
Science and
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Facilities Council
Hartree Centre
Welcome
Vassil Alexandrov
STFC Hartree Centre, CSO

What is the Hartree Centre?

- STFC’s high performance computing, data analytics and AI technology centre
- Provides businesses (and applied researchers) with collaborative access to powerful technologies, facilities and scientific computing expertise
- Based at Sci-Tech Daresbury in North West England
- Around 100 staff

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Hartree Centre

The Mission of the Hartree Centre

“Transforming UK industry by accelerating the adoption of high performance computing, high performance data analytics and cognitive technologies (AI, ML, DL) through (industry) challenge-led research and innovation”

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Network of expertise

Government & public sector

Local business networks

Technology partners

Universities

Academia

UK Research and Innovation

LCR4.0 START

IBM

HALTON BOROUGH COUNCIL

Cheshire & Warrington CW4.0

SIEMENS

Science and Technology Facilities Council

Horizon Europe

NVIDIA

UK Atomic Energy Authority

Sci-Tech DARESBURY

Atos

International research communities

Liverpool City Region Local Enterprise Partnership

VEC VIRTUAL ENGINEERING CENTRE

intel

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Our platforms

Intel Platforms

Bull Sequana X1000 (4.3PFlop/s, ~80000 cores)
Lenovo NeXtScale | 8,192 cores
Lenovo System x iDataPlex system | 2048 cores
Intel Xeon Phi | Knight's Corner
IBM big data analytics cluster | 288TB

IBM Data Centric Platforms

IBM Power8 + NVLink + Tesla P100
IBM Power8 + Nvidia K80

JADE – Oxford University

Tier 2 Regional Deep Learning Supercomputer
Atos Bull 22x Nvidia DGX1 – DL supercomputer

- 176 V100 GPUS, Deep Learning Frameworks
- In excess of 630,784 CUDA Cores

Atos Quantum Learning Machine (QLM)

Discovering and delivering next-generation algorithms for future quantum computers

Cloud Computing Platforms

We have access to multiple cloud vendor platforms. We are vendor agnostic, so can deploy to a variety of different cloud runtimes during and after projects. Post project, this can simplify handover of solutions into customer production environments.

Visual Computing Suite

Collaborative visual computing technologies enabling exploration of data analytics and computational modelling

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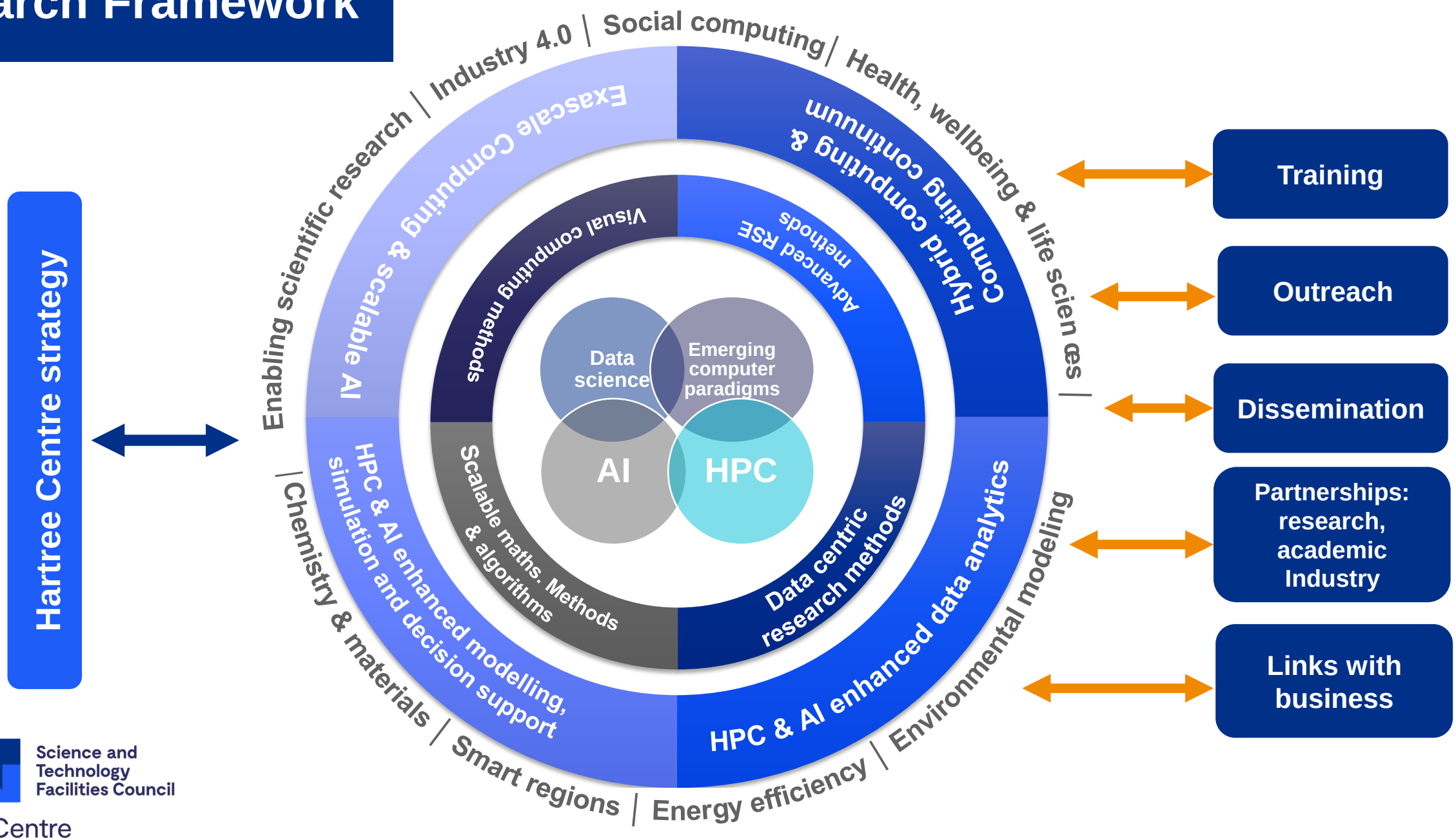
Research Framework



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Hartree Centre and the Hartree National Centre for Digital Innovation

2021: Hartree National Centre for Digital Innovation

Mission: Position the UK as a global leader in the applications of AI and HPC by industry.

