

EXCALIBUR
10

BASE-II BLUEPRINTING AI FOR SCIENCE AT EXASCLE

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UK Research
and Innovation



UK Atomic
Energy
Authority

Scope

BASE-1 vs BASE-II

- BASE-I (Phase 1a), **Benchmarking** for AI for Science at Exascale
 - Very dense landscape
- BASE-II (Phase-II): **Blueprinting** AI for Science at Exascale
 - Aims to identify / develop reusable AI4S patterns / templates



AI Labs.tw



Alibaba



AMD



Andes Technology



Aon Devices



BAAI



Cadence



Calypso AI



Centaur Technology



Cerebras



Cisco



Code Reef



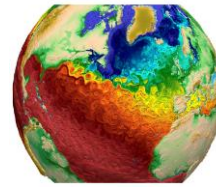
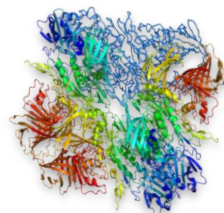
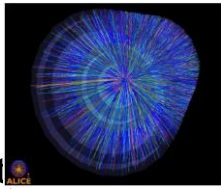
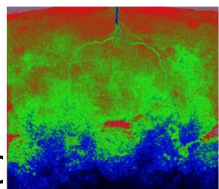
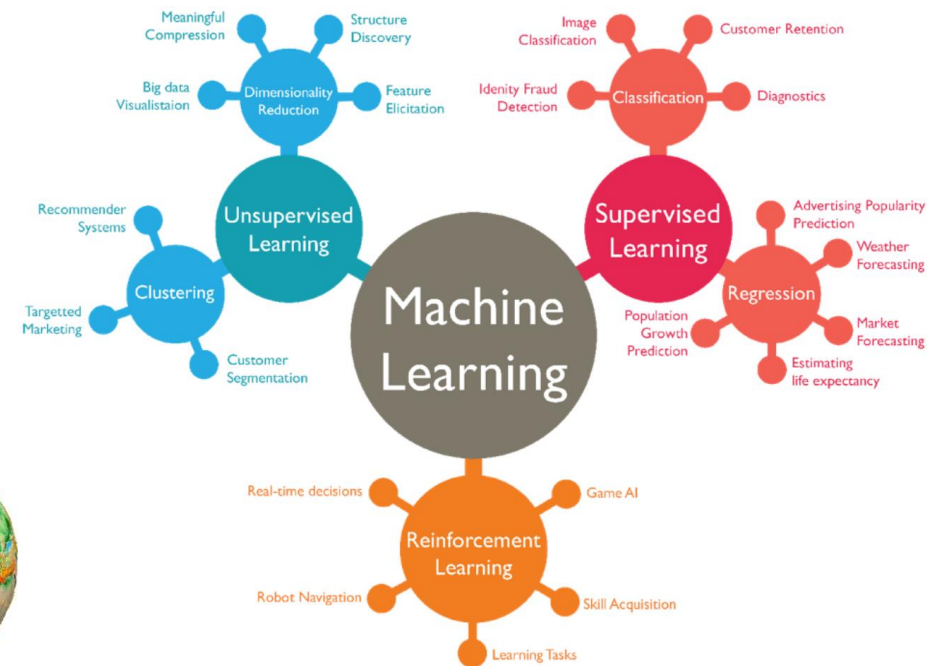
Cray



CTuning Foundation



Dell



BASE-II Work Packages: **Progress**

WP1 AI for Science Benchmarks	WP2 AI/HPC Convergence at the Software Level	WP3 HW/SW Co-Design	WP4 Knowledge Exchange
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*Scalable AI for
Science Benchmarks*

*AI for accelerating
supporting HPC*

*Support Exascale
science cases*

Learn and Share

BASE-II Work Packages: Progress

WP1

AI for Science
Benchmarks

*Scalable AI for
Science Benchmarks*

- Released a pre-exascale suite 1.2.0
- Surveyed a wide range of exascale candidates.
- Gearing for next release with one exascale case.

WP2

AI/HPC Convergence
at the Software Level

*AI for accelerating
supporting HPC*

- Compatibility between NNs and PDEs (Out-Layer Hypersurface NNs)
- Padding Free Convolution
- Zero Coordinate Shift (ZCS)

