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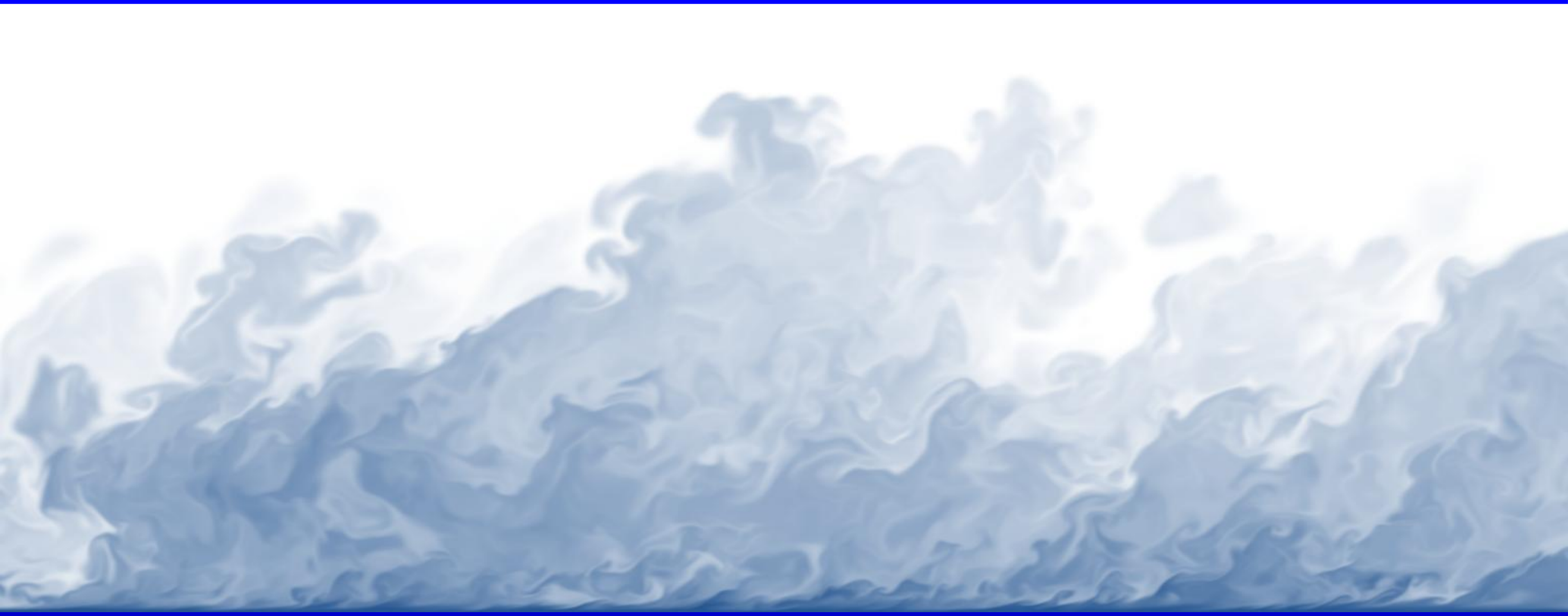

One Year of HUNTER from a User Perspective: Progress, Performance, and Patience with NS3D

Christoph Wenzel

WSSP 2026

April, 2026

Introduction – Boundary-layer group

Christoph Wenzel

Boundary Layers

Tobias Gibis

DNS Compressible Turbulence

Jason Appelbaum

DNS Compressible Turbulence

Abissan Suntharajan

DNS Compressible Turbulence

Leander Düntsch

DNS Transition Control

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EXPERIMENT Transition Control

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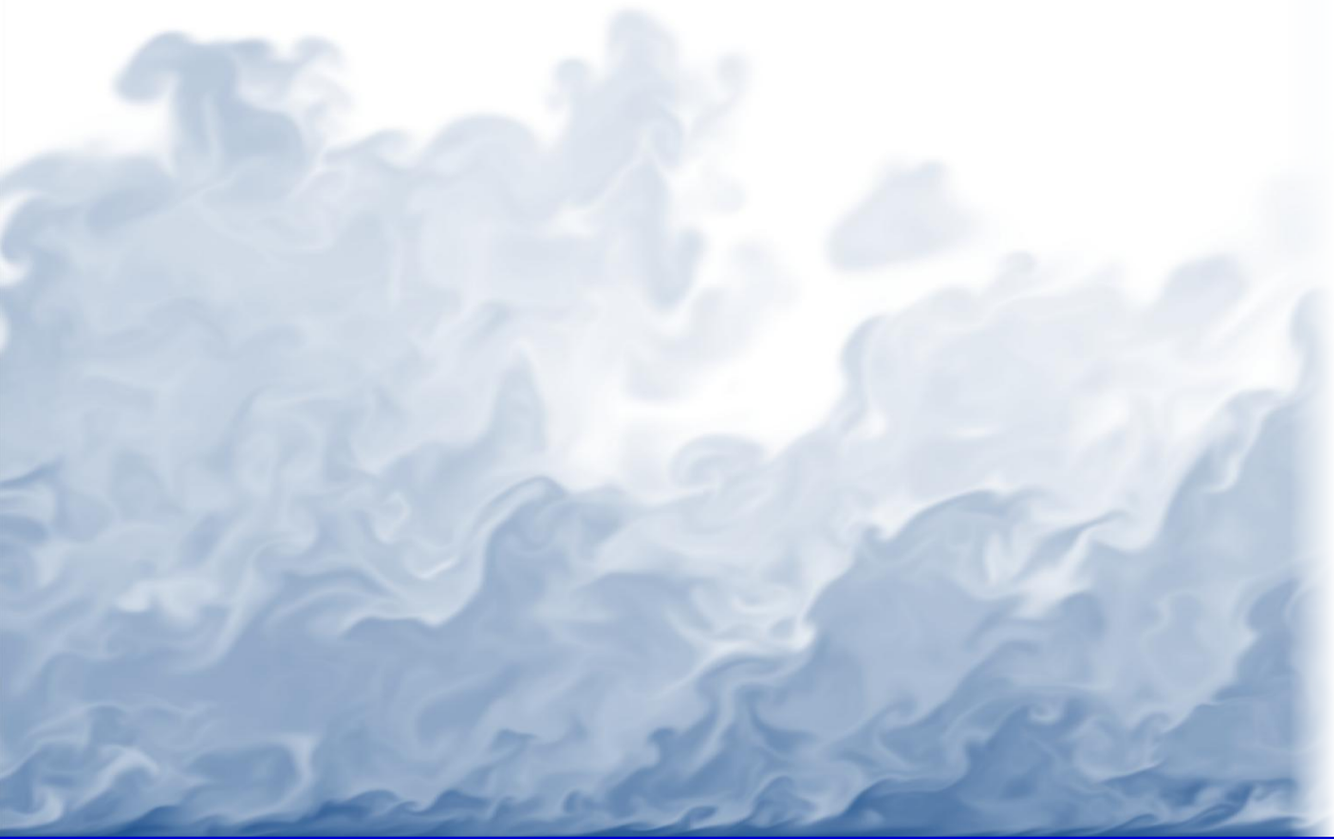

Introduction

NS3D GPU Porting Status

Performance insights

- Performance sensitivity to
  - MPI decomposition
  - Rank ordering
- Scaling behaviour

Summary/Conclusions

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Rendering: Wenzel

Christoph Wenzel

Paradigm

In a certain sense, understanding boundary layers can be assessed by the ability to predict their behavior for arbitrary boundary conditions.

Task:

Solve the governing equations:

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j\right) = 0$$

Conservation of momentum:

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_j}\left(u_i \rho u_j\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}$$

Conservation of total inner energy:

$$\frac{\partial}{\partial t}\left(\rho E\right) + \frac{\partial}{\partial x_j}\left(u_j \rho H\right) = \frac{\partial}{\partial x_j}\left(u_i \sigma_{ij}\right) + \frac{\partial q_j}{\partial x_j}$$

with: $\sigma_{ij} \approx 2\mu\left(S_{ij} - \frac{1}{3} S_{kk}\delta_{ij}\right)$ $S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ and: $q_j = -k\frac{\partial T}{\partial x_j}$