- A five-year, £172M government investment which brings high-tech jobs and skills to the North West of England
- HNCDI will provide UK companies with access to leading edge super-computing and AI technology which can help them develop new products and processes
- Economic impacts will result from productivity uplifts and upskilled UK workforce in AI and computing technologies
- Support for companies of all sizes with regional partnerships to support SMEs

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Strategic R&D&Technology Areas for HNCDI

- **AI enhanced modelling, simulation and decision support**
  - Combining modelling and simulation with the latest developments in AI and machine learning in order to aid decision making for scientific and industrial challenges
- **AI enhanced data analytics**
  - Enhancing data analytics using the latest developments in AI and machine learning
- **Exascale and scalable AI**
  - Pushing the limits of computing and expanding the scale and scalability of AI
- **Hybrid computing and the computing continuum**
  - Exploring the integration of cloud, high performance computing and accelerators (e.g. GPUs, quantum) in a hybrid fashion

Thematic Application Areas

Hartree is looking to support digital innovation in the following thematic application areas with a sector based approach, underpinned by transferable technologies and skills.

Materials	Transport	Health, Wellbeing & Life Science
Environment, Energy and Smart Regions	Industry 4.0	Process Engineering

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Hartree National Centre for Digital Innovation

Help to realise the industrial, economic and societal potential associated with AI and digital technologies

Translate high performance and cloud computing, AI, quantum computing and capabilities associated with related technologies into scalable tools and techniques for industry.

Build widely adopted solutions to drive digital innovation

Accessible training and understanding	Translating research to generate solutions	Embedding AI and digital solutions	Driving future investment in key technologies

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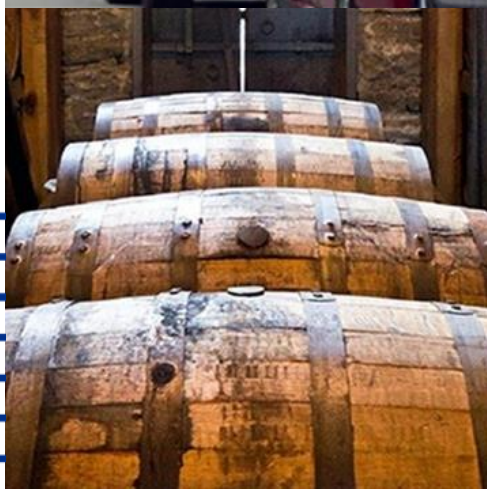
What does a typical project with the Hartree Centre look like?

- Addresses industrial & scientific, economic or societal challenges while advancing UK capabilities in digital innovation
- Leads to the development of new capability in the core technology and application areas
- Has strong engagement from external organisations



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Exascale Computing

Exascale Computing

- Work in partnership with ECP (Exascale Computing Project) – USA to advance the state-of-the-art
- Collaborate with UKAEA in the area of Fusion modelling and simulation at scale
- Collaborate with MetOffice in the area of performance portability
- Through partnership in several ExCALUBUR EPSRC projects work with partners to advance state-of-the-art in particular areas and domains.

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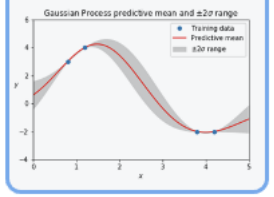
Collaboration with UKAEA

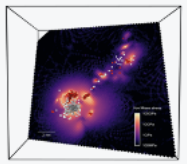
Fusion – a long established ‘exascale’ simulation challenge

For modelling plasma turbulence, designing materials and for Digital Twinning

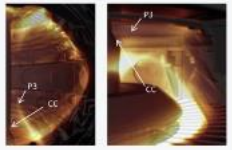
Emulators and UQ solutions for exascale era

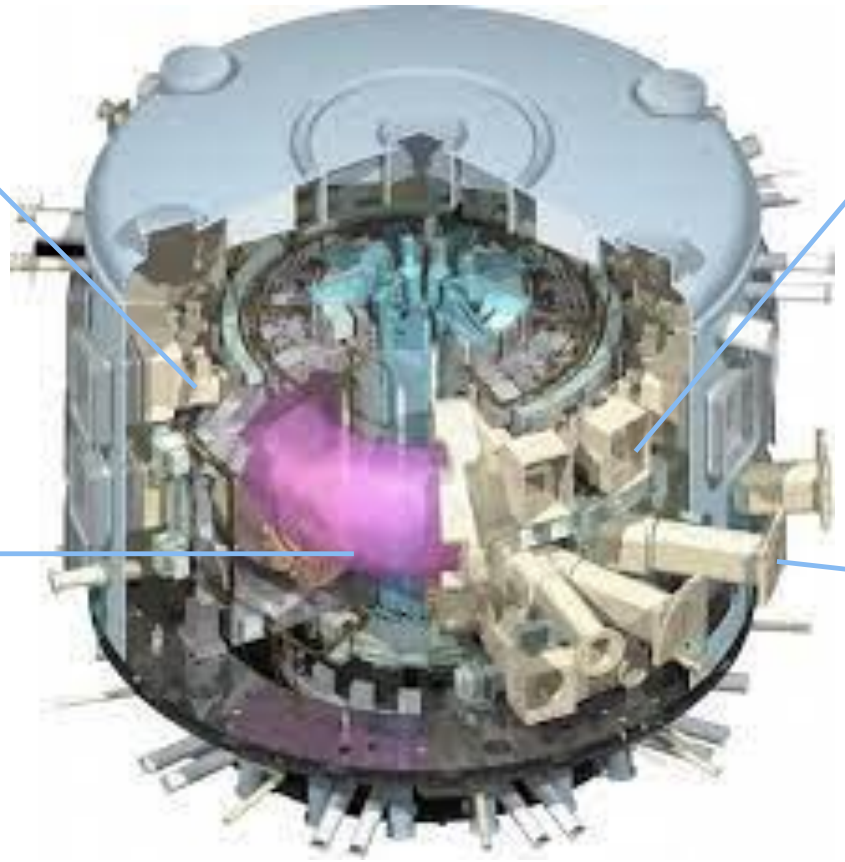


Exascale scalable stress-strain simulator

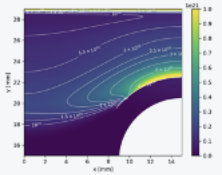


Modelling the complex physics of the plasma exhaust

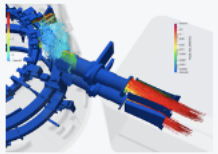




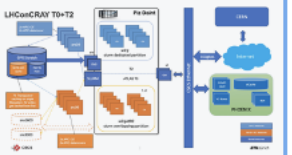
High fidelity model of Tritium retention & release



