Science and Technology Facilities Council

Hartree Centre

Performance Portability for Existing Weather & Climate Models using PSyclone

Application to the NEMO Ocean Model

Chris Dearden and **Andy Porter**, STFC Hartree Centre
Wayne Gaudin, NVIDIA

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CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

Acknowledgements

PSyclone is developed by a growing number of people:

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Overview

1. The Problem: Performance, Portability and Productivity
2. The PSyclone tool
3. PSyclone: revolution versus evolution
4. Results of Applying PSyclone to NEMO
5. Next Steps

The Problem

- 3P's : Performance, Portability and Productivity
  - Maintainable high performance software
  - Single-source science code
  - Performance portability
- Complex parallel code + Complex parallel architectures + Complex compilers = Complex optimisation space => unlikely to be a single solution
- Single-source optimised code is unlikely to be possible
- So … separate science specification/code from code optimisation

- A domain-specific compiler for embedded DSL(s)
  - Configurable: FD/FV NEMO, GOcean, FE LFRic
  - Currently Fortran -> Fortran/OpenCL
  - Supports distributed- and shared-memory parallelism
  - Supports code generation and code transformation
- A tool for use by HPC experts
  - Hard to beat a human (arguably)
  - Work round limitations/bugs
  - Optimisations encoded as a ‘recipe’ rather than baked into the scientific source code
  - Different recipes for different computer architectures
  - Enables scriptable, whole-code optimisation
  - Support for profiling, debugging and kernel extraction

PSyclone: Two Modes of Operation

Revolution

Process code written in a DSL

Currently two Domains supported:

- LFRic - Mixed finite elements, mesh unstructured in horizontal, structured in vertical, embedded in Fortran
- GOcean - DSL for 2D, finite difference, stretched, structured grid, embedded in Fortran

Evolution

Process existing code that follows strict coding conventions

Recognise certain code structures and construct higher-level Internal Representation

Transformations applied to this IR

In development for NEMO (plus associated models, e.g. SI3, MEDUSA). Also applied to ROMS.

