Prototyping an in-situ visualisation mini-app for the LFRic Project

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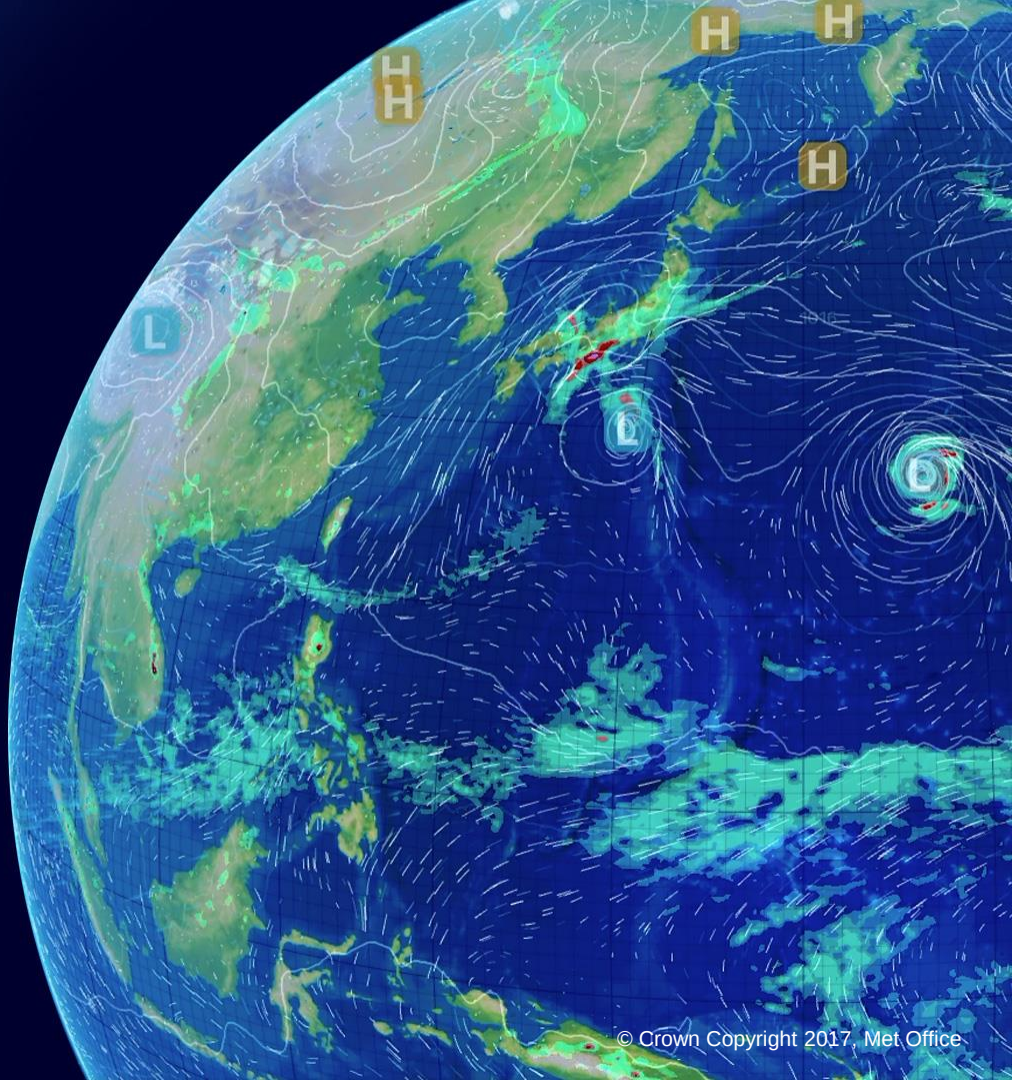
18th Workshop on high performance computing in meteorology

24th-28th September 2018, ECMWF, UK.