Exascale modelling of fast particle MHD



Big Data infrastructure for ITER era



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Dr. Rob Akers – UKAEA

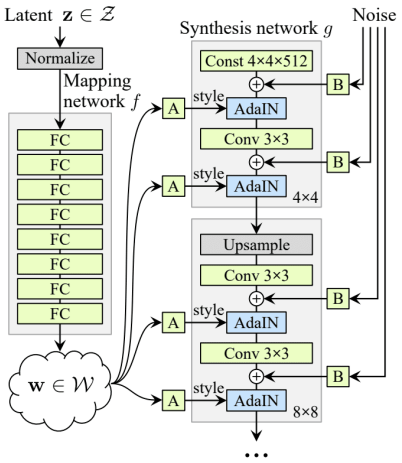
UK Atomic Energy Authority

Net Zero timeline dictates that we must design under uncertainty ‘in-silico’

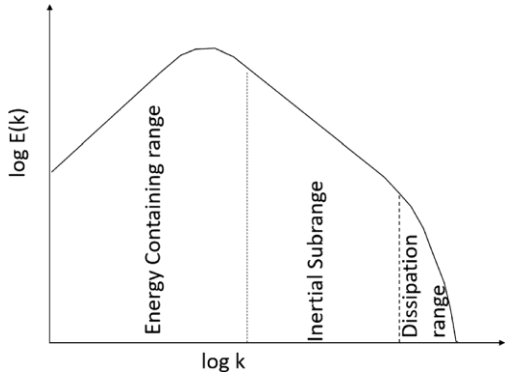
Turbulence with Style

Jony Castagna - Francesca Schiavello

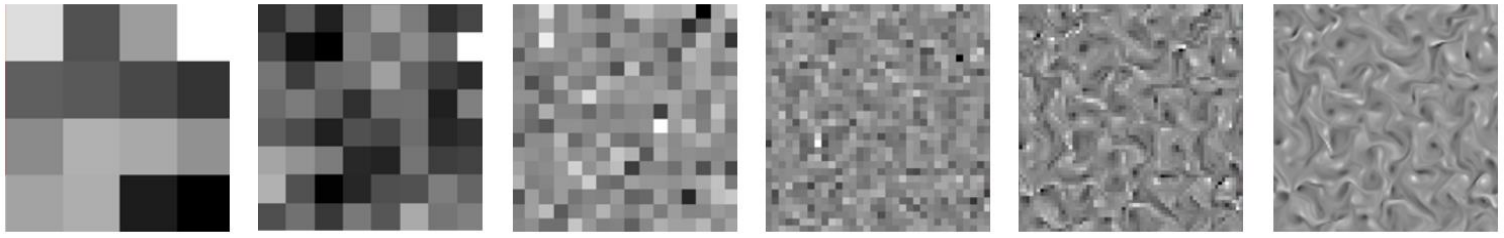
StyleGAN is a powerful Generative Adversarial Network (GAN) for face synthesis



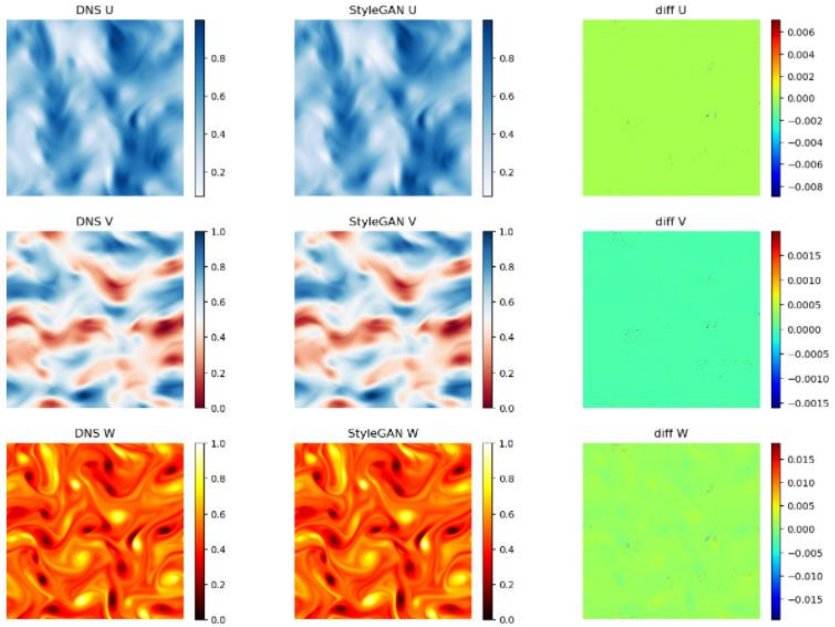
Kolmogorov energy spectrum



We use StyleGAN to learn the cascade of energy and reproduce isotropic turbulence



