Grand Challenges

Numerical Relativity in the UK (UKNR)

Over the next five to ten years, UKNR will maintain and extend the UK's scientific leadership in gravitational wave science and support the UK's Science and Technology Framework by building the necessary software infrastructure to keep pace in a rapidly changing world

The Community

www.uknumericalrelativity.org

Numerical Relativity (NR) refers to the solution of Einstein's equations on a computer, and ranges from simple laptop calculations in spherical symmetry, to large-scale simulations that require several million core hours each. Simulations of orbits and the merger of black holes and neutron stars have played a central role in the breakthrough results in gravitational-wave astronomy over the last decade, including the dynamics of exotic objects and spacetimes and new areas of exploration in fundamental physics beyond general relativity. UKNR's vision is to bring together all NR groups within the UK to form a collaborative community with a shared vision and speaks with one voice. This community will be both inward looking and outward looking. For the former, UKNR will foster collaboration in code development/exploitation with code sharing and training and identify the UK's future digital infrastructure needs as a community. UKNR will survey the current and future global digital infrastructure landscape to formulate a UK-wide strategic plan for NR code development as they move into the exascale era.

The Challenge

Increasing the precision of numerical output to keep up with Big Data and development of new techniques that work beyond Einstein's theory

The detection of gravitational waves 10 years ago by the Laser Interferometer Gravitational Observatory (LIGO) heralded a golden age of gravitational wave physics, allowing us to probe hitherto unreachable regimes of fundamental physics such as the nature of gravity, black holes and the origins of the Big Bang. To make these discoveries requires precise theoretical predictions, but since the Einstein equations are famously intractable analytically, NR is key to solving the Einstein equations and making theoretical predictions. As major participants in many international multi-billion-pound experiments with a legacy of gravitational breakthroughs, and scientific leadership in numerical relativity, the UK plays key roles in this worldwide endeavour to understand the nature of our universe. There are two major scientific challenges in numerical relativity today: increasing the precision of numerical output to keep up with the inevitable deluge of high precision data from future detectors, and the development of new methodologies to compute

predictions of fundamental physics beyond Einstein's theory. To meet these challenges requires significant breakthroughs in the development of computational techniques and compute infrastructure.

A major strength of UKNR is its scientific nimbleness, responding quickly and decisively to the rapidly changing digital infrastructure landscape and constantly shifting scientific frontiers. UKNR code developers led the international NR community in transitioning from CPUs to GPUs and pioneered the first codes to probe theories beyond Einstein's and other new physics. In parallel, we have played a key role in developing the flagship waveform models that have been used in all LIGO-Virgo-KAGRA observations to date. As the international scientific community braces itself for a momentous few decades of discoveries with gravitational wave astronomy, maintaining and extending this scientific lead is key to ensure that UK science remains at the forefront. Beyond the scientific challenges outlined in the UK Compute Roadmap, creating a sovereign digital infrastructure is key to remain resilient in the face of global instability. While scientific computing often relies on open-source libraries, many of these libraries were developed in non-UK national labs. The NR community is no different as almost all their codes rely on extensive libraries that they do not fully control. Finally, and perhaps most importantly, the dizzying rise of AI has significant implications across all scientific disciplines, and NR will be no exception. While standard neural networks have been applied in data analysis in astrophysics for many years, its use in NR is nascent. This provides a huge opportunity for UKNR scientists to assume leadership in this field.

The Solution

Achieving high precision with less, integrating AI and machine learning methodologies into NR and achieving software sovereignty

Over the next decade, UKNR aims to maintain and extend their international lead in the development of cutting-edge numerical relativity codes, building on three interconnected principles: achieving high precision with less, integrating AI and machine learning methodologies into numerical relativity and achieving software sovereignty.

Achieving high precision with less: UKNR will reach the required precision for the next generation gravitational wave detectors by adopting more energy efficient technologies (e.g. our recent transition from CPUs into GPUs), seeking efficiency gains from refining present computational methodologies (such as factoring codes to take advantage of much lower energy single precision compute units), and building completely new numerical methodologies such as the Physics-Informed Neural Networks (PINN) to allow upscaling of low resolution simulations.

Incorporating AI and machine learning into numerical relativity: UKNR will leverage the rapid advances of AI and machine learning techniques to achieve precision goals, solve presently intractable scientific problems, and improve their code development workflow. However, achieving consistency, reliability and

explainability is a key requirement for any successful integration of AI into numerical relativity. UKNR intend to collaborate with AI and machine learning experts to achieve this goal.

Achieving software sovereignty: In an increasingly uncertain world, it is crucial that the UK achieves digital sovereignty. In particular, the UK needs to be at the forefront of code development, steering the direction of research, and becoming independent of hardware developments -- a goal that aligns with EU initiatives around homegrown hardware from the ARM and RISC-V ecosystem. In the context of NR where many codes still rely on non-UK compute libraries (e.g. the US ECP-based AMReX), UKNR plan to build a UK base capability to develop our own compute libraries for adaptive mesh finite difference solvers, seeking out collaboration with other CoSeC CCPs which require such technology.

The Outcome

To maintain and extend UK's scientific leadership in the present golden age of gravitational wave science

Over the next 10 years, UKNR aims not only to maintain the UK's scientific leadership in the present golden age of gravitational wave science, but to extend it. It will support the UK's Science and Technology Framework by building the necessary digital software infrastructure and developing the human capital, keeping pace in a rapidly changing world and digital landscape. The coalescing of the UKNR as a community has opened multiple avenues of code sharing and consolidation, such as the joint use of underlying libraries. This consolidation is a force multiplier within the community. Participating in the CoSeC framework has provided, and will continue to provide, the opportunity to contribute and benefit from cross-cutting knowledge transfer, and the community fully intends to participate in the process to make the UK HPC community more than the sum of its parts.

More Information

CoSeC
www.CoSeC.ac.uk
CoSeC@stfc.ac.uk

UKNR
www.uknumericalrelativity.org