
 524 PCM (OpenFOAM) and copper (CalculiX). a) The temperature scale is adapted to the PCM
 525 temperature. b) The temperature scale is adapted to the solid temperature.

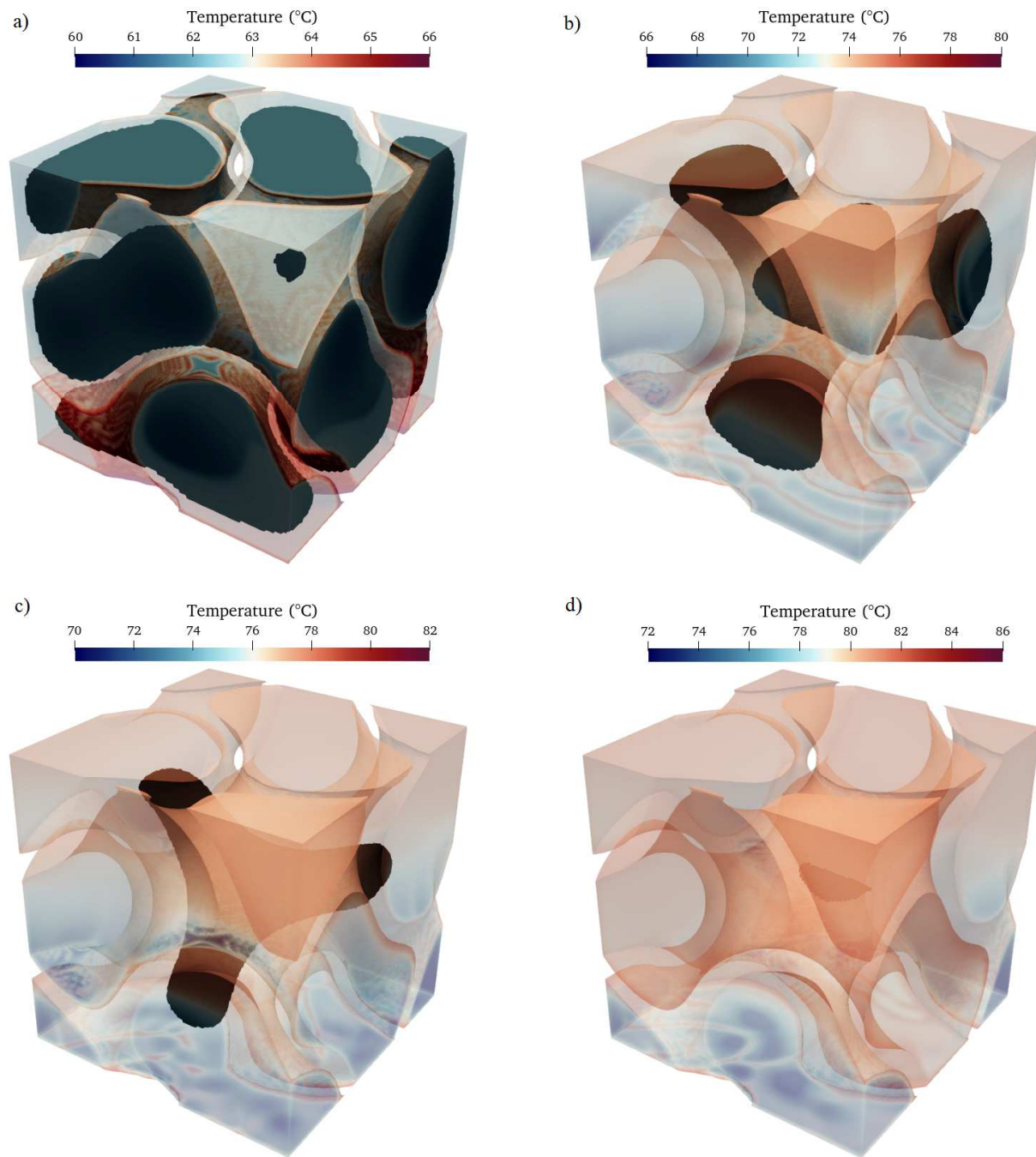
526 The convection process thus begins only from approximately 15 minutes after the start of
 527 heating, when the PCM close to the solid interface is melted. Fig. 12 shows local velocity
 528 vectors within the liquid PCM at the same time as in Fig. 11. Due to temperature gradients,
 529 the hot liquid moves upward, following the winding structure geometry. The top part of the
 530 PCM therefore melts faster than the bottom, despite the fact it is the bottom face that is
 531 heated. This process is also observed in Fig. 11.a, in the top left and right corners of the PCM.
 532 The upper parts of these areas melt while the lower parts are still solid. The velocities remain
 533 smaller than $4 \text{ mm} \cdot \text{s}^{-1}$ at this time but can exceed $1 \text{ cm} \cdot \text{s}^{-1}$ during the simulation.