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Talk Overview

- Background and Motivation
- LFRic ‘mini-apps’
- In-situ analysis and visualisation
- Overview of Paraview/Catalyst
- Example outputs from the LFRic Paraview/Catalyst mini-app

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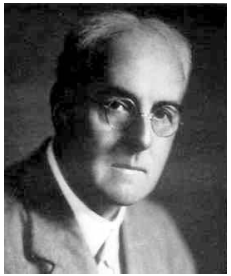
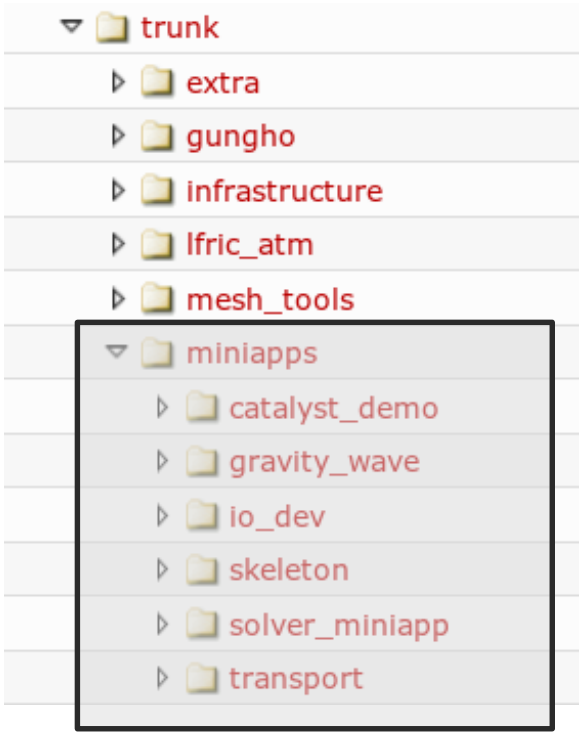
Background and Motivation



- LFRic - a project to rewrite Met Office modelling infrastructure in preparation for the Exascale challenge
- Precursor project GungHo (*Met Office, NERC, STFC*)
- LFRic aim is to work in collaboration with others in the community
- UM partner collaborations have been extended to LFRic/Exascale
- Mini-apps are a useful tool for enabling collaborators to more easily develop within LFRic
- This talk concentrates on a in-situ visualisation mini-app developed in conjunction with Wolfgang Hayek at NIWA

LFRic mini-apps

- Definition is quite flexible:
  - They could be a model (e.g. gungho dynamical core)
  - They could be a some science or infrastructure functionality (e.g. gravity wave test case, I/O)
  - They could be a demo/prototype application that is new functionality (e.g. the visualisation mini-app)
- Currently all mini-apps live inside the main LFRic repository
  - They have their own Makefile and can be built as entirely standalone executables
  - They can pull in LFRic core infrastructure and science
  - They can have their own specific code components
  - They can have their own unit tests and test suites



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In-situ Analysis and Visualisation

- Looking towards Exascale, the increasing volume of data to be processed and stored will become an issue
- Maybe we don’t always have to write full data to disk, before analysis and visualisation?!
- Some benefits of the in-situ approach:
  - “FLOPS are free” – better to process data while it is still “hot” (near the processor)
  - Gives scientists a way to quickly look at results or debug a model run without necessarily writing and post-processing data
  - Avoids having to write specific file formats

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Paraview/Catalyst Overview

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Paraview

- High-performance 3D visualisation tool
- Scales to billions of unstructured grid cells and 100,000 cores
- Client-server architecture
- Parallel processing with MPI, multithreading, and GPU
- Graphics rendering on CPUs and GPUs

