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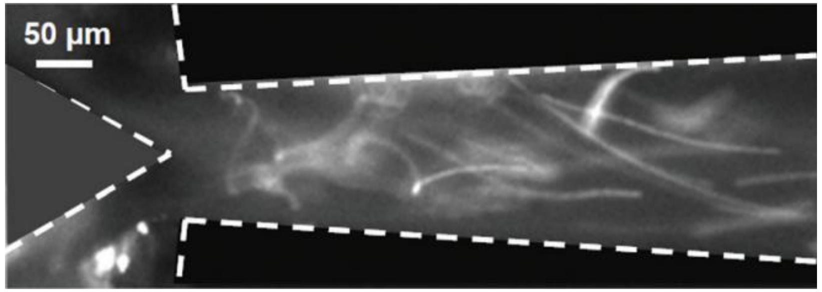
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

TURBO: GPU accelerated simulations of 2D incompressible Turbulence

Victor de J. Valadão
University of Torino

Spoke 3 General Meeting, Elba 5-9 / 05, 2024

Physical Motivation



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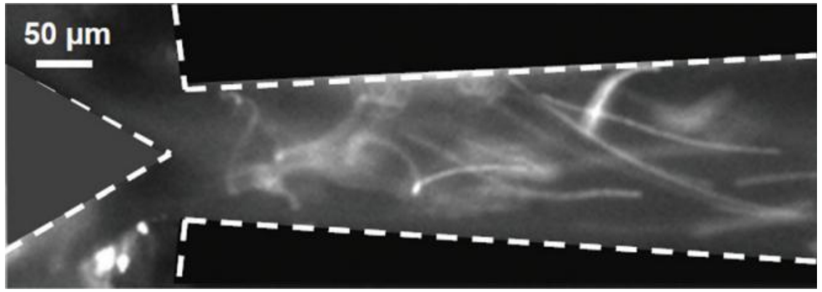

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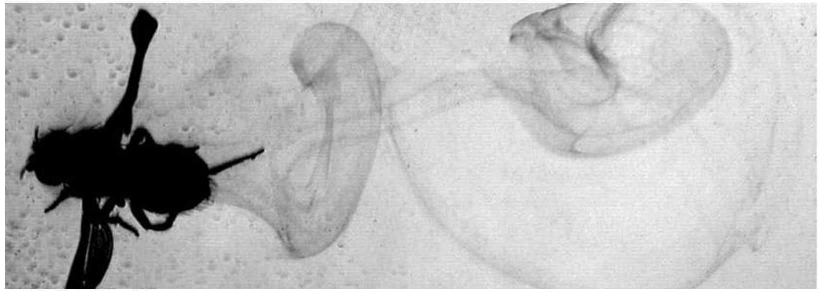
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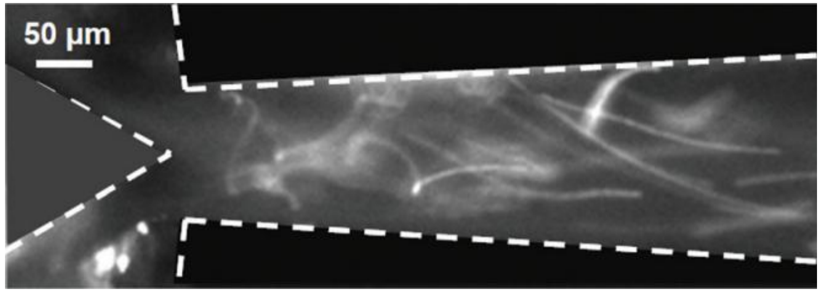

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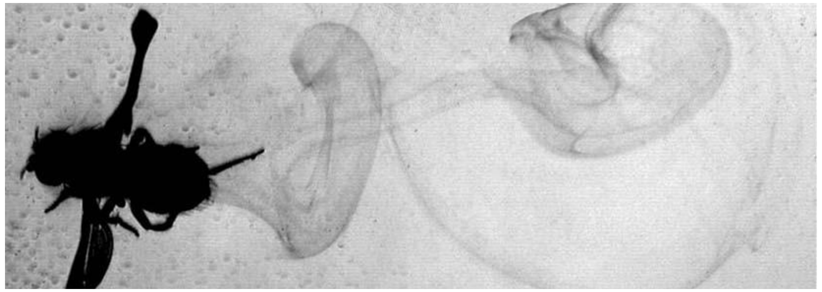

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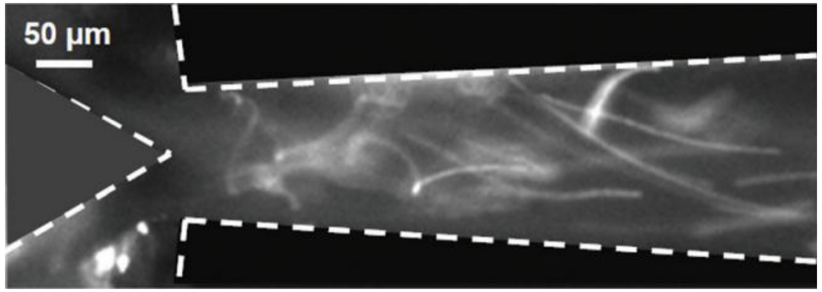