534

535 **Fig. 12.** Velocity vectors in a melting area of the PCM, 17 minutes after the start of heating
 536 the structure composed of an 8% thickness gyroid.

537 Fig. 13 shows the change in the solid PCM inside the gyroid structure composed of 6% thick
 538 branches. Following the previous results, a melting process starting from the PCM-copper
 539 interface towards the center of the PCM is expected. This behavior is observed in Fig. 13.
 540 After 10 minutes (Fig. 13.a), only the PCM close to the edges begins to melt, as in Fig. 10.
 541 Note that the temperature in the liquid PCM exceeds 65°C. Seven minutes later (Fig. 13.b),
 542 the upper part of the PCM is hotter than the lower part, due to convection. The volume of the
 543 solid PCM has decreased drastically. Three minutes later (Fig. 13.c), the solid PCM is
 544 shrinking sharply, while the temperature varies weakly in comparison with Fig. 13.b. Only the
 545 central part of the PCM remains solid after 20 minutes. Finally, after 23 minutes, only a small
 546 part of the PCM is still in the solid state. The temperature will then increase faster without
 547 PCM to melt. A few seconds later, the solid PCM disappears.

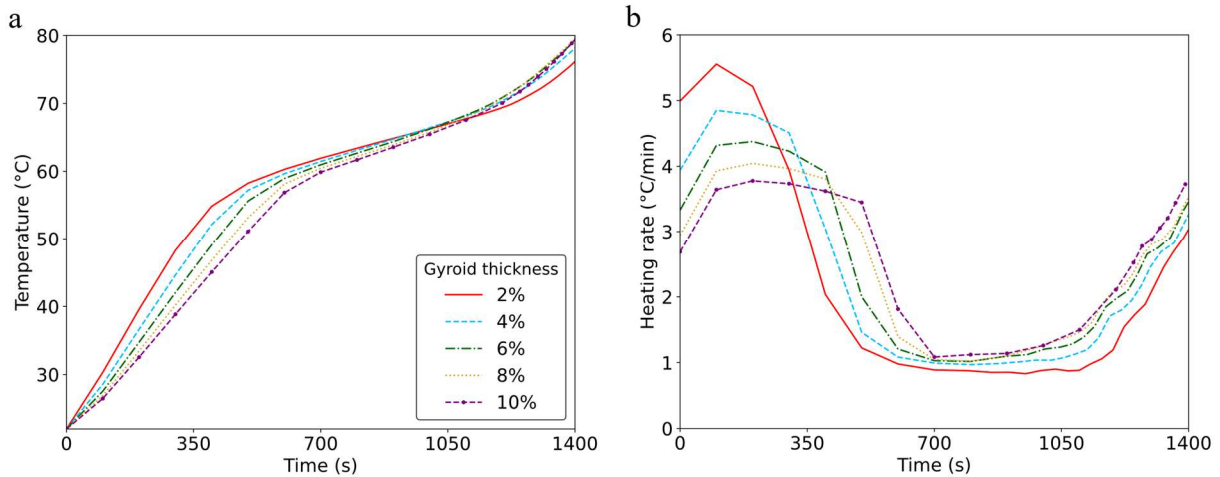


548

549 **Fig. 13.** OpenFOAM temperature field and solid PCM (in black) in a copper gyroid structure
 550 consisting of 6% thick branches. a) 10 minutes; b) 17 minutes; c) 20 minutes; d) 23 minutes;
 551 after the start of heating.

