Short Term Scientific Mission Report

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1 Summary

In January 2016, I was awarded a 3-week STSM Grant to visit Professor Tim Myers at the Centre de Recerca Matematica (CRM) in Barcelona, Spain. The visit took place on June 2016 and consisted in spending the first and third weeks at the CRM and the second week at the ECMI conference in Santiago de Compostela (Spain). The main objectives of my research proposal were: continue unfinished work with Prof. Myers on the mathematical modelling of heat transfer and phase change at the nanoscale, dissemination of my current research and sketch a plan to apply for a Marie-Sklodowska Curie Individual Fellowship to work with Prof. Myers in the CRM.

In Section 2 I provide details on the progress achieved with respect the initially planned objectives and in Section 3 I give my conclusions and an overall assessment of my visit to the CRM.

2 Progress

2.1 Continuation of previous work

As specified in the research proposal, I planned to continue unfinished work that we started before my departure from the CRM in July 2014. This was originally organized in two parts: *The hyperbolic Stefan problem* and *Theoretical and Practical Stefan problems*. I cover the progress of these two items in the sections 2.1.1 and 2.1.2, respectively. In addition, I include a third section (2.1.3), titled *The Stefan problem with a size-dependent thermal conductivity*, where I present a new research project that we discussed during the last week of my visit and was not included in the original research proposal.

2.1.1 The Hyperbolic Stefan problem (HSP)

Most of the time of my visit was spent working on this topic. During the first two days, we derived a formulation of the HSP slightly different from the original form (derived in 2014). We assumed that the heat flux, q_i, satisfies the modified Fourier law

$$q_i = k_i \frac{\partial T_i}{\partial x} + l_i^2 \frac{\partial^2 q_i}{\partial x^2} \tag{1}$$

where k_i is the thermal conductivity, T_i the temperature and l_i the mean free path of the heat carriers. The subscript i takes the value 's' or 'l' if one refers to solid or liquid, respectively. In this case, the heat equation does not contain hyperbolic terms, and the nondimensional two-phase Stefan problem can be written as

$$u_t = u_{xx} + u_{txx} \quad \text{on} \quad 0 < x < s(t)\,, \tag{2}$$

$$v_t = \alpha v_{xx} + l v_{txx} \quad \text{on} \quad s(t) < x < \infty\,, \tag{3}$$

$$(\beta + u_{xx}\big|_s - l^2 \alpha v_{xx}\big|_s) s_t = (u_x - k v_x)\big|_s\,, \qquad s(0) = 0\,, \tag{4}$$

$$u(0,t) = -1\,, \qquad u(s,t) = v(s,t) = 0\,, \qquad v \to v_0 \text{ as } x \to \infty\,, \tag{5}$$

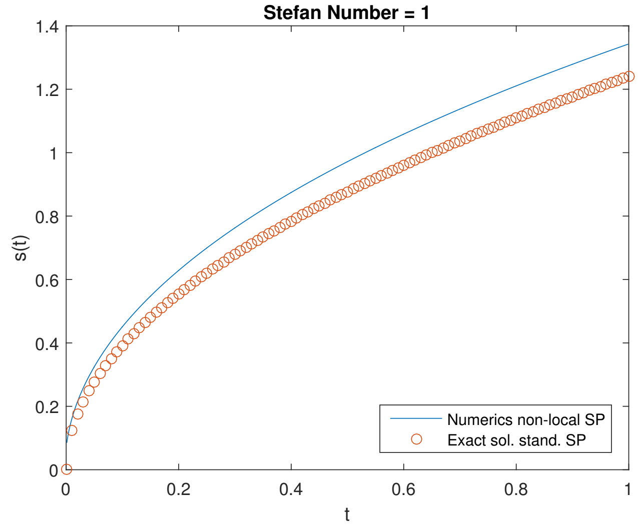
where u and v are the temperatures of the solid and the liquid phase, respectively, and β, k, l and α are non-dimensional parameters. The nondimensional far-field temperature of the liquid is represented by v_0.

