Exploring the Ultimate Regime of Turbulent Rayleigh-Bénard Convection through Unprecedented Spectral-Element Simulations

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Team


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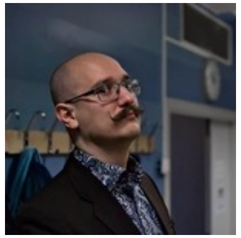
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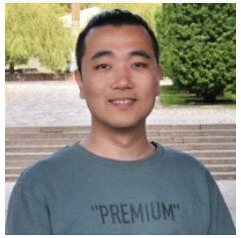
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Turbulent thermal convection

- Applications in nature and technology
  - From chip cooling, heat exchanges in power plants, to heat convection in the Earth's mantle and the sun.
- **Rayleigh-Bénard convection**: Canonical turbulent convection with fundamental open question: **Is there an ultimate regime,** i.e. anomalous scaling of Nusselt number (heat transfer) and Rayleigh number (buoyancy)?
  - Long-standing open issue in turbulence (Kraichnan 1962)
  - Difficult to conduct controlled experiments at high Rayleigh numbers $Ra > 10^{15}$
- Challenges with direct numerical simulations
  - **Large computational cost** due to resolution needs: $(H/\eta)^3 \sim Ra^{9/8}$
  - Numerical method with **minimal dissipative and dispersive errors** to capture and track small scales in time
  - Produces **unmanageable volumes of data**
  - **Long integration** times for steady state statistics
  - **Efficient implementation** on modern hardware

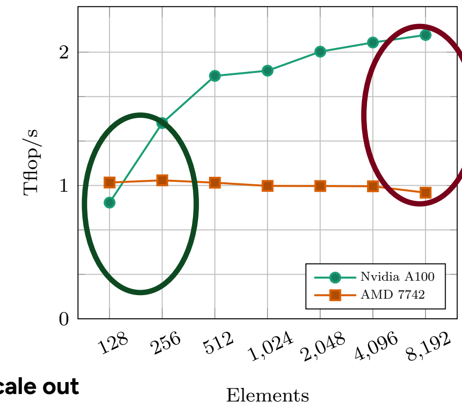
Illustration of the canonical problem at $Ra = 10^{13}$, iso-surfaces of temperature

Introduction

- Exascale will require either **unreasonably large problem** sizes or **significantly improved efficiency** of current methods
  - Finite-Volume LES of a 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 309 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**

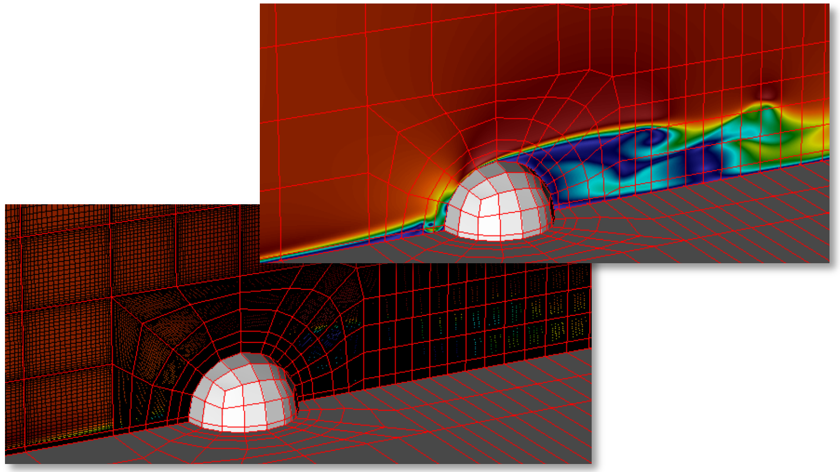


Accelerators works best with a lot of data!

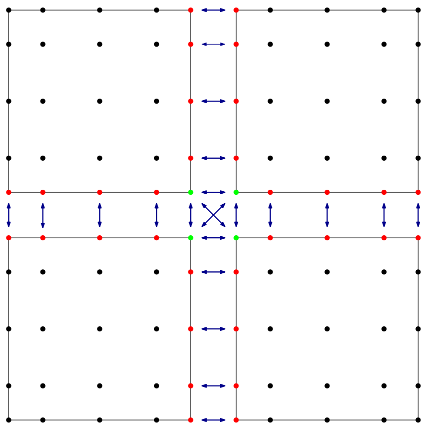
...but we rather scale out our problems...