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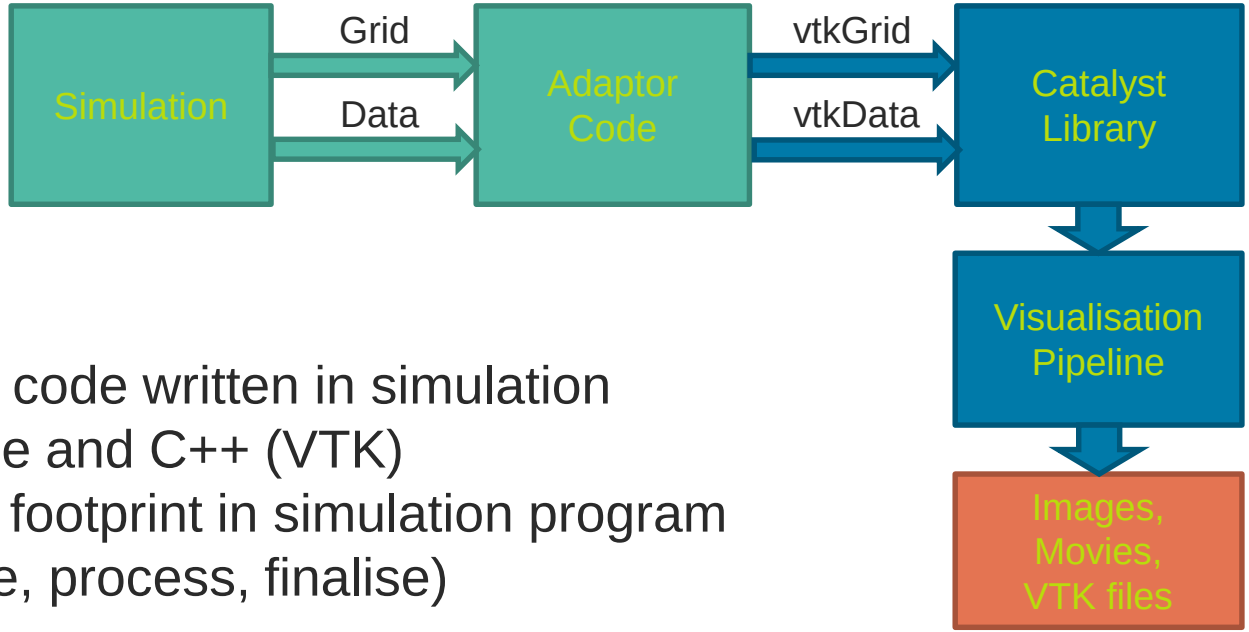
Catalyst

- Is a library that is part of Paraview codebase
- Forms the bridge between the science simulation code and Paraview visualisation
- Enables access to full Paraview capabilities for any simulation code
- Possibilities
  - Render images while the simulation runs
  - Convert and output native simulation format as VTK (e.g. for later analysis)
  - Possible to output every timestep
  - Paraview Live: pause, analyse, resume

Paraview / Catalyst Workflow



- Adaptor code written in simulation language and C++ (VTK)
- Minimal footprint in simulation program (initialise, process, finalise)

Image courtesy of Wolfgang Hayek

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In-situ visualisation methods

Various interactions are possible:

- Via the Python pipeline
  - Create standard scripts for end users to edit
  - End users can create their own Paraview workflow and export script
  - Minimal programming required (but need to learn some Paraview)
- Create specialist ‘adaptor’ code in C++. More programming skills required but have access to full power of Paraview.
- Paraview ‘live’ – Paraview running simultaneously with live model