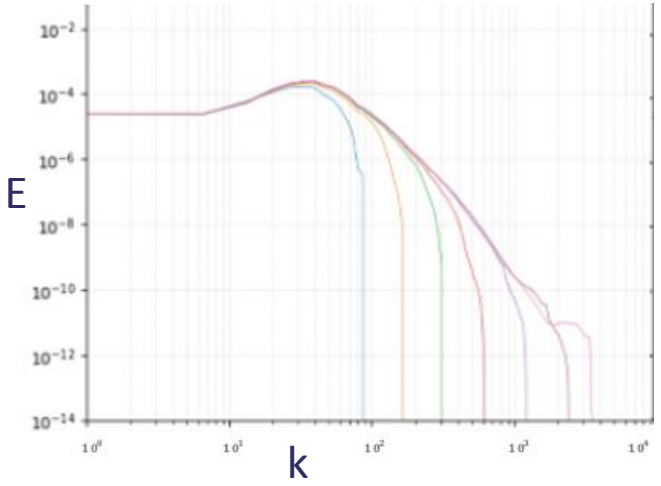
Preliminary results



MSE 0.006%

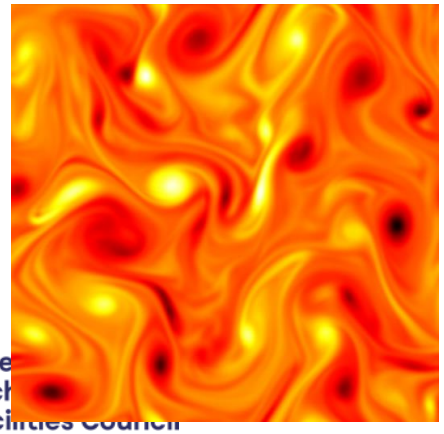
SSIM 0.993

- trained with 2625 DNS images of 2D-HIT
- 100k steps
- 11h on 1 GPU (V100)
- resolution 256x256
- filter at 32x32
- $Re_\tau = 60$, $t > 500\ \tau_e$

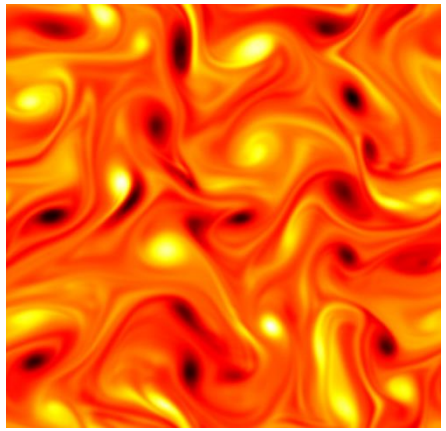


Match with Energy spectrum up to 10^{-10}

Trained on a single image



able to adapt to a different flow



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Collaboration with ECP

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Collaboration with ECP

Objectives:

- Develop and enhance further variety of hybrid stochastic/deterministic methods for Linear Algebra and integrate them into relevant ECP libraries
- Explore integration of ECP technology stack, particularly the Kokkos programming model.
- PSyclone is available on the Spack package manager.
- Share knowledge and best practices with the ECP partners.

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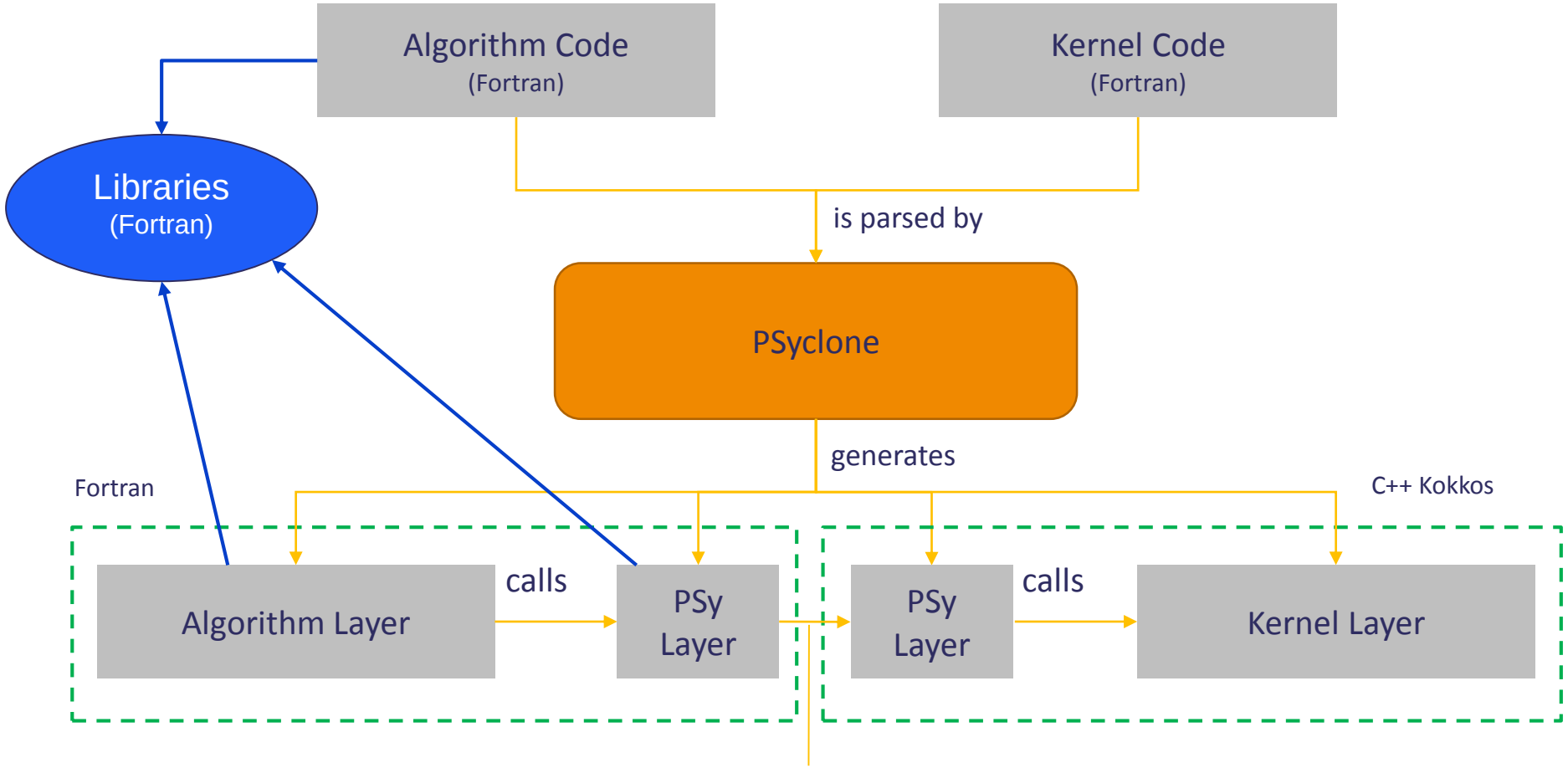
Initial exploration with Kokkos

- Fully integrate with Kokkos (adopt View containers)
  - Assume data duplication (Fortran Array <-> Views)
  - Use all Kokkos functionality.