Spectral Elements

- Finite Elements with high-order basis functions
  - N-th order Legendre-Lagrange polynomials $l_i(\xi)$
  - Gauss-Lobatto-Legendre quadrature points ξ_i
  - Fast tensor product formulation
    - $u^e(\xi,\eta,\gamma) = \sum_{i,j,k}^{N} u_{i,j,k}^e l_i(\xi) l_j(\eta) l_k(\gamma)$
  - High-order at low cost! (**Level 3 BLAS!**)



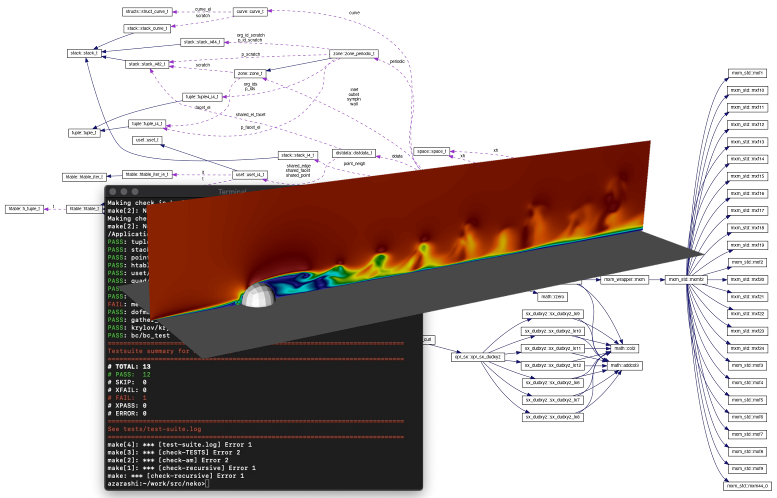
- Too expensive to assemble matrices
  - Element stiffness matrices $A_{i,j}^k$ with $\boldsymbol{O}(\boldsymbol{N}^6)$ **non-zeros**
- Matrix free formulation, key to achieve good performance in SEM
  - Unassembled matrix $A_L = \text{diag}\{A^1, A^2, \dots, A^E\}$ and functions $u_L = \{u^e\}_{e=1}^E$
  - Operation count is **only** $\boldsymbol{O}(\boldsymbol{N}^4)$ **not** $\boldsymbol{O}(\boldsymbol{N}^6)$
  - Boolean gather/scatter matrix Q^T and Q
    - Ensure continuity of functions on the element level $u = Q^T u_L$ and $u_L = Qu$
- Q and Q^T formed, only the action QQ^T is used
  - Matrix-vector product $w = Au \Rightarrow w_L = QQ^T A_L u_L$



1: A.T. Patera, A spectral element method for fluid dynamics: Laminar flow in a channel expansion, J. Comput. Phys. 1984
2. M. O. Deville, P. F. Fischer, E.H. Mund, High-Order Methods for Incompressible Fluid Flow, 2002
3: P.F. Fischer, J.W. Lottes, S.G. Kerkemeier, Nek5000 Web page: http://nek5000.mcs.anl.gov, 2008
4: H.M. Tufo, P.F Fischer, Terascale Spectral Element Algorithms and Implementations, Gordon-Bell prize 1999

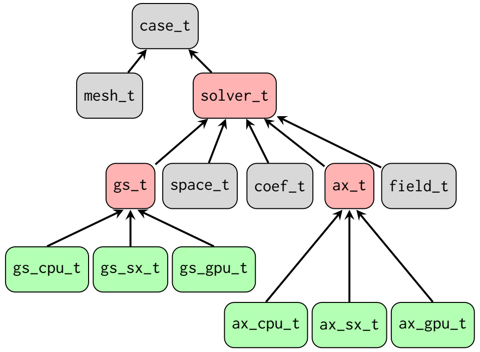
Portable Spectral Element Framework NEKO

- High-order spectral element flow solver
  - Incompressible Navier-Stokes equations
  - Matrix-free formulation, **small tensor products**
  - **Gather-scatter** operationst 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
```

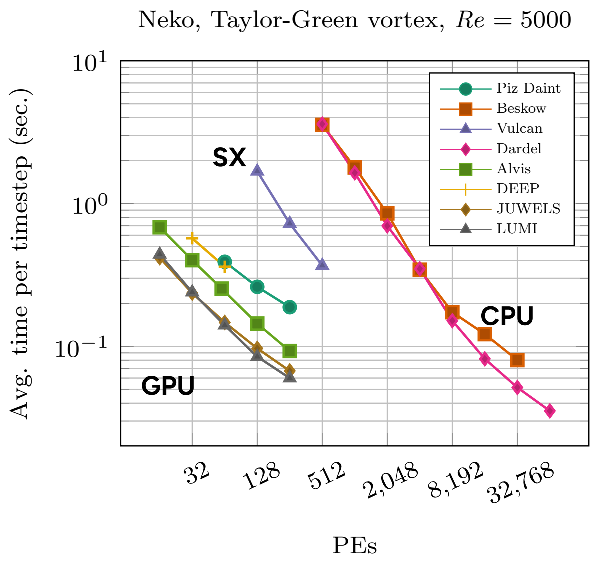


- Various hardware-backends
  - CPUs, GPUs down to exotic vector processors and FPGAs
    - **Device abstraction layer** for accelerators (CUDA/HIP/OpenCL)
  - Modern software engineering (pFUnit, ReFrame, **Spack**)

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

ExtremeFLOW/neko

www.neko.cfd



Device Abstraction Layer

How to interface Fortran with accelerators?

- Native CUDA/HIP/OpenCL implementation via C-interfaces
- Device pointers in each derived type