552 Fig. 14.a shows the average temperature in the whole PCM according to time, for the five
 553 thickness configurations. Before most of the PCM has melted, the lower the thickness, the
 554 higher the temperature. During this conduction time, the energy is transferred through the
 555 interface. The lower the thicknesses, the greater the exchange interface area. Therefore, there
 556 is more conductive heat transfer for copper gyroid structures with thin branches. In addition,
 557 for thick gyroid structures, the bounding box is also thicker, so energy coming from the
 558 bottom face must diffuse in a thicker copper volume before reaching the PCM. Energy thus
 559 attains the PCM faster in thin gyroid structures. Very quickly, however, after several hundreds
 560 of seconds (Fig. 14.b), the heating rate becomes lower for thin gyroid structures. Since there is

561 more PCM, the melting process plays a more significant role than in thicker configurations.
 562 The heating rate thus reduces substantially down to a quasi-constant heating rate of around
 563 $1^{\circ}\text{C}\cdot\text{min}^{-1}$. This second phase (melting phase) occurs earlier for thin copper gyroid structures
 564 since there is more PCM. Due to the quantity, the melting phase is also longer in thin
 565 configurations. Fig. 14.a shows greater damping of temperature variation inside thin copper
 566 gyroid structures, thanks to the PCM. Finally, a third phase happens, when the PCM is mostly
 567 or totally liquid. The heating rate increases again (Fig. 14.b). Since this last phase begins later
 568 for the 2% thick gyroid, the temperature is lower than in the other simulations. At the end, the
 569 thinner it is, the colder the temperature.

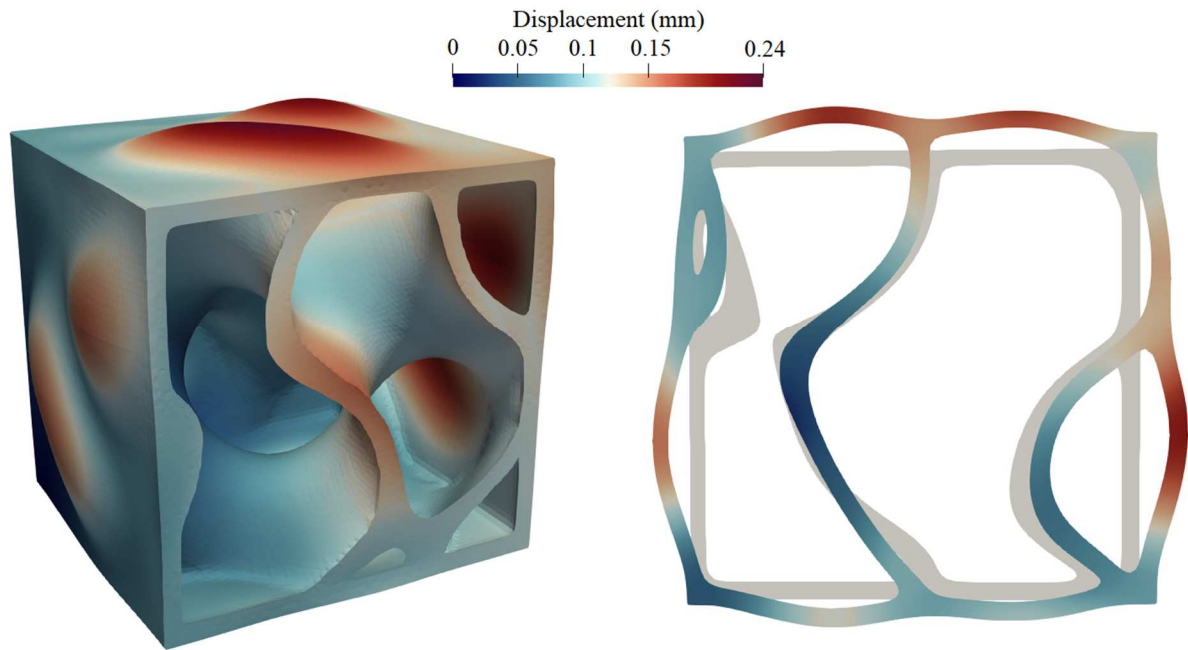


570
 571 **Fig. 14.** a) Average temperature in the PCM according to time for the five thickness cases. b)
 572 Heating rate (time derivative of temperature) in the PCM according to time.