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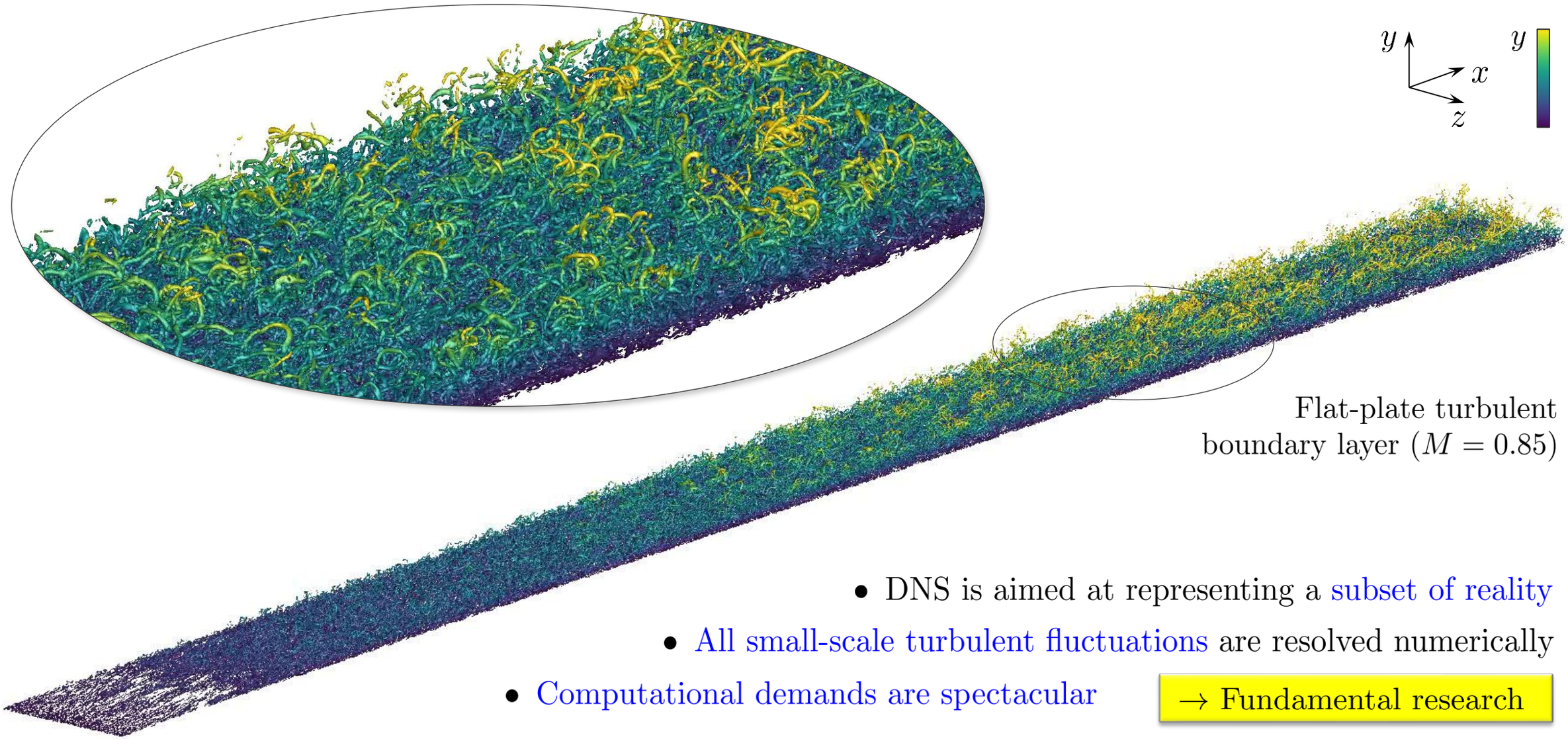
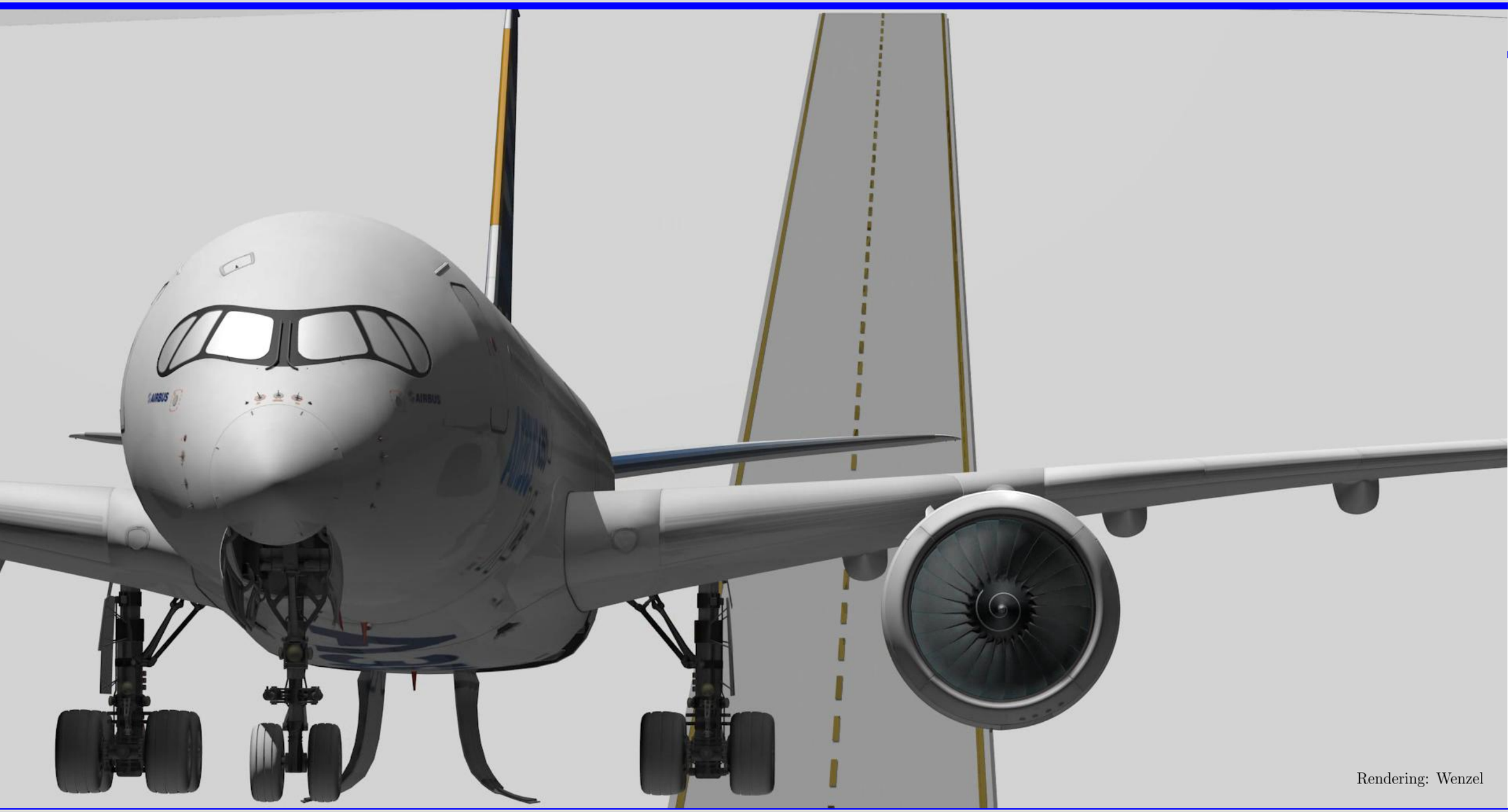


Flat-plate turbulent
boundary layer ($M = 0.85$)

- DNS is aimed at representing a subset of reality
- All small-scale turbulent fluctuations are resolved numerically
- Computational demands are spectacular

→ Fundamental research



Rendering: Wenzel

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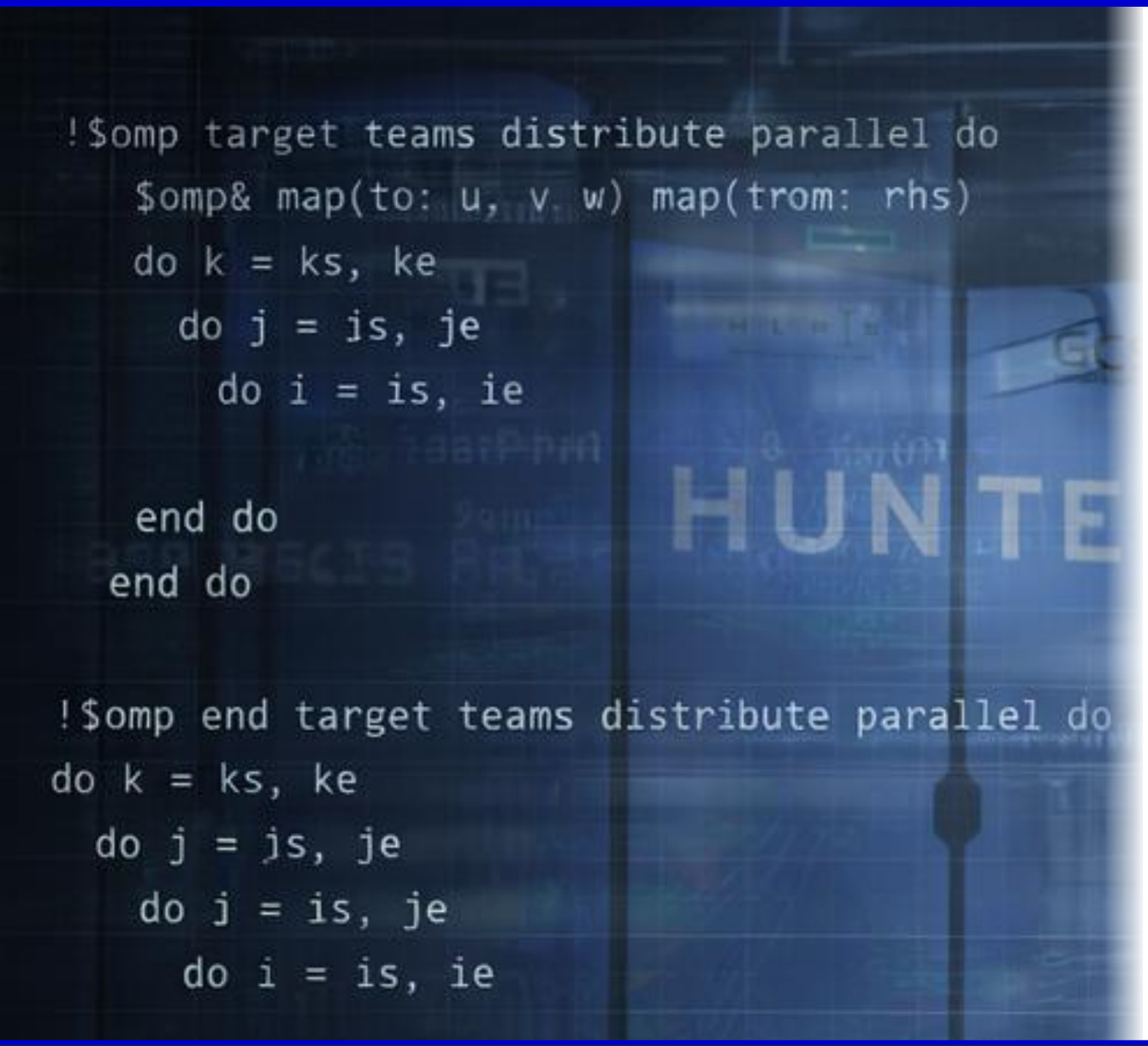
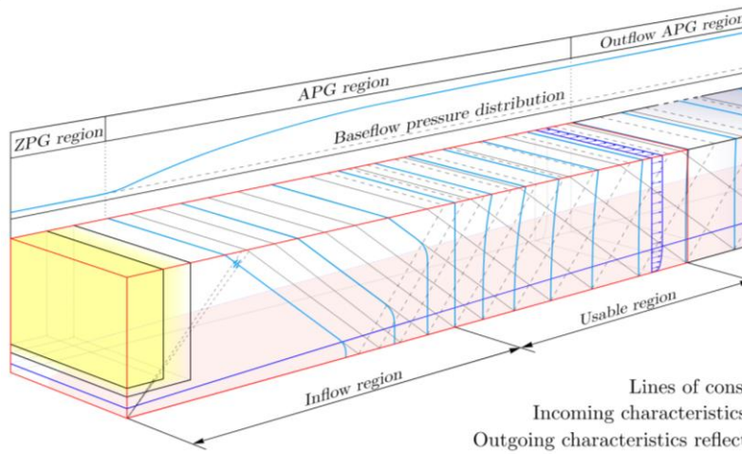


NS3D: Basic information

- NS3D is a compressible Navier–Stokes finite-difference solver for fundamental research
- First version developed between 2005–2008
- Current version stems from a major rewrite and refactoring (2017–2018)

Language	Modern Fortran
Domain Decomposition	Full 3D domain decomposition
Parallelization (CPU)	Hybrid: MPI + OpenMP
GPU Porting	staying with OpenMP



NS3D: Porting to GPU

- **Setup and early decisions (2024)**
  - GPU port of NS3D using OpenMP, with support from HLRS, HPE, and AMD
- **September 2024**
  - Start of porting effort using partially ported version for Hawk AI (NVIDIA A100) by HPE
  - Major issues: differences between NVHPC, Cray, and AMD compilers
  - AMD ecosystem (Cray, AMD) less mature
  - Many compiler bugs and missing features significantly slowed development
- **March 2025**
  - First correct Taylor–Green vortex with all numerical schemes
- **June 2025**
  - First correct turbulent boundary layer case
- **August 2025**
  - First stable GPU version for production-case development
- **September 2025: Status at WSSP**
  - Some rare issues remain
  - Workarounds still present in parts of the code

2 days per week each

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- **Status September 2025**
  - Production cases are running stably (small and large scale)

?

2 days per week each

- Many setbacks e.g. due to software-stack updates exposing previously hidden bugs in our code (mainly affecting large cases), along with limited MPI decomposition robustness
- Extensive debugging effort, largely relying on trial-and-error (and a fair amount of guesswork)
- Mystery bugs: random NaNs or Infs in major arrays, HDF5 interface randomly fails

- **Today (April 2026)**
  - Production cases are running stably (small and large scale)

A small collection of problems

- Derived types (e.g. `Pvec%u`) not reliably usable inside kernels
  → Solution: Use pointer-based access before entering kernels (e.g. `u` → `Pvec%u`)
- Cray compiler has a limited number of arrays per kernel (≈ 120 arrays)
  → Solution: Split very large kernels
- NaNs/Infs are not reliably detected by the compiler
  → Solution: Custom GPU kernels to check for NaNs at regular intervals
- `firstprivate` scalars are not passed correctly to `declare target` functions
  → Solution: Use the `value` attribute
- Arrays slicing in kernel routines causes issues
  → Solution: Avoid slicing inside kernels
  → Note: Rewrite critical parts (e.g. reduced I/O) using explicit loops
- ...