Paraview/Catalyst Python pipeline

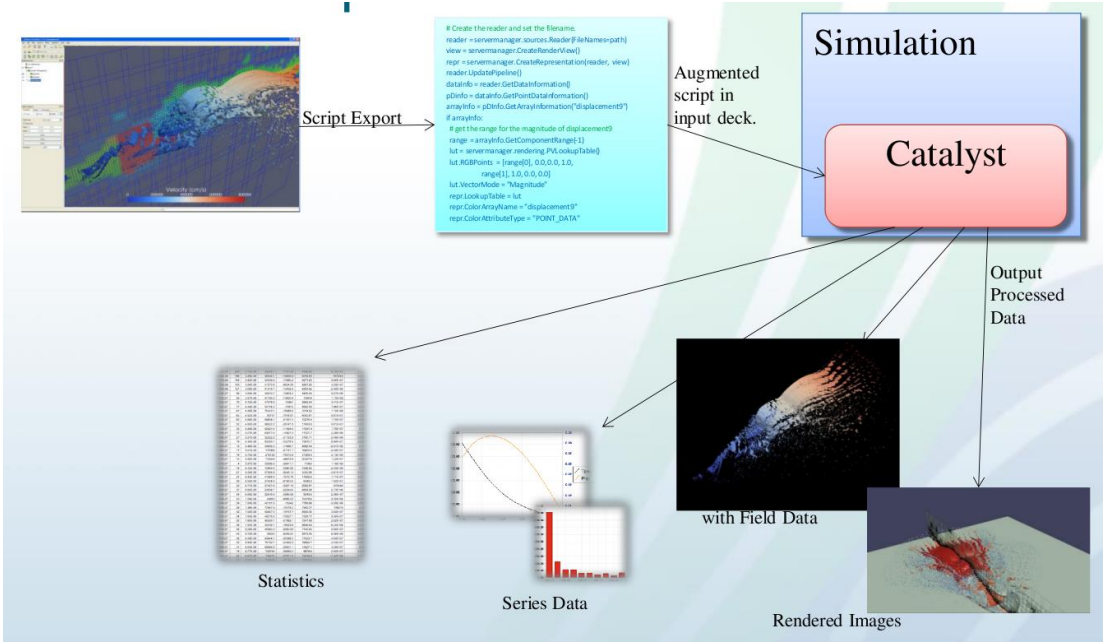


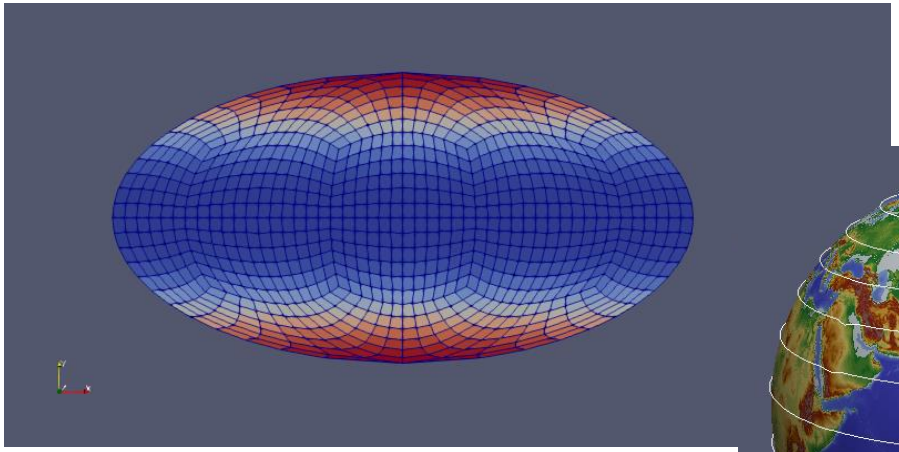
Image courtesy of Kitware Catalyst Tutorial