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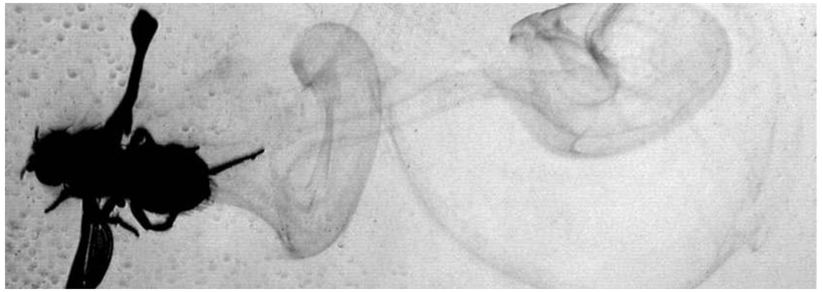

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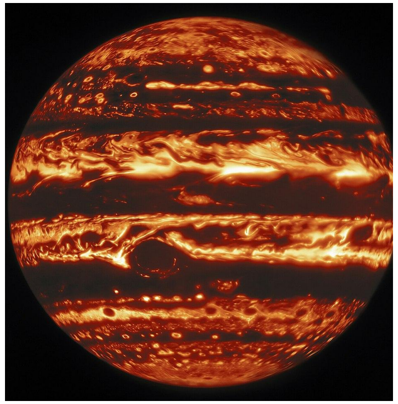

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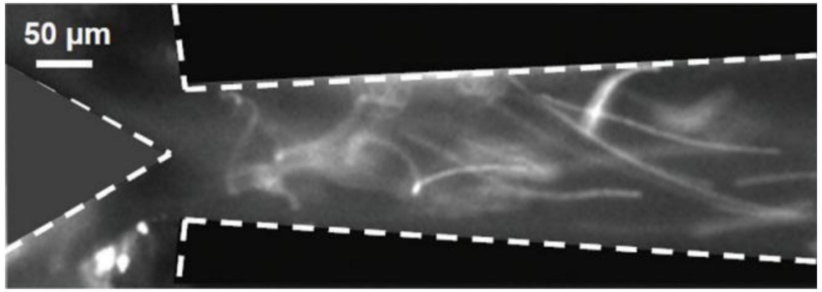

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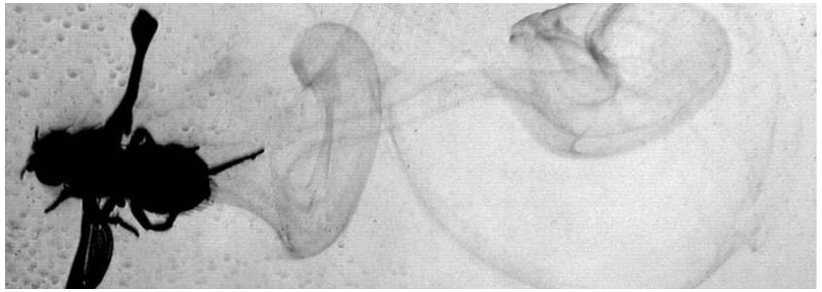
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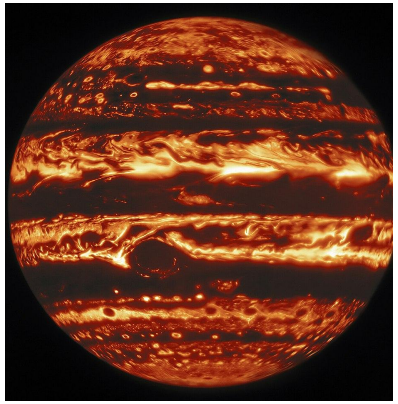
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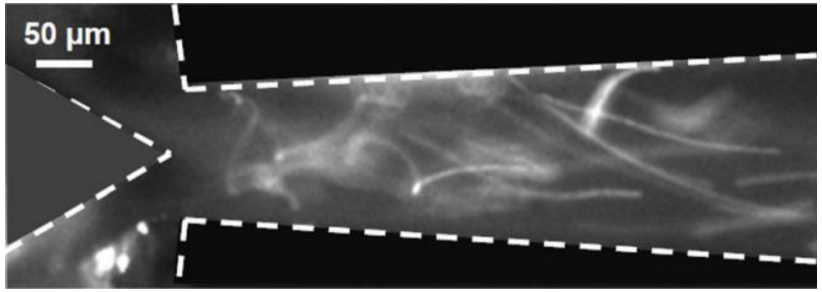

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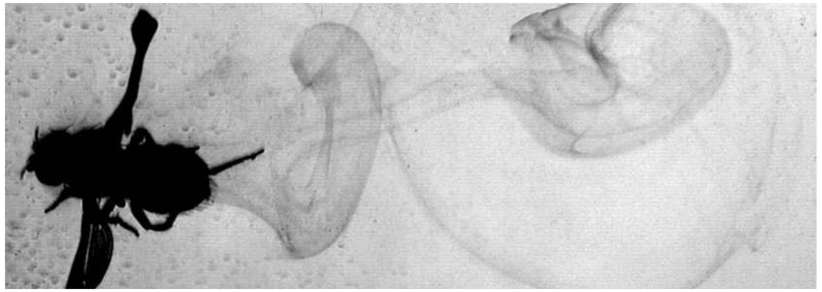

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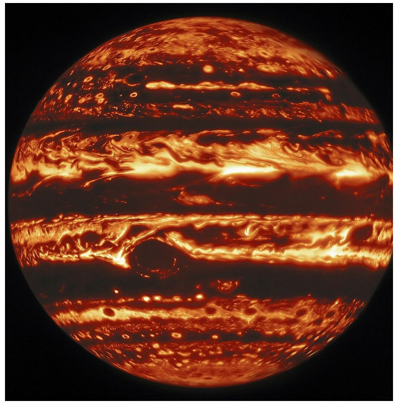