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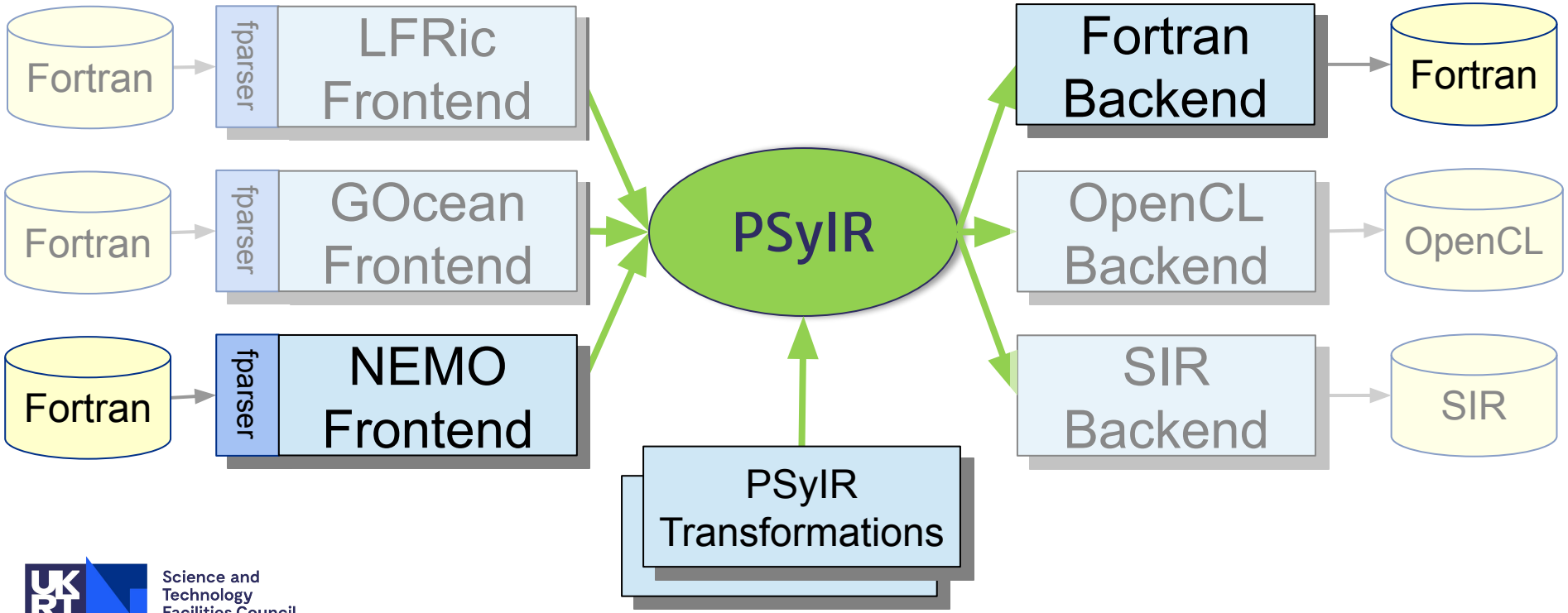
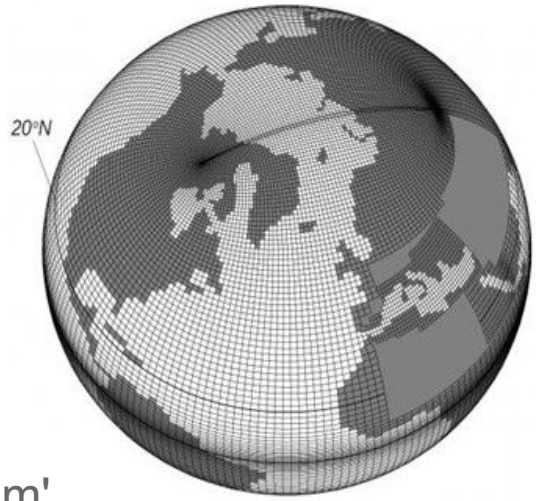
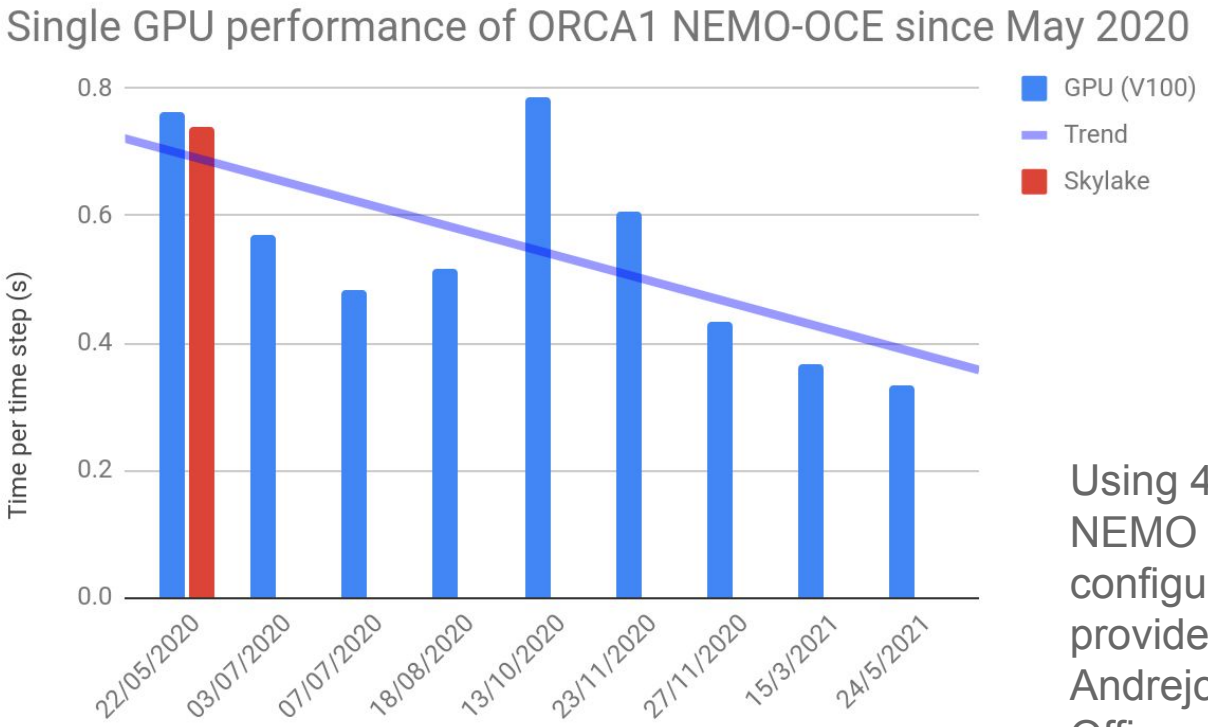
PSyclone: Basic Architecture