To start with the simplest possible physical scenario, we considered the one-phase solidification problem by assuming the liquid phase initially at the freezing temperature, $v = v_0 = 0$. In this case (2)–(5) reduces to

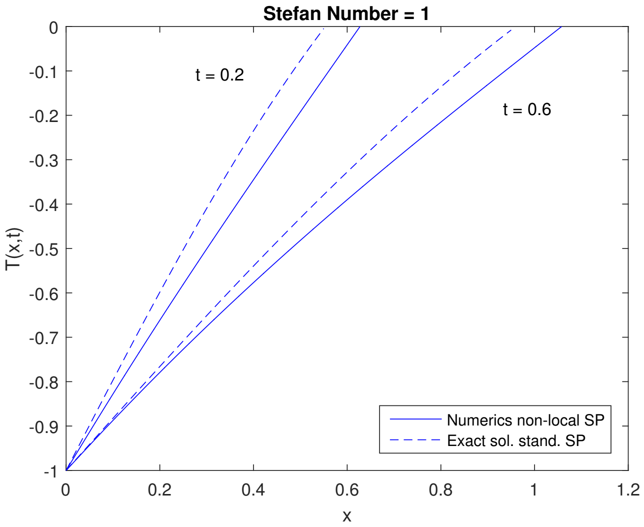
$$u_t = u_{xx} + u_{txx}\,, \qquad (\beta + u_{xx}\big|_s) s_t = u_x\big|_s\,, \tag{6}$$

$$u(0,t) = -1\,, \qquad u(s,t) = 0\,, \qquad s(0) = 0. \tag{7}$$

In the following days, I started working on the numerical solution of (6)–(7). During the first week Prof. Myers, myself and his PhD student, Marc Calvo, who was working on the asymptotic solution of the problem, met everyday to discuss the progress made. Prof. Myers and his group also attended the ECMI conference, where continued working on the problem. By the end of the third week, we obtained the first sensible set of results, which are shown in Figure 1.



(a)



(b)

Figure 1: Position of the phase change front (a) and temperature profiles (b) for $\beta = 1$.

The results in Figure 1 show how the non-local terms (6)–(7) introduce a delay in the propagation of the solidification front, which in turn affects the temperature profiles. Theses results provide enough motivation to continue the study of this model and, possibly, to extend the research to the case where the hyperbolic terms cannot be neglected.

2.1.2 Theoretical and practical Stefan problems

At the final stage of my PhD we had the idea of working towards an extensive monograph on the theoretical bases and the application of modern Stefan problems. This study would gather our research done during the four years of my postgraduate research, the previous research in the field by Prof. Myers and the main contributions by other authors in recent times.

During my visit we had the opportunity to review the content structure of the monograph and start distributing tasks. My first task will consist on writing and presenting approximate solutions for the classical Stefan problem in the sphere, which will later help to introduce our models on the melting of spherical nanoparticles (in the practical applications section of the monograph). Prof. Myers will start working on the introduction and the derivation of the Stefan problem in Cartesian coordinates.

2.1.3 The Stefan problem with a size-dependent thermal conductivity

Several experimental studies have provided evidence of the variation of the thermal conductivity with the size of the physical system. A simplified model for the thermal conductivity that takes into account the size effect is given by

$$k_s = \frac{2k_s^* L^2}{l^2}\left(\sqrt{1+\frac{l^2}{L^2}}-1\right) , \qquad (8)$$

where k_s^* is the bulk thermal conductivity, L the size of the phsyical system and l the mean free path of the heat carriers [1, 2].

Before my departure from the CRM in 2014, I proposed to investigate the impact of introducing a size-dependent thermal conductivity on the Stefan problem and discuss the implications that this would have on the solidification of nanofilms, nanoparticles and nanowires. In this situation, the expression of the thermal conductivity for the growing solid phase will be

