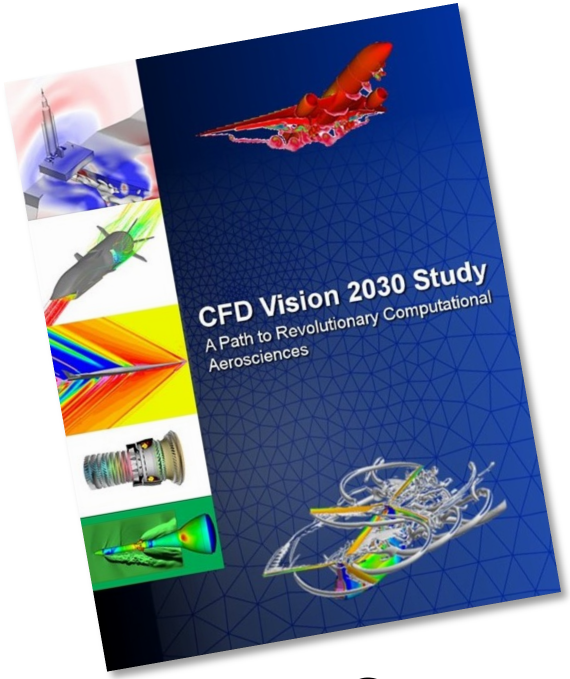
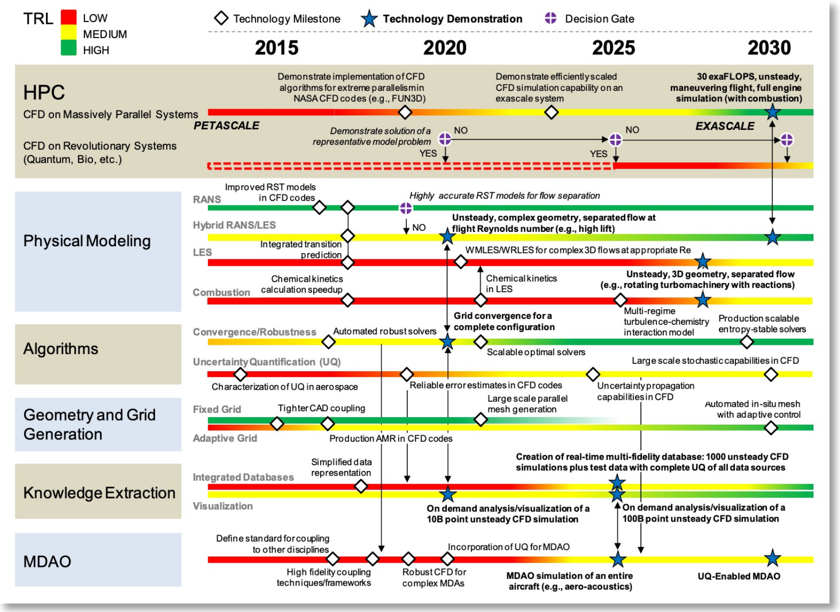
CEEC

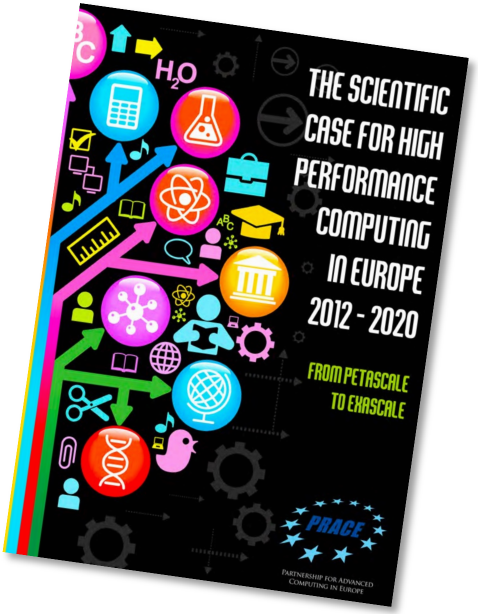
Centre of Excellence in Exascale CFD

Introduction

About 10% of the energy use in the world is spent overcoming turbulent friction







No upper limit in fluid dynamics to the size of the systems to be studied via simulations