WP3

HW/SW Co-Design

*Support Exascale
science cases*

- Developed a range of storage, network and compute test-beds

WP4

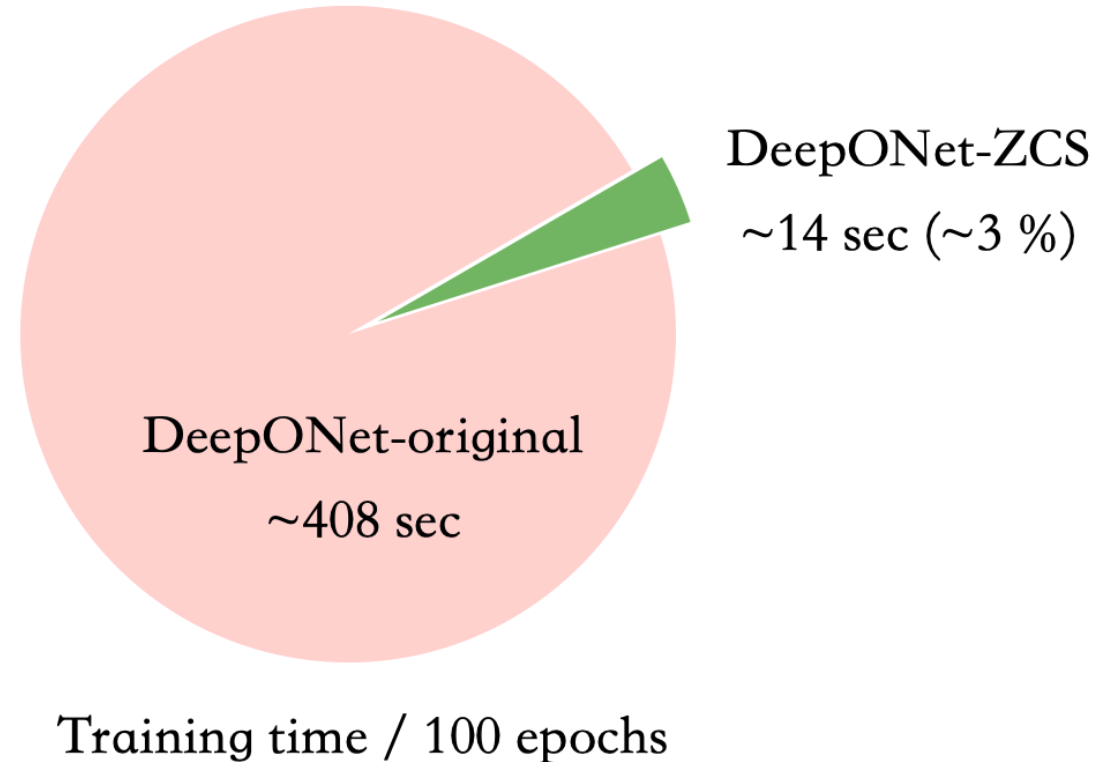
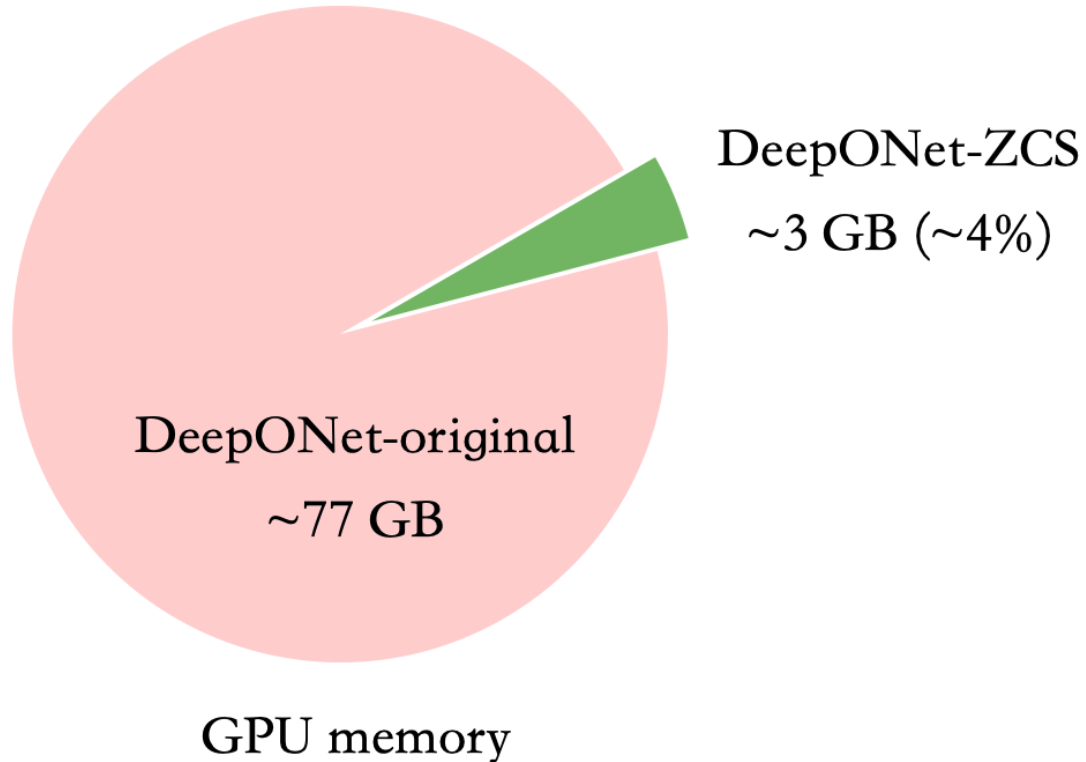
Knowledge Exchange

Learn and Share

- Seminars on AI for Science
- ML For Science Training
- Engagements with partner organisations
- Plans for wider KE across ExCALIBUR

Some Sample Results (See Our Poster)

Training a DeepONet with DeepXPE for bending of Kirchhoff-Love plates (4th-order PDE)



Current Challenges

- Identifying AI+HPC Cases
- Identifying scientifically *meaningful* scalable AI for Science cases (other than LLMs)
- Performance modelling of large-scale AI models
- Recruitment!