573 5.2 Fluid-structure interaction simulations

574 As described in section 2, we consider a fluid-structure simulation at the end of the melting
 575 process of the PCM, when the temperature is almost homogeneous. In the simulation, the final
 576 temperature field in the porous architected structure is considered while the liquid
 577 temperature is assumed to be equal to 85°C . The liquid temperature is indirectly involved in
 578 equation (8) through the density, and thus has a significant impact on thermal volume
 579 expansion. The copper temperature is also involved in the thermal dilatation and generates
 580 mechanical stresses in the structure.

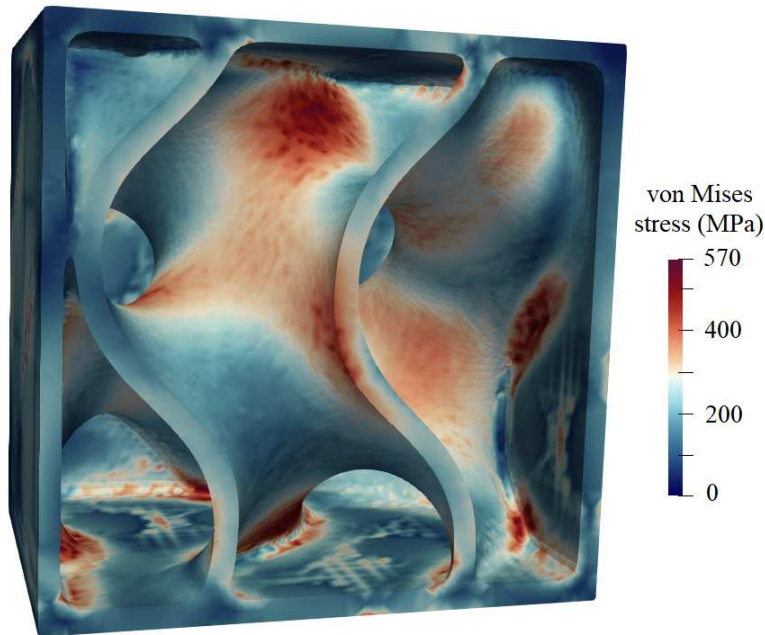
581 The deformation of the porous architected structure (4% thick), completely filled with PCM
 582 ($\xi_0 = 100\%$), is presented in Fig. 15 with a scale factor of 30. Fig. 15.b compares a section
 583 before and after deformation. The greatest displacements occur at the box sides due to the
 584 pressure gradients. The pressure is indeed significant inside the box while the atmospheric
 585 pressure is negligible outside. Instead, the pressure is constrained inside gyroid branches on
 586 both sides. Note that the side displacement remains relatively small ($240\ \mu\text{m}$).



587

588 **Fig. 15.** Displacement field of the 4% thick gyroid structure initially fully filled with the PCM
 589 ($\xi_0 = 100\%$), from CalculiX. The deformations presented here correspond to the genuine
 590 deformation multiplied by 30. a) Displacement of the 3D copper gyroid structure. b)
 591 Comparison of the deformed structure with the initial geometry in the central section of the
 592 copper gyroid structure.

593 Fig. 16 displays the von Mises stresses inside the porous architected structure for the same
 594 configuration. The greatest stresses do not occur at the box sides but in the thick branches,
 595 especially close to the junctures. These parts undergo compressive forces due to the pressure.
 596 The stresses reach as much as 570 MPa at several locations. The value of the compressive
 597 yield strength of copper can vary according to the material properties. In the paper, we assume
 598 that its value is 138 MPa [51]. Based on the von Mises criterion, this configuration thus
 599 widely exceeds safe stresses and should lead at least to plastic deformations and perhaps
 600 failures.



601

602 **Fig. 16.** The von Mises stresses from CalculiX in the 4% thick gyroid structure initially fully
 603 filled with the melted PCM ($\xi_0 = 100\%$).