```
type field_t
   real(kind=rp), allocatable :: x(:,:,:,:) !< Field data
   type(space_t), pointer :: Xh     !< Function space
   type(mesh_t), pointer :: msh     !< Mesh
   type(dofmap_t), pointer :: dof   !< Dofmap
   type(c_ptr) :: x_d = C_NULL_PTR !< Device pointer
end type field_t
```

- Abstraction layer hiding memory management
- Hash table associating x with x_d
- Kernels invoked from the object hierarchy via C interfaces (Ax, vector ops)
  - **Wrapper functions** for each supported accelerator backend
  - **Templated** (CUDA/HIP) or **pre-processor macros** (OpenCL) for runtime parameters
- **Auto/runtime tuning** based on polynomial order

```
src/
|
|-- math
|    `-- bcknd
|         |-- cpu
|         |-- device
|         |    |-- cuda
|         |    |-- hip
|         |    `-- opencl
|         |-- sx
|         `-- xsmm
```

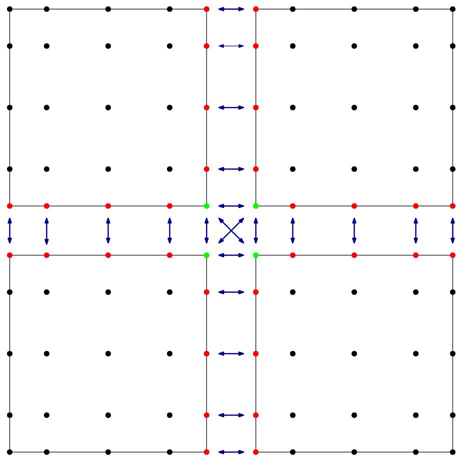
```
!> Enum @a hipError_t
enum, bind(c)
   enumerator :: hipSuccess = 0
   ...
end enum

!> Enum @a hipMemcpyKind
enum, bind(c)
   enumerator :: hipMemcpyHostToHost = 0
   enumerator :: hipMemcpyHostToDevice = 1
   ...
end enum