NS3D modernization for heterogeneous GPU systems

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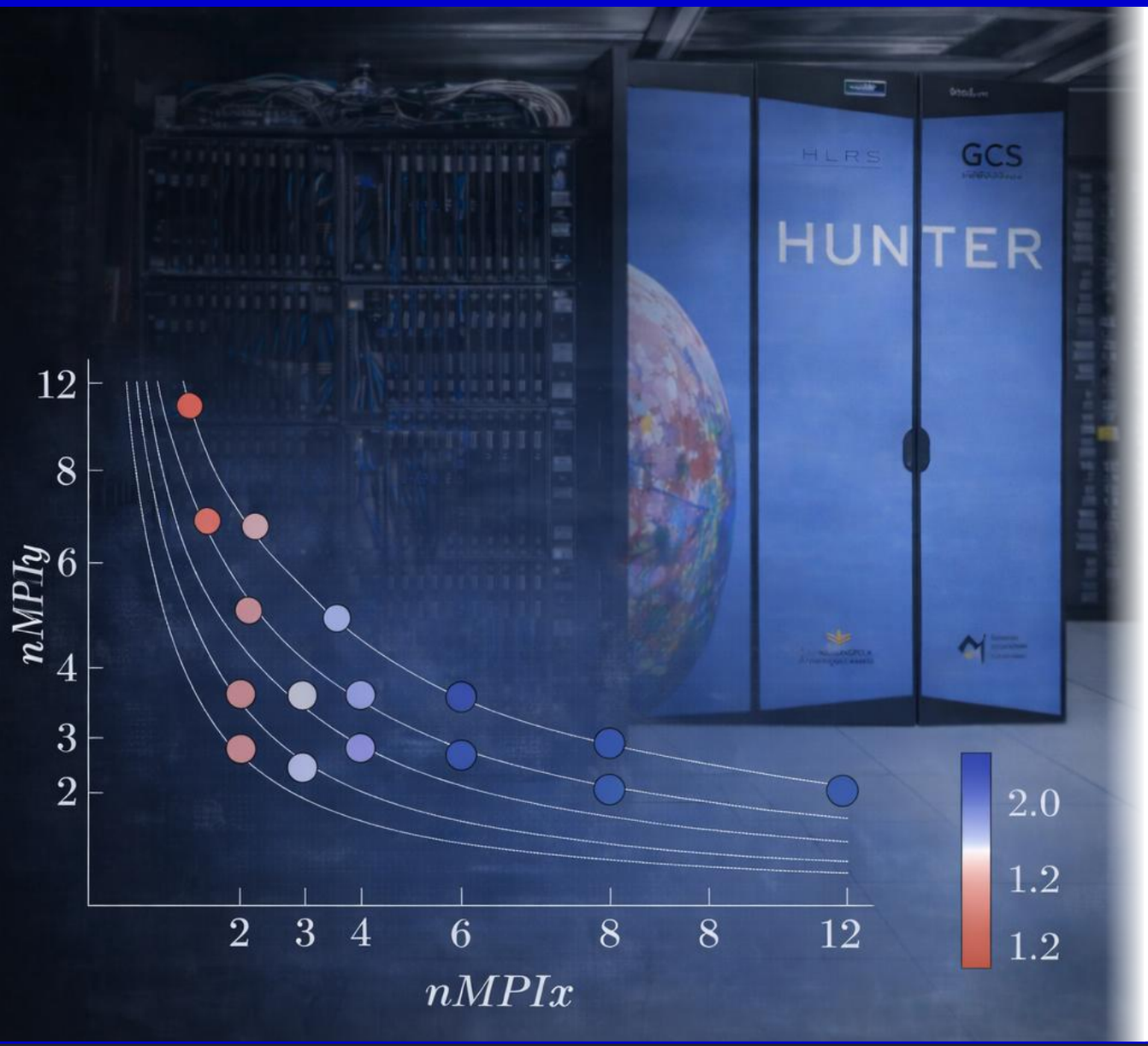
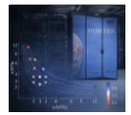
- Ported NS3D to multiple GPU platforms (LUMI, Leonardo)
  - Extended support beyond USM-based architectures
  - Introduced a new memory management strategy
  - Addressed compiler differences in OpenMP offloading
  - Enabled modern Fortran data structures on GPUs
  - Improved code stability through systematic debugging and runtime checks
  - Started performance optimization focusing on the main bottlenecks

- **Current status:** Stable production runs established; final NS3D_{neo}.develop version expected soon
- NS3D_{neo}.develop runs in both USM and non-USM modes





Characterization of NS3D$_{neo}$.develop on HUNTER

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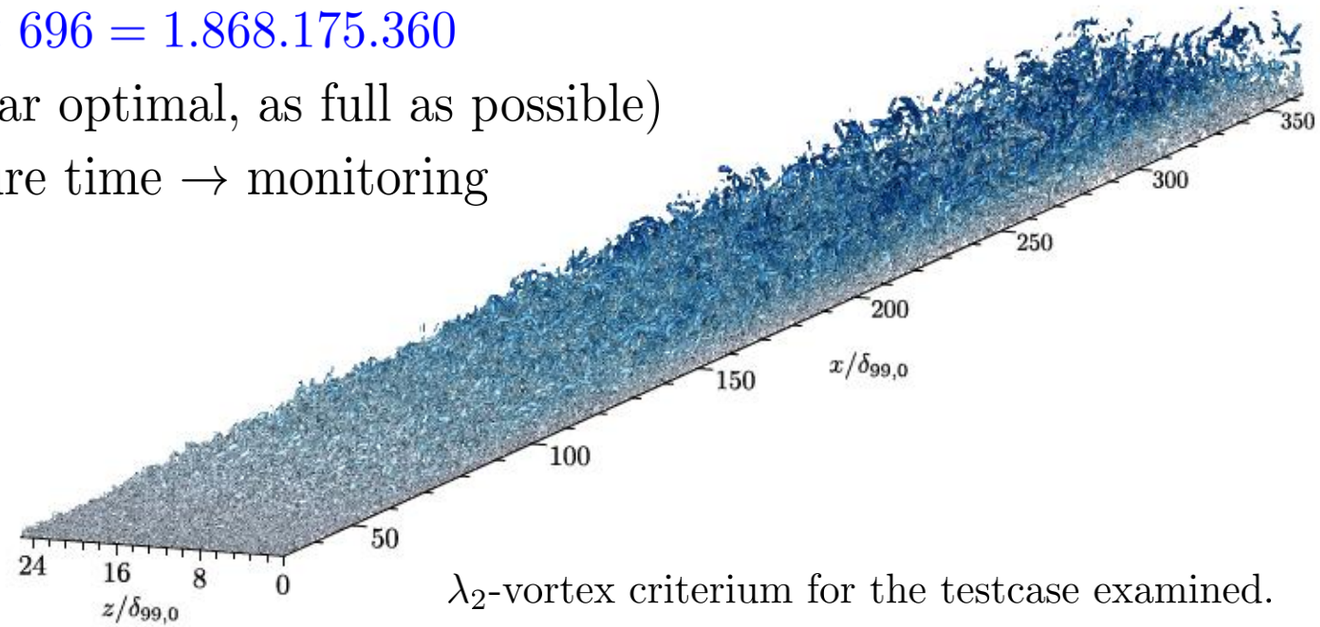
- DNS of a spatially developing turbulent boundary layer
- Grid stretching in streamwise and wall-normal direction (requiring grid transformations)
- Turbulent inflow condition (random-number-based)
- Spatial filtering is applied

Domain size has been chosen to fit on 12 nodes (48 MPI ranks, 1 MPI rank per APU):

- Total number of grid points: $5592 \times 480 \times 696 = 1.868.175.360$
- Grid points per MPI rank: 38.920.320 (near optimal, as full as possible)
- Procedure: Run 1000 time steps → measure time → monitoring
- Postprocessing



λ_2-vortex criterium for the testcase examined.

Performance Sensitivity: MPI Decomposition and Rank Ordering

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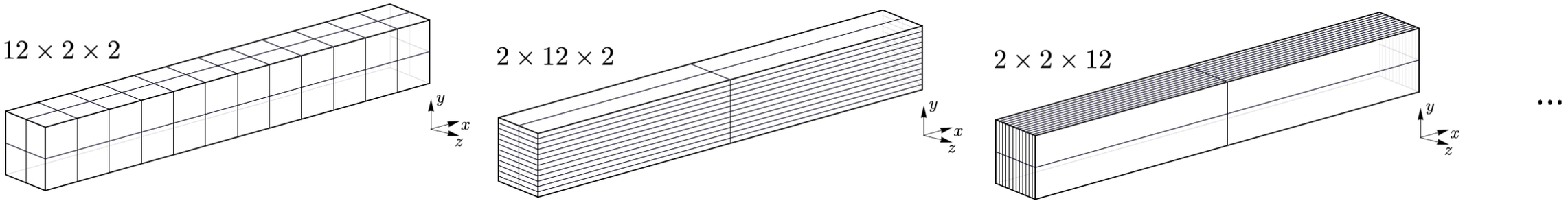
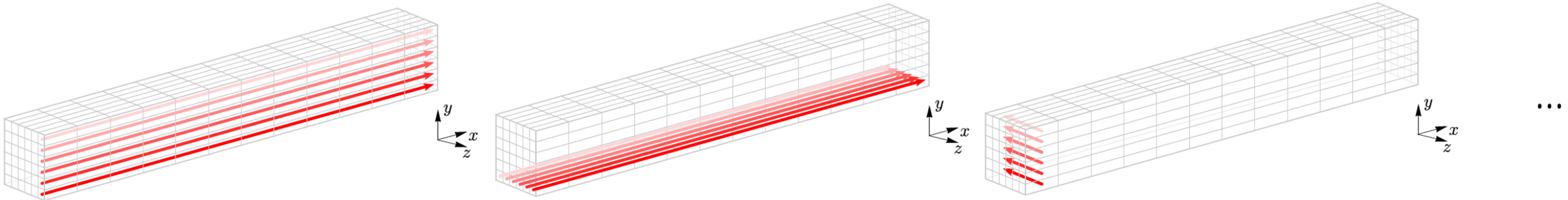
All permutations of the 3D MPI domain decomposition were tested ($12 \times 2 \times 2$, $2 \times 12 \times 2$, ...), with a fixed total of 48 MPI ranks:



All permutations of the 3D MPI rank ordering were tested (`xyz`, `xzy`, ...):



Total: 108 cases

MPI decomposition: $12 \times 2 \times 2$ (xyz-ordering)