- Use UnmanagedViews and Kokkos Fortran interface
  - Some Kokkos functionality like acceleration available but PSyclone still in charge of the data-layout.

- Use Kokkos with rawpointers from Fortran Arrays
  - No automatic device acceleration or data-layout abstraction.
  - We can still use Kokkos parallel execution model.

Plans for C++ frameworks



Prepare all needed functionality with raw pointers and function wrappers and use a single Fortran C_ISO_BINDING call.

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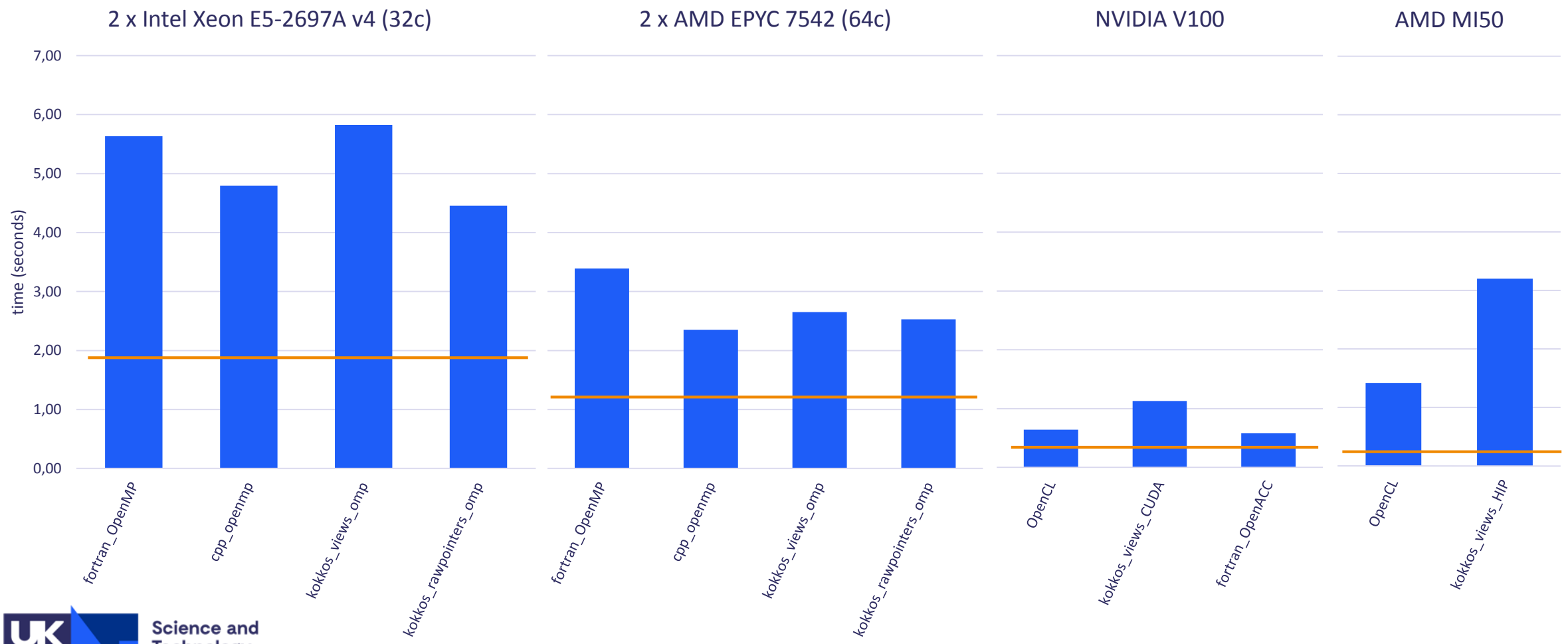
NemoLite2D manual implementations



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bandwidth roofline

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Collaboration with EXCALIBUR (NEPTUNE and other) projects

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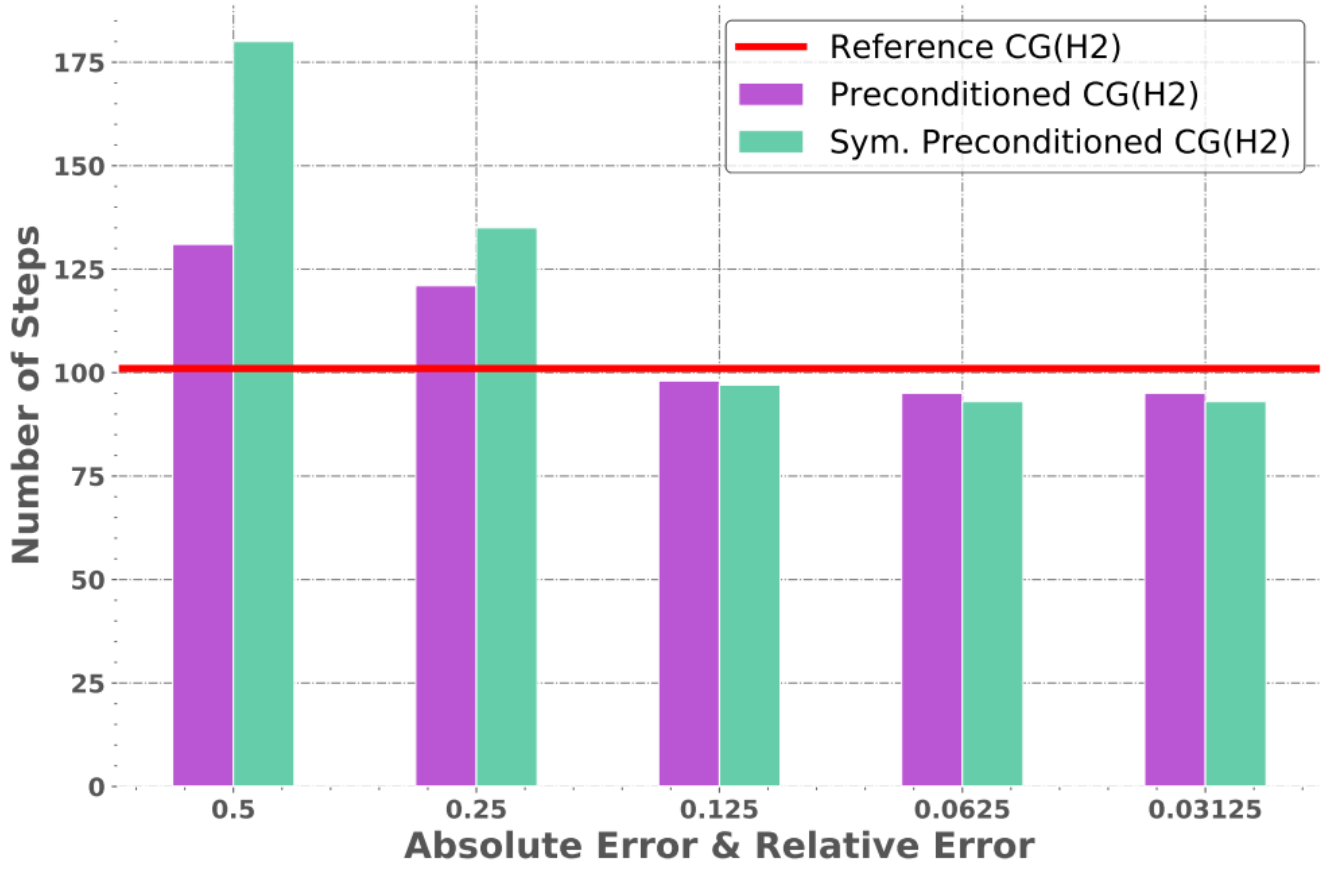
Set of matrices used