Visualisation in LFRic

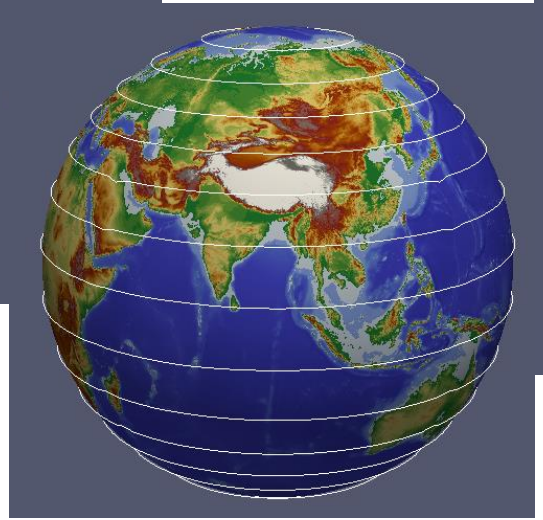
- 3D visualisation is part of a UM partner Exascale collaboration visualisation work package
- Complements existing 2D visualisation development for Exascale
- Aims:
  - Gather requirements for 3D visualisation
  - Explore in-situ visualisation, create a demo mini-app for evaluation
  - Provide reader plugin(s) for LFRic output data (UGRID) for relevant 3D visualisation tools

Results

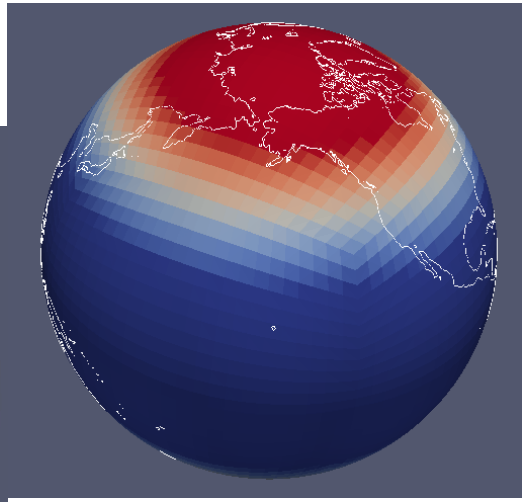
Static images rendered directly from LFRic via Paraview/catalyst



Density field as Mollweide projection



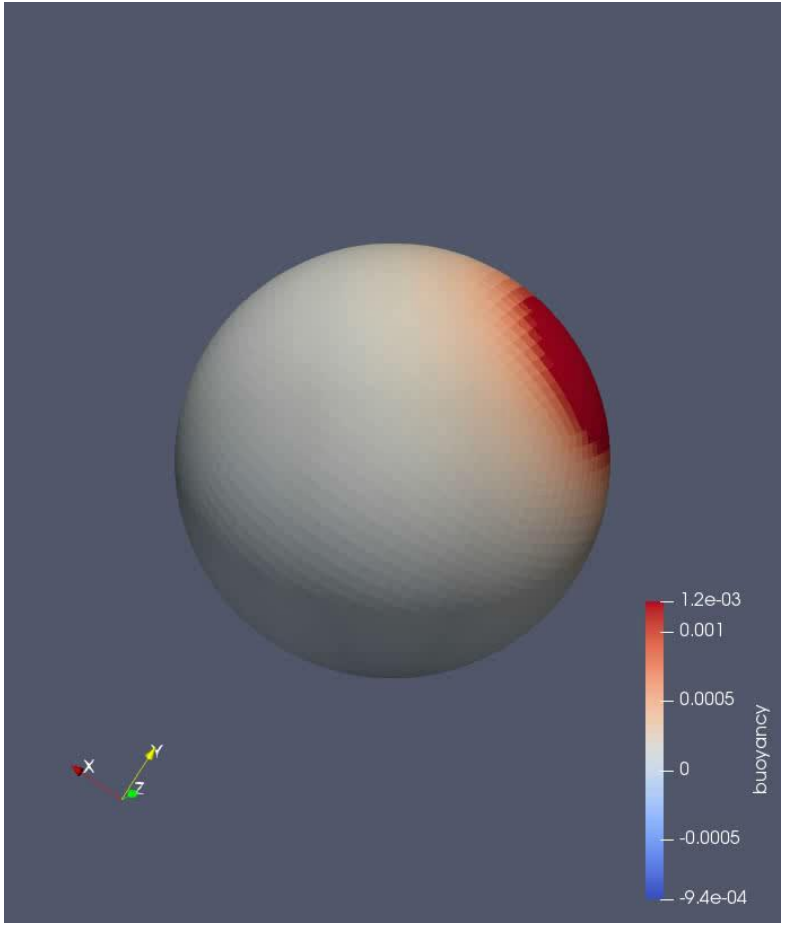
Density field as contours plus topography