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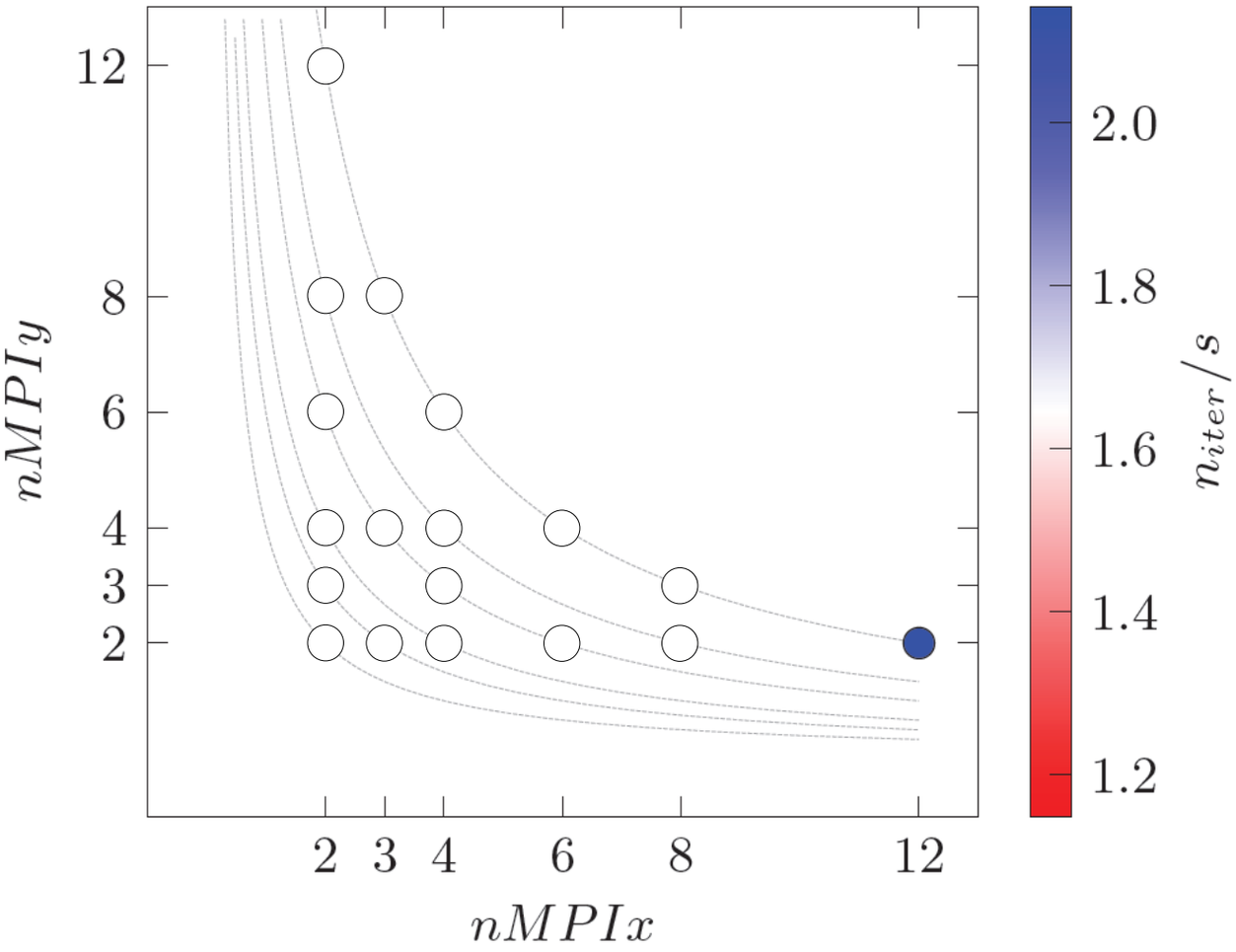
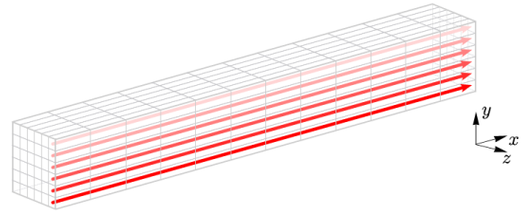
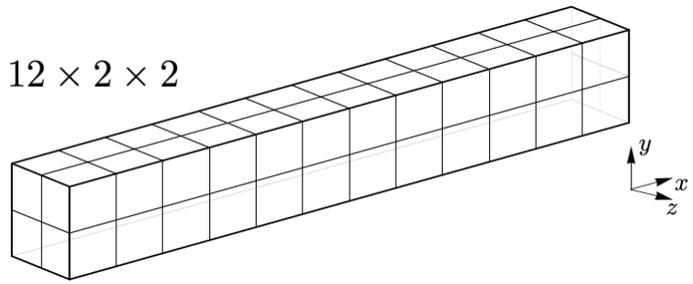





```
1  do k = 1, ...
2     do j = 1, ...
3        do i = 1, ...
4                 ...
5        end do
6     end do
7  end do
```



MPI decomposition: $2 \times 12 \times 2$ (xyz-ordering)

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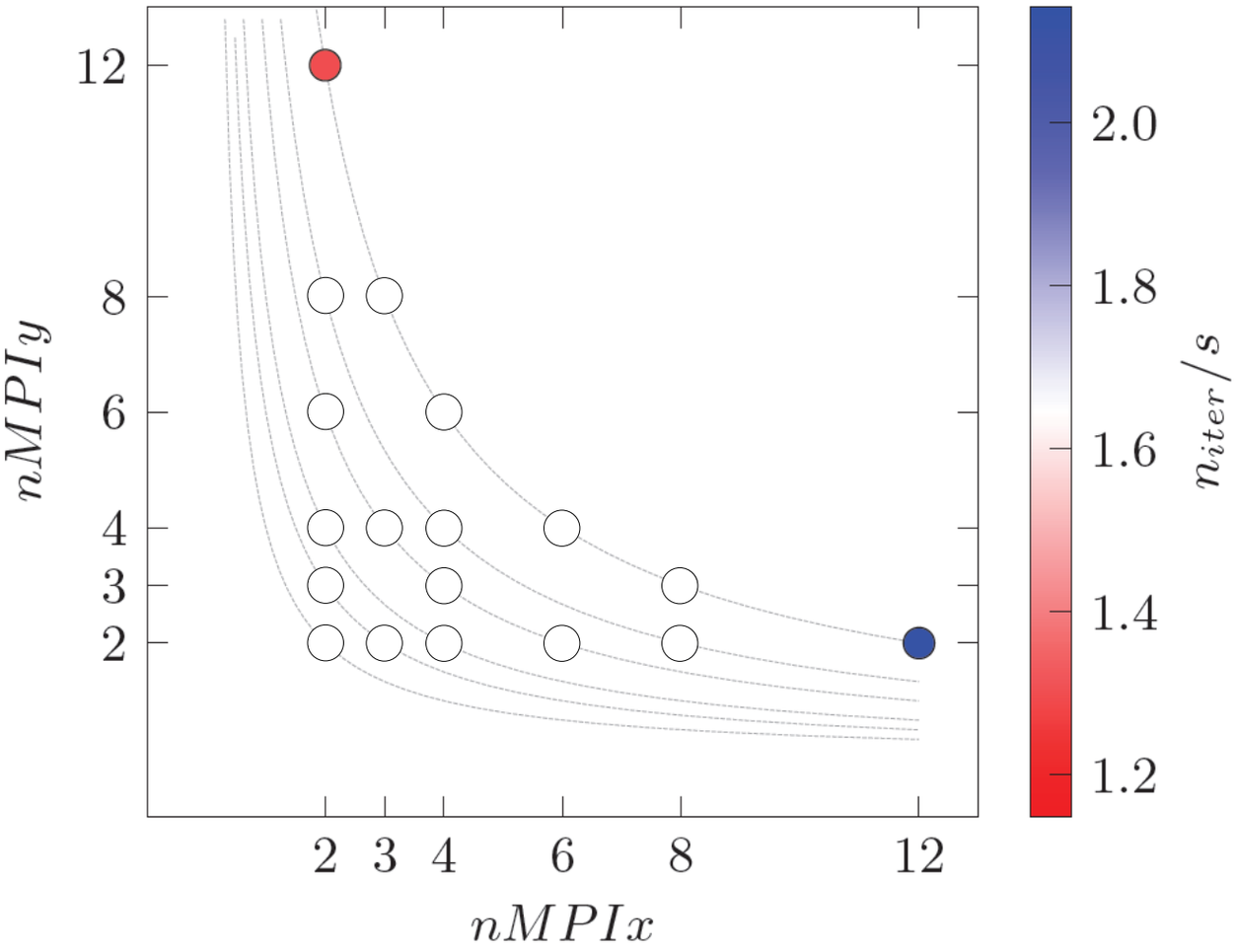

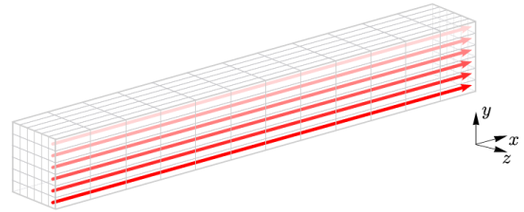


```
1  do k = 1, ...
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3        do i = 1, ...
4                 ...
5        end do
6     end do
7  end do
```
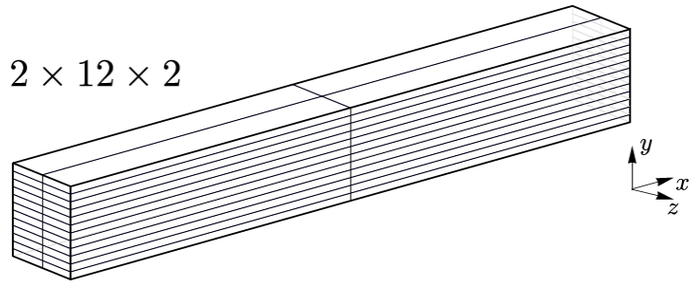

$2 \times 12 \times 2$



MPI decomposition: $2 \times 2 \times 12$ (xyz-ordering)

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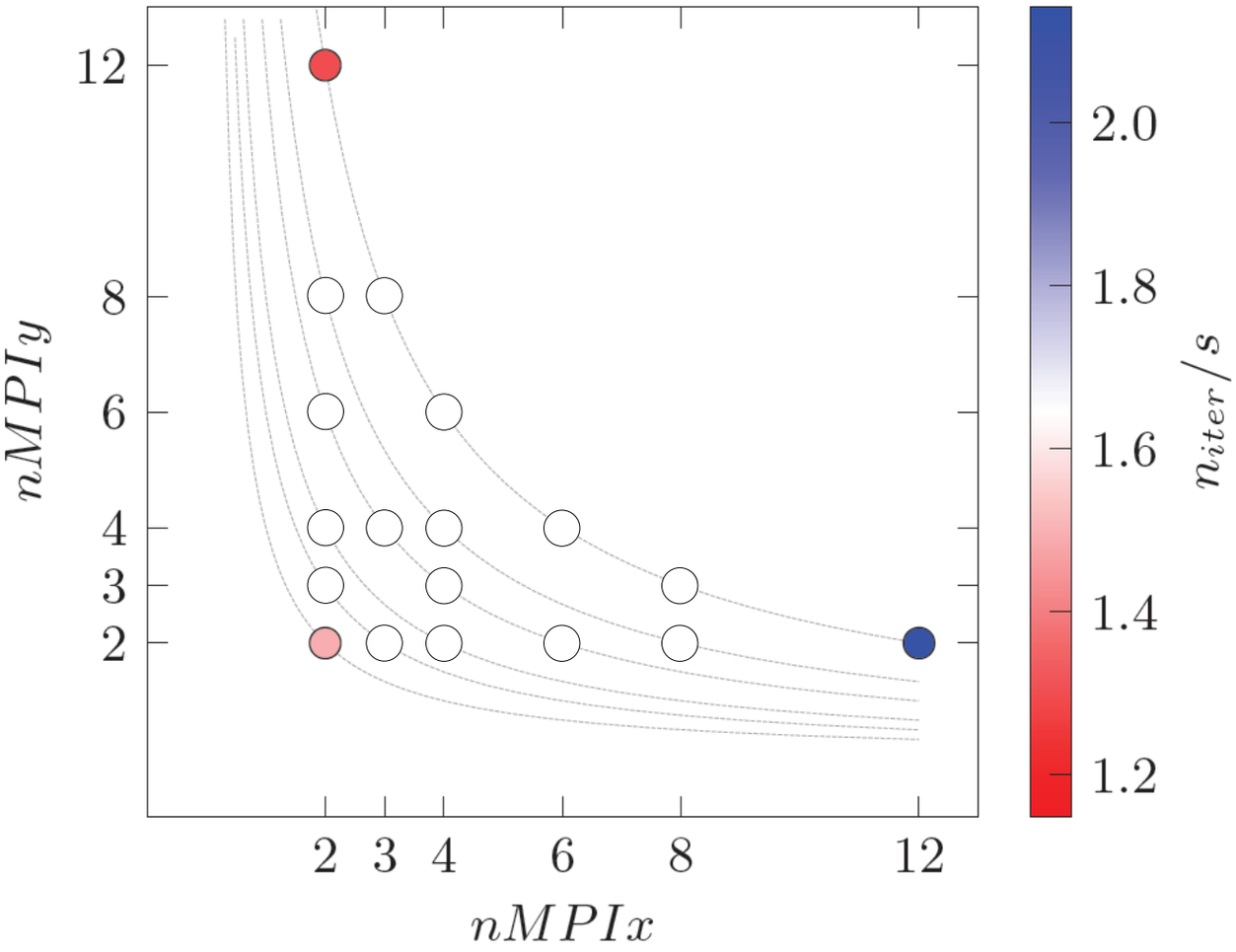