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Adding complexity

- Boundaries;
- Multi-phase fluid;
- Thermal / Electromagnetic coupling;
- Rotation;
- Stratification;
- Compressibility;
- So on …

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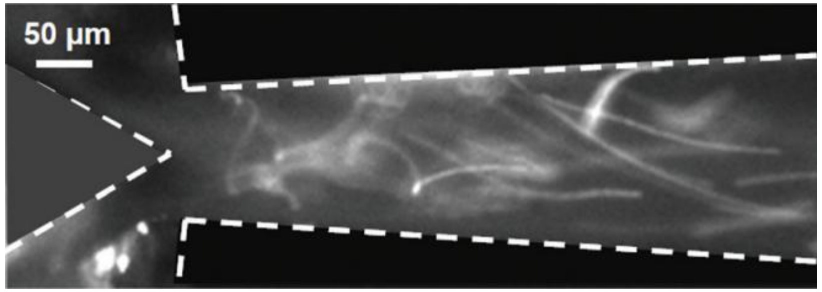

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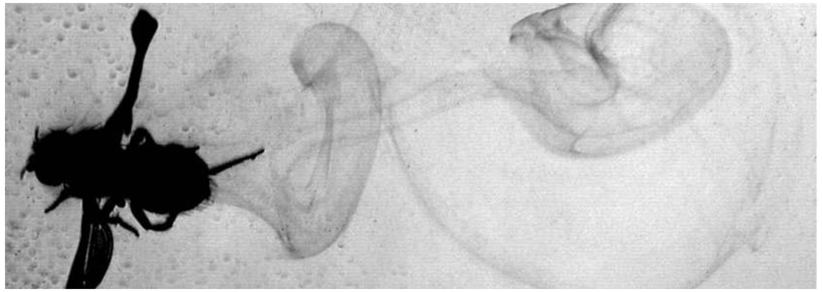

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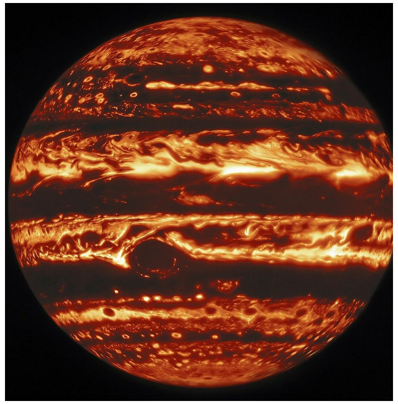

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$$Re = \frac{UL}{\nu} \to \infty$$

Simple case is already challenging

- No general solution (existence => Millenium Problem);
- Anomalous behavior when viscosity vanishes;
- Formation of structures at several spatial scales;
- Huge gap between different time scales of the problem;
- Displays rare Intermittent events;
- Multifractal Statistics;

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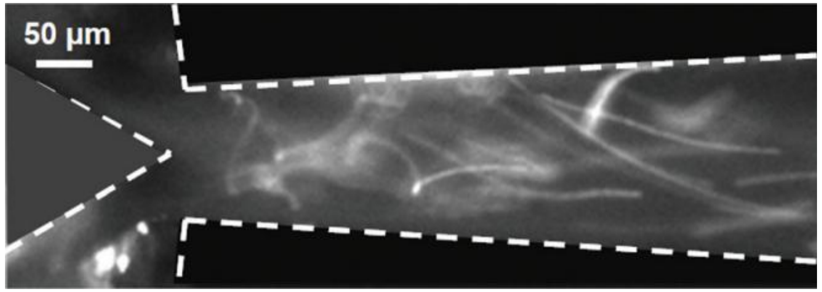

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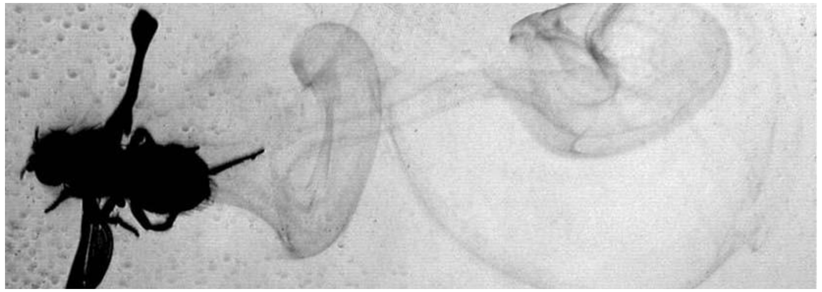

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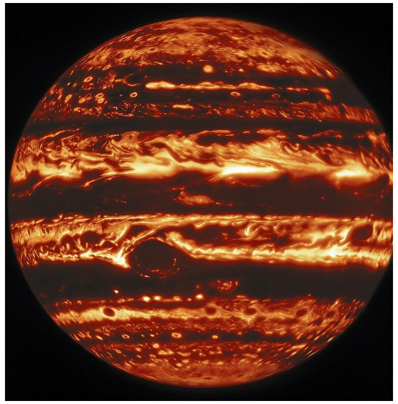

