# Don't be phased

Attempts to speed up numerical simulations of multiphase microstructures are opening up fertile ground for new research, as **Dr Maya Neytcheva** describes

**Can you outline the background to your research?**

Multiphase processes involve interactions between several different phases, such as fluid to fluid or fluid to solid. Multiple phases constitute a very important area of research with many highly prioritised and important applications, such as droplet deposition, underwater explosions and micro-jetting devices. When studying such processes with the aim of ultimately utilising them in practice, numerous difficulties are faced due to the variety of scales in space and time. One of the most important features of multi-phase flow processes is the dynamics of the interfaces between the materials. Understanding, predicting and controlling this is crucial. However, the interfaces between the phases are sharp, ie. of zero thickness, requiring advanced computer simulations to produce accurate results.

**Can you explain the 'diffuse-interface phase-field' approach?**

When studying multiphase problems, one very important task is to locate and accurately trace the sharp interfaces between the phases and their dynamics in space and time. In addition to the sharpness of those interfaces, the characteristics of the phases (such as density or viscosity) change abruptly across the interfaces. As numerical simulations provide approximations of the solution in only a finite number of space points, it becomes clear that in order to 'see' (resolve) the interfaces and their evolution, we need many points along them. Special attention is also needed to handle properly the discontinuities of the parameters.

One way to circumvent the sharp interfaces and the jumps in the parameter values is to assume that the interfaces have a thickness we can control in the model and make as small as possible. Thus, in two dimensions, instead of lines we could think of stripes. A model, based on the above assumption, is the so-called 'diffuse interface phase-field' model. This is one of the possible mathematical abstractions proposed to describe multiphase phenomena.

**In what context are you employing iterative solution methods? What challenges do they bring?**

The chain of objectives that leads to choosing iterative methods for the numerical simulations of multiphase flow processes is complex. The numerical simulations objective – to follow the dynamics of the interfaces between different phases and to provide sufficient accuracy in the simulation process – requires that the diffusive interface be thin enough. In order to achieve this, the resolution of the discretisation of the computational domain (at least along the interfaces) has to be fine enough, and this leads to algebraic systems of very large dimensions. Such complexity rules out direct solution techniques, and the iterative methods become the only viable alternative. Straightforwardly applying iterative methods to solve the resulting linear systems may, in general, require a large number of iterations.

**What do you hope to achieve in the project?**

The aim of the project is to speed up the simulations of multiphase flow processes by constructing a preconditioner for the arising linear systems. To construct a very efficient preconditioner that fully utilises the properties of the corresponding discrete model and its structure, we have to combine knowledge about the nature of the original problem, the discretisation method, the inherent structures and, last but not least, about the architecture and the characteristics of the computer where the numerical simulations are to be performed. We also had to come up with an algorithm that decomposes into sub-problems, which can be efficiently solved via highly optimised and broadly available program tool boxes.

**What have been the project's main activities so far? Have you encountered any notable hurdles, and if so, how have these been addressed?**

The main aim of the project is to figure out how to speed up the numerical simulations, provided that we use the diffuse-interface model. This goal has been achieved to a very large extent.

The project activities are manifest in the cooperation between an engineer, who is an expert on the physics behind multiphase flow problems and the phase-field model, and a numerical analyst, whose expertise is in efficient preconditioning techniques. This collaboration has made it possible to discover the inherent properties (structures) of the discrete model and has brought to life a numerical algorithm which fully utilises those structures, speeding up the simulation process significantly. An additional effect was to enable the usage of highly optimised general-purpose solution methods, which are not efficient when applied on the whole algebraic system but are very suitable when solving sub-systems in the so-discovered algebraic structures. The suggested algorithms are implemented and can be ported, and run on various computer platforms, including parallel high performance computers.

# Computational issues

The flourishing science of numerical simulations is presenting opportunities for detailed interdisciplinary work, and Uppsala University's **Department of Information Technology** has harnessed this with its project on the diffuse-interface phase-field approach

**IN THE PAST** decade computational science has emerged as the third branch of scientific endeavour, alongside the theoretical and experimental areas. The complexity of problems investigated by scientists means that laboratory experiments are frequently unfeasible, and instead computer simulations (also known as numerical simulations) must be used, tackling problems ranging from the reduction of air pollution and the storage of nuclear waste to cell biology and quantum mechanics. As numerical simulations have developed, computation has led to novel theoretical results and methodological approaches, and has fostered a symbiotic relationship with the other branches of investigation.