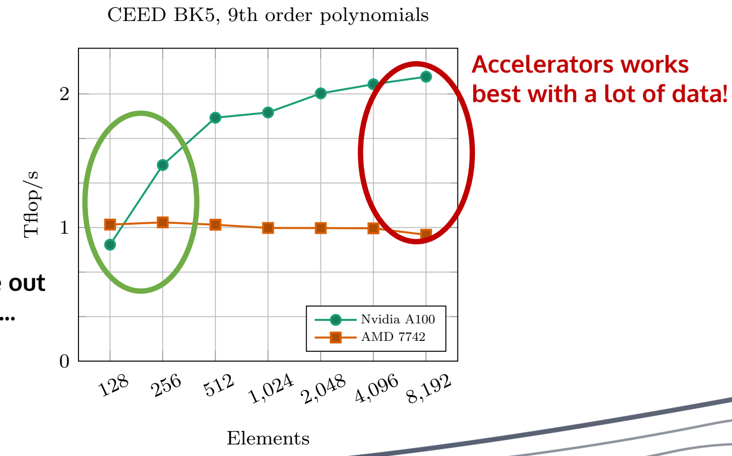
Computational Fluid Dynamics is one of the areas with a clear need and **great potential to reach exascale**

Introduction

- Exascale will require either **unreasonable large problem** sizes or **significantly improved efficiency** of current methods
  - Finite-Volyme LES of full car on the entire K computer (京) required **more than 100 billion grid points** to run efficiently
  - What problem size is needed to fill the 379 PFlop/s LUMI…
- High-order methods
  - Attractive numerical properties, **small dispersion** errors and more "accuracy" per degree of freedom
  - Better suited to take advantage of **modern hardware** (accelerators)

京: 82944 nodes, 663552 Cores, **10 PFlop/s**

Dardel: 56 nodes, 448 MI250X GCDs, ≈**10 PFlop/s**



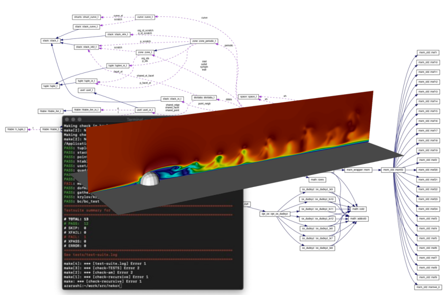
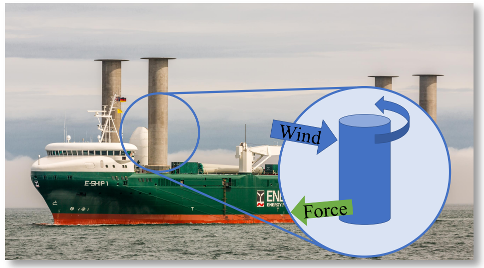
…but we rather scale out our problems in CFD…

