UK Research and Innovation

Met Office

UK Atomic Energy Authority

ExCALIBUR

Exascale Computing ALgorithms & Infrastructures Benefiting UK Research (ExCALIBUR)

ExCALIBUR is a UK research programme that aims to deliver the next generation of high-performance simulation software for the highest-priority fields in UK research. It started in October 2019 and will run through until March 2025, redesigning high priority computer codes and algorithms to meet the demands of both advancing technology and UK research.

excalibur.ac.uk

ExCALIBUR is led by:

The Met Office and the Engineering and Physical Sciences Research Council (EPSRC) along with the UK Atomic Energy Authority (UKAEA) and UK Research and Innovation (UKRI) research councils; including the Natural Environment Research Council (NERC), the Medical Research Council (MRC) and the Science and Technologies Facilities Council (STFC).

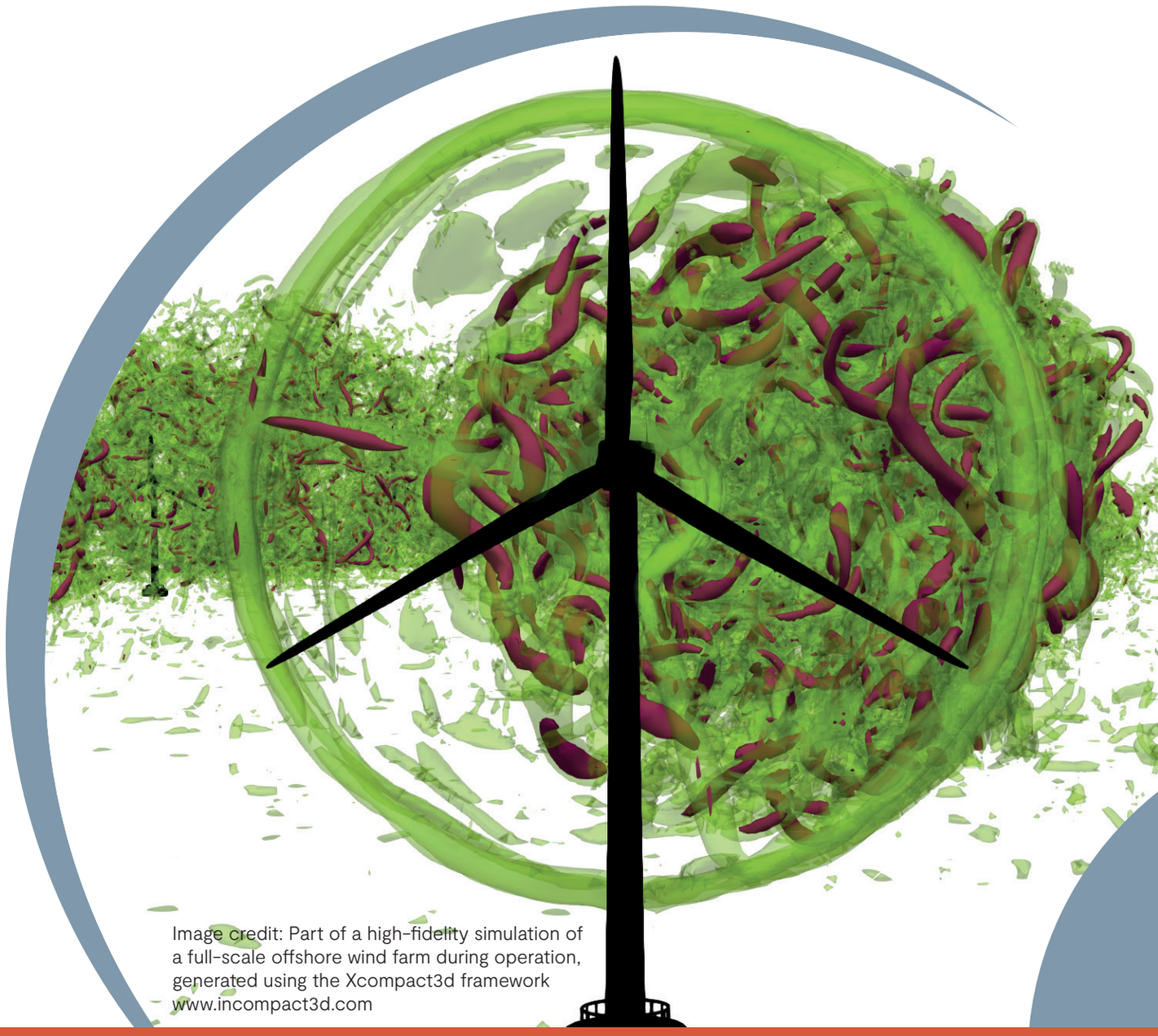

Image credit: Part of a high-fidelity simulation of a full-scale offshore wind farm during operation, generated using the Xcompact3d framework www.incompact3d.com

EXCALIBUR 10

Radical changes to supercomputer architectures are on the horizon. To continue to make scientific advances on some of the most challenging physical problems, such as weather forecasting, engine design, astrophysics, particle physics and fusion energy, it is essential that the UK fully harnesses the power of those supercomputers.