The work of Dr Maya Neytcheva focuses upon a group of computer models of particular complexity. The diffuse-interface phase-field approach is a specific type of numerical simulation, and one which is broadly applicable due to its basis on the 'total free energy' of the physical system. The approach has been found to be a powerful mathematical model for simulating the creation and evolution of both morphological patterns and interface motion. This allows it to be a single theoretical framework underpinning investigations from the micro- to the macroscale. The applications include (but are not limited to) crystal growth and spinodal decomposition, capillary phenomena, oil recovery, and the dynamics of two or more populations.

The power of the diffuse-interface phase-field approach is matched by its complexity and the size of the arising numerical models, meaning that an alternative to analytical solutions is the only practicable approach. Techniques must be used to make the dynamics of interface movement accessible in a discreet form. This allows the discovery of the solution at some points in space and time only, and the movement from continuous to discreet entails an error in the solution, albeit an estimable one. The finite element method (FEM) is a well-established flexible discretisation technique that is being utilised at the Division of Scientific Computing at the Department of Information Technology, Uppsala University. This method is based on the pioneering work of Alexander Hrennikoff and Richard Courant, which was codified by Olgierd Zienkiewicz. Starting in 1947, Zienkiewicz published a number of works on FEM, which recognised the potential of the approach to areas beyond solid mechanics. The methodology allows the approximate solution to partial differential equations (PDEs) – equations which often model multidimensional systems. The strength of FEM is that it allows the complex geometries to be treated as a union of individual (small) elements, which are much more easily handled in the analysis and the error estimates of the so-computed approximate solutions.

## NO EASY SOLUTION

Uppsala's Scientific Computing division, with its broad scope of research areas, provides an excellent environment for Neytcheva and her group to work on and prove the efficacy of preconditioning methods. These are necessary for the processing of complex models near the point of solution. Once the FEM, or other such technique, has produced discrete points, the resulting algebraic systems need to be solved. These linear systems are the main burden which must be dealt with by the researchers and applied scientists, and for which the preconditioning methods are so important. Systems of small dimensions are able to be approached using the 'direct' method, a technique which produces an exact result to machine accuracy. However, direct methods have extremely high computational demands, which grow exponentially with the number of degrees of freedom in the discreet models. The problem is that the calculations at the forefront of research require millions or even billions of degrees of freedom, and are well beyond the computer resources available today. As such, 'iterative methods' are essential for large-scale scientific computations. These methods converge upon results, as the name suggests, through multiple

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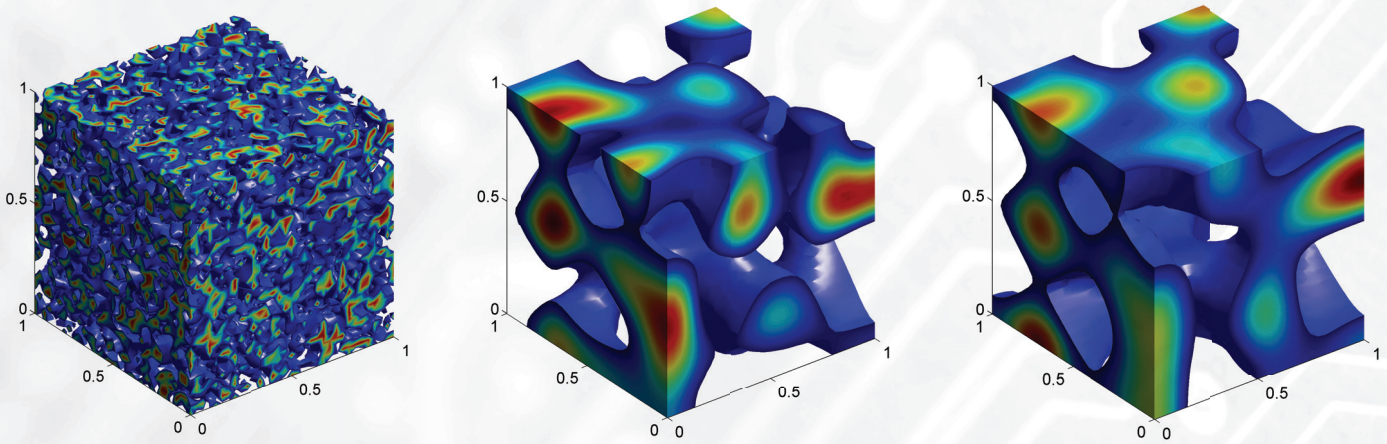