Matrix	Dimension	Non-zeros	Sparsity (%)	Type
circuit5M-dc	3,523,317	19,194,193	1.5×10^{-6}	symmetric
nonsym_r3_a11	20,930	638,733	0.15	nonsymmetric
sym_r6_a11	1,314,306	36,951,316	0.02	symmetric
H2hat	6,144	11,501,568	30.47	hermitian
H2	12,288	4,202,496	2.78	hermitian
NLD	8,192	24,576	4.66×10^{-2}	nonsymmetric

MCMCMI creates a non-symmetric preconditioner at very low precision may worsen CG convergence.



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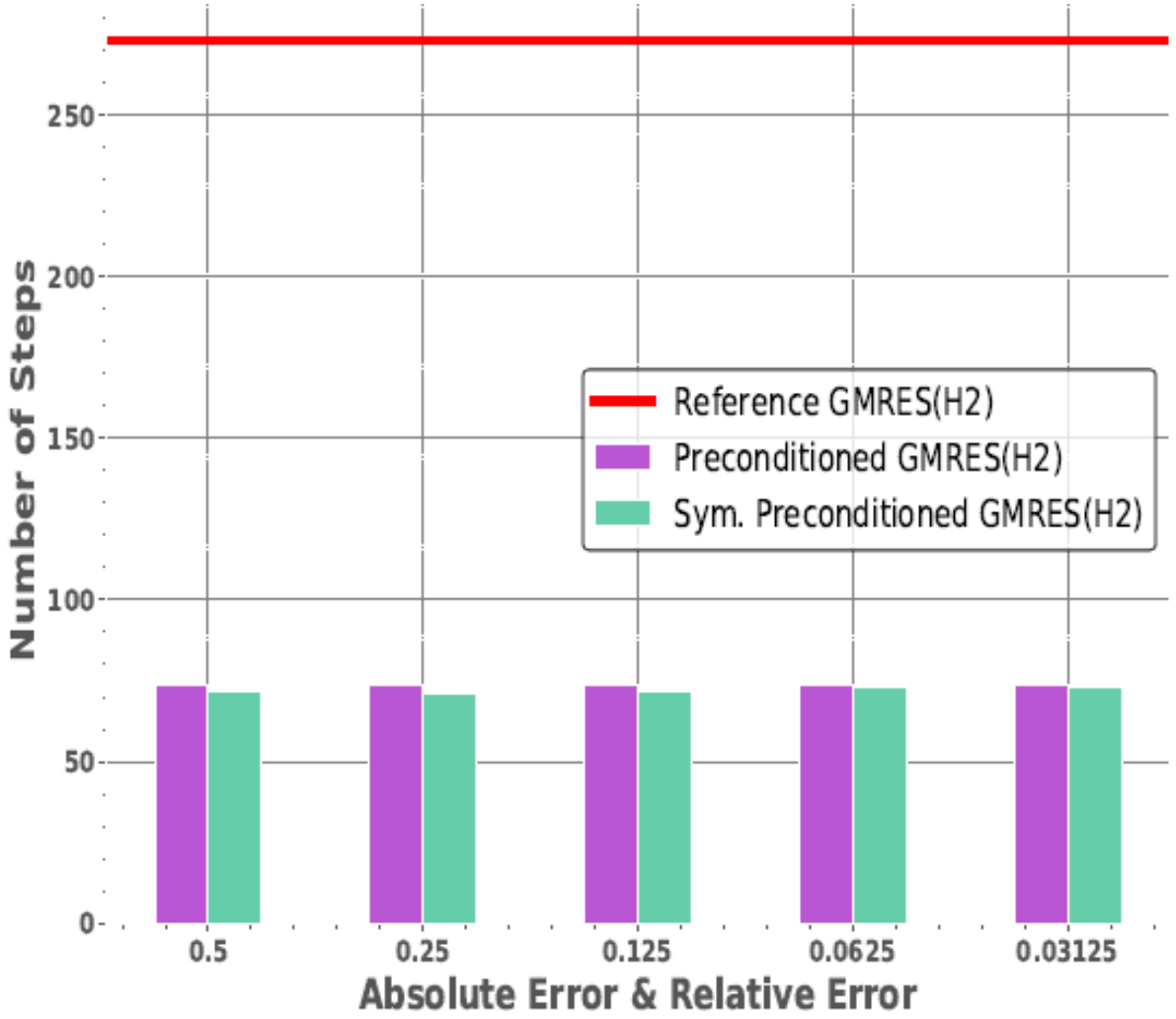
MCMCMI / GMRES hybrid approach for H2 matrices