ExCALIBUR is addressing this challenge by redesigning high priority computer codes and algorithms, keeping UK research and development at the forefront of high-performance simulation science.

Its Hardware and Enabling Software (H&ES) programme provides early access to novel hardware and software technologies that may play a part in future exascale systems and services. Researchers can use the H&ES testbeds to validate the portability and performance of their codes, and to explore the potential of new paradigms such as workflow offload to data processing units, or wafer scale computer engines.

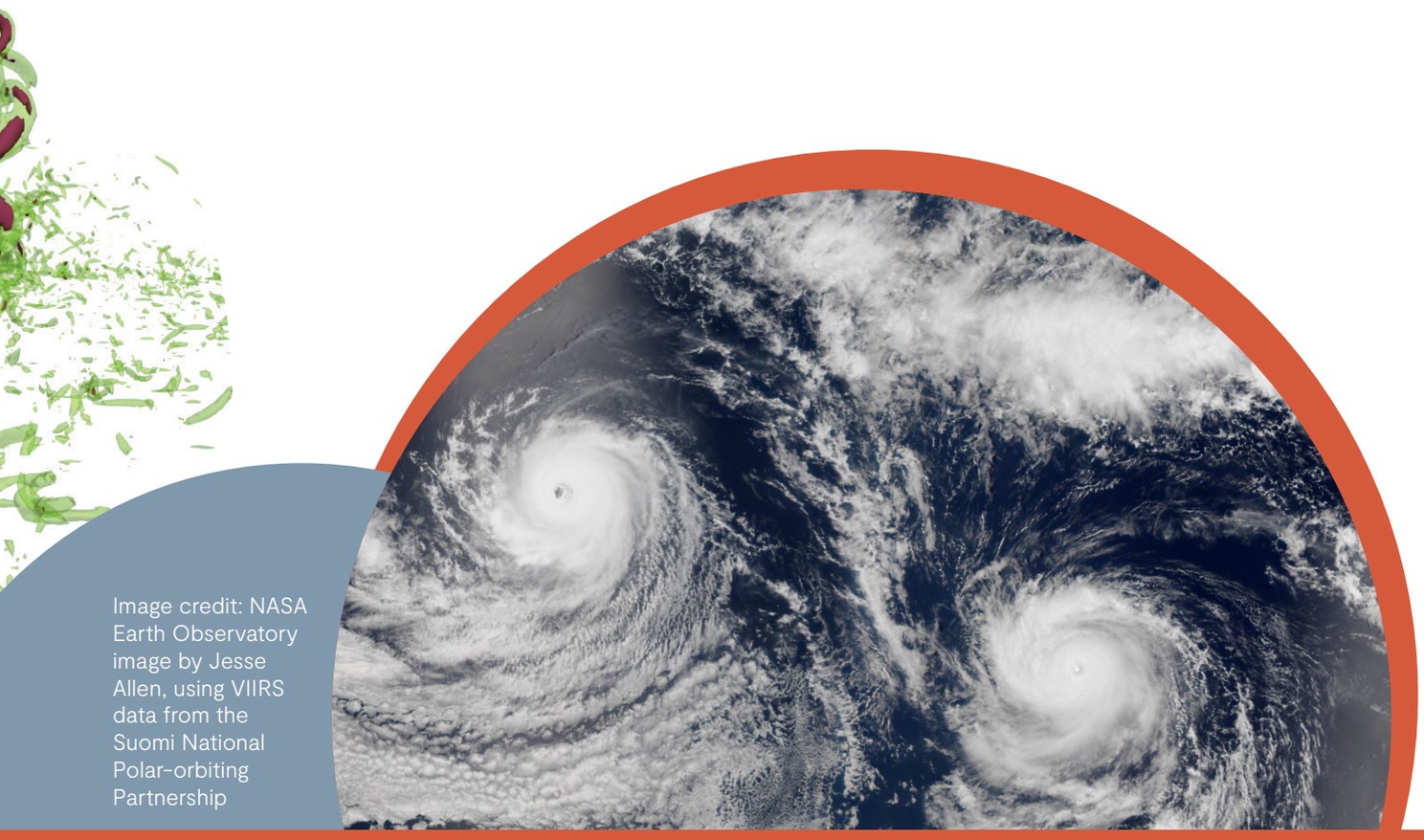

Image credit: NASA Earth Observatory image by Jesse Allen, using VIIRS data from the Suomi National Polar-orbiting Partnership

ExCALIBUR is built on four pillars:

Separation of Concerns

The algorithms that encapsulate the mathematics and physics of the problem are separated from the computational science of their implementation.