**FIGURE 1**. INTERFACE EVOLUTION OF A TWO-PHASE MIXTURE

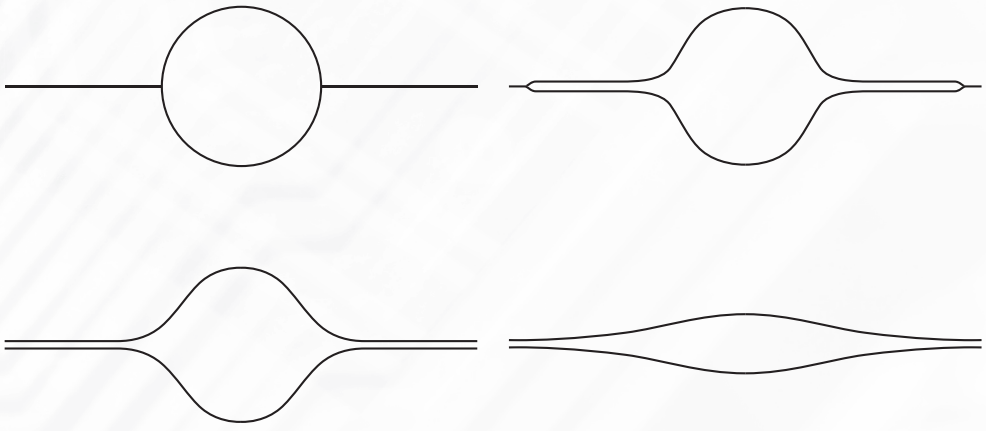

**FIGURE 2**. INTERFACE EVOLUTION IN A THREE-PHASE FLUID SYSTEM

iterations. Each individual iteration uses only a small amount of computational power relative to direct methods, but may have to go through very large numbers of iterations in order to achieve results of sufficient accuracy. Preconditioning can enhance this process, thereby utilising the available technology in the most efficient manner.

## THE BURDEN OF TECHNOLOGY

The continual improvement of computer technology is essential to the development of more complex models for multiphase microstructures. Yet this also makes the role of the researcher more difficult. Whilst more powerful computers have the resources to consider densely elaborate problems, the architecture of the computers themselves has become increasingly heterogeneous. Since the researchers involved must understand the architecture of the computers in use in order to efficiently implement the iterative solution methods, and in particular regarding preconditioning strategies, computer resourcefulness becomes a central issue. This can be seen as the overlap between computational and computer science.

The preconditioner selected must take into account the computational architecture in order to be of use. The essential factor is the trade-off between the numerical efficiency (number of iterations) and the computational efficiency (difficulty of each iteration). 'Optimal' preconditioning techniques achieve both aims, but must necessarily act closely within the structures of the computer. Uppsala's developed preconditioning technique has been extremely successful, producing a flexible tool which works across large time steps without degrading the convergence rate of the iterations. Furthermore, large-scale tests have been performed with up to 270 million degrees of freedom. Utilising a high performance parallel computing platform, this checked the robustness as well as the performance and scalability of the numerical method. Neytcheva is pleased with the results that have been produced: "The preconditioning method is tested against other methods, often used by applied scientists, and has confirmed the theoretical expectations being both robust with respect to problem parameters and faster in overall computing time". Such a result demonstrates the success of the project.

## THE FUTURE OF THE DISCIPLINE

Neytcheva is in agreement with Professor Volker Mehrmann of the Technische Universität Berlin, who prophetically remarked that "the golden age of numerical analysis has not yet started". In order to continue to pursue the possibility of ever more powerful modelling requires an investment in the students who are currently going through university. Neytcheva thinks it should be a high priority of institutions to educate and bring forward the young researchers who are capable of addressing new issues in the computational science domain. It is imperative that research is conducted not only in the theoretical disciplines, such as mathematics, but in the application-driven areas of research. It is only through such interdisciplinary work that significant progress will be made within the field. Furthermore, there is a strong need to develop novel methods, given the continuously growing complexity of the models that are being brought forward from engineering and science.

## INTELLIGENCE

### FINITE ELEMENT BASED PRECONDITIONING METHODS FOR SOLVING ALGEBRAIC PROBLEMS ARISING IN MODELLING OF MULTIPHASE MICROSTRUCTURES

### OBJECTIVES

The project considers numerical simulations of interface motion in multiphase flow dynamics. The aim is to enable fast and reliable numerical solutions of large algebraic problems arising from finite element discretisations of those models. The project aims towards the construction, analysis and implementation of a fully robust, preconditioned iterative solution method that utilises the inherent structure of the arising matrices.

### KEY COLLABORATORS

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### FUNDING

Swedish Research Council

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