Enter the flow state —

what the atomic world could teach us about the future of batteries and more

Project Leader: Professor Debra Bernhardt, Senior Group Leader/ARC Australian Laureate Fellow, The Bernhardt Group

Partner Institutions: University of Queensland
System: Setonix (Phase 1)
Areas of science: ATOMIC PHYSICS, Energy and Resources, Material Science, Visualisation

30
researchers and more working together

4
million dollars in funding

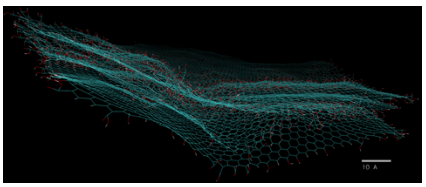
335,975
core hours in 2022

The Challenge

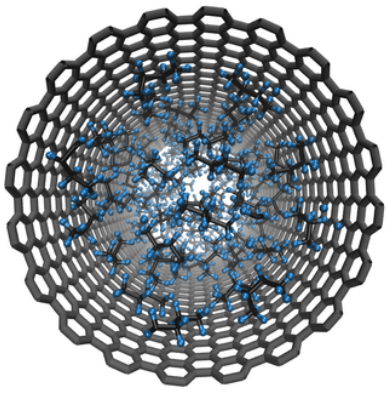
While scientists have long studied theories and algorithms on the simulation of molecular flow rates, this research is often not easily accessible to other researchers. Some questions on the behaviour of matter — such as how molecules behave under extreme conditions — is still unknown.

While they are studying the world at nanoscale, researchers require massive compute power to properly simulate the world at the scale and detail necessary for these breakthroughs.

Professor Bernhardt, research software engineer Dr Emily Kahl, and team, wanted to tap into higher computer power to more effectively, and quickly, simulate the world at nanoscale.



Visualisation of some graphene-oxide flakes clumping together, which is directly related to the project on flow-driven self-assembly we have with PaCER (credit: Dr Amy Geddes).



Butane flowing through a carbon nanotube. This is not directly related to the PaCER grand challenge, but is a cool visualisation of nano-confined flow, which is an important component of our research using nonequilibrium molecular dynamics (credit: Dr Emily Kahl and Michelle Hunter).

The Solution

Video games have long tapped into graphical processing units, or GPUs, to bring their virtual worlds to life and make them more realistic, something that requires significant computing power to achieve. With increasing focus on using GPUs for academic research, that same type of computing power has had a significant impact for researchers like Professor Bernhardt and Dr Kahl.

Just like creating realistic water in video games, the team are able to tap into the modern GPU clusters on Pawsey's Setonix HPC to simulate, study and research how different atoms and molecules interact at an unprecedented scale at higher speed yet a fraction of power use. For instance, they can better understand how different types of 2D materials like graphene, filter out different molecules, and ultimately determine which types of material are better suited for real-world applications like seawater desalination.

The new architecture of Setonix will enable Professor Bernhardt and Dr Kahl to scale up their projects to study systems much larger than before. The simulation of molecular dynamics can easily result in hundreds of millions of patterns with Setonix's increased computing power allowing for calculations to be done more quickly.

Because they're faster, the team can operate more simulations with the same research funding, enabling faster and more discoveries. Access to a larger scale supercomputer also allows the team to simulate systems and processes that would be completely inaccessible for smaller computers.

While high-performance computing algorithms often require complex development pathways and unique tools, Professor Bernhardt and Dr Kahl have entered the Pawsey Centre for Extreme Scale Readiness (PaCER), a program designed to help computational researchers prepare for the next era of supercomputing. Through this, the team have been able to optimise their algorithms and workflows to be used on Setonix more effectively, helping them to study systems that were inaccessible previously , as well as complete their project faster.

The Outcomes

With Setonix, Professor Bernahrdt and Dr Kahl are hoping to unlock many of the mysteries we still face on how the world works at an atomic level. By understanding and developing new molecular structures, the research could help create new filtration systems to enable accessibility to clean water more widely and new battery types that ultimately fuel our homes, cars and day-to-day lives.

Importantly, Professor Bernhardt and Dr Kahl want to share their knowledge and findings with the broader research community to ensure the fundamental molecular simulations have the highest possible impact. With this in mind, the team are producing a plugin to enable their simulations to be used by more researchers in an array of areas and encourage widespread adoption in fields such as biomedical science, chemical engineering and materials science.