Density field with coastline overlay

Images courtesy of Wolfgang Hayek, NIWA

gravity wave miniapp data output as VTK and rendered as an animation within Paraview



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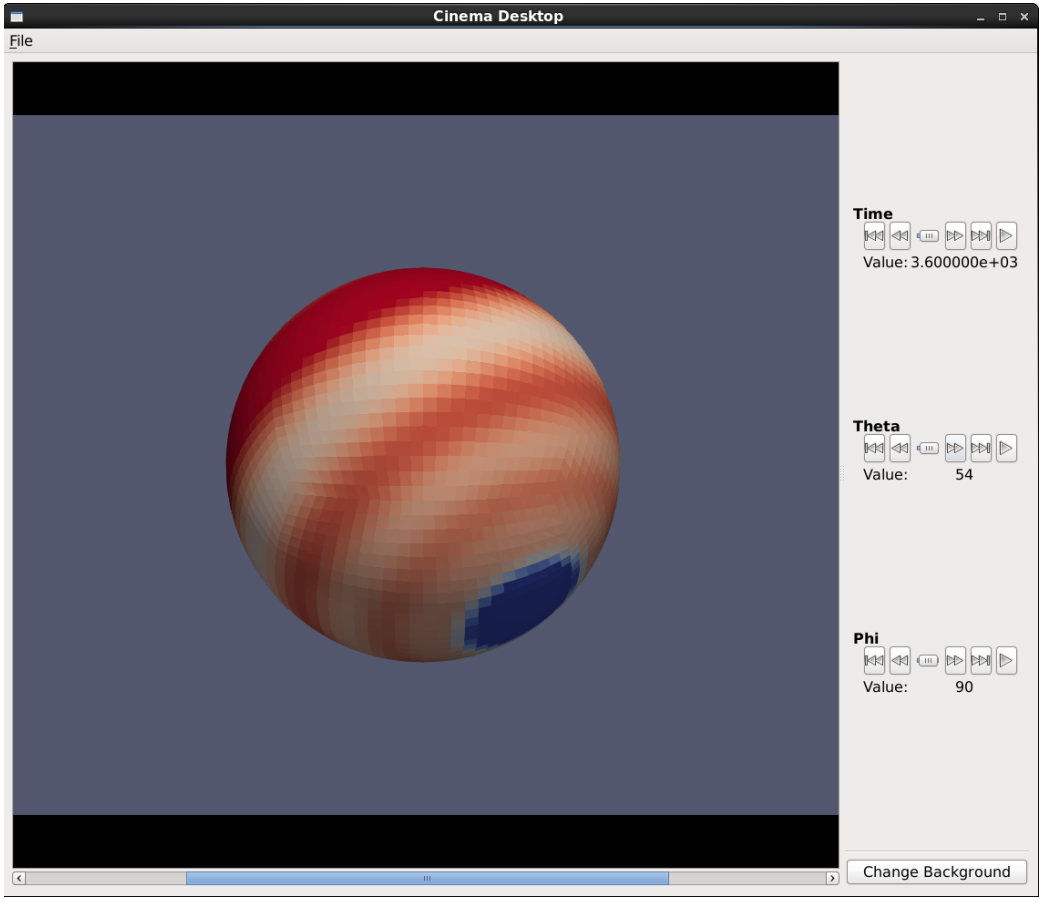
Browsing a Cinema database output from LFRic via Paraview/Catalyst