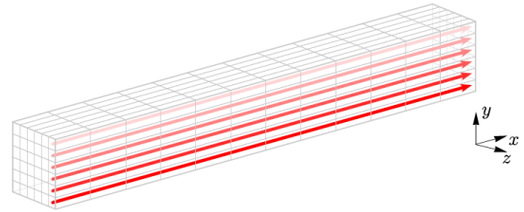


```
1  do k = 1, ...
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6     end do
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```
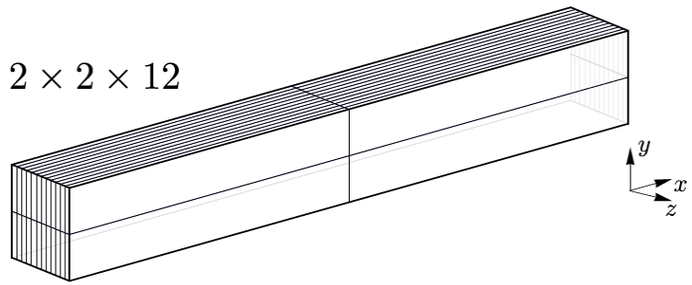

$2 \times 2 \times 12$



MPI decomposition (xyz-ordering)

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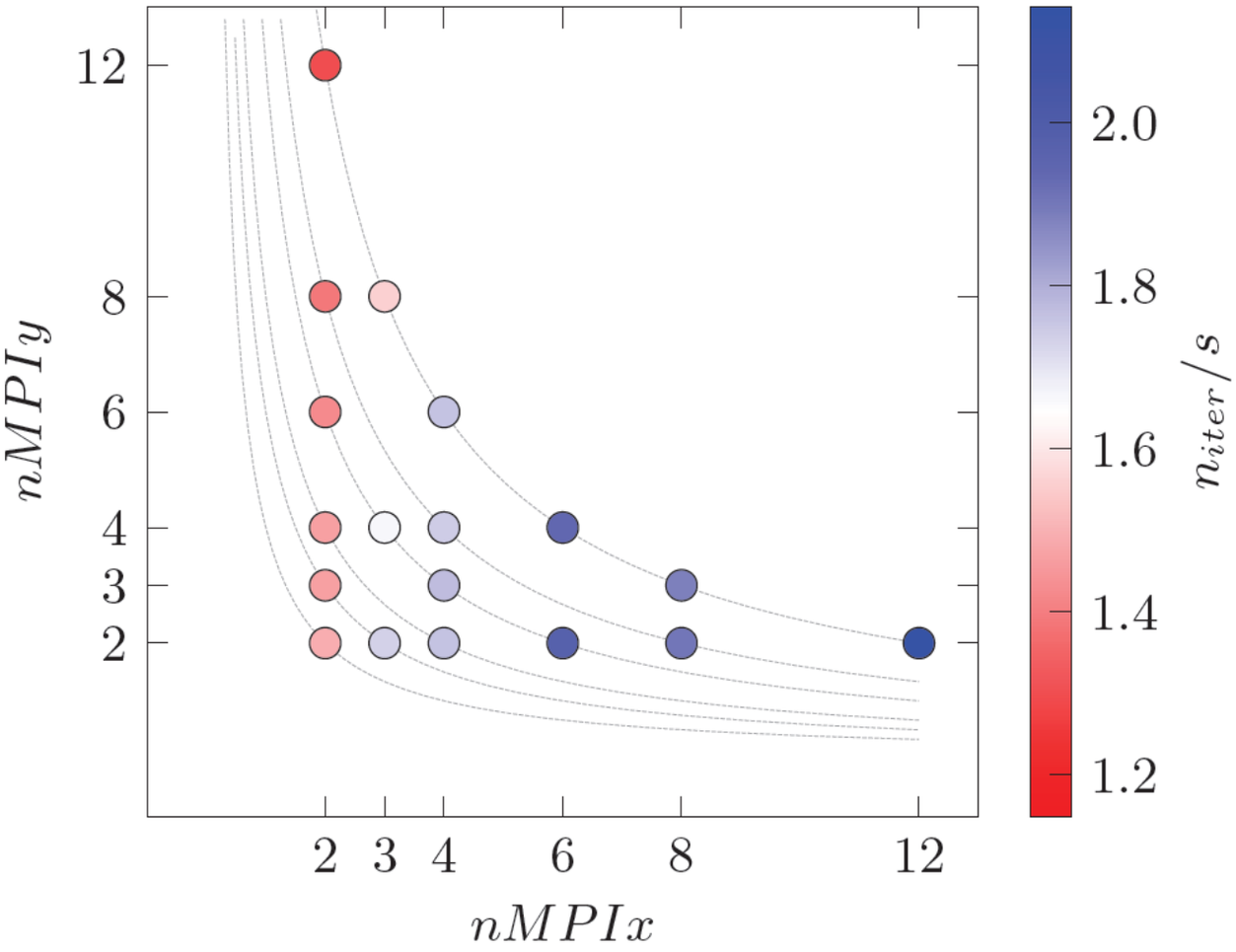

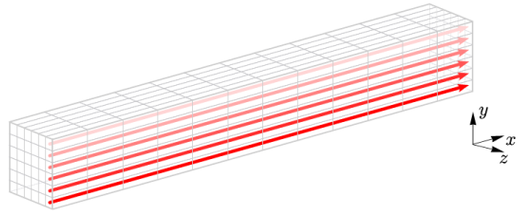