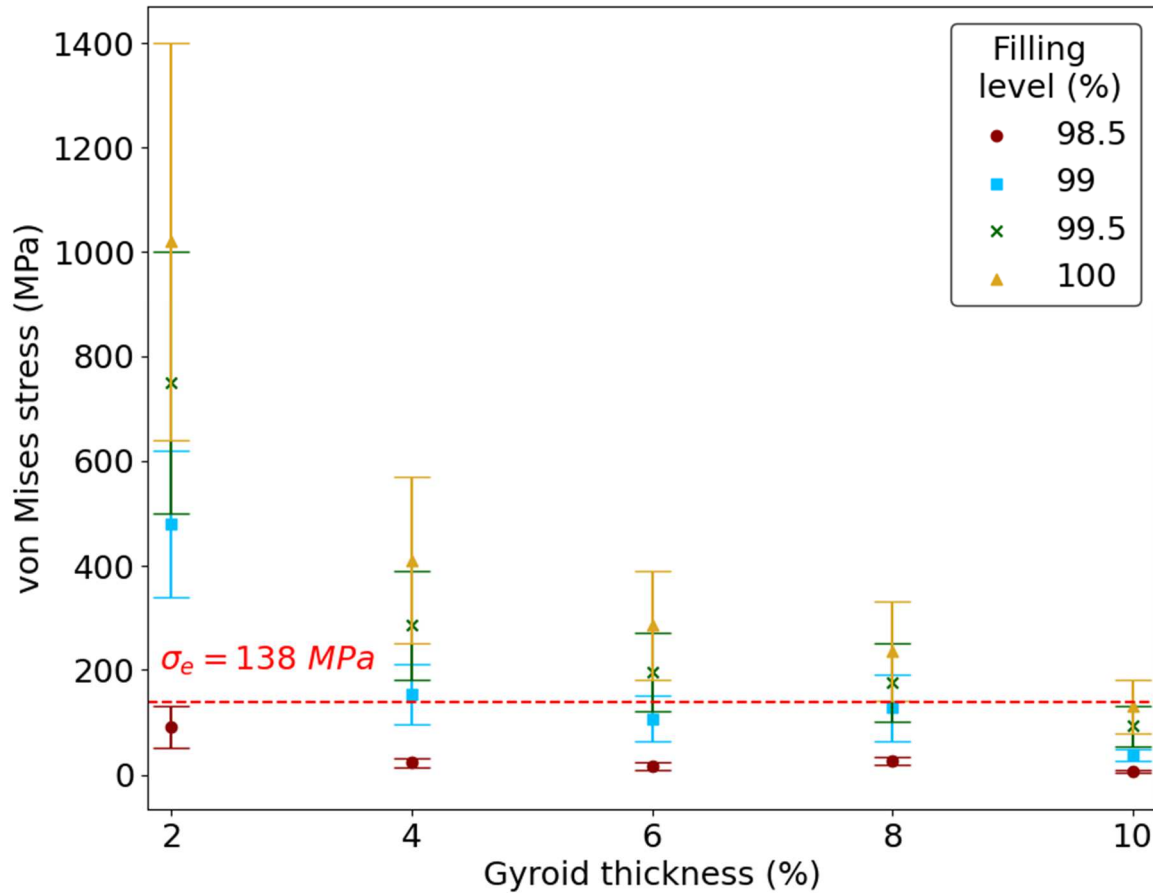
604

605 6. Discussion

606 6.1 Stresses involved in the encapsulating solid

607 The model presented allows us to compute the stresses generated by the thermal expansion of
 608 the PCM in the encapsulating structure. Based on these results, it is possible to predict
 609 whether a configuration is reliable or not from this point of view. In the paper, we focus on
 610 the yield stress and not on failure. Since such a product must undergo several cycles, plastic
 611 deformation should not occur for safe and efficient use. Like in the prior section, we follow
 612 the von Mises criterion. Fig. 17 displays the maximal von Mises stress in copper for each
 613 configuration that was tested. We recall that simulations with different filling levels and
 614 thicknesses of gyroid branches were carried out. For each configuration, a range is provided
 615 for the maximal von Mises stress, corresponding to the FSI simulations with two values of
 616 adiabatic compressibility $\chi_T = 4 \times 10^{-10} Pa^{-1}$ and $\chi_T = 10^{-9} Pa^{-1}$ (§4.1). With a branch
 617 thickness of only 2% of the box size length, the stresses are very high and exceed the yield
 618 stress for every filling level greater than 99%. With less PCM in the host architecture matrix,
 619 its volume expansion does not involve sufficient stresses to deform the copper plastically.
 620 This is an important issue since this geometry is the hollowest one, so filled with the greatest
 621 amount of PCM. With a thickness of 4% to 8%, the stresses decrease, as expected, but to a
 622 level which is not sufficient to change the previous conclusions on 2% thick gyroids. Indeed,
 623 from a filling level of 99%, a risk of plastic deformation still exists. With a thickness of 10%,
 624 the solid structure can undergo high pressures with von Mises stresses remaining smaller than
 625 the yield stress. With this thickness, only a completely filled structure could be deformed
 626 plastically. However, such a geometry contains a smaller amount of PCM than for a gyroid
 627 composed of 2% thick branches. Considering the maximum filling level of each geometry
 628 without jeopardizing the structure, the 2% thick geometry remains the structure that can be
 629 filled with the greatest amount of PCM. With a filling level of 98.5%, this geometry can

