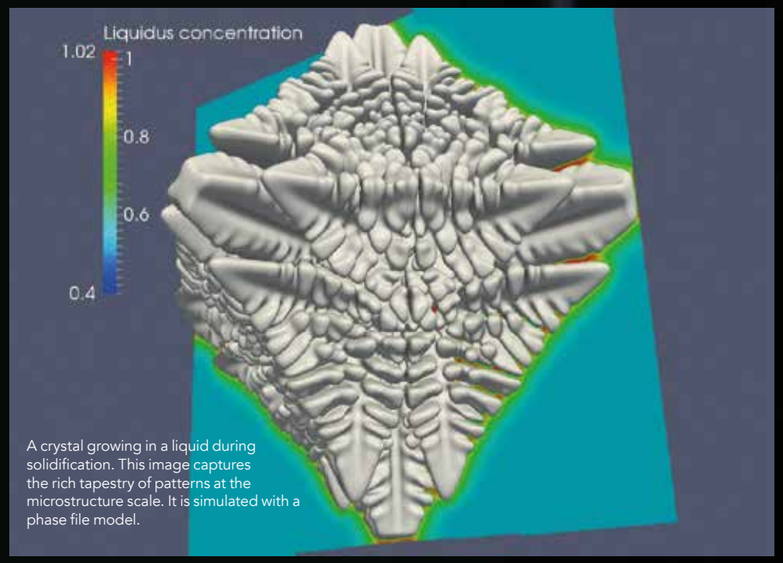
Predicting new materials and processes: the power of computer simulations

In the world of materials science, the structure of a material is key to its function. This material structure can be defined through various processes occurring from the atomic to micron scales. To predict these intricate interactions is a difficult task and has been a long-term effort for **Professor Nikolas Provatas**, theoretical physicist and director of the High-Performance Computing Center at McGill University. His group has created new simulation model techniques to understand exactly what happens during the formation of a material. This method of exploration is cheap and can significantly quicken discovery times by predicting targeted experiments for laboratory development.

Materials science is at the core of modern technology. Now ubiquitous devices such as laptops, tablets, or smart phones, rely on small chips to process information. Without scientific breakthroughs in the field of materials science, these chips would not exist, and neither would our relied-upon devices. The growing demand for new products generates a growing demand for new materials with improved properties, to be used in everyday applications. But the processes for developing these materials are extremely complicated and difficult to understand. When different types of elements are combined to make a new structure, and therefore a new material with different properties, the outcome is unknown: the system may not be stable or exhibit the desired property. The final result depends on interactions occurring at small length scales that are not easy to visualise or access experimentally.



A crystal growing in a liquid during solidification. This image captures the rich tapestry of patterns at the microstructure scale. It is simulated with a phase file model.

Professor Nikolas Provatas, from McGill University, leads a team of scientists that try to elucidate the processes that occur at multiple scales during material growth. The group specialises in the development of a new class of microscopic models that, with the aid of High-Performance Computing (HPC) simulations, will improve understanding of the underlying process mechanisms during material development. These models could enable prediction of novel materials and their properties, which depend on the material growth conditions. For example, when rapidly cooled, a material may develop voids and cracks at the micrometre domain which result in it being too fragile for engineering applications. In work funded by both industry and the Canadian government, Dr Provatas aims to explain why some materials behave differently to others. This is a crucial question to answer if we are to create new materials with desired properties such as increased strength or improved electrical conductivity, to name a few.

WHY SIMULATIONS?

Metal alloys belong to a class of materials that contains metals and several other elements. A notable example is steel, a combination of the elements iron and carbon. The development of a new and more efficient way to manufacture steel revolutionised the construction industry. Nowadays, various

The team use computer simulations to determine the conditions under which a specific type of material can form

Graphene has a two-dimensional structure with atoms arranged in a hexagonal pattern.

Inset shows graphene sample simulated with an XPFC model that shows the structure of defects.

industries, particularly aerospace and military, have created an increased demand for new materials that exhibit enhanced properties. For example, high-speed airplanes require materials that are tolerant to extreme temperatures and resistant to corrosion.

When building a new material, there are endless possibilities: multiple elements can be employed in different combinations and using different processes. This makes for a costly, time-consuming research effort which cannot account for all possible combinations of materials and processes. But what if we could explore and synthesise new materials virtually, just by defining input parameters in a computer model?

Dr Provatas' group works at the interface of materials science, condensed matter physics and computer modelling. They focus on using computer simulations to determine the conditions under which a specific type of material can exist. Often, such conditions can involve various mechanisms occurring during solidification. Solidification is the process by which a liquid changes into a solid, by varying conditions such as temperature or density. While this is still difficult to achieve, new models and high computation power have led to advances in simulations. The group's work has started to shed light on the various mechanisms responsible for materials' evolution at the critical microstructure domain.