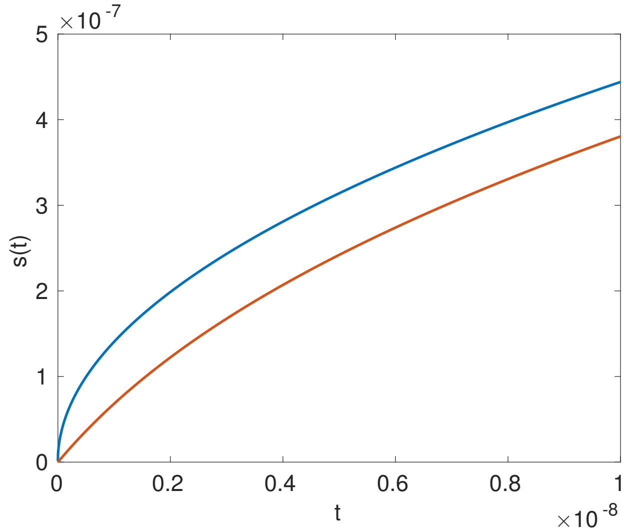


Figure 2: Evolution of the solid-liquid interface. The physical parameters used correspond to Silicon. The red line is the solution to the model with varying thermal conductivity and the blue line to the problem with bulk thermal conductivity.

given by

$$k_s = \frac{2k_s^* s(t)^2}{l^2}\left(\sqrt{1+\frac{l^2}{s(t)^2}}-1\right), \tag{9}$$

where $s(t)$ is the position of the solid-liquid interface. In figure 2, I present the numerical solution of the one-phase Stefan problem for a solidifying Si nanofilm. The blue line represents the solution of the standard problem with constant thermal conductivity and the red line the solution of the problem with (9). These preliminary results show a remarkable difference between the two cases. For instance, at $t = 10$ ns the interface position pedicted by the two different models differs by ≈ 90 nm.

During the last week of my visit we had the opportunity to briefly comment these results and concluded that it would be very interesting to further investigation the problem. A Skype meeting between me, Prof. Myers and Mr. Marc Calvo, will be scheduled soon to organise this project.

2.2 Dissemination of my research

In the second week of my visit I attended the 19th European Conference on Mathematics for Industry in Santiago de Compostela, Spain. I had the pleasure to receive the prestigious Anile-ECMI Prize for the best PhD in Europe on an industrial mathematics related topic. As the prize winner, I was entitled to give the *2016 Anile Prize Lecture*, where I presented the research done in my PhD and part of my current work on laser-induced melting. In addition, I participated in the mini-symposium 'Mathematics in nanotechnology' organized by Prof. Myers, where part and extensions of our work on nanoparticle melting was presented and discussed.

The conference was full of interesting talks related to my research, on topics such as numerical approaches to laser melting of metals, mathematical modeling of Lithium-Ion batteries and moving boundary problems in industrial applications. This provided an ideal enviroment for networking, giving me the opportunity to meet local and international reserachers in industrial and applied mathematics.

Given that my visit was limited to 3 weeks, I used the free time left during the conference to make progress on the numerical solution of (6)–(7). I also met with Prof. Myers everyday to discuss the problem.

2.3 Marie-Sklodowska Curie Individual Fellowship

In May 2016, I was offered a 2 year postdoctoral position at McMaster University (Hamilton, Canada), which I accepted. As a result, me and Prof. Myers agreed on postponing the application for the Marie-Sklodowska Curie Individual Fellowship for the next round of applications in September 2017.

3 Conclusion

The initial objectives of the research proposal were accomplished and the final balance is very positive. Visiting Prof. Myers was crucial to follow up with the unfinished work on *the hyperbolic Stefan problem* and the organization of tasks for our monograph *Theoretical and practical Stefan problems.* In addition, we had the opportunity to discuss a new research project on the Stefan problem with size-dependent thermal conductivity. It is envisaged that this study will represent an original piece of work which will very likely be submitted for publication in a high impact factor journal.

At an individual level, the visit allowed me to attend and give a talk at the ECMI conference in Santiago de Compostela, where I presented part of the work done in collaboration with Prof. Myers and part of my work in the field of laser-induced melting. During the conference, I was awarded with the prestigious Anile-ECMI Prize for the best PhD in Europe on an industrial mathematics related topic. In addition, I had the opportunity to attend many interesting talks and network with top-notch European researchers in industrial and applied mathematics.

References

[1] D. Jou, J. Casas-Vazquez, G. Lebon, M. Grmela, *A phenomenological scaling approach for heat transport in nano-systems*, Applied Mathematics Letters 18, 963–967, 2004.

[2] F.X. Alvarez and D. Jou, *Memory and nonlocal effects in heat transport: From diffusive to ballistic regimes*, Journal of Applied Physics 90, 083109, 2007.