630 contain 113 cm^3 of PCM while remaining safe according to the simulations. In comparison,
 631 the thicker geometry filled to a level of 99.5% can only contain 82 cm^3 of PCM. It appears
 632 that the filling level is a more interesting parameter since it drastically impacts the stresses
 633 involved, while decreasing the quantity of PCM only slightly.

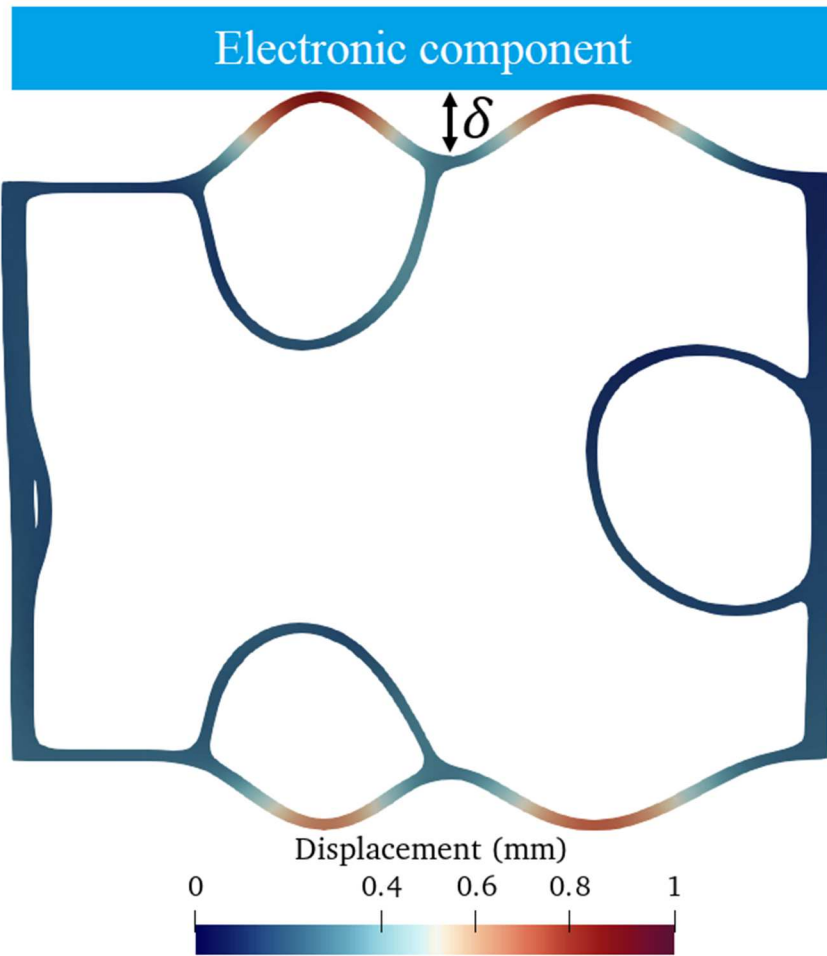


634
 635 **Fig. 17.** von Mises stresses for each configuration. The yield stress is displayed in red. The
 636 error bars are associated with the uncertainties on adiabatic compressibility. They correspond
 637 to two FSI simulations based on two different values of adiabatic compressibility.