Cinema is an initiative for big scientific data. The approach is to capture images in an 'image database' at a range of view angles to enable browsing the data without creating a full-resolution dataset



https://cinemascience.org/

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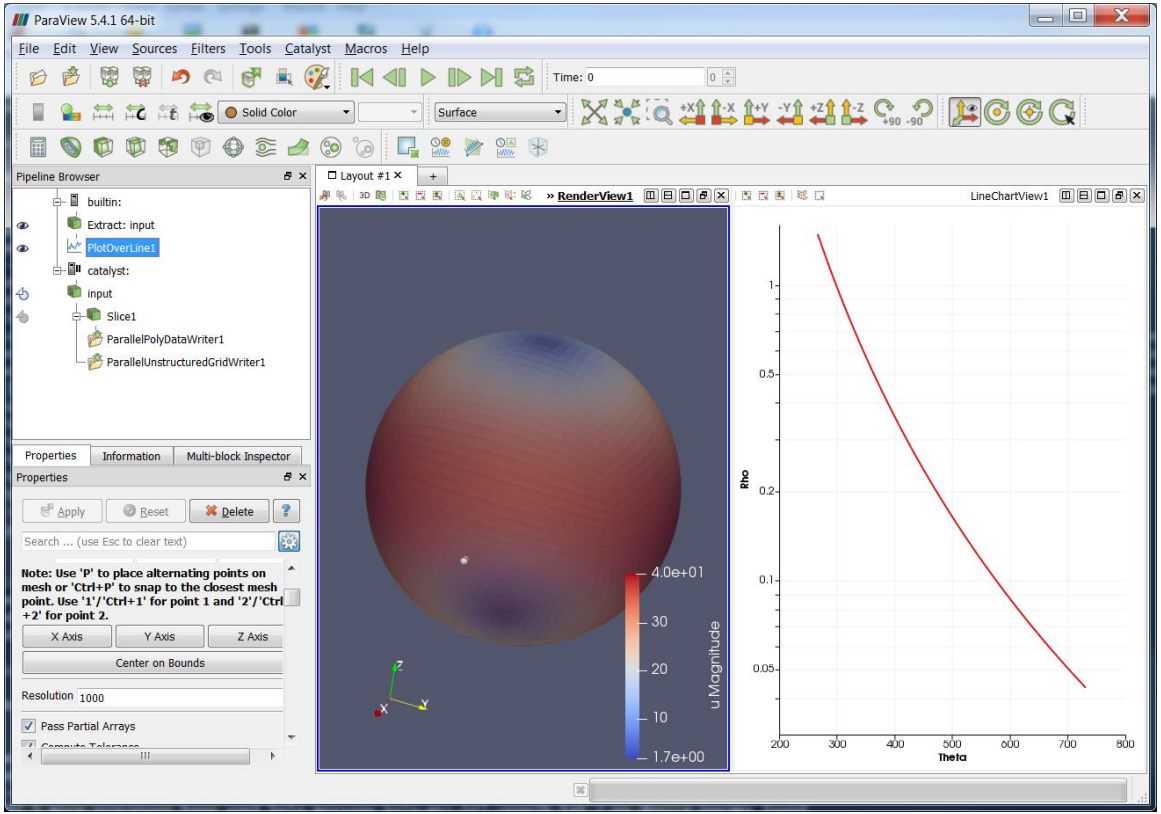
Paraview Live



Next Steps

- Evaluation of the mini-app by scientists and gather requirements and use cases for further development
- Trials running on HPC (server) with visualisation on desktop (client)
- Create Paraview plugin for LFRic UGRID data to facilitate general evaluation of Paraview
- Possibly trial other tools based on VTK such as Vapor, Visit