MODELLING USING HIGH PERFORMANCE COMPUTING

One of the most important steps in performing computer simulations is associated with the length scales involved. Dr Provatas' team has made significant contributions both to the micrometre and nanometre scale domains. Firstly, at the micron scale domain, the adaptive-mesh refinement technique (termed "AMR") is used to resolve models. What is interesting about this technique is that it selects the levels of precision dynamically in a simulation. It will focus only on certain areas that require precision. This allowed the team to investigate new insights such as how matter selects its length scale in the micrometre regime. The outcome of these studies is crucial as it directly relates to the manufacturing process of many metal alloys.

These models could enable prediction of how novel materials and their properties depend on their growth conditions

On the other hand, different types of microscopic models have been developed to predict interactions between the atomic and micrometre scale. The advantage of using these types of models (termed 'XPFC'), is that many microstructure phenomena can be modelled that simultaneously involve atomic scale effects. This involves, for example, phenomena associated with two-dimensional materials such as graphene. Dr Provatas' group also pioneered using these models to explain how the process of nucleation (synthesis) of solid nanoparticles in solution works, and how defects facilitate particle nucleation in alloys.

THE IMPORTANCE OF THE RESEARCH

Professor Provatas' research has shown that it is possible to understand important processes responsible for developing new materials. Molecular dynamics models are the usual method of choice for investigating precise properties at the atomic scale, but they are typically not able to access time scales relevant to experimentally obtained results, correlated to manufacturing processes. The researchers believe that their models could compliment molecular dynamics approaches to assist the metal alloy industry in finding the appropriate routes for producing low price materials with properties that would outperform the state-of-the-art materials that are used today.

Currently, there are various factors that affect the numerical simulations. Most of them are related to the use of the mathematical appropriate model. In some instances, the model can be a combination of two different models. The first will be used to pre-calculate output data. In turn, these can be used as input parameters in the second model. With this approach it is possible to arrive at more reliable results and predict materials' properties. This is an approach being used by Dr Provatas, for example, to study Hot Cracking Susceptibility of metal alloys (the tendency of a material to form cracks under extreme cooling in 3D laser printing).

Dr Provatas' team expects that the models they use will be improved with time. Before any improvement the team will test its ability to predict experimentally measurable quantities. If the predicted values deviate from the experimental values, then the model will undergo modifications to include further complex processes. New composite models could also arise from the combination of two different models. The most important part of the simulations is to retain the salient physics while being simple enough to deploy on fast running algorithms. This will pave the way in understanding the main processes responsible for material development and will be a strong industrial asset for future manufacturing.

Q&A

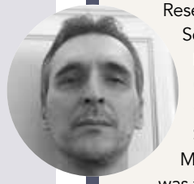
What makes your models better than the already existing molecular dynamics models?
Our models are actually connected intimately to molecular dynamics models. Where they differ is that they retain only the salient atomic scale features that are required to explain many emergent material properties, while washing out others that occur on too short time scales. This strategy allows us to be able to access experimentally relevant time scales.

Why is it difficult to predict a material's structure with a good degree of accuracy?
There are too many variable and processes interacting in unknown ways.

Why is such intense computation power required in the simulations?
Matter is comprised of an incredibly large number of atoms that co-interact with each other. Our models simulate equations that play out the physics of many millions of interacting atomic-scale regions and evolve these regions (and their interactions) one tiny time step at a time. As a result, immense computer power is required to compute all these interactions at each time step, and a large computer memory (100s of GB per file sometimes) is required to store this information over the many millions of time steps that represent a material's path in time.

Do you think your models will lead to the prediction of any possible material structure in the future?
Yes, we are presently collaborating with about three projects which aim to develop a know-how on what process will lead to improved strength in 3D laser printing of metal alloys.

How do you see the field progressing in ten years' time?
With the combination of more cost-effective cloud-based multi-processor computing, the ability to process and mine large sets of computed and experimental data, and the advance of improved mathematical models that contain richer physics of internal processes going on in matter, I believe that groups like ours will be able to predict pathways to advanced materials effectively, thus reducing the idea-to-innovation time for new materials in unprecedented ways.



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Detail

RESEARCH OBJECTIVES

Professor Provatas uses High Performance Computing to better understand the structure and properties of materials.

FUNDING

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COLLABORATORS

Professor Provatas acknowledges the invaluable contributions of his collaborators and students, with specific mention of **Drs Nana Ofori-Opoku** and **Sami Majaniemi** and **Professor Ken Elder**.

BIO

Nikolas Provatas is a professor of physics at McGill University, holds a Canada Research Chair (Tier 1), and is the Scientific Director of the McGill High Performance Computing Centre. From 2001 – 2012, he was a professor of Materials Science and Engineering at McMaster University. In 2016 he was awarded the Metallurgical and Materials Society (Met Soc of CIM) Metal Physics Award.

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