

*Prototype 12:*

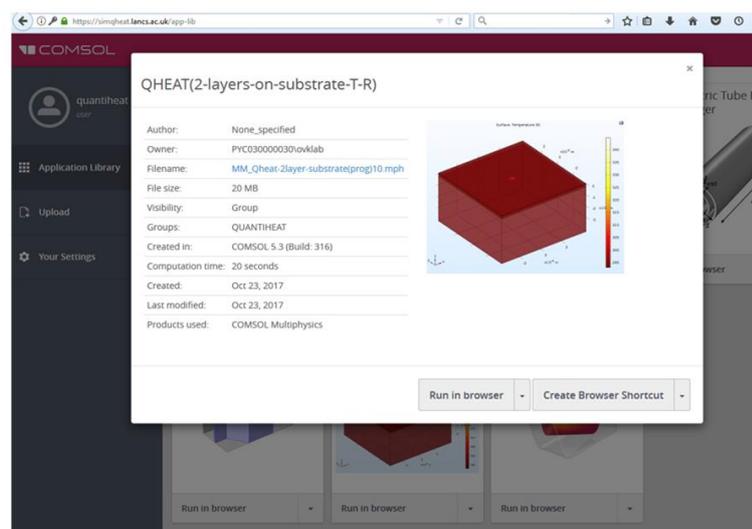
# **Simulation Tool for Heat Transfer within Nanomaterials**

*Lead Partner: CNRS (Centre National de la Recherche Scientifique) – CETHIL (Centre d’Énergétique et de Thermique de Lyon), France*

Heat conduction on the nanoscale may be described differently to the way it is at macroscale mainly due to the failure of Fourier’s law in crystalline materials [1]. Furthermore, thermal boundary resistances (TBR) between materials become significant and cannot be neglected in front of the bulk thermal resistances in many configurations at the sub-micrometer scale [1]. Accounting for these effects can be done semi-analytically in simple geometries by some researchers and engineers (not everyone!), but not at all in complex ones such as those encountered often in current nanomaterials and nanodevices. Complex simulation tools based on the Boltzmann Transport Equation (BTE) [2] is a solution, which are however often hindered by its usual complexity. As a consequence, there is a lack of tools making it possible to get a quick estimate of the flux exchanged from a hot spot on surface to the bath, a situation often met in nanometrology involving techniques such as scanning thermal microscopy or photothermal heating and in industry, especially in electronics.

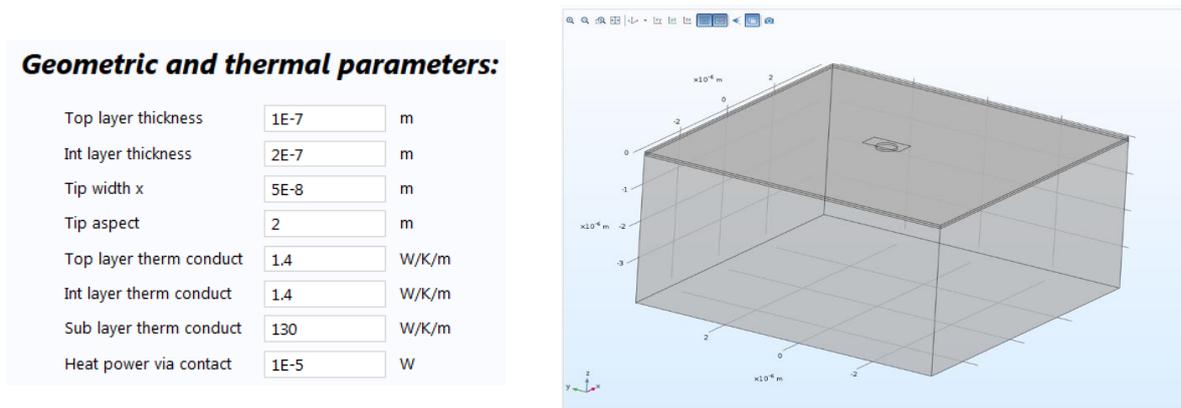
To mitigate this issue, we have developed a free online software based on Finite Element Modeling (FEM) where effective thermal conductivities accounting for the phonon confinement can be included. The tool is based on the COMSOL software [3] that solves heat transfer in the diffusive regime through a Finite Element Method (FEM) and that is well-known in academia and industry. A server performs the calculations entered remotely by the user. Various computations can be performed in the same time. A limited number of configurations are available currently, but it is hoped that more will be added in the future.