Acknowledgements

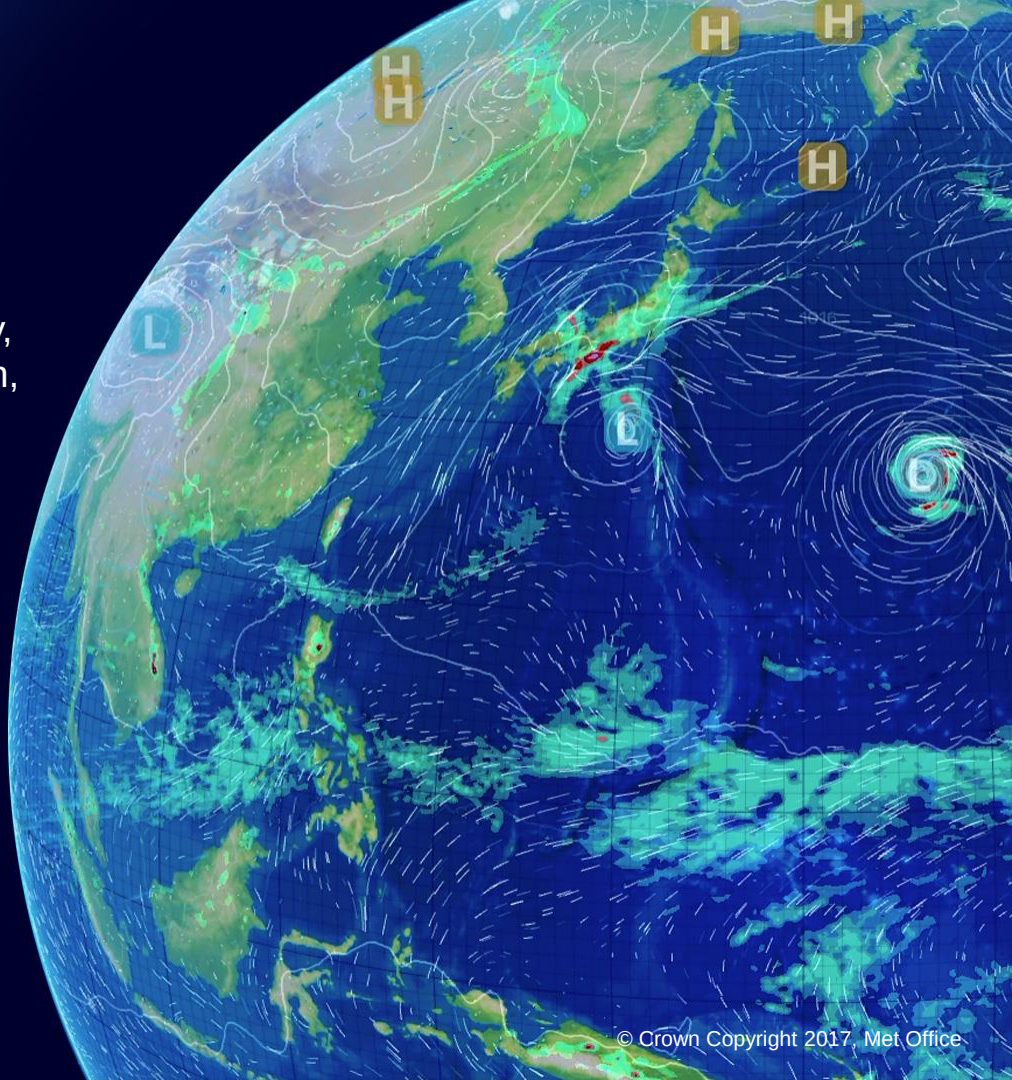
Met Office UK LFRic team:
Sam Adams, Tommaso Benacchio, Matthew Hambley, Mike Hobson, Iva Kavcic, Chris Maynard, Tom Melvin, Steve Mullerworth, Stephen Pring, Steve Sandbach, Ben Shipway, Ricky Wong

LFRic Collaborators:
STFC (Hartree Centre), UK:
Rupert Ford, Andy Porter

NIWA / NESI, NZ:
Wolfgang Hayek, Alex Pletzer

Monash University, Australia: Mike Rezny

IPSL (LSCE/CEA), France:
Olga Abramkina, Yann Meurdesoif



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Thank You!

Questions?