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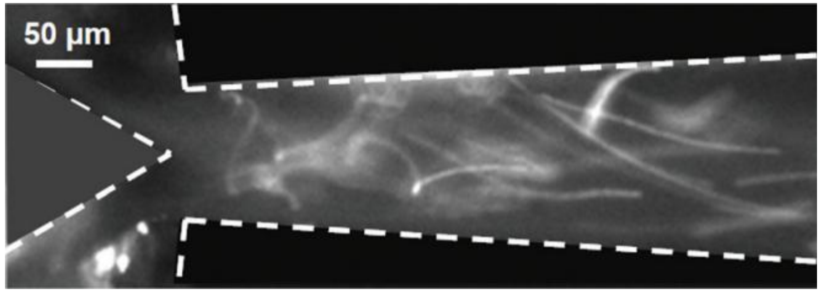

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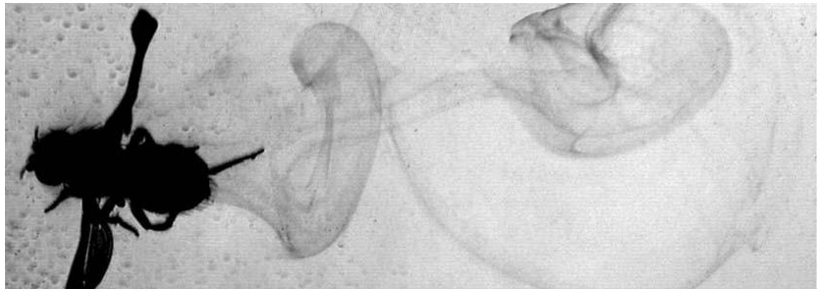

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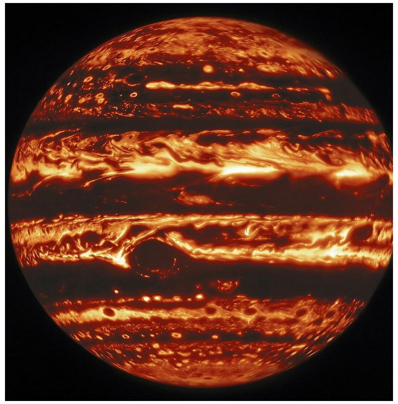

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Pseudospectral approach

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- Solves NSE in the Fourier space;
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It is fully parallelizable!!!

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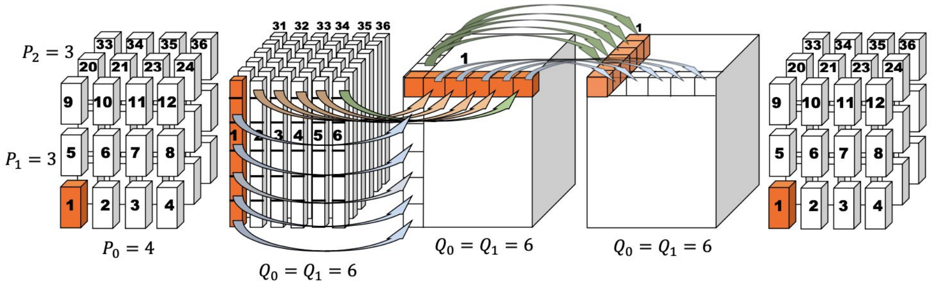

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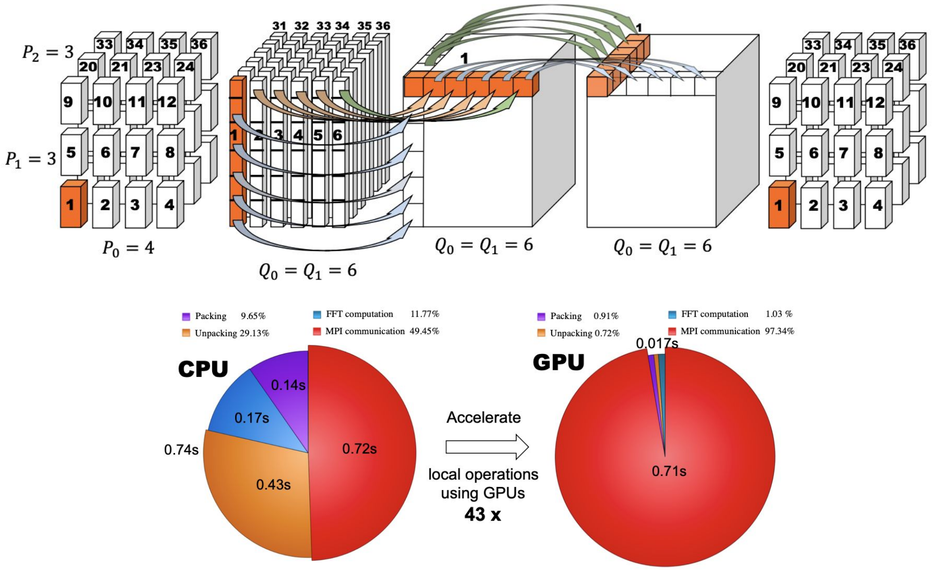