**Figure 1.** Main window of the online tool once the user is logged and has selected the multilayer-on-substrate configuration

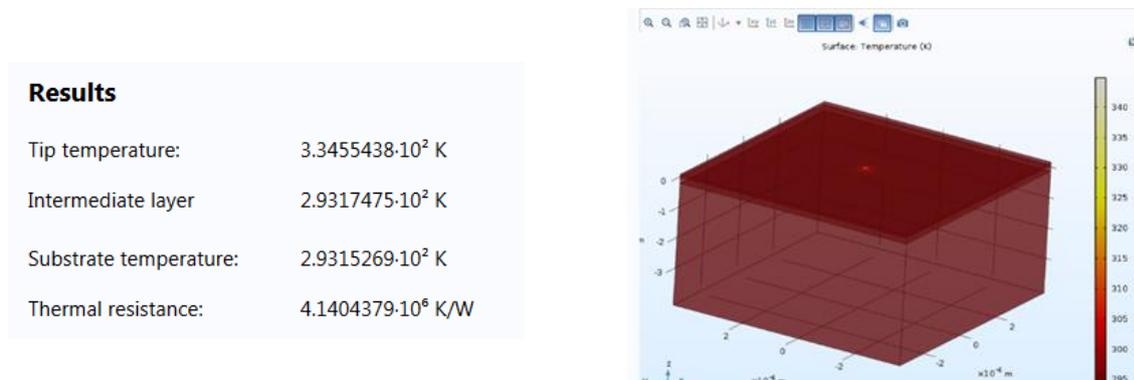


## How to access and use the online simulation tool?

The web address is <https://simqheat.lancs.ac.uk/>. A login and a password are then required to enter into the system. A list of possible computations for various configurations appears on the screen in addition to the list of current computations performed by the server (see Fig. 1). Once the user has selected the configuration of choice, a window with the parameters that the tool allows to select – only a limited amount are manageable – appears on the screen as shown on Fig. 2. Thin-films-on-substrate are typical geometries considered, as they encompass many of the situations of interest in a simplified way. Once the user has entered the parameters, in particular the size of the source and the heat flux dissipated from it, the computation takes place. In the easiest cases it lasts few seconds before the temperature field in the system starts to be displayed. The key quantities that are given by the software are the maximal temperatures at the surface and in the layer below the top one, and the thermal resistance from the maximal temperature to bath (see Fig. 3). This is the key quantity to be determined in many situations. While the size of the simulation domain is fixed and the top surface is considered as insulated, parametric studies are possible by modifying the other input parameters. The online tool is hosted and maintained at the University of Lancaster (ULANC).



**Figure 2.** Example of parameters selected in the online tool, here in a layer-on-substrate geometry with an elliptic hot source