638

639 6.2 Thermal contact resistance

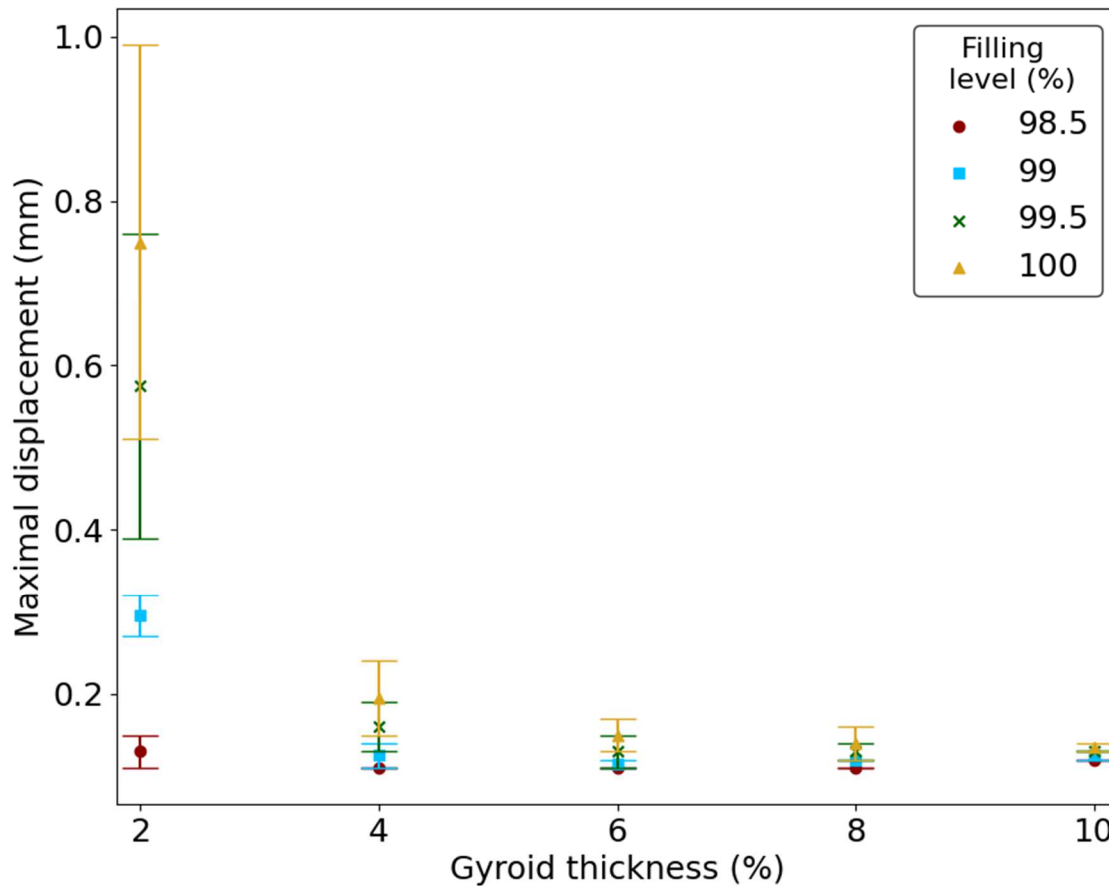
640 Excessive heat can severely impact electronic devices. The proposed geometry filled with
 641 PCM is used to reduce the temperature. However, to be efficient, the contact between the
 642 innovative composite and devices must be efficient, i.e., the contact surface must be
 643 maximized. The deformation of the solid structure decreases the exchange area and leads to a
 644 loss in heat transfer (Fig. 18). Thermal contact resistance is defined as the ratio between the
 645 peak and valley δ (see Fig. 18) and the thermal conductivity of the medium between the
 646 innovative composite and the electronic component (often air) $R_{th} = \frac{\delta}{\lambda_{air}}$. On the example in
 647 Fig. 18, $\delta \sim 1 \text{ mm}$, the temperature is approximately 85°C , which yields a thermal
 648 conductivity of $\lambda_{air} \sim 0.03 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, and $R_{th} \sim 0.033 \text{ K}\cdot\text{m}^2\cdot\text{W}^{-1}$. The thermal contact
 649 resistance is very significant in this configuration which is the worst one tested in the paper
 650 and the most adverse case from electronic devices. Fig. 19 displays the displacements
 651 according to the gyroid thickness for every filling level.



652

653 **Fig. 18.** Deformed 2% thick gyroid structure completely filled with PCM (scaled up by a
 654 factor of 10). The contact with an electronic component is less efficient due to deformation. δ ,
 655 the so-called peak to valley, is the distance between the component and the structure.