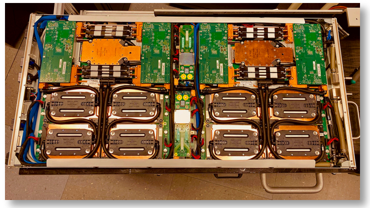
Overview

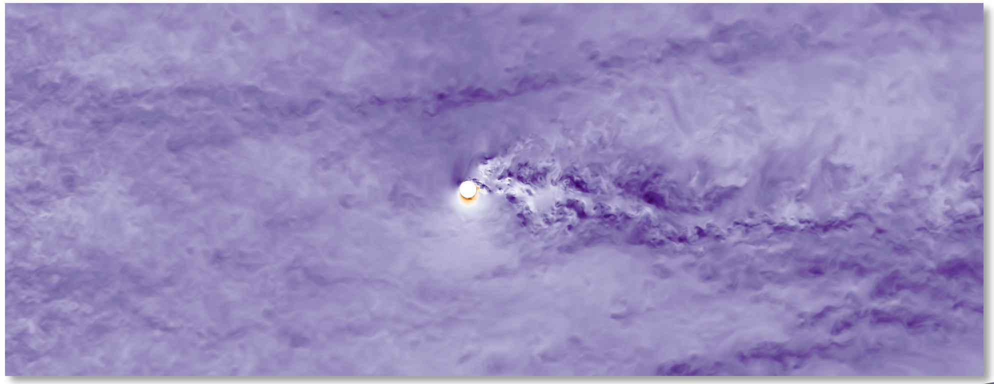
CEEC

The main goal of CEEC is to address the extreme-scale computing challenge to enable the use of accurate and cost-efficient high fidelity computational fluid dynamics (CFD) simulations at exascale

- Implement **exascale-ready workflows** for addressing grand challenge scientific problems
- Develop **new or improved algorithms** that can efficiently exploit exascale systems.
- Significantly improve **energy efficiency** of simulations
- Demonstrate workflows on **lighthouse cases** relevant for both academia and industry