interface
   integer (c_int) function hipMalloc(ptr_d, s) &
        bind(c, name='hipMalloc')
     use, intrinsic :: iso_c_binding
     implicit none
     type(c_ptr) :: ptr_d
     integer(c_size_t), value :: s
   end function hipMalloc
end interface
```

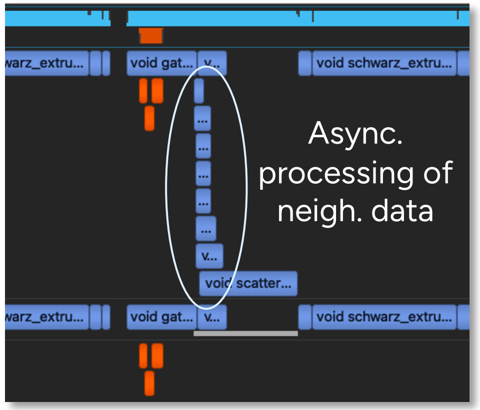
```
subroutine field_init(f,…)
type(field_t) :: f
...
call allocate(f%x(…,…,…,…,)
call device_alloc(f%x_d, size)
call device_associate(f%x, f%x_d)
```

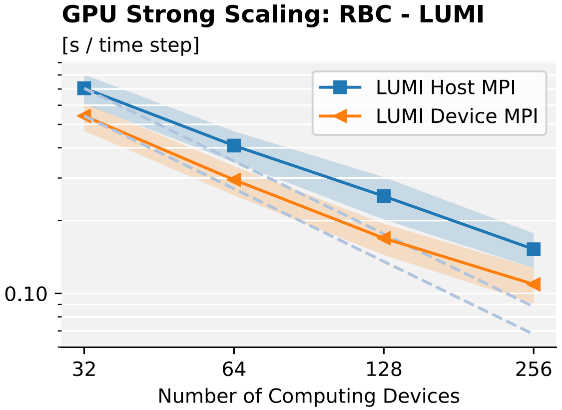
`cudaMalloc` `hipMalloc` `clCreateBuffer`

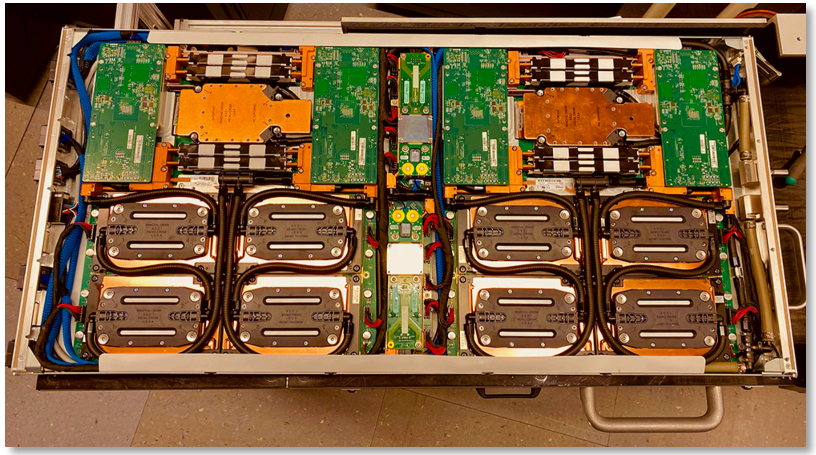
Gather-Scatter

- Uses indirect addressing and are (mostly) non-injective
- Topology aware optimisations
  - Facets (single neighbour), red points
    - Injective, **vectorizable** (always operating on **sorted** tuples)
  - Non facets (arbitrary number of neighbours), green points
    - **Cannot** be made injective, **not vectorizable** (small amount)
- Multiple levels of overlapping communication and computation
  - Overlapping with **non-blocking MPI** (device aware)
  - **Asynchronous** GPU kernels (neighbours in streams)
  - **Auto/runtime** tuning of all combinations



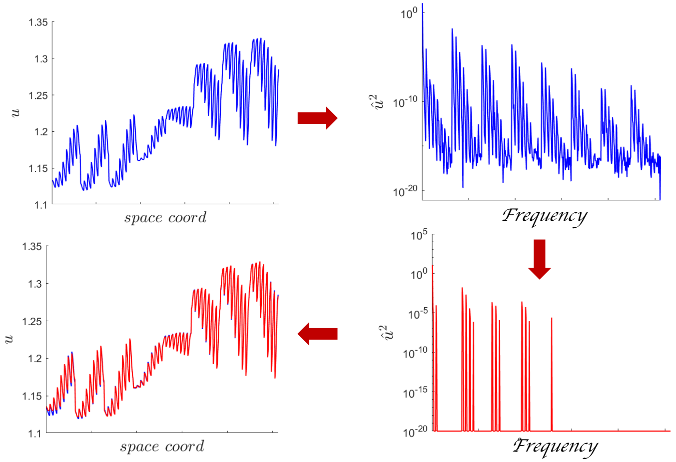






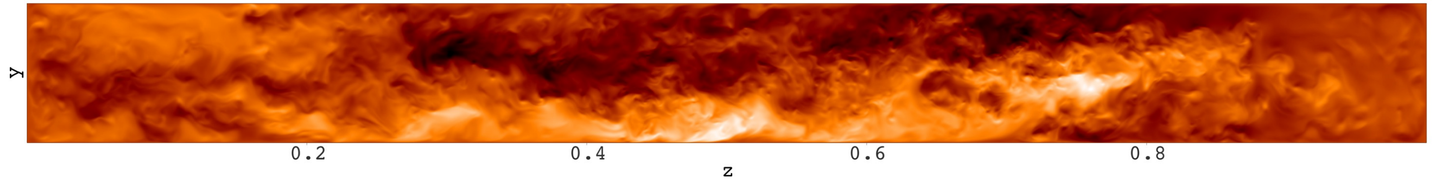
Synchronous and Hybrid Data Compression

- **Lossy compression, physics-based method:**
  discard data not associated with the most energetic flow motions[1]