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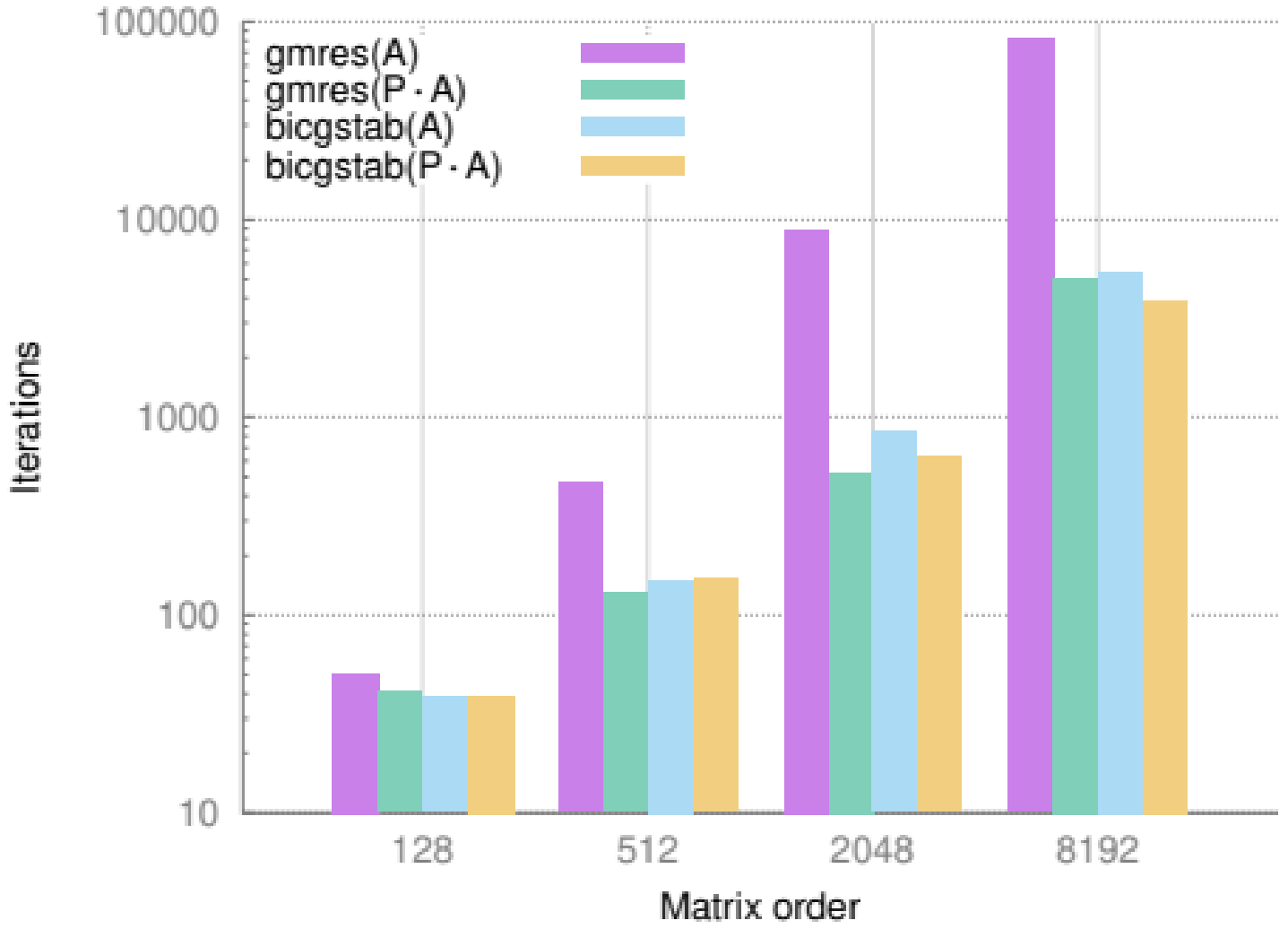
MCMCMI is effective in reducing the number of iterations for a non-linear diffusion problem



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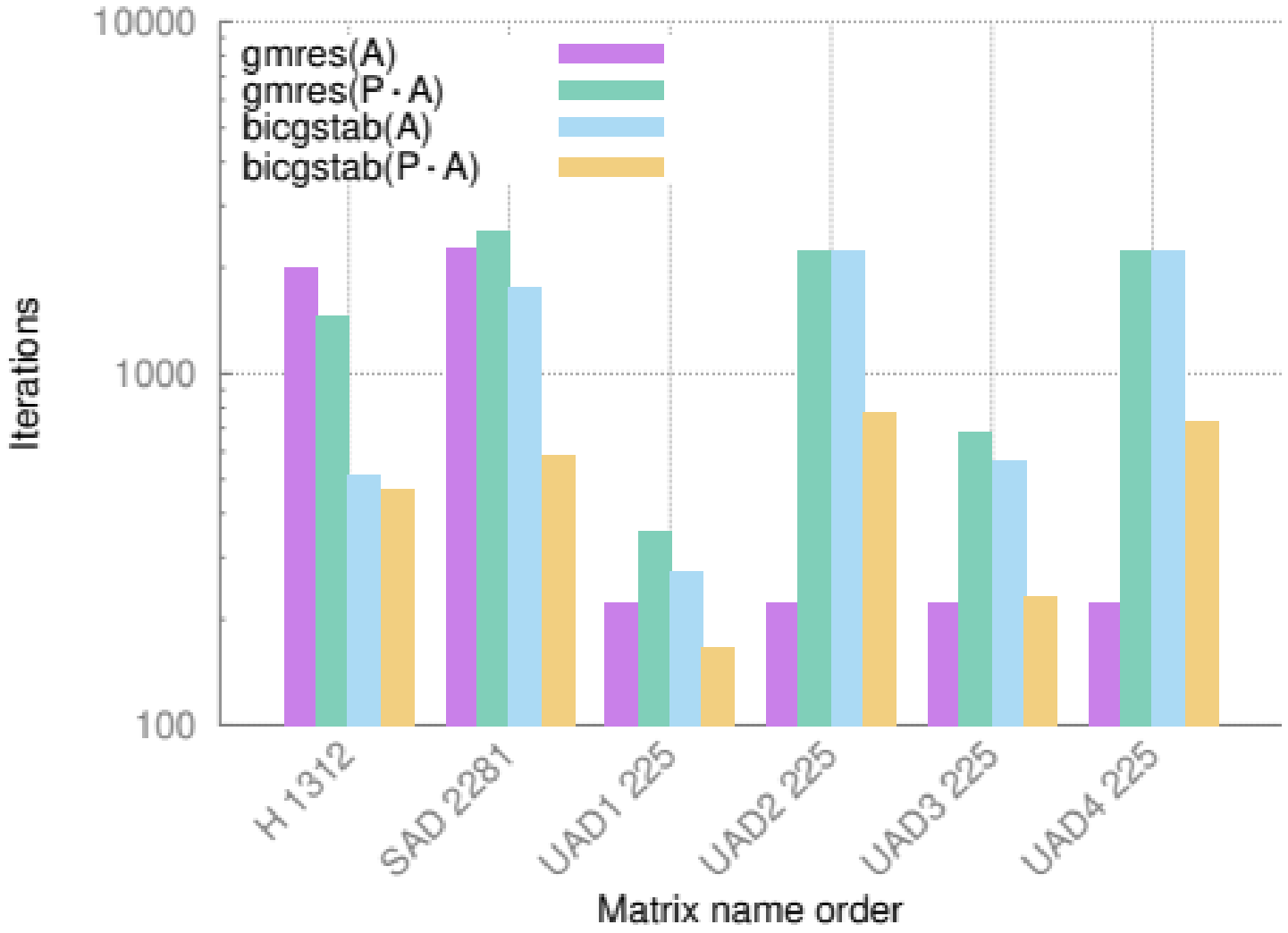
MCMCMI apparently more suitable in combination with BiCGstab than with GMRES for matrices considered