```
1  do k = 1, ...
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5        end do
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7  end do
```

MPI decomposition: $12 \times 2 \times 2$ (xyz-ordering)

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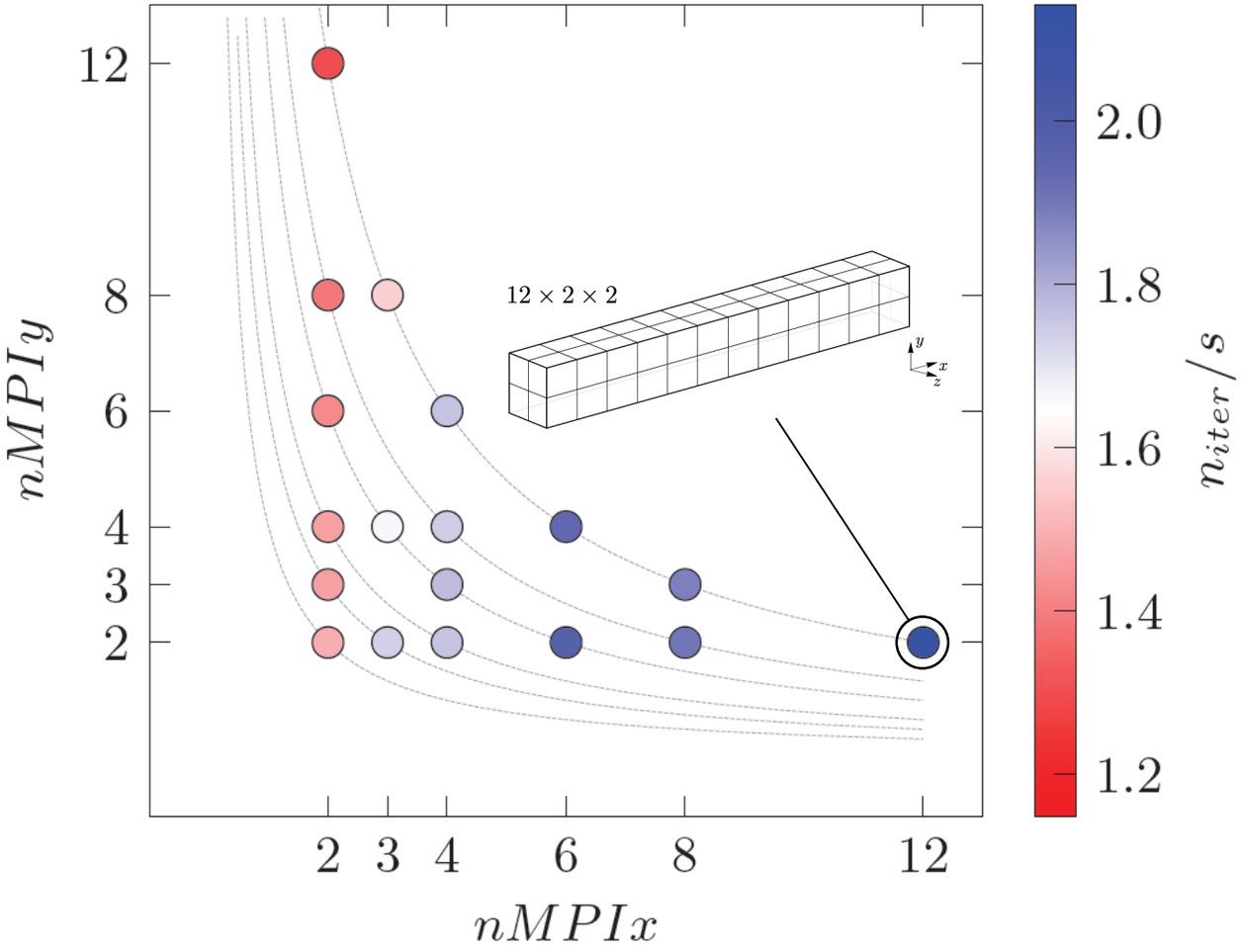

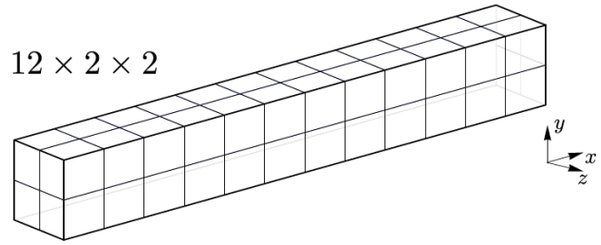

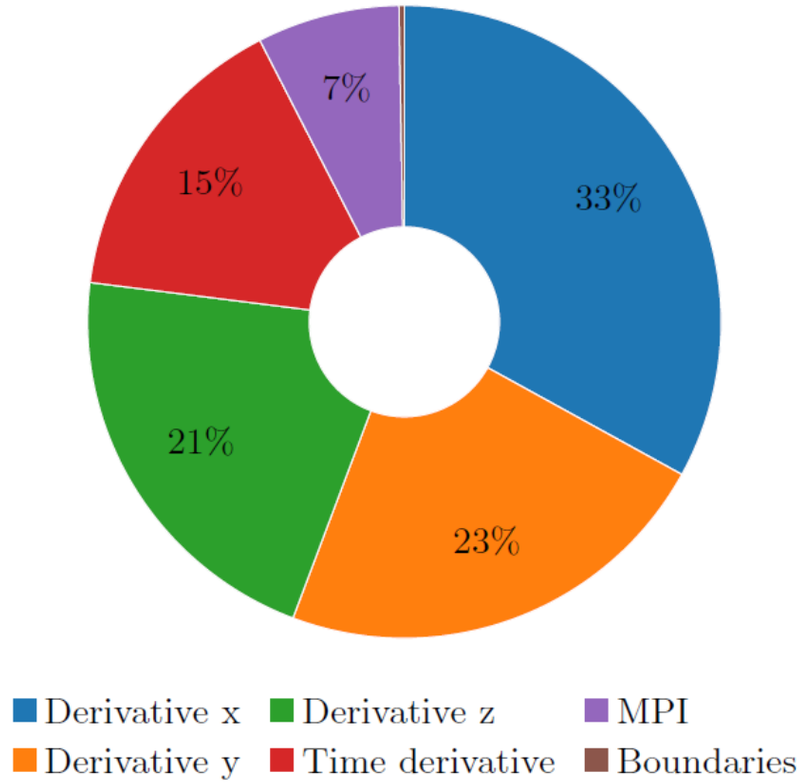

MPI decomposition: $12 \times 2 \times 2$ (xyz-ordering)

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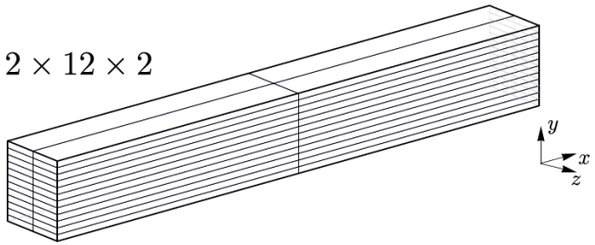
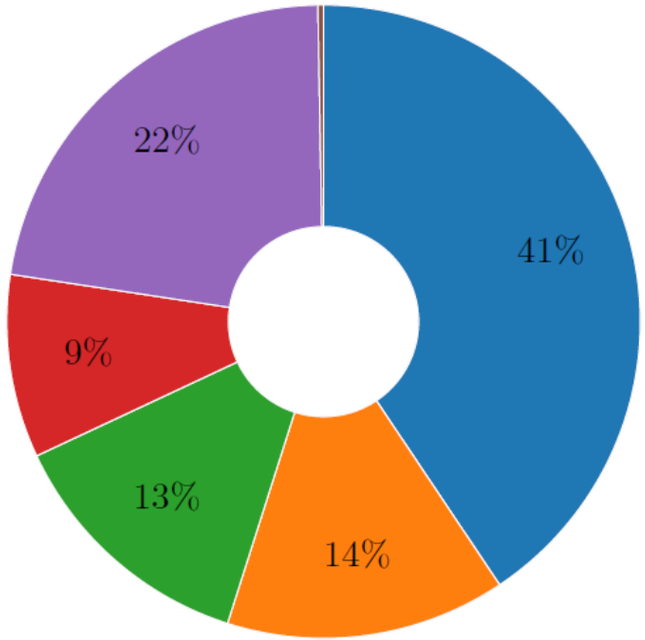
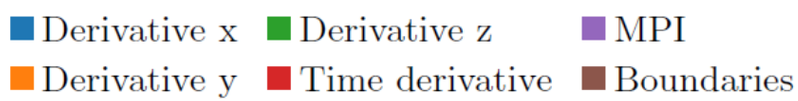
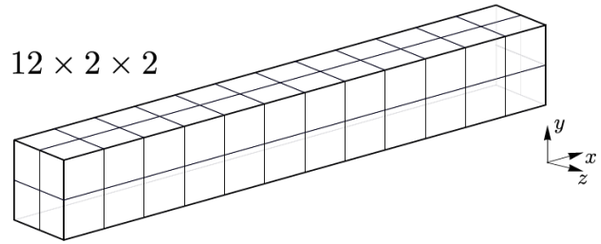
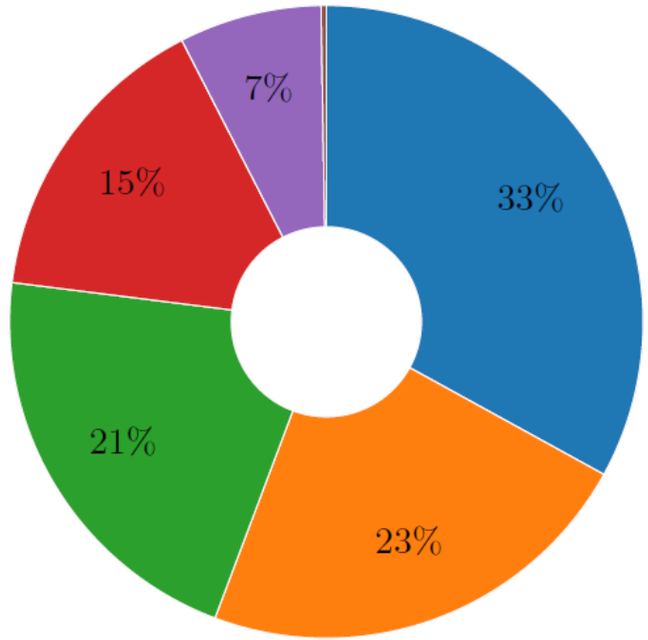
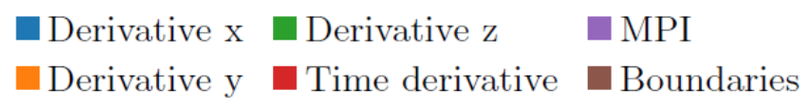




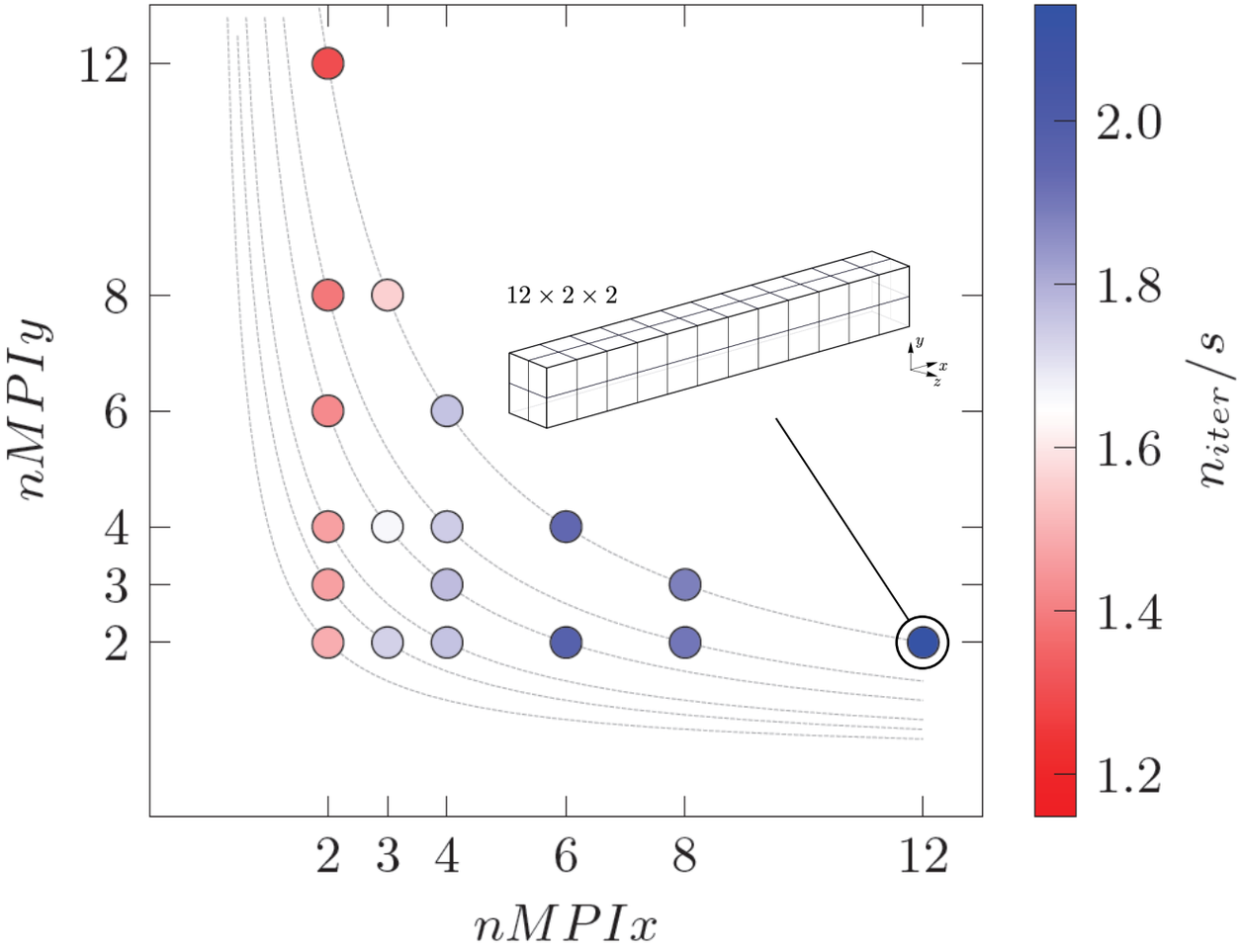


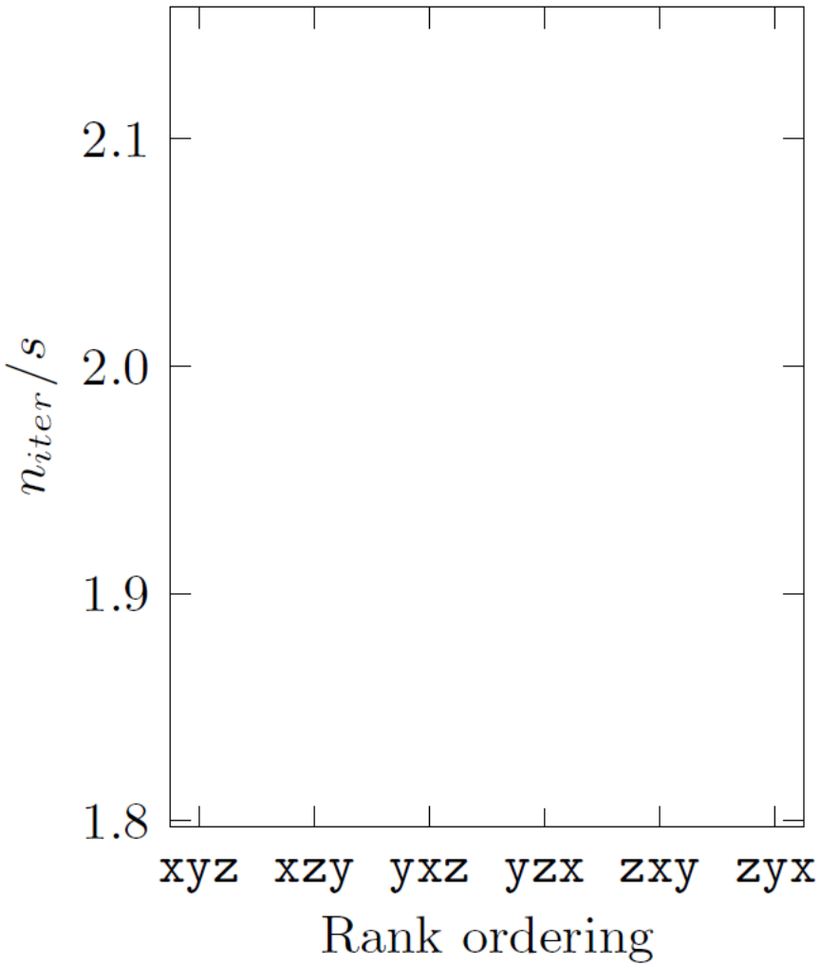






MPI decomposition: Influence of rank ordering





MPI decomposition: Influence of rank ordering

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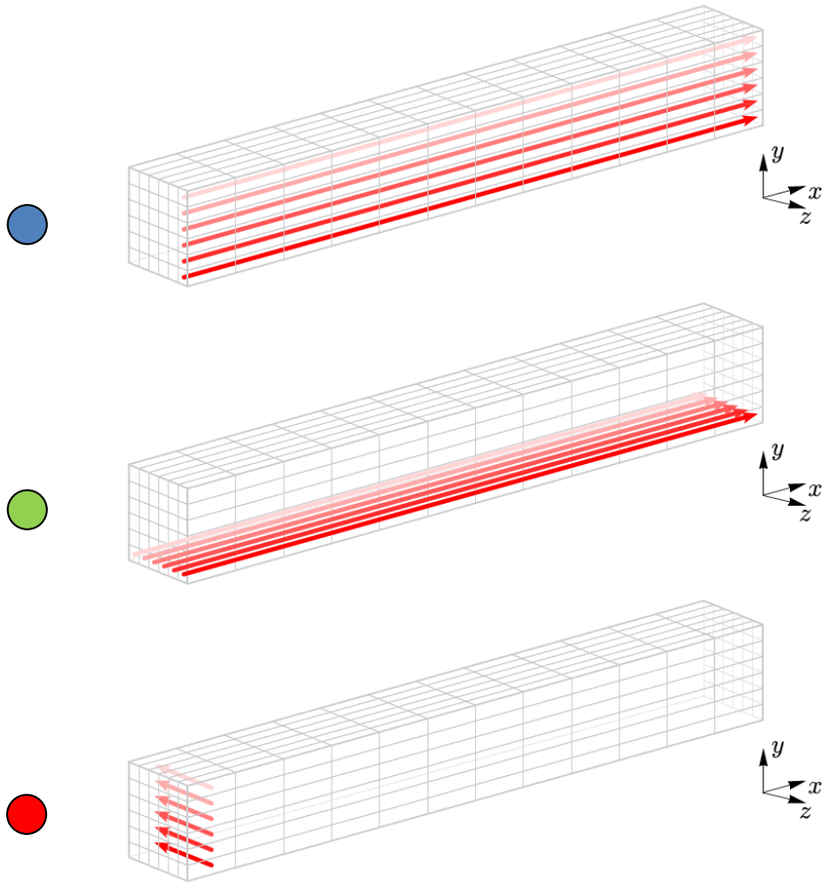

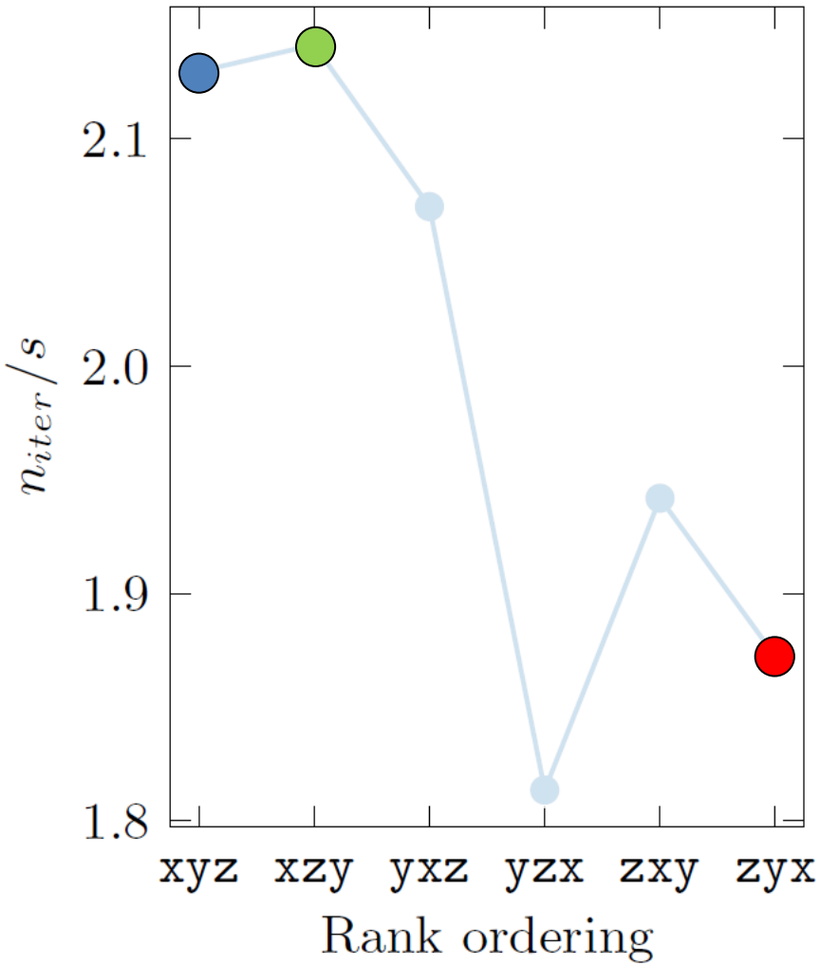

Summary: Bringing everything together...

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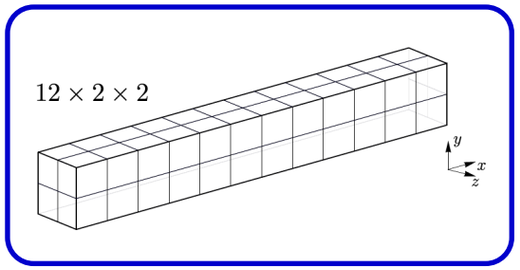

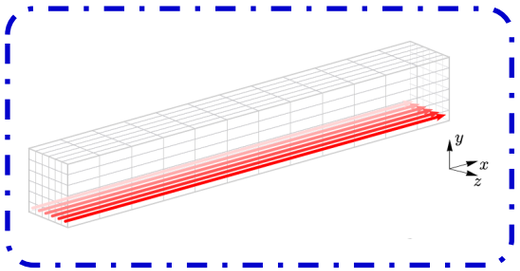

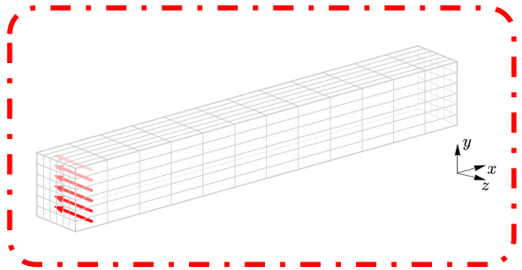

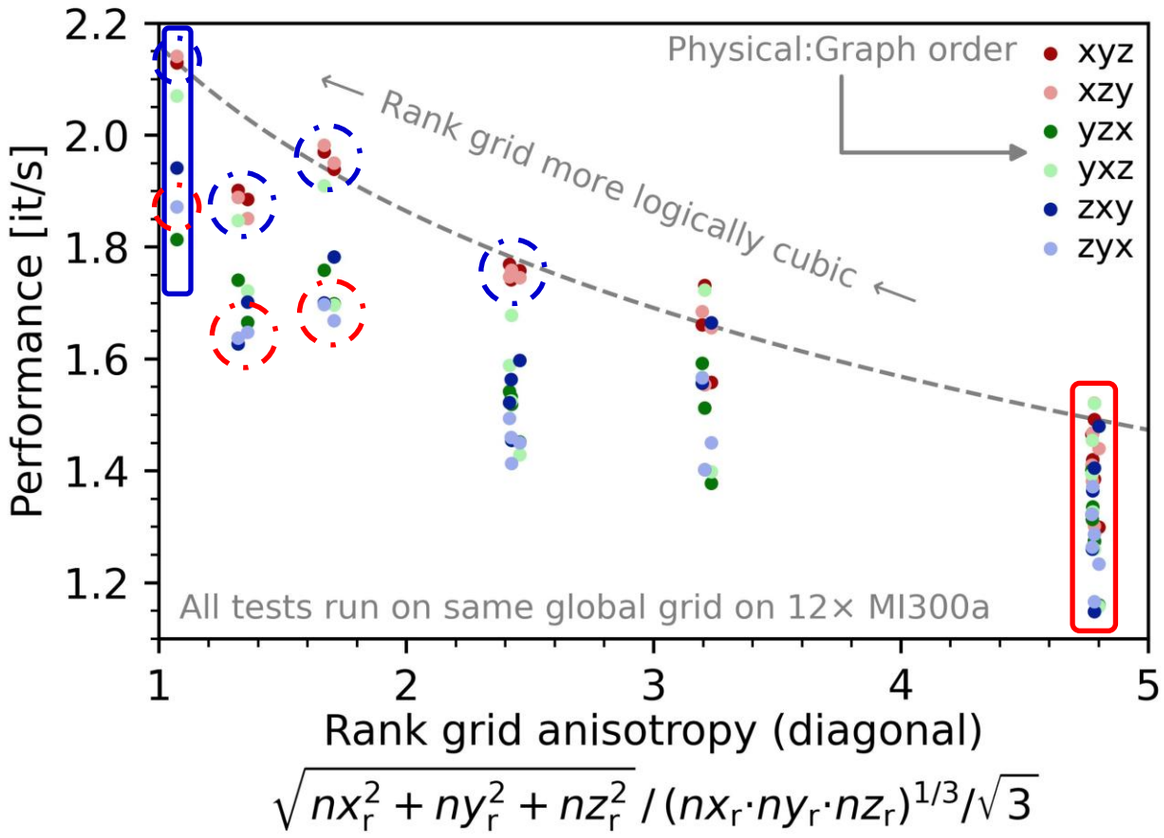