Co-design

Holistic design of the software of the entire simulation system involving innovative collaborations between mathematicians, domain scientists and computational scientists.

Data Science

Research to design new workflows adapted to managing & analysing vast volumes of data ingested and produced by simulations.

Investment in People

Improved career development driven by professional forward-looking approach to scientific software design of simulation codes.

ExCALIBUR Science Use-case Plans

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The UK has a highly skilled and growing Research Software Engineering (RSE) Community. However, at this critical moment in the development of large-scale supercomputing there is significant growth in the demand for both the skills and size of this community.

ExCALIBUR will provide training (encompassing both technical and professional development) to enable the UK Research Community to embrace the acceleration in research enabled by Exascale Systems.

There will be a strong focus on the development of activities to facilitate both the cross fertilisation of knowledge and the movement of people within and academia and industry.

A unique aspect of the project is that every component has a designated Knowledge Exchange Coordinator, which has led to the formation of a dedicated knowledge exchange network throughout the ExCALIBUR programme.

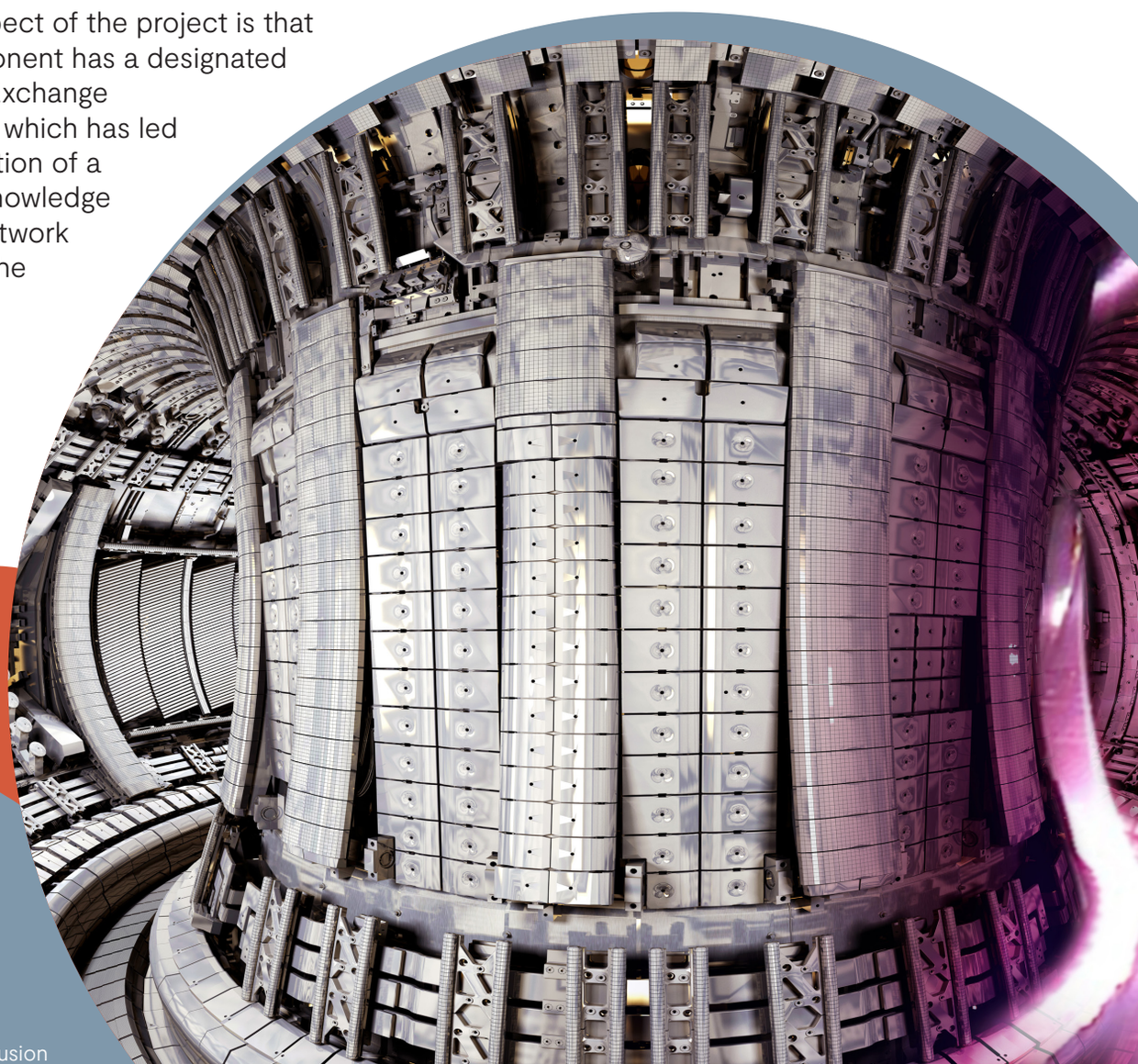


Image credit: EUROfusion

Key UK-related ExCALIBUR Software

uDALES
(urban Dutch Atmospheric Large Eddy Simulation)
Large-eddy-simulation software for urban flow, dispersion and microclimate modelling.
https://github.com/uDALES