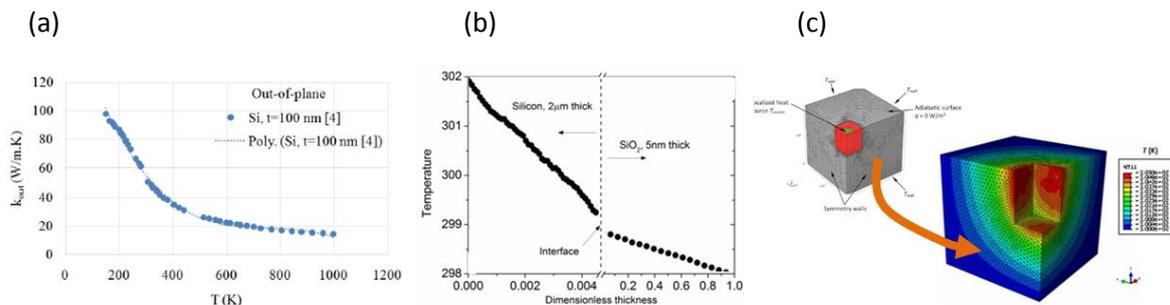


**Figure 3.** Example of results and temperature field in the volume

## Including nanoscale effects in the simulation of heat conduction

At first sight, the COMSOL software allows only to consider diffusive heat conduction, while it is now well-established that heat transfer on the nanoscale can be much more complicated [1]. A way to include nanoscale effects is to consider size-dependent effective thermal conductivity. As a result, such quantity has been computed within the Quantiheat collaboration. The results are proposed in the form of a library of data that allow for the calculation with the online software. In particular, a Monte Carlo method solving the Boltzmann Transport Equation [2] has been used at the University of Reims-Champagne Ardennes (URCA) as shown in Fig. 4. Some of the calculations could be performed by means of a new tool developed within the Quantiheat collaboration, where FEM and BTE solvers are coupled as a single tool in order to be able to consider very large simulation domains [4] (see Fig. 4c). Ballistic constrictions (i.e. configurations beyond 1D) are included in the results. For more simple geometries, semi-analytical solutions have been computed at the Catalan Institute of Nanoscience and Nanotechnology (ICN2) and the Centre for Energy and Thermal Science (CETHIL) of the CNRS.

In addition to the phonon confinement effects, a library of Thermal Boundary Resistances is also provided. For situations where phonon-based thermal conduction occurs, the TBR values have been computed by means of the Acoustic Mismatch Model (AMM) and the Diffuse Mismatch Model (DMM) [5] at CETHIL for the most common materials. It is known that these data allow estimating the impact of the surface within some uncertainty on the order of unity. For metal-dielectric interfaces, the computations require to include electron-phonon coupling phenomena. Semi-analytical computations performed at the VTT Technical Research Centre of Finland are able to provide some estimates, based on comparison with literature [6]. While all these data may not provide an exact value, they already give estimates which are way better than erroneous ones based on Fourier's law.



**Figure 4.** Few examples of tools developed and results obtained within the Quantiheat collaboration for feeding the library of data within the project involving the Monte Carlo solver of URCA. (a) Fitting of the Monte-Carlo BTE results as function of temperature at a given layer thickness for determining the size-dependent thermal conductivity. (b) Monte Carlo result showing the temperature jump (discontinuity) typical of ballistic transport of boundary resistance. (c) Coupling between BTE solver and FEM to perform multiscale simulation up to arbitrary-large computational domains from sub-mean free path heat source.

If some external contributor proposes to add a simulation program or data associated with another geometry, it will be positively valued. However, only a limited number of such proposals can be accepted.



Note that the same online tool can be used for computation of the tip-sample flux exchange in scanning thermal microscopy. This is the object of a separate Application Note<sup>1</sup>.

## **References**

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- [2] J. Randrianalisoa and D. Baillis, *Monte Carlo simulation of steady-state microscale phonon heat transport*, ASME Journal of Heat Transfer 130, 072404 (2008)
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- [5] E.T. Swartz and R.O. Pohl, *Thermal boundary resistance*, Reviews of Modern Physics 61, 605 (1989)
- [6] Quantiheat consortium Report, Deliverable D5.2, *Thermal boundary resistances calculated from different methods. Simulations and comparison with experimental data*, 2016

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<sup>1</sup> Prototype 11: Modelling Tool for SThM Tip and Sample Interaction