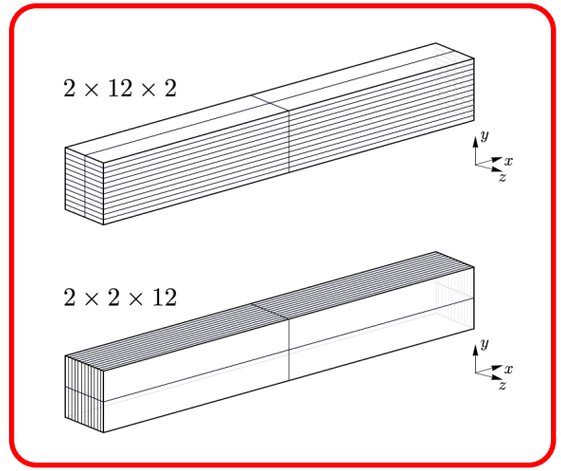

Summary: Bringing everything together...

If you are looking for long hanging fruits in performance, check you case design!

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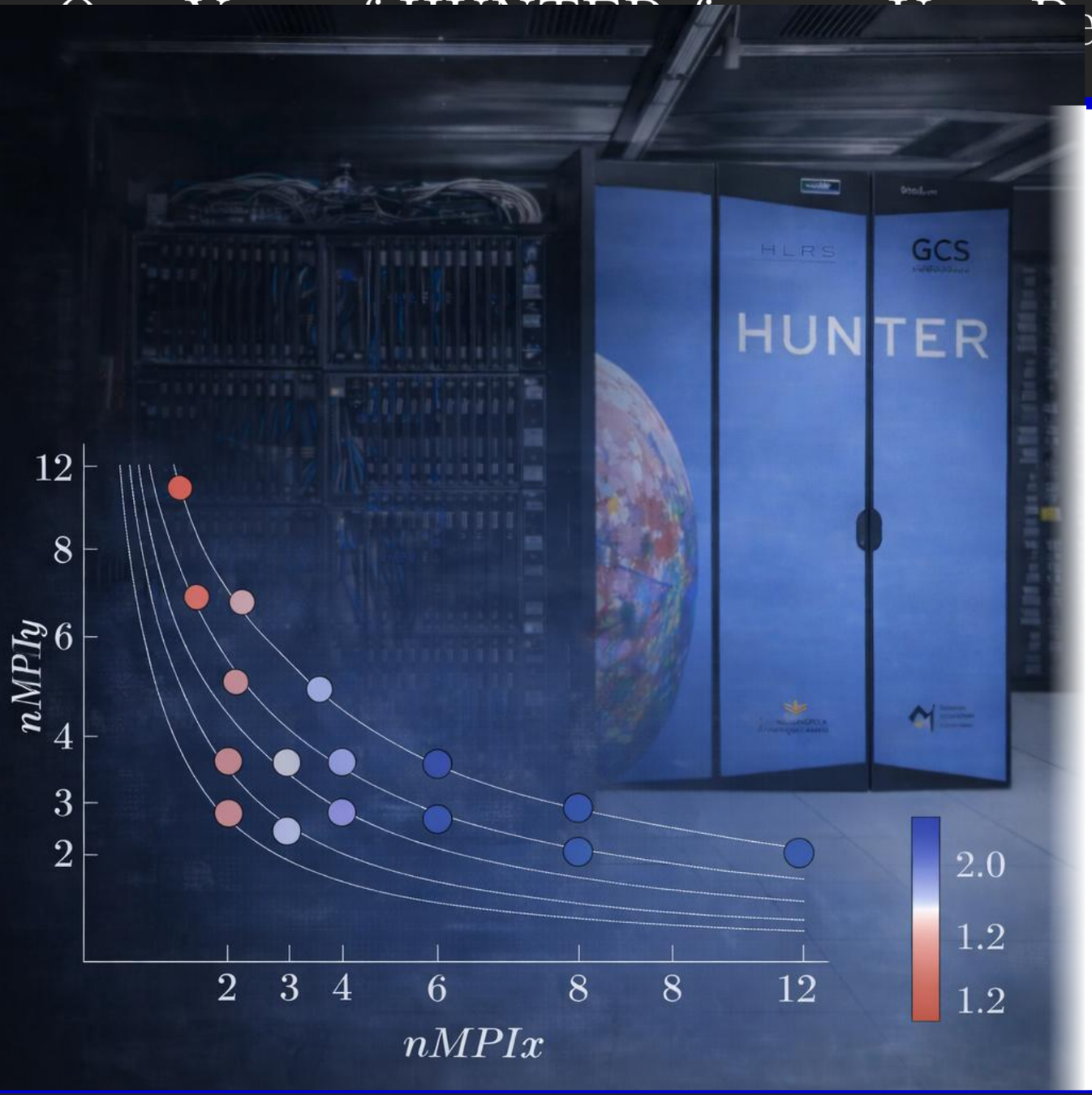

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- Same near-production test case as before:

n_{nodes}	$n_{\text{gridPoints}}$	n_x	n_y	n_z	$n_{\text{MPI},x}$	$n_{\text{MPI},y}$	$n_{\text{MPI},z}$	$n_{x,\text{rank}}$	$n_{y,\text{rank}}$	$n_{z,\text{rank}}$
12	1.868.175.360	5592	480	696	12	2	2	466	240	348
36	5.604.526.080	7456	720	1044	16	3	3	466	240	348
54	8.406.789.120	8388	720	1392	18	3	4	466	240	348
80	12.454.502.400	9320	960	1392	20	4	4	466	240	348
92	14.322.677.760	10718	960	1392	23	4	4	466	240	348
128	19.927.203.840	14912	960	1392	32	4	4	466	240	348

- Same test procedure as before
- All cases were computed twice for consistency
- Different MPI rank orderings were tested with consistent results, therefore only results for (`xyz`) are shown
- Lessons learned previously were applied, resulting in MPI domains that are as cubic as possible (in terms of n_x, n_y, n_z per MPI rank)

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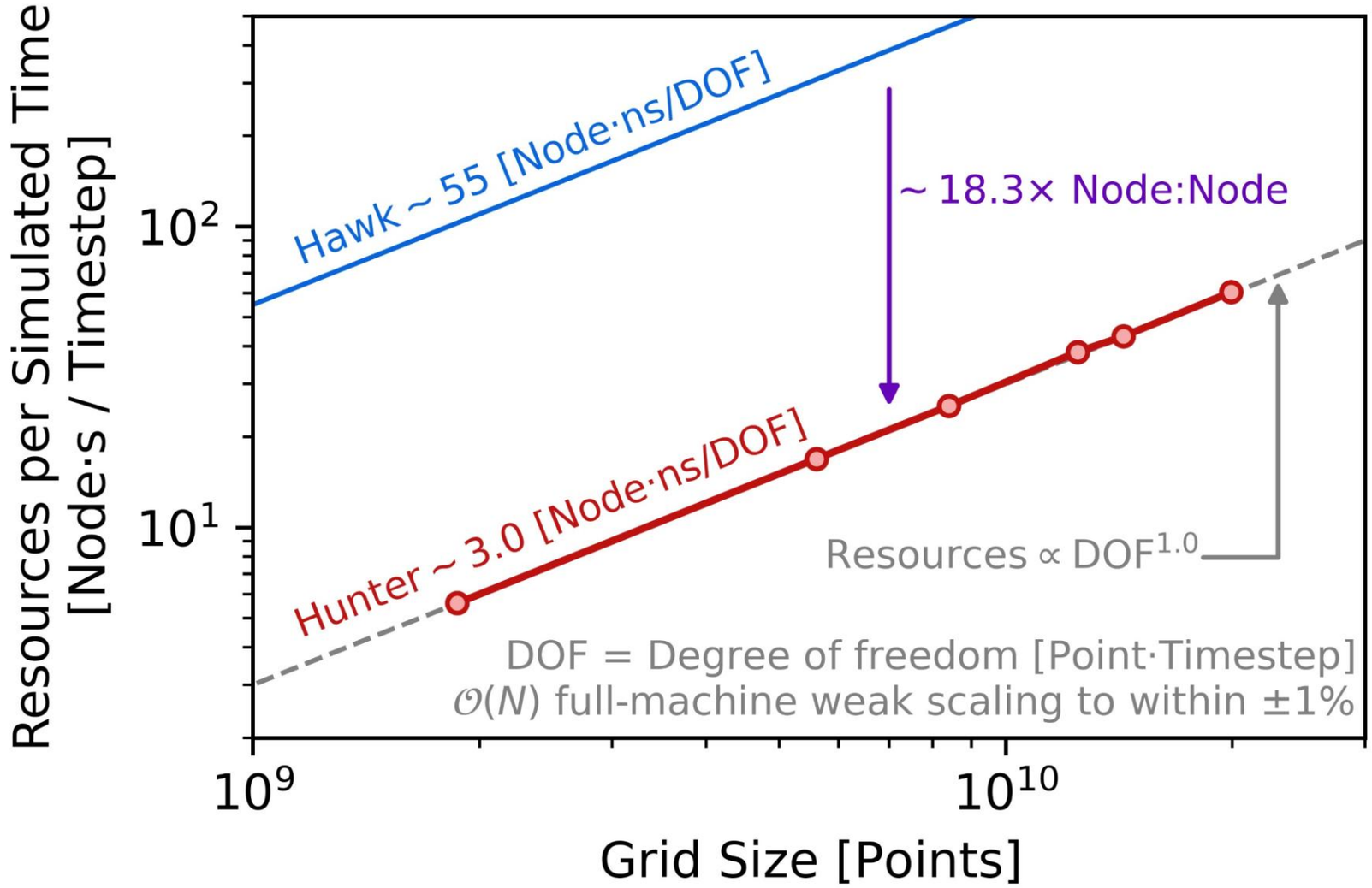

Introduction

NS3D GPU Porting Status

Performance insights

- Performance sensitivity to
  - MPI decomposition