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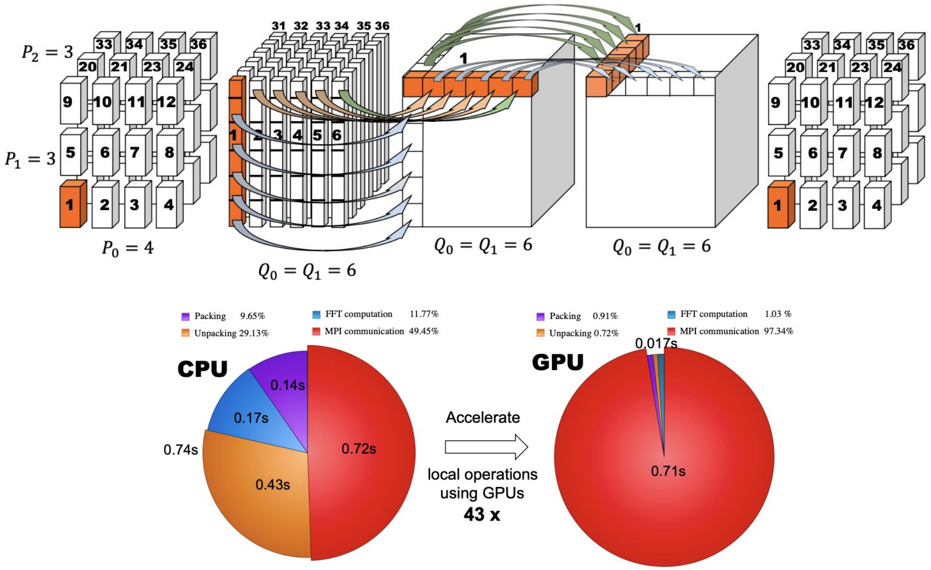

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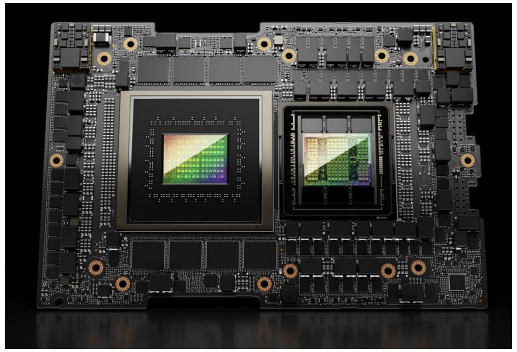

Nvidia H200

Unreleased - 141 GB

"Small sized" problems: 2D turbulence models

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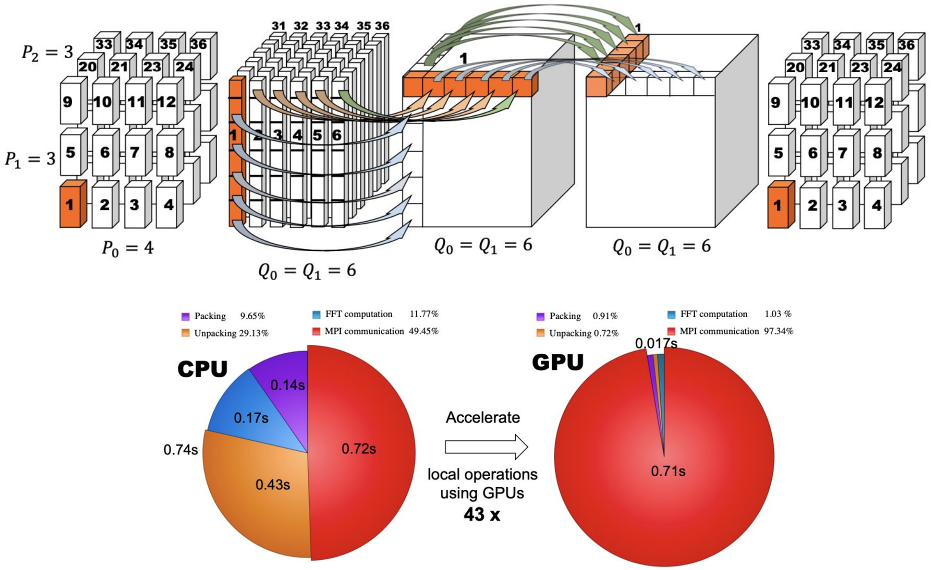

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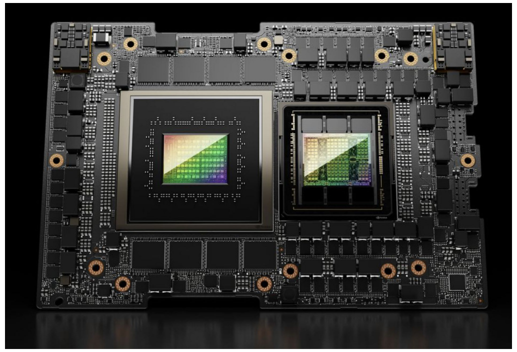

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"Small sized" problems: 2D turbulence models

$$\partial_t \omega + v_i \partial_i \omega + (-1)^n \nu \partial^{2n} \omega + (-1)^m \mu \partial^{2m} \omega = F$$

$$v_i = \epsilon_{ij} \partial_j \psi \qquad \hat{\omega}(k,t) = k^{\alpha} \hat{\psi}(k,t)$$

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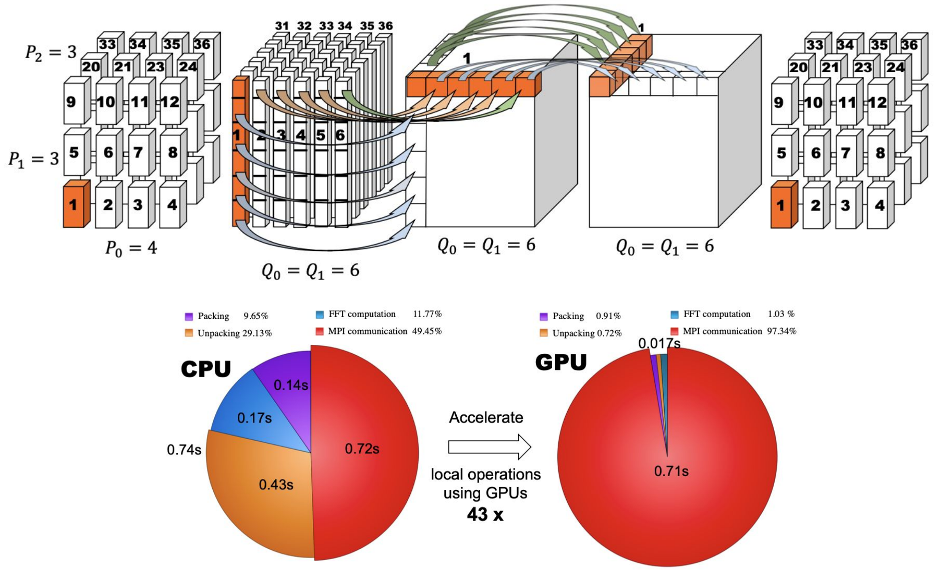

