Scientific report

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1 Purpose of the STSM

The goal of this STSM was to attend the doc-course "Applied Mathematics and Optimization" that took place at IMUS in the University of Seville (Spain). The main objectives of this activity were:

- To provide an intensive training in scientific areas of interest, including non-linear optimization.
- To initiate the students in a research topic by developing a training research work, that eventually can result in an article or even further.
- To identify students of high scientific quality that could carry on a PhD Thesis under the direction of researchers of the organizing centers.

The program was composed of three different formative activities: 4 courses, a series of lectures and a supervised research stage under the guidance of individualized tutors. All participants also to attended two workshops that were scheduled during the doc-course: Workshop on Mixed Integer Non-linear Programming, held in Seville March 30-April 1, 2015; and Final Workshop on Applied Mathematics, held at BCAM in Bilbao May 26-27, 2015. The courses were organized in March and April 2015 and the topics were the following:

1. Advanced course in Nonlinear Optimization,
2. Multiscale and Multiphysic Computational Mathematical Modeling,
3. Computational fluid dynamics,
4. Modelling and optimization algorithms in networks design and energy planning.

The courses took place during the first month of the program and each one last 15 hours long. The research seminar consisted of a number of two-hour sessions and took place during the second and third month of the program. In each session a specialist on the selected topic presented recent research related to the contents of the program. Finally, each attendant developed a supervised research work on a specific project chosen among a list of proposals under the guidance of a personalized tutor per student. The topic assigned to Martin Michalek was supervised by Prof. Dr. Francisco Guillén and was focused on: *Analysis and numerical study of some solidification models.*

2 Description of the work carried out during the STSM

The applicant participated on the DOC COURSE in Sevilla 2015 and obtained the final participant diploma. During the course, the applicant participate on The Second Sevilla Workshop on Mixed Integer Nonlinear Programming (March 30 – April 1 2015, Sevilla) and the BCAM Workshop on Mathematics and its Applications (May 26-27, 2015, Bilbao) with short talk on the topic: "Phase field modeling of melting and solidification" During the DOC COURSE the applicant satisfied all given goals. The course consisted of two parts – in the first one, he attended lectures on recent topics in applied mathematics (optimization, numerical computation, stochastic optimization and applied graph analysis on transportation problems). The applicant also wrote brief lecture notes (20 pages) introducing "Finite element method". The second part of the course (2 months) was dedicated to cooperation with prof. Francisco Guillen on the given problem (Caginalp-like model of melting and solidification).

3 Description of the main results obtained

Nowadays, pure and applied mathematics is losing connection. However, any of these two scientific branches cannot survive alone. In modelling of real phenomena, many different approximations can be constructed which are then numerically computed. Without deeper analysis, one might construct unstable or inconsistent approximations.

The studied phenomena was the phase change of a material (e.g. water (or ice) or steel being solidified or melted). We have considered a thermodynamically consistent model based on ideas of R. Caginalp [Cag86] which describes dynamics (in time evolution) of phase changes.

The model was described in [BGCJV12] with an extra second order quadratic term. Due to the extra term, only local in time existence was shown because of absence of global in time energy estimates.[1] The phenomenon is mathematically posed as partial differential equaiton

$$\partial_t \theta = K \triangle \theta - \frac{\ell}{2} g(\phi) \partial_t \phi \tag{1}$$

$$\varepsilon^2 \partial_t \phi = \varepsilon^2 \triangle \phi - f(\phi) + \frac{\varepsilon \ell}{2} g(\phi) \theta. \tag{2}$$

[1] The model is also used in the theory of feromagnetic fluids according to [Mir14].

Where θ is temperature, ϕ is description of phase (solid fraction). These two function on a time space $[0, T] \times \Omega$ are unknown and complemented by initial data in time zero. The nonlinear function f is derivative of bi-stable potential and g gives interpolation between states of entropy during a phase change.[2] Similar models were also treated analytically (not numerically) in [Mir14] and [QB10].

We provided existence and uniqueness results of solutions of the continuous equation. Also some specific properties of solutions were obtained.

Based on the mathematical analysis, few computational (numerical) schemes were proposed. A

- Nonlinear stable - for which stability of approximations and convergence to a continuous solution were shown (however, for computational reasons is the nonlinear scheme badly applicable).
- Linear scheme 1 - which was shown to be conditionally stable and convergent and the condition given was very mild.
- Linear scheme 2 - which was shown to be optimally behaving with respect to approximation of the physical phenomena (optimally numerically dissipating), however, only conditionally stable under quite strong conditions.

The main novelty was an introduction of a new idea how to use analytical results (maximum principles) inductively to show the stability of the scheme. This idea was used in the case of the Linear scheme 1.

It is worth to be noted that in numerical literature results on stable and convergent linear approximations of a nonlinear differentail equations are very uncommon.

The linear schemes were then programmed using Finite Element Method approximations and computing language FEniCS. Numerous numerical experiments were done (melting, solidification, "fight" of phases, etc.). The numerical results were consistent with the given analysis and numerical errors corresponded with the classical approximation errors.

4 Future collaboration with the host institution and forseen publications

In the future, we plan to extend the result and release the mild condition on the stability of the linear scheme 1. This would lead to an interesting example of (for small time step) stable linear approximations of nonlinear equations, which is very rare and would lead to successful publication.

There are also few other models which are more complex - e.g. dealing with alloys solidification or solidification/melting in a moving fluid. Mathematical and numerical analysis of such models would be very reasonable topic for future collaboration.

[2] Exhausting description can be found in the referenced articles.

References

[BGCJV12] Sylvie Benzoni-Gavage, Laurent Chupin, Didier Jamet, and Julien Vovelle. On a phase field model for solid-liquid phase transitions. *Discrete Contin. Dyn. Syst.*, 32(6):1997–2025, 2012.

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[Mir14] Alain Miranville. Some mathematical models in phase transition. *Discrete Contin. Dyn. Syst. Ser. S*, 7(2):271–306, 2014.

[QB10] R. S. Qin and H. K. Bhadeshia. Phase field method. *Materials Science and Technology*, 26(7):803–811, 2010.

Sevilla, 29 june 2015

Confirmation by the host institution of the successful execution of the

DOC-COURSE on Applied Mathematics and Optimization,

hold at IMUS, Universidad de Sevilla (Spain). Mars-May 2015

Student: Martin Michalek

Supervisor: Francisco Guillen-Gonzalez

The considered problem:

Title: Analysis and numerical study of some solidification models.

Abstract: Some parabolic partial differential equations modelling solidification processes will be studied from the analytical and numerical point of view. In particular, the dissipativity of these problems is used to obtain a-priori estimates of the adequate approximative solutions that allows to obtain a solution via a limit process. This fact must also be profited to design stable and convergent numerical schemes. Some numerical simulations will be made to compare with the analytical results.

The achievements:

Martin Michalek has attended satisfactorily all courses and has developped the research period.

He has got a very good background in all the points treated in the research period, like

1. documentation and comprensión of some fundamental physical situations behind solidification problems

2. a good knowledge of mathematical results of Canigalp's model, which is a energy-phase field model, accounting latent heat effects, maximum principie for the phase variable and energy dissipation.

3. The design of energy-stable schemes, determining some constraints to get time schemes conserving the maximum principle property.

4. The realization of numerous numerical simulations to compare the numerical analysis and to provide numerical comparations with respect to changes in some physical parameters of the problem

Sincerely,

Francisco Guillen-Gonzalez, Full professor at EDAN and IMUS, Universidad de Sevilla

UNIVERSIDAD DE SEVILLA
Dpto. Ecuaciones Diferenciales y Análisis Numérico