  - Rank ordering
- Scaling behaviour

Summary/Conclusions

Summary and conclusions

- **Starting point (Sept. 2025):** First production cases available, but limited robustness
- Many setbacks e.g. due to software-stack updates exposing previously hidden bugs in our code (mainly affecting large cases), along with limited MPI decomposition robustness
- Extensive debugging effort, largely relying on trial-and-error (and a fair amount of guesswork)
- Remaining mystery bugs: random NaNs or Infs in major arrays, HDF5 interface randomly fails

- **Current status:** (Largely) stable production runs; final NS3D_{neo}.develop version expected soon
- NS3D_{neo}.develop runs in both USM and non-USM modes

- **Performance insights (non-optimised version!):**
  - Strong sensitivity to MPI decomposition and rank ordering (up to $\times 2$)
  - Excellent weak scaling for near-optimal setups ($\sim$40M grid points per MPI rank)
  - Near-cubic MPI subdomains significantly improve performance
  - `xyz` rank ordering advantageous for current implementation

→ Next steps: Optimization!

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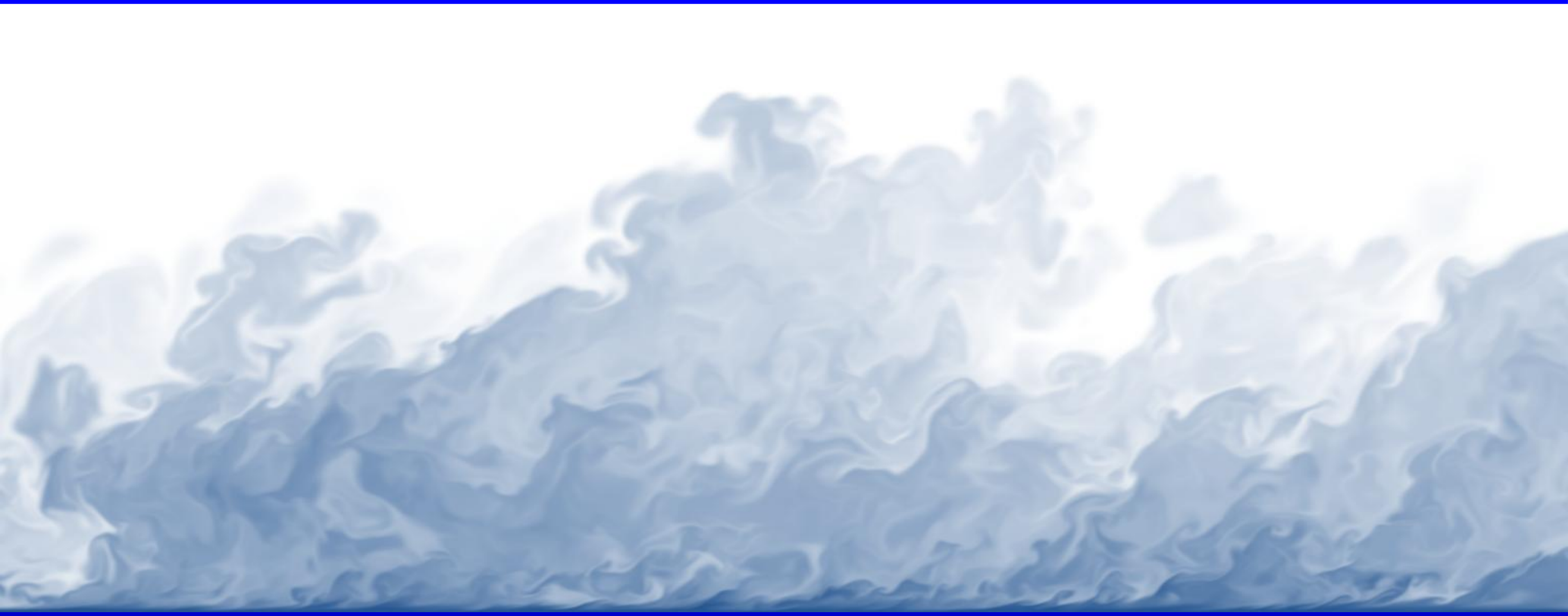

One Year of HUNTER from a User Perspective: Progress, Performance, and Patience with NS3D

Christoph Wenzel

WSSP 2026

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