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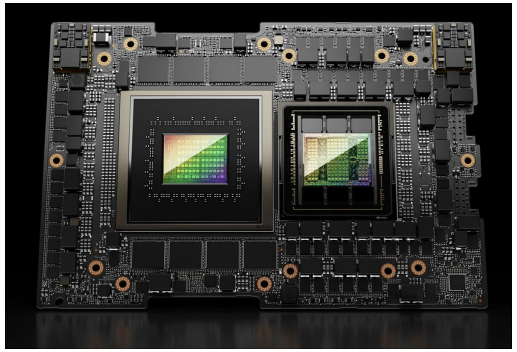

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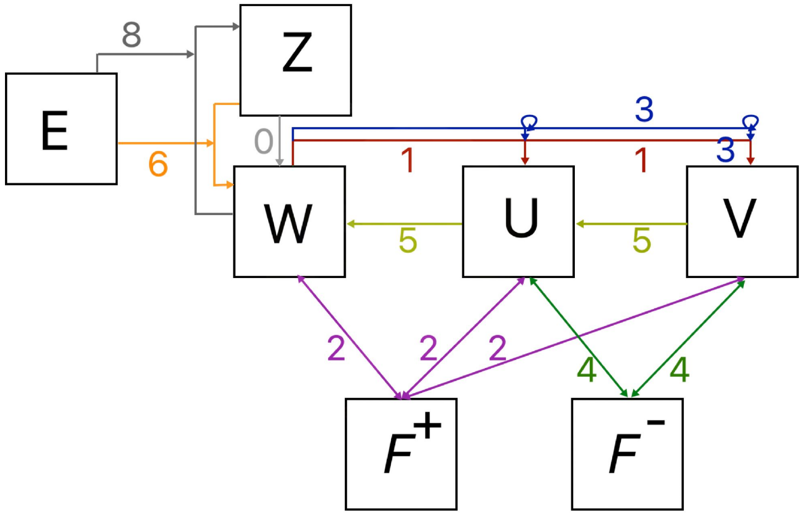
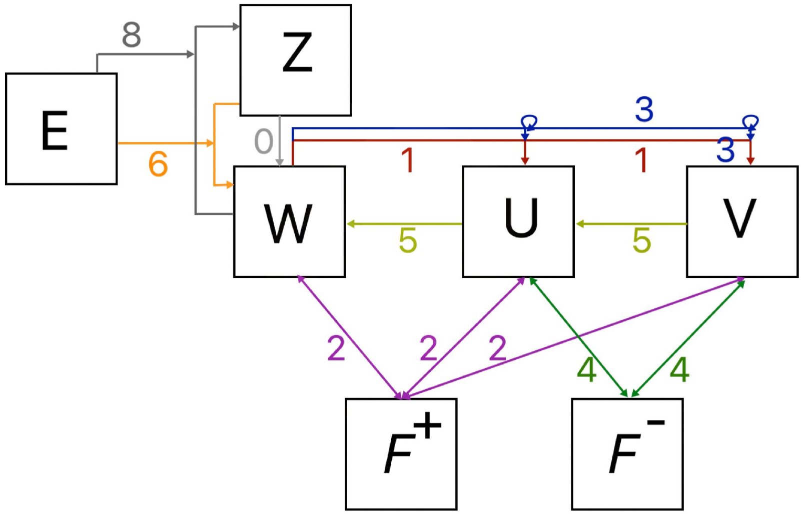
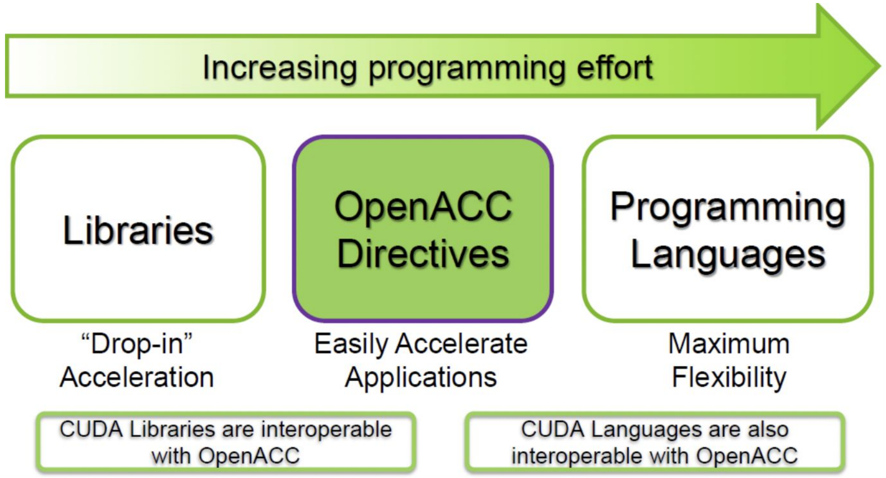
- Same degree of physical/mathematical complexity;
- Reduces the spatial dimensions of all 2;
- Reduces dimensionality by solving scalar equations;
- Same algorithm with very little adaptations;