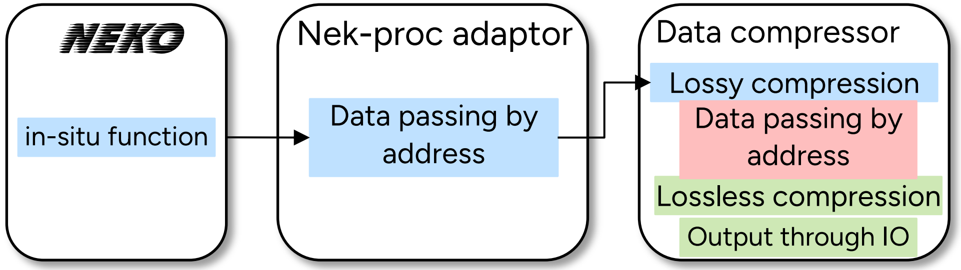


- **Lossless compression:**
  ADIOS2 operator with runtime configuration
- **97% data reduction** with a **relative error of 2.5%**

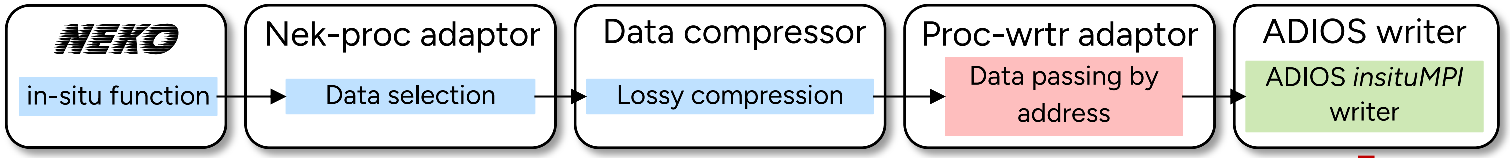
Compressed velocity field $Ra = 10^{11}$



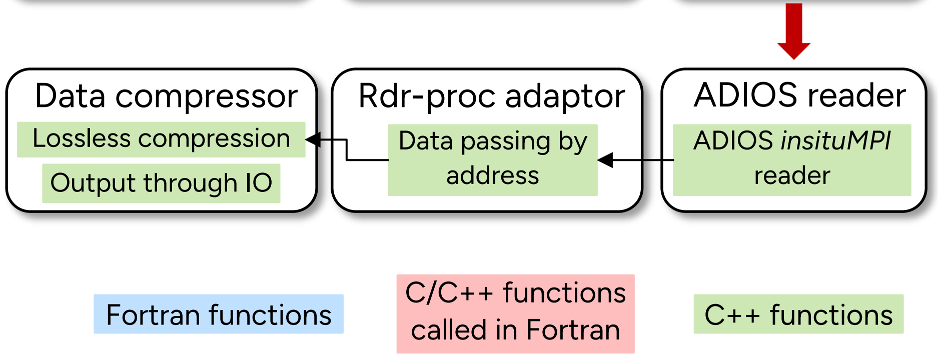
In-situ approach[2]



Synchronous compression



Hybrid compression

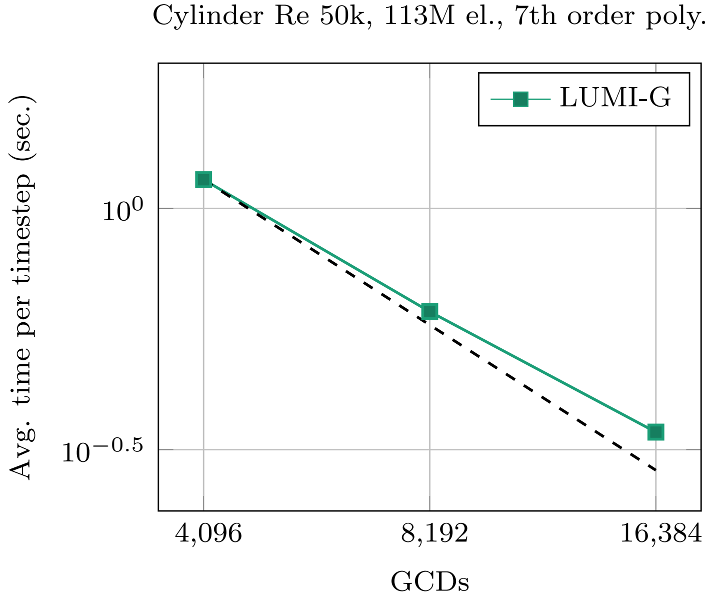


1: E. Otero et al., "Lossy data compression effects on wall-bounded turbulence: bounds on data reduction," Flow, Turbulence and Combustion, vol. 101, no. 2, pp. 365– 387, 2018.

2: Y. Ju et al., "In-Situ Techniques on GPU-Accelerated Data-Intensive Applications," eScience, 2023.

Performance Baseline

- Full machine runs towards the end of the LUMI-G pilot phase
- DNS of flow past a circular cylinder at $Re = 50{,}000$
  - 113M elements
  - 7^{th} order polynomials (8 GLL points)
- Simulation restarted from prebaked low-order runs
  - Restart checkpoint: 453GB
  - Extrapolated to 7^{th} order polynomials
  - Computed solution (snapshot): 1.5TB
- Preliminary results
  - Achieved close to 80% parallel efficiency
  - Using 20%, 40% and 80% of the entire machine



Numerical Method $P_N - P_N$

- Time integration is performed using an implicit-explicit scheme (BDFk/EXTk)

$$\sum_{j=0}^{k} \frac{b_j}{dt} u^{n-j} = -\nabla p^n + \frac{1}{Re} \nabla^2 u^n + \sum_{j=1}^{k} a_j \left(u^{n-j} \cdot \nabla u^{n-j} + f^n \right)$$