- **Finite-difference** model using a tripolar, stretched latitude, longitude mesh ('ORCA')
- Three core components:
  - NEMO-OPA: ocean dynamics, thermodynamics
  - NEMO-SI3: sea-ice (thermo)dynamics, brine inclusions...
  - NEMO-TOP/PISCES: tracer transport and biogeochemistry
- Mesh rotated so that poles are over land
  - Can go to high resolution without the 'pole problem'
- Relatively large (core of ~100K lines of Fortran)

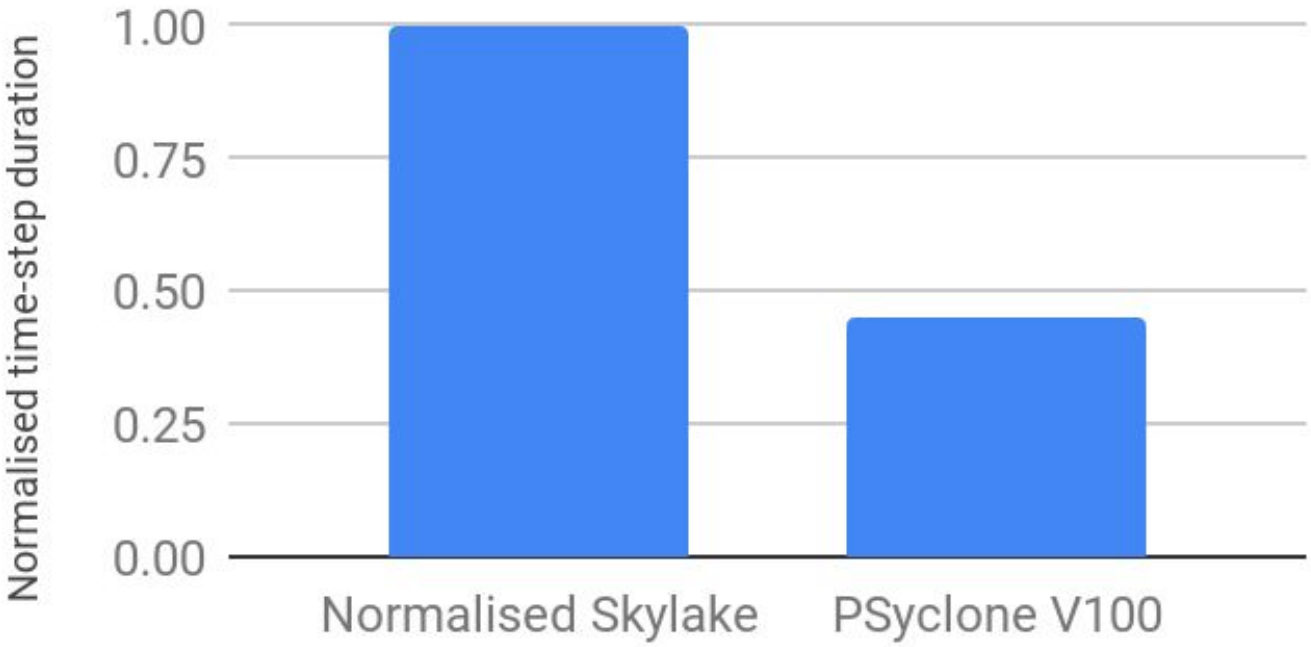


Results - ORCA1 ocean, OpenACC