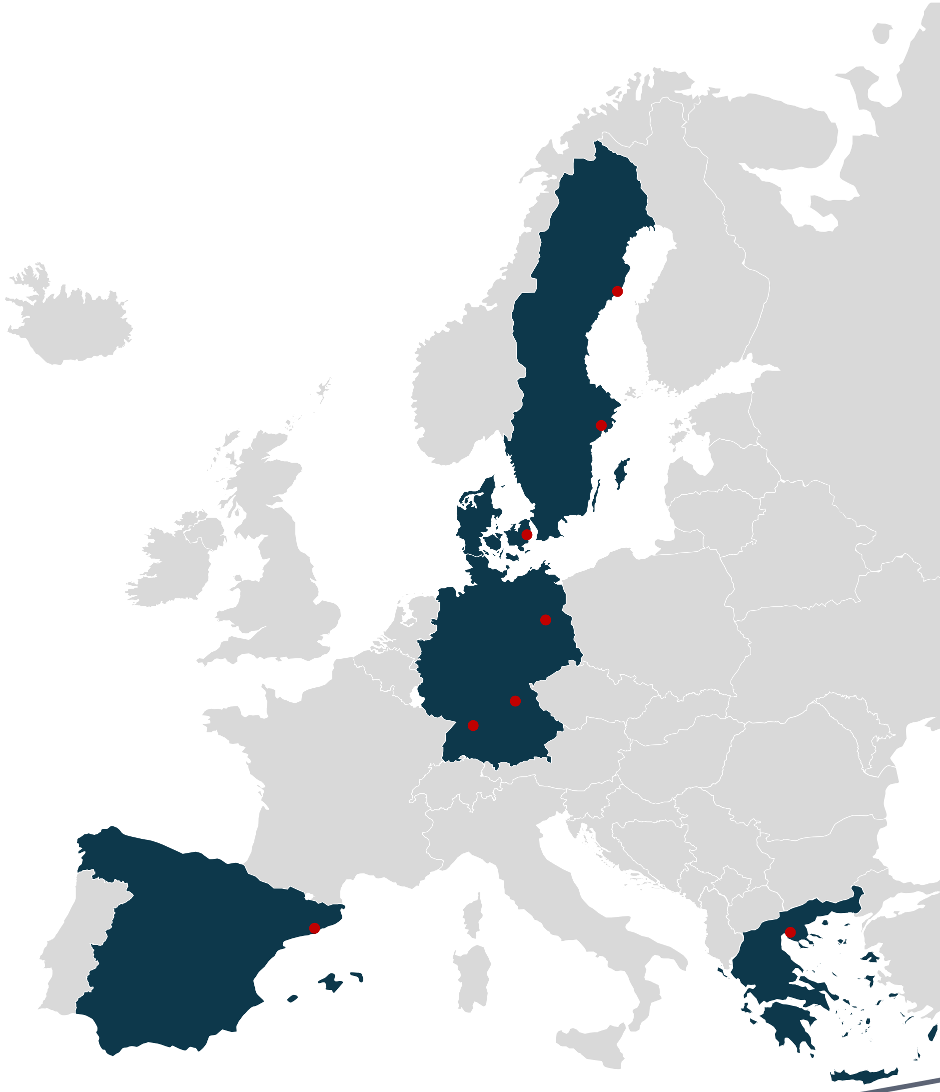




Partners

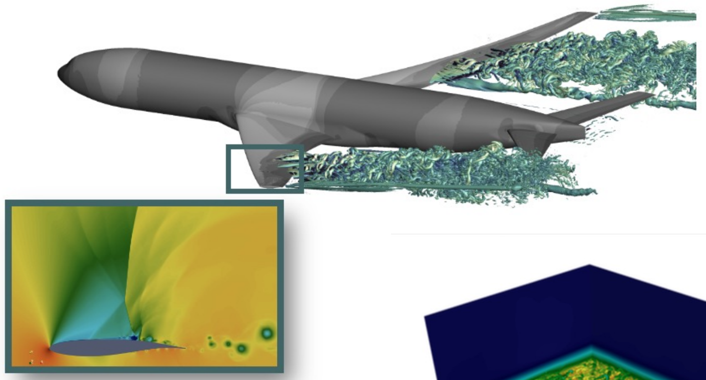
Eight partners from five European countries

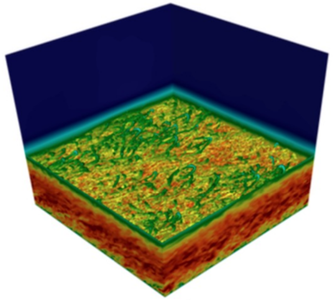
- KTH Royal Institute of Technology (Coordinator)
- Umeå University
- Technical University of Denmark
- University of Erlangen-Nuremberg
- University of Stuttgart
- Barcelona Supercomputing Center
- Aristotle University of Thessaloniki
- Federal Institute for Materials Research and Testing

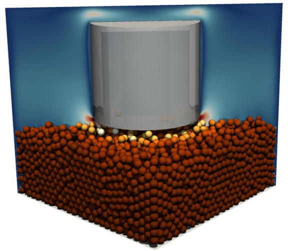


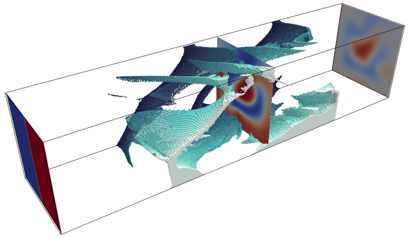
Lighthouse Cases

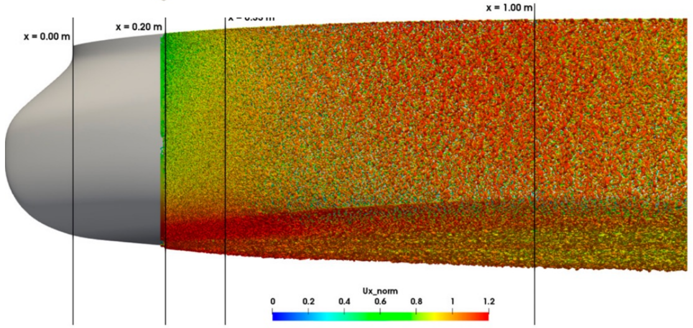
- **Shock-boundary layer interaction and buffet on wings at the edge of the flight envelope**
  - Codes used: FLEXI
- **High fidelity aeroelastic simulation of the SFB 401 wing in flight conditions**
  - Codes used: Alya
- **Topology optimisation of static mixers**
  - Codes used: Neko
- **Localized erosion of an offshore wind-turbine foundations**
  - Codes used: waLBerla
- **Simulation of Atmospheric Boundary Layer flows**
  - Codes used: NekRS/Nek5000
- **Merchant ship hull**
  - Codes used: Neko