with b_k and a_k coefficients of the implicit-explicit scheme, solving at time-step n

$$\Delta p^n = \sum_{j=1}^{k} a_j \left(u^{n-j} \cdot \nabla u^{n-j} + f^n \right)$$

$$\frac{1}{Re} \Delta u^n - \frac{b_0}{dt} u^n = \nabla p^n + \sum_{j=1}^{k} \left(\frac{b_j}{dt} u^{n-j} + a_j \left(u^{n-j} \cdot \nabla u^{n-j} + f^n \right) \right)$$

- Three velocity solves using CG with block Jacobi preconditioner (**fast**)
- One Pressure solve using GMRES with an additive overlapping Schwarz preconditioner (**expensive**)

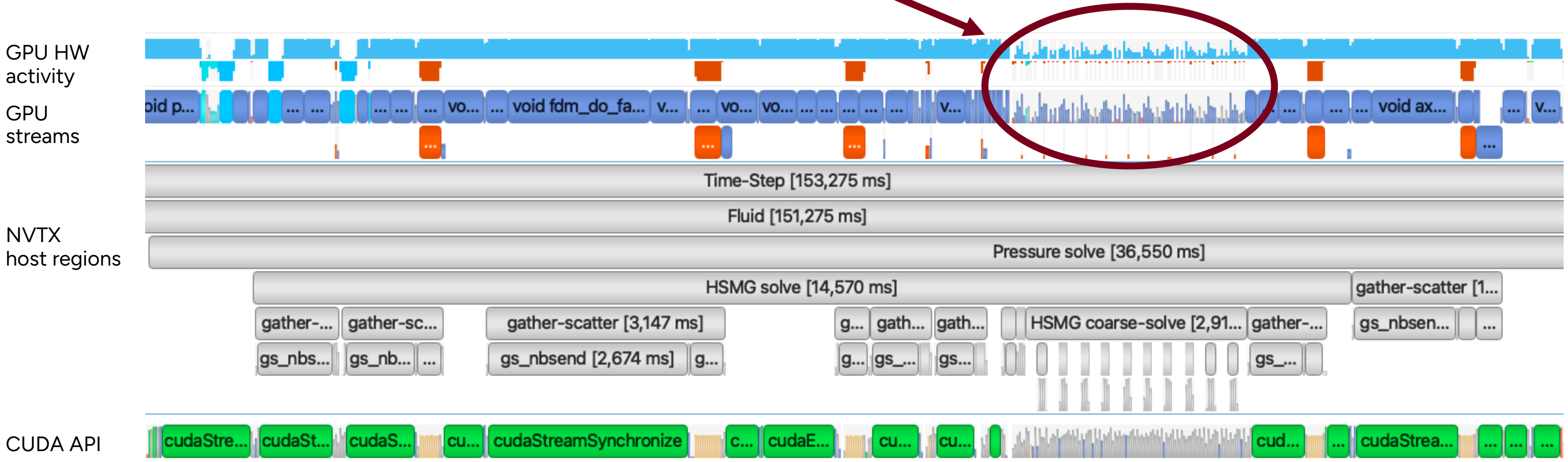
$M_0^{-1} = \underbrace{R_0^T A_0^{-1} R_0}_{\text{Coarse grid (linear elements)}} + \sum_{k=1}^{K} R_k^T \tilde{A}_k^{-1} R_k$, key is to have a **scalable coarse grid solver**

1. G.E. Karniadakis, M. Israeli, S.A. Orszag, High-order splitting methods for the incompressible Navier-Stokes equations, J. Comput Phys, 1991

Additive Schwarz Preconditioner on GPUs

- Coarse grid solved using an approximate Krylov solver
  - Preconditioned Pipelined Conjugate Gradient with a low, maximum iteration limit
- Low computational efficiency on GPUs
  - A_0 is on linear elements, too little data to keep the GPU busy.
  - Many small kernels, dominated by kernel launch latency

$$M_0^{-1} = R_0^T A_0^{-1} R_0 + \sum_{k=1}^{K} R_k^T \tilde{A}_k^{-1} R_k$$



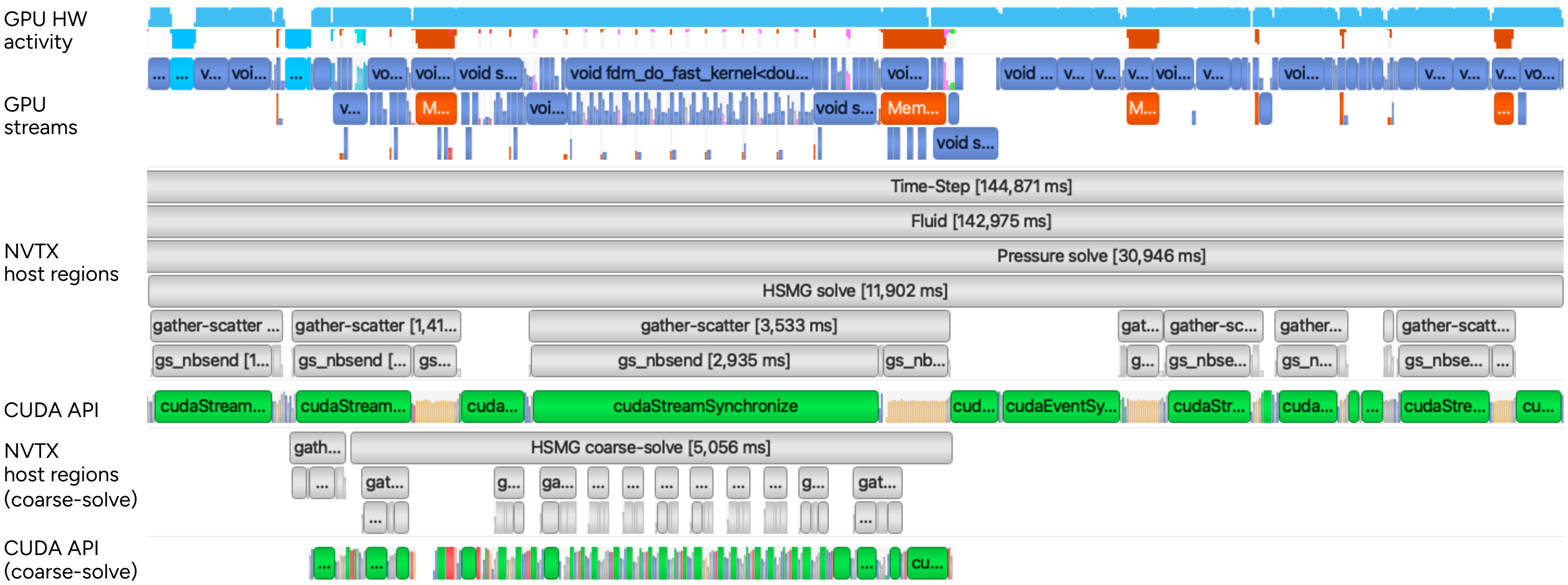
Task-decomposed Overlapped Preconditioner