656 As seen in the previous section, the gyroid with 2% thick branches is the most efficient from
 657 the stress point of view. However, with greater displacements, one could expect significant
 658 thermal contact resistance. Fig. 19 shows that displacements are indeed far larger in this
 659 configuration than with thicker gyroids, except with a filling level of 98.5%. The
 660 displacements are of the order of $10^{-4} m$, like in every other configuration with thicknesses
 661 of 4 to 10%. With such displacements, the thermal contact resistance is approximately $R_{th} \sim$
 662 $0.0033 K.m^2.W^{-1}$. Note that this value remains an important issue and must impact the
 663 experimental performance. In our model, this feature is not considered and some differences
 664 between the theoretical results presented in the paper and experimentation could occur on
 665 account of this. Similarly, the contact between the PCM and copper before melting is not
 666 taken into account in the model. The heat transfer between every part of the device could
 667 therefore be slower than in the simulation, but should modify neither the structure
 668 displacement nor the stresses significantly.



669

670 **Fig. 19.** Maximal displacement for each configuration. The error bars are associated with the
 671 uncertainties on adiabatic compressibility. They correspond to two FSI simulations based on
 672 two different values of adiabatic compressibility.

673

674 7. Conclusion

675 Electronic cooling relies on different techniques. Among them, PCMs mitigate temperature
 676 increases. This approach is therefore widely used experimentally and is a subject of huge
 677 interest in the community. However, the theoretical modeling of the coupled physical
 678 phenomena remains a challenge. We have addressed this very complex problem and proposed
 679 a complete 3D model involving CHT and FSI simulations, based on 3 open-source software
 680 codes: OpenFOAM, CalculiX and preCICE. The PCM model, which has been implemented in
 681 OpenFOAM, takes account of phase changes, conduction and convection. This model has
 682 been validated on the analytical solution of the Stefan problem and experimental data of a 2D
 683 configuration. The CHT simulations relied on the PCM model (OpenFOAM) and the
 684 conduction in the solid architected structure (CalculiX). The interface coupling between the
 685 two codes was managed by preCICE. The FSI simulations aimed to compute the structure
 686 displacements and induced stresses. Such information is very useful to prevent mechanical
 687 failures and improve the efficiency of heat transfer at the interface with electronic
 688 components, as deformation of the structure can worsen the contact.

689 This modeling was applied to gyroid structures, triply-periodic minimal surfaces, which are
 690 expected to behave efficiently. Such shapes do maximize the exchange surface, thus

691 intensifying heat transfer during heating and improving thermal damping in electronic
692 components. We have simulated several configurations with different geometry thicknesses
693 and various filling levels of PCM (from 98.5 to 100%). The thicknesses of the gyroid
694 branches ranged from 2% to 10% of the container box side length. Depending on the filling
695 rate, thermal expansion of liquid PCM led to pressure increases inside the 3D architected
696 porous conductive matrix, and therefore significant mechanical stresses. For the first time, we
697 have shown that the filling ratio has a notable impact on the stresses that are induced. Only
698 1% short of the maximum volume reduces the mechanical stresses and failure risk
699 considerably. Compared to this low value, increasing the thickness of the container cuts a lot
700 more the PCM volume, and thus thermal performance. To optimize thermal management,
701 decreasing the quantity of PCM is thus preferable to strengthening the container geometry,
702 which scales the volume down too much. As the fluid pressure remains low, the solid
703 deformation is found to be small even for thin gyroids. The simulated maximal displacement
704 with 2% thick branches is of the same order (0.1 mm), as with consolidated gyroids filled
705 with more PCM. The contact thermal resistance is therefore also of the same order of
706 magnitude.

707 With this 3D fluid-structure modeling of the heat and mass transfers in a complex system
708 dedicated to the thermal management of electronic devices, we were able to select the 2%
709 thick gyroid as the most efficient configuration. A future study based on both experimentation
710 and simulation will be carried out with this design of architected porous structures based on
711 metallic additive manufacturing impregnated with palmitic acid. This innovative composite
712 will be characterized to specify the input parameters of the simulations and validate the
713 theoretical results. Following this study, the material will be integrated into a power supply in
714 order to evaluate its performance and its capacity to manage power peaks more effectively.

715

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720 **8. References**

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