Time integration



Time integration and porting method





Chen S., *"Introduction to OpenACC"* (2016) @ bu.edu

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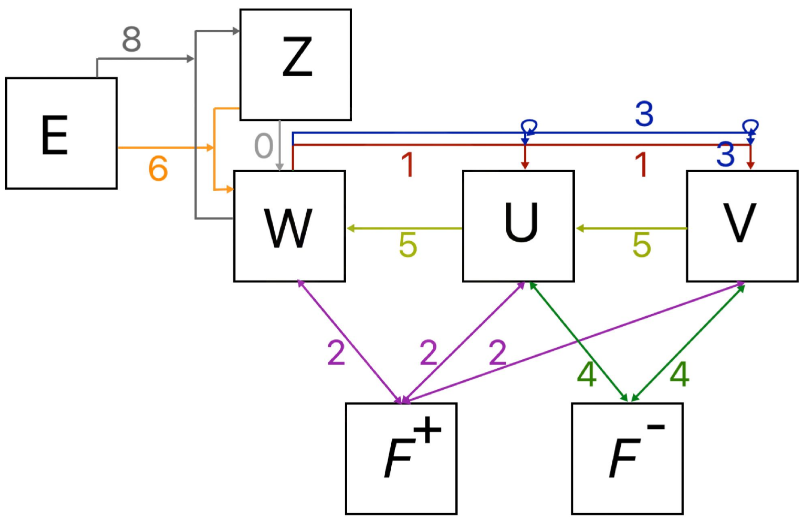

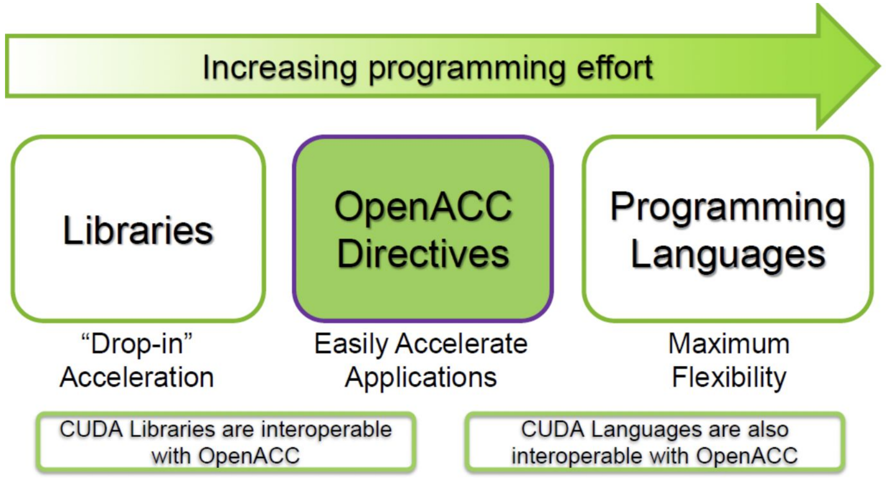

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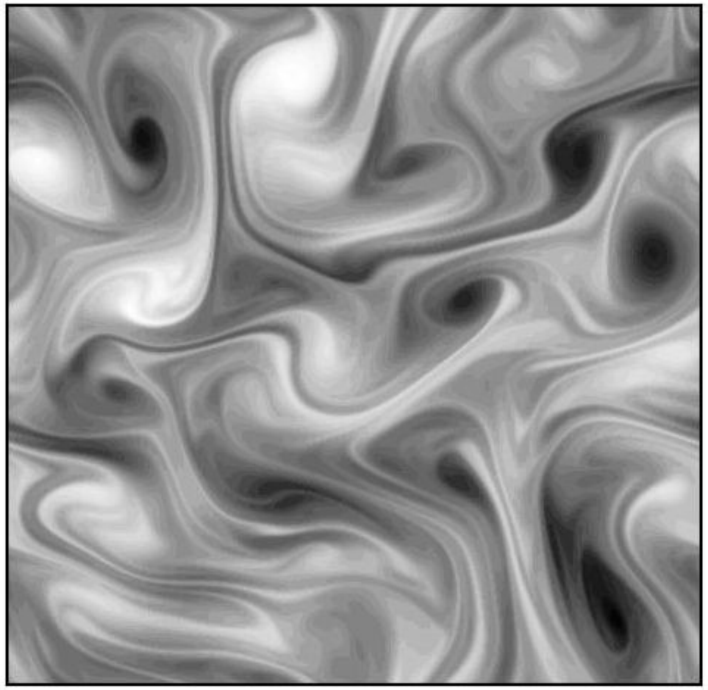
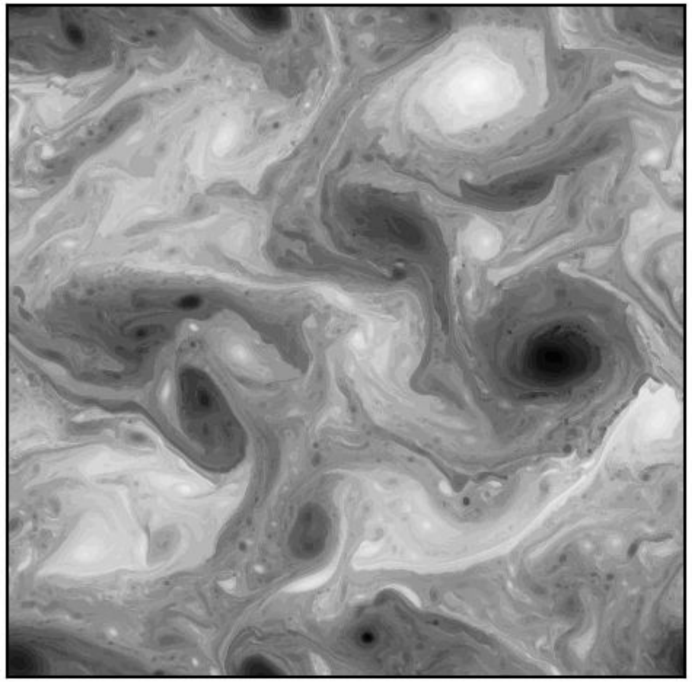
```
!$acc parallel loop collapse(2) present(z, u, v, fkx, fky)
do j=1,NY
do i=1,NX2P1
  z(1,i,j)=+fkx(i)*u(2,i,j)+fky(j)*v(2,i,j)
  z(2,i,j)=-fkx(i)*u(1,i,j)-fky(j)*v(1,i,j)
end do
end do
!$acc end parallel loop
```