- Exploit available **task-parallelism**
  - Launch the left and right part of M_0^{-1} in parallel on the device
  - Launch independent work in parallel from **different threads** in an OpenMP region
  - Launch tasks in **separate streams** to allow overlap and increase GPU utilization
  - Maximise kernel overlap using **stream priority** to ensure progress in both stream

Thread 0   Thread 1

$$M_0^{-1} = R_0^T A_0^{-1} R_0 + \sum_{k=1}^{K} R_k^T \tilde{A}_k^{-1} R_k$$

Stream 1   Stream 2



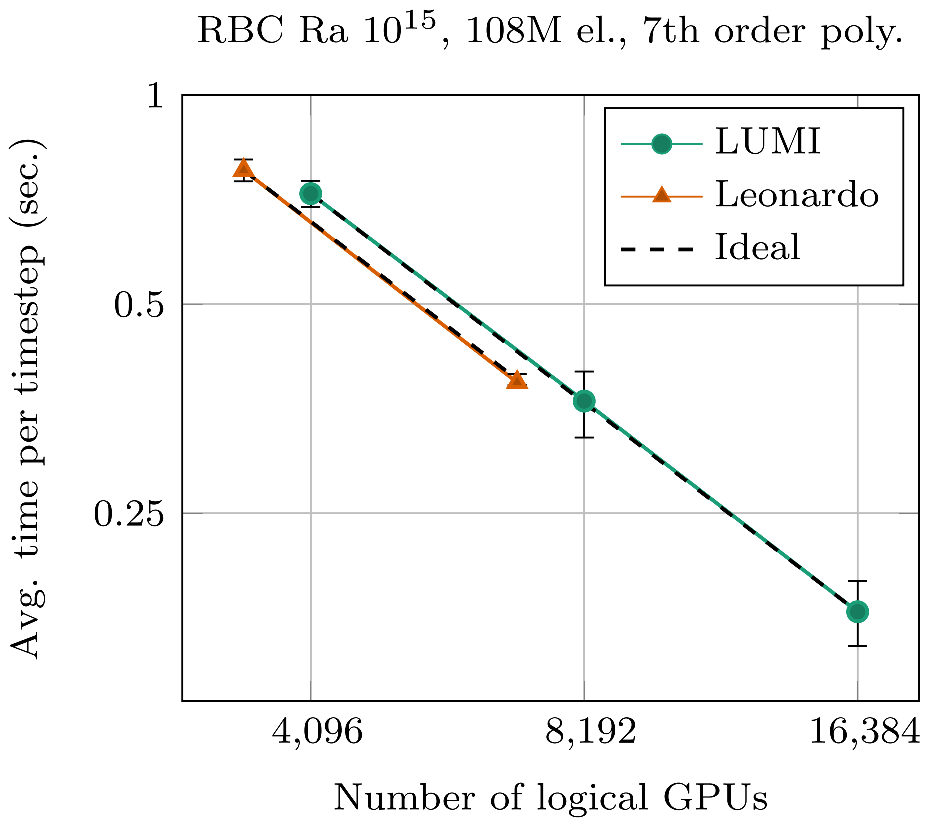
Performance Results

- Performance measurements on two of the EuroHPC-JU pre-exascale supercomputers **LUMI** and **Leonardo**
- Experiments were performed between
  - March–April 2023 on LUMI
  - April 2023 on Leonardo (pre-production)
- RBC in a cylinder with aspect ratio 1:10
  - $Ra = 10^{15}$
  - 108M elements, 7^{th} order polynomials
  - 37B unique grid points and more than 148B degrees of freedom
- Strong Scalability
  - Average time per timestep (after transient)
- One MPI rank per logical GPU
  - One rank per GCD (AMD)
  - One rank per device (Nvidia)

System	**LUMI**	**Leonardo**
Computing device	AMD MI250X	Nvidia A100 (custom)
Peak Tflop FP64/s	47.9 (95.7 Matrix)	11.2 (22.4)
Peak BW/s	3300	1640
No. devices	10240	13824
Interconnect	HPE Slingshot 11 200 GbE NICs (4x200 Gb/s)	Nvidia HDR 2x(2x100 Gb/s)
MPI	Cray MPICH 8.1.18	OpenMPI 4.1.4