EasyVVUQ
(Easy verification, validation and uncertainty quantification)
EasyVVUQ is a Python library designed to facilitate verification, validation and uncertainty quantification (VVUQ) for a wide variety of simulations. It was conceived and developed within the EU funded VECMA (Verified Exascale Computing for Multiscale Applications) project.
https://easyvvuq.readthedocs.io/

SENGA+
SENGA+ is a compressible three-dimensional Direct Numerical Simulation code written in FORTRAN, and is one of the major workhorses in the UKCTRF community.
https://www.ukctrf.com/index.php/senga/

Xcompact3d
Xcompact3d is a suite of high-order finite-difference flow solvers dedicated to the study of turbulent flows. Incompact3d is the flagship solver of the ecosystem Xcompact3d and is designed to study incompressible flows.
https://www.incompact3d.com/

SWIFT
(SPH With Inter-dependent Fine-grained Tasking)
SWIFT is a hydrodynamics and gravity code for astrophysics and cosmology.
https://swift.dur.ac.uk/

DualSPHysics
DualSPHysics is based on the Smoothed Particle Hydrodynamics model named SPHysics (www.sphysics.org). The code is developed (GNU Lesser General Public License) to study free-surface flow phenomena where Eulerian methods can be difficult to apply. DualSPHysics is a set of C++ and CUDA codes designed to deal with real-life engineering problems.
https://dual.sphysics.org/

Nektar++ SPECTRAL/HP ELEMENT FRAMEWORK

Nektar++ is a tensor product based finite element package designed to allow one to construct efficient classical low polynomial order h-type solvers (where h is the size of the finite element) as well as higher p-order piecewise polynomial order solvers.
https://www.nektar.info/

MUI

(Multiscale Universal Interface)

The Multiscale Universal Interface (MUI), provides a C++ header-only implementation that is based around the MPI Multiple-Program Multiple-Data (MPMD) paradigm using a particle-based approach for discretisation and quickly embeds into new and existing codes. It enables either tight or loose coupling of the physics of a problem by creating an interface between software.
https://mxui.github.io/

FEniCSx

(Finite Element ni Computational Software)

FEniCSx is a popular open-source computing platform for solving partial differential equations (PDEs). FEniCSx enables users to quickly translate scientific models into efficient finite element code.
https://fenicsproject.org/

ExaHyPE

(Exascale Hyperbolic PDE Engine)

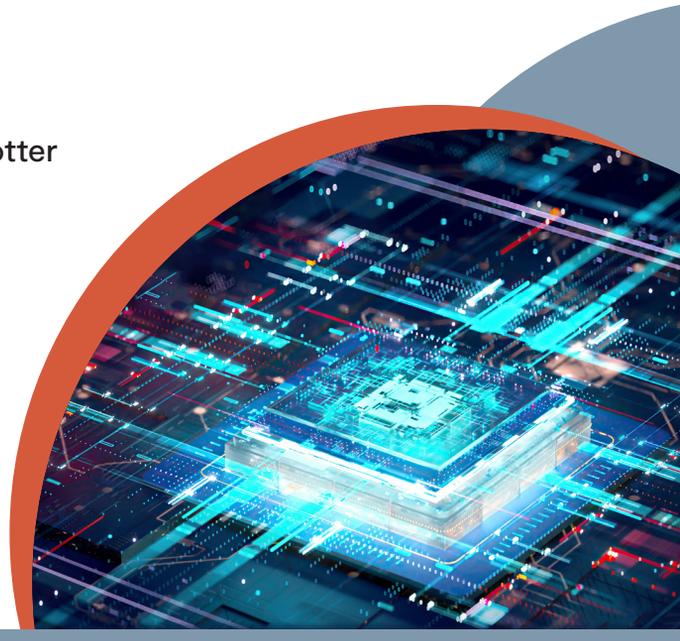
ExaHyPE is an open source simulation engine to solve hyperbolic PDE systems using high-order ADER-DG discretisation.
http://www.exahype.org

Otter

A data-driven taskification tool.
https://github.com/Otter-Taskification/otter

Psyclone

A code generation system developed to support domain-specific languages (DSLs) for finite element, finite volume and finite difference codes.
https://psyclone.readthedocs.io/en/stable/index.html



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