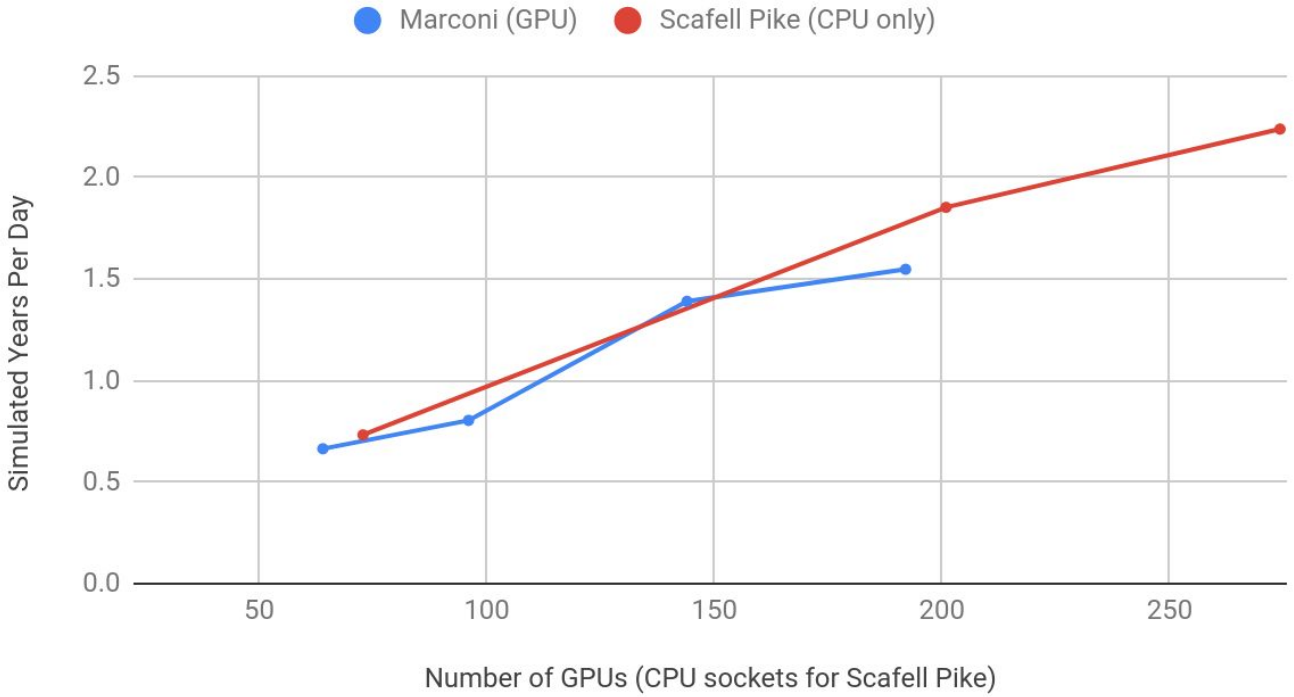
Using 4.0.2 of NEMO & G08 configuration provided by Mirek Andrejczuk, Met Office

Results - ORCA1 ocean, GPU



Results - ORCA12 ocean, GPU + MPI

Large-scale resources accessed through **ESiWACE2**
Run on up to **192 GPUs** on **Marconi** (V100) and JUWELS Booster (A100)
Scaling performance still under investigation



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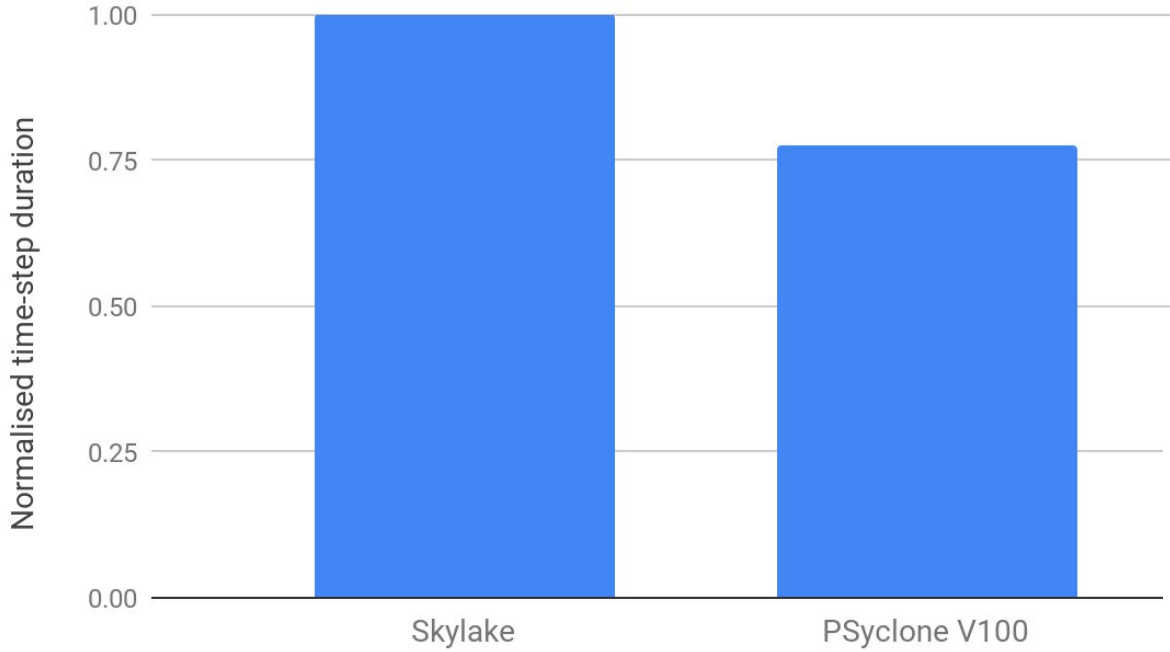
Ongoing - ORCA1 ocean+sea ice, GPU