Compiler	CCE 14.0.2	GCC 8.5.0
GPU Driver	5.16.9.22.20	520.61.05
CUDA/ROCm	ROCm 5.2.3	CUDA 11.8

Performance Results

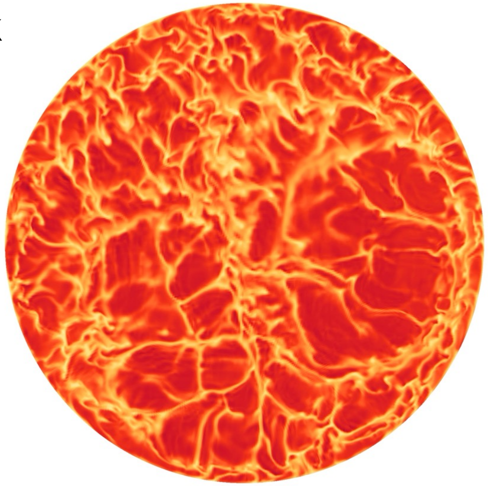
- Close to perfect parallel efficiency on both LUMI and Leonardo
- Close to perfect parallel efficiency with less than 7000 elements per logical GPU
- Significantly reducing the smallest required problem size for strong scalability limits
- Improvements mainly due to the new overlapped pressure preconditioner



99% confidence intervals is illustrated as error bars

Summary

- Insight into Rayleigh-Bénard convection
  - The question about an ultimate regime can only be settled through simulations made possible through the developments in this work
- In-situ data processing
  - Hybrid data compression, streaming data to the CPU for online post-processing
    while the simulation continues to run on the GPU
  - New ways of analysing and processing data from simulations
- Task-decomposed overlapped pressure preconditioner
  - Expressing more of the available concurrency of the application
  - Key ingredient to achieve good strong scalability on LUMI and Leonardo



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NEKO

SeRC Swedish e-Science Research Centre

Swedish Research Council

CEEC

DEEP-SEA

EXCELLERAT

LUMI

LEONARDO

EuroHPC Joint Undertaking

ADMIRE malleable data solutions for HPC

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