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Areas of Interests

- Performance portability
- Scalable AI – surrogate modelling, AI for Fusion, etc.
- General Inverse Problems
- Separation of concerns
- Applied to variety of application areas

Summary

- Fully engaged with ECP (Exascale Computing Project) – USA to advance the state-of-the-art – over areas of particular strong collaboration
- Established strong collaboration with UKAEA in the area of Fusion modelling and simulation at scale
- Enhanced the collaboration with MetOffice in the area of performance portability
- Through partnership in several ExCALUBUR EPSRC projects work with partners helped to advance the state-of-the-art in particular areas and domains.

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Collaboration with industry - selected case studies

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Case study

Computer aided formulation

Faster development process for products like shampoo, reducing testing

"The Hartree Centre's high performance computing capabilities help us achieve better design solutions for our consumers, delivered by more efficient, cost-effective and sustainable processes."

− Paul Howells, Unilever

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Unilever

Collaborative R&D

Case study

Forecasting energy use

South West Water manages waste water treatment
– each plant is a unique environment

Challenge: Forecast energy use for each plant, and make a fair comparison of different sites' efficiency

Solution:

- Machine learning model which allowed forecasting of energy consumption
- Time series techniques to extract long-term trends in energy use
- Metrics to help SWW make a fair comparison between sites.

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South West Water

python™

R

Big data analytics

Case study

Designing safer vehicles

Access to compute capability reduced time to run vehicle simulation models by 50%

“Access to high performance computing with the convenience of operating from our own office is a real game-changer, helping us meet customer cost and timescale requirements and enabling us to thrive in a global market.”

− Tim Williams, Simpact Engineering Ltd.

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simpact® superior impact solutions

Platform as a service

Case study

Code optimisation for aerospace engines

Codes for modelling component design made to run ~ 20% to 40% faster

“Working with the Hartree Centre, we have quickly made significant improvements to our code, delivering faster turnaround and more capability to our engineers.”

− Matthew Street, Rolls-Royce

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Rolls-Royce

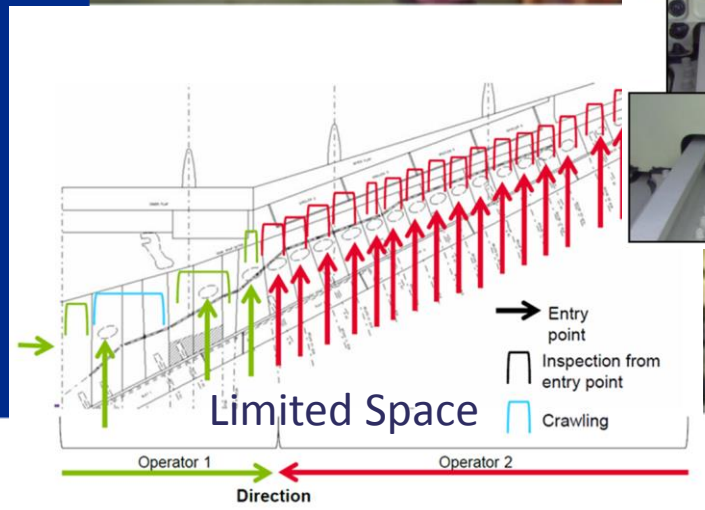
Collaborative R&D

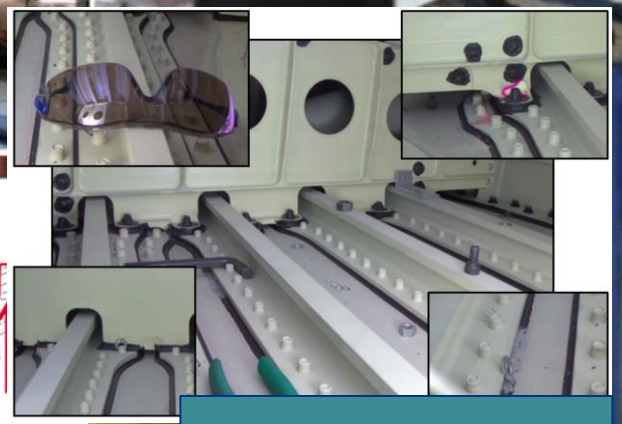
Case study

Airbus | Deep Learning for Wing Tank Inspection

Faster quality control process for wing tank inspection (A320 & A321)

- Check correct standard of: sealant, fasteners, paint, adhesion, liquids
- Detection of flaws: Missing/damaged sealant, excess paint, scratches and foreign objects (nuts, bolts, misc tools, swarf, safety glasses, wire, etc.)





Model Creation with >1000 Images

Train/Validate 80:20

Test Set >50 Images

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AIRBUS

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Questions?

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Thank you

Vassil Alexandrov

vassil.alexandrov@stfc.ac.uk

hartree.stfc.ac.uk @HartreeCentre STFC Hartree Centre hartree@stfc.ac.uk