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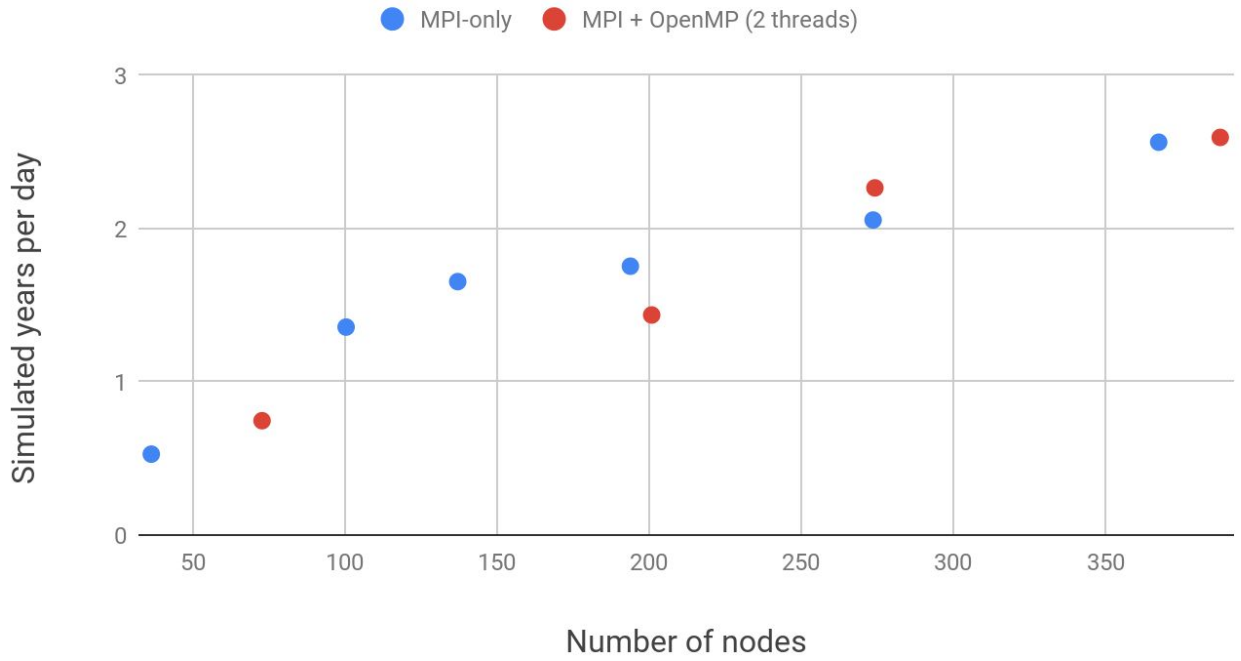
Results - ORCA12 ocean, OpenMP+MPI



Loops over **vertical levels** parallelised using OpenMP.
More work to be done...

Next Steps

- Other GPU hardware (OpenMP Offload)
- Optimise OpenMP CPU performance
- Data Movement
  - Explicit management instead of unified memory
- Investigate applicability to NEMOVAR and WAVEWATCH III
- Adjoint Generation

Summary

- **PSyclone** is a tool for code-generation and transformation
- Aimed at the HPC expert
- Supports revolution (e.g. **LFRic**) and evolution (e.g. **NEMO**)
- Used with NEMO to add **OpenACC** or **OpenMP** directives
- Good single GPU performance obtained for NEMO
- Work in progress on multi-GPU performance
- Work in progress on application to **SI3**, **MEDUSA** and **NEMOVAR**
- Support for **OpenMP offload** in development

Thank you

User, Developer and Reference Guides are available:

psyclone[-dev,-ref].readthedocs.io

For more information please contact:

rupert.ford@stfc.ac.uk
andrew.porter@stfc.ac.uk

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