Some nice images

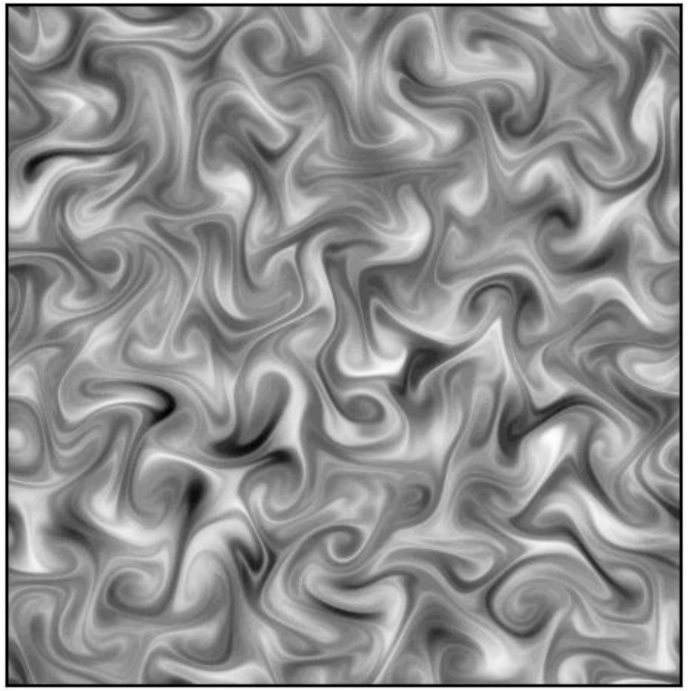


Navier-Stokes Turbulence



Surface Quasi-geostrophic Turbulence

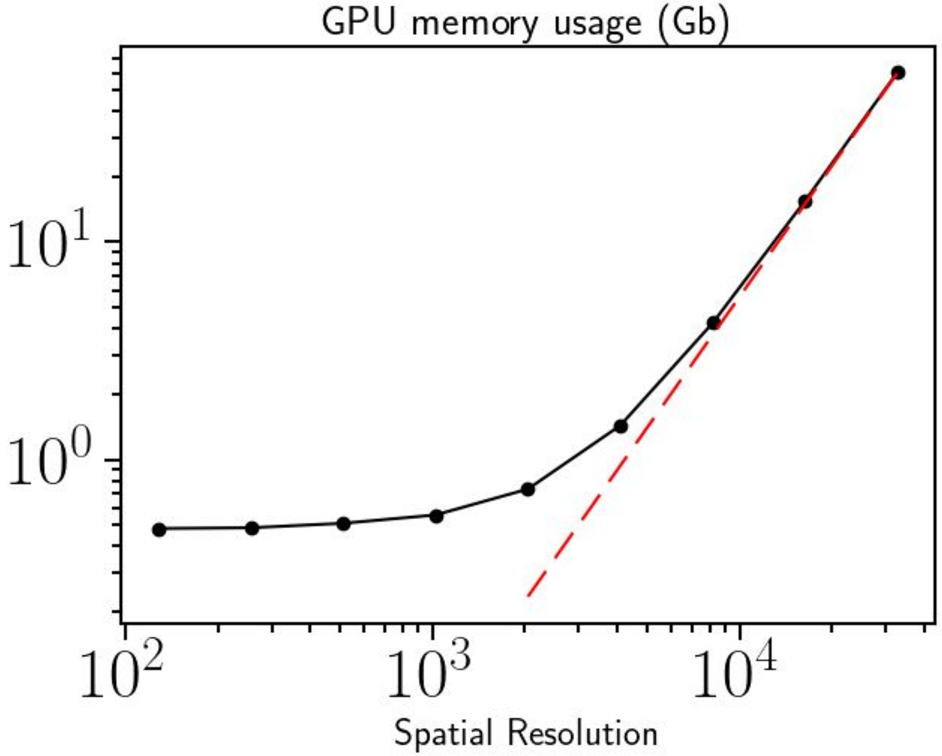
2 papers in preparation



Passive-scalar advection

Up to (32768)^2

Preliminary performance tests @ Leonardo



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