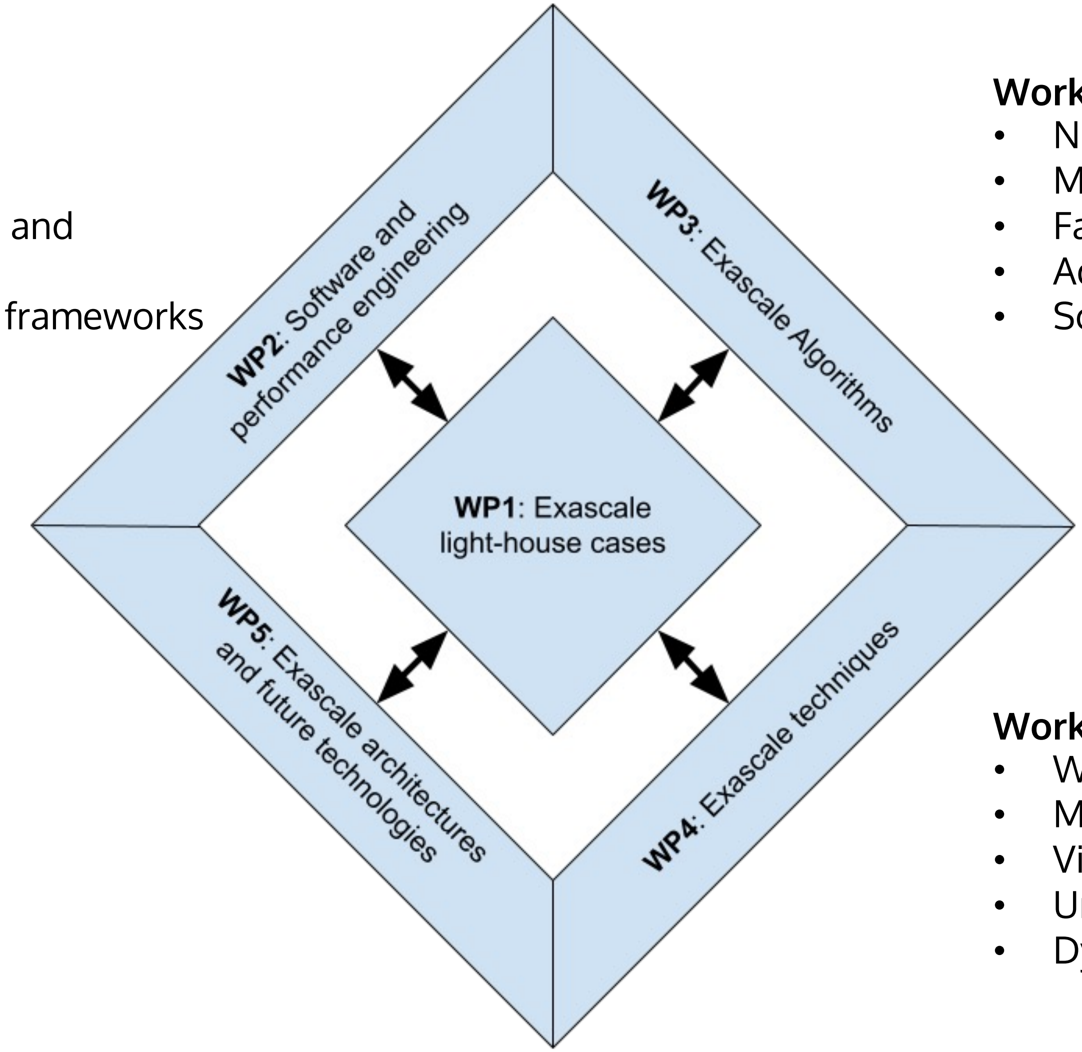




Technical Work

Work package 2
- Performance engineering
- Code generation techniques
- Continuous integration, testing, and performance tracking
- Integration with fault-tolerance frameworks
- Software deployment

Work package 3
- Numerical methods and solver for exascale
- Mixed-precision algorithms
- Fault-resilient algorithms
- Adaptivity and error control
- Scalable optimization algorithms



Work package 5
- Evaluation of EPI and EUPilots
- Quantum Computing

Work package 4
- Workflows
- ML-based sub-models
- Visualization and data mangement
- Uncertainty quantification
- Dynamic resource mangement

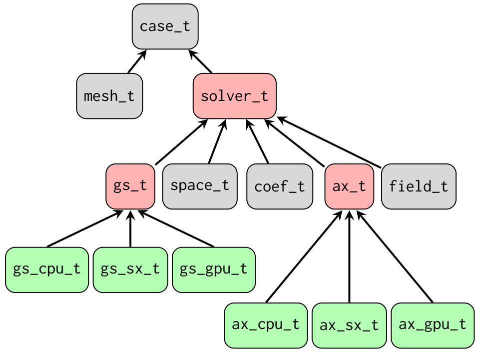
Portable Spectral Element Framework NEKO

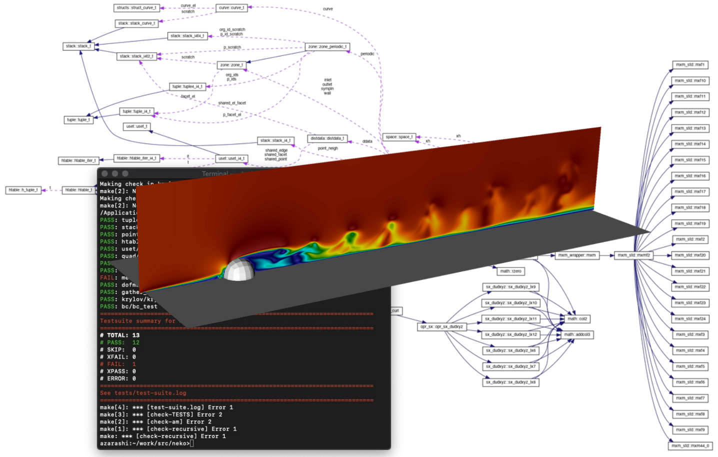
CEEC

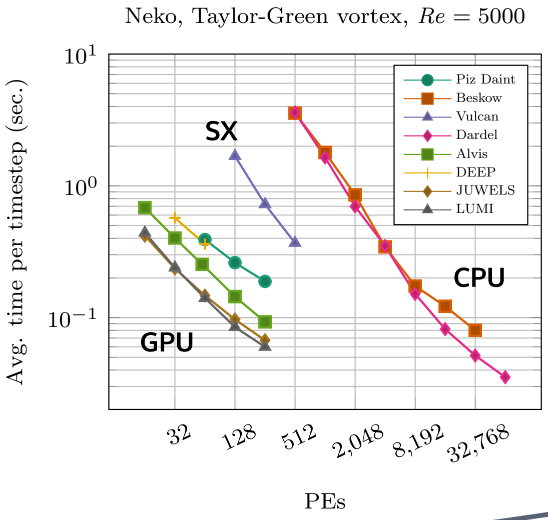
- High-order spectral element flow solver
  - Incompressible Navier-Stokes equations
  - Matrix-free formulation, **small tensor products**
  - **Gather-scatter** operations between elements
- Modern **object-oriented** approach (Fortran 2008)

```fortran
! Base type for a matrix-vector product providing Ax
type, abstract :: ax_t
 contains
   procedure(ax_compute), nopass, deferred :: compute
end type ax_t

! Abstract interface for computing Ax
abstract interface
   subroutine ax_compute(w, u, coef, msh, Xh)
     implicit none
     type(space_t), intent(inout) :: Xh
     type(mesh_t),  intent(inout) :: msh
     type(coef_t),  intent(inout) :: coef
     real(kind=dp), intent(inout) :: w(:,:,:,:)
     real(kind=dp), intent(inout) :: u(:,:,:,:)
   end subroutine ax_compute
end interface
```







- Various hardware-backends
  - CPUs, GPUs down to exotic vector processors and FPGAs
    - **Device abstraction layer** for accelerators (CUDA/HIP/OpenCL)
- Modern Software Engineering (pFUnit, ReFrame, **Spack**)

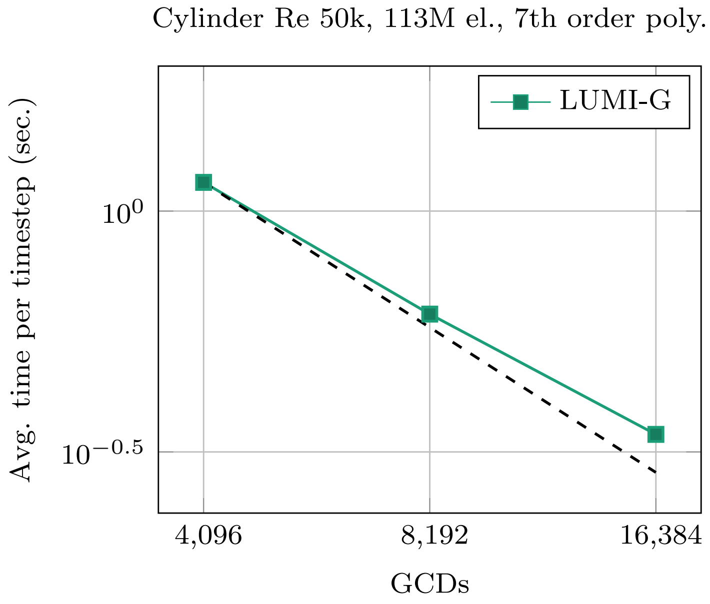
```
> spack install neko+cuda
```

ExtremeFLOW/neko

www.neko.cfd

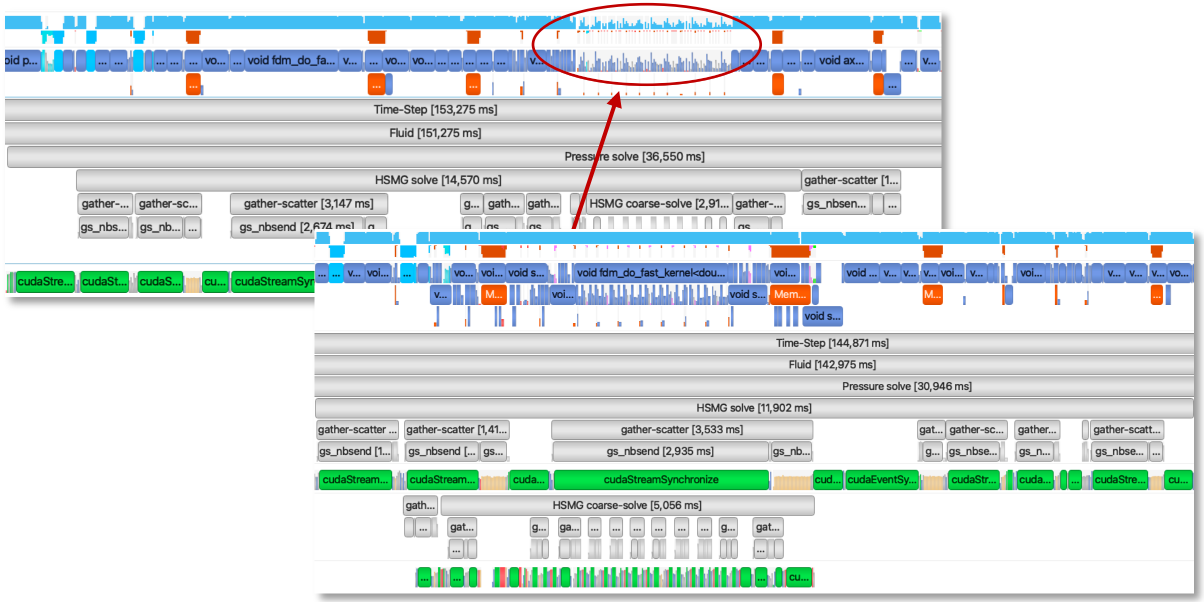
LUMI Hero Run

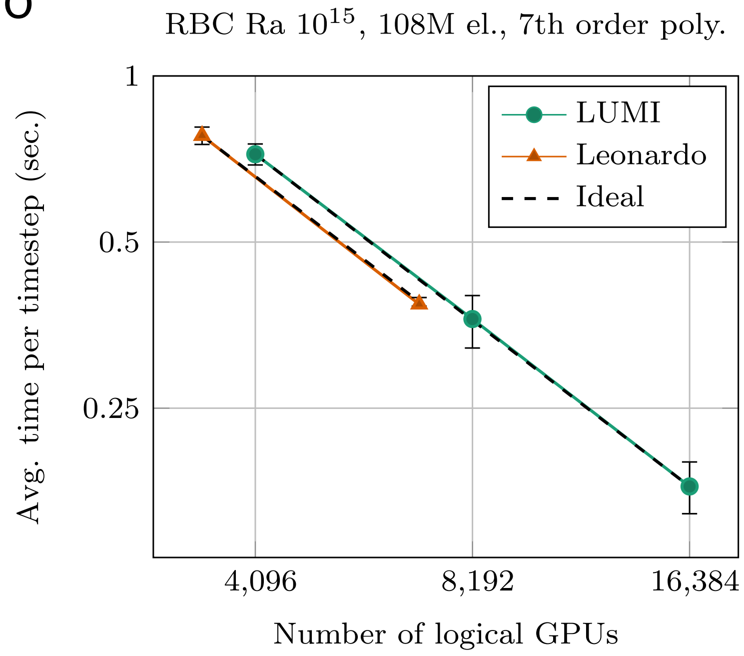
- Twelve-hour of exclusive access to the world's third-fastest supercomputer
- DNS of flow past a circular cylinder at Re = 50,000
  - 113M elements
  - 7th order polynomials (8 GLL points)
- Simulation restarted from prebaked low-order runs
  - Restart checkpoint: 453GB
  - Extrapolated to 7th order polynomials
  - Computed solution (snapshot): 1.5TB
- Preliminary results
  - Achieved close to 80% parallel efficiency
  - Using 20%, 40% and 80% of the entire machine



Extreme-scale High-Fidelity Simulations of Turbulent Rayleigh-Bénard Convection

- Exploring the ultimate regime of turbulent RBC
- The first Swedish lead ACM Gordon Bell Finalist
- Excellent strong scaling on both LUMI and Leonardo
  - Up to 80% of LUMI and 50% of Leonardo
- Novel task-parallel preconditioner





Cooled wall

Heated wall

Summary

- High-order methods are **essential** on current HPC machines
  - More suitable for current hardware and improved accuracy for "free"
- The heterogenous HPC landscape is a **nightmare**
  - Find a suitable level of **abstraction**
  - Use the best tools, **mix langauges and programming models**
- Modern software engineering approaches to **ensure (performance) portability**
  - **Automate testing** across various architectures and programmig models
  - Deployment: **Spack,** verification & validation: **Reframe**

Thank you for your attention!

CEEC
Centre of Excellence in Exascale CFD

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Sweden, Germany, Spain, Greece, and Denmark under grant agreement No 101093393.

Co-funded by the European Union

EuroHPC Joint Undertaking

Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European High Performance Computing Joint Undertaking (JU) and Sweden, Germany, Spain, Greece, and Denmark. Neither the European Union nor the granting authority can be held responsible for them.

CEEC

Centre of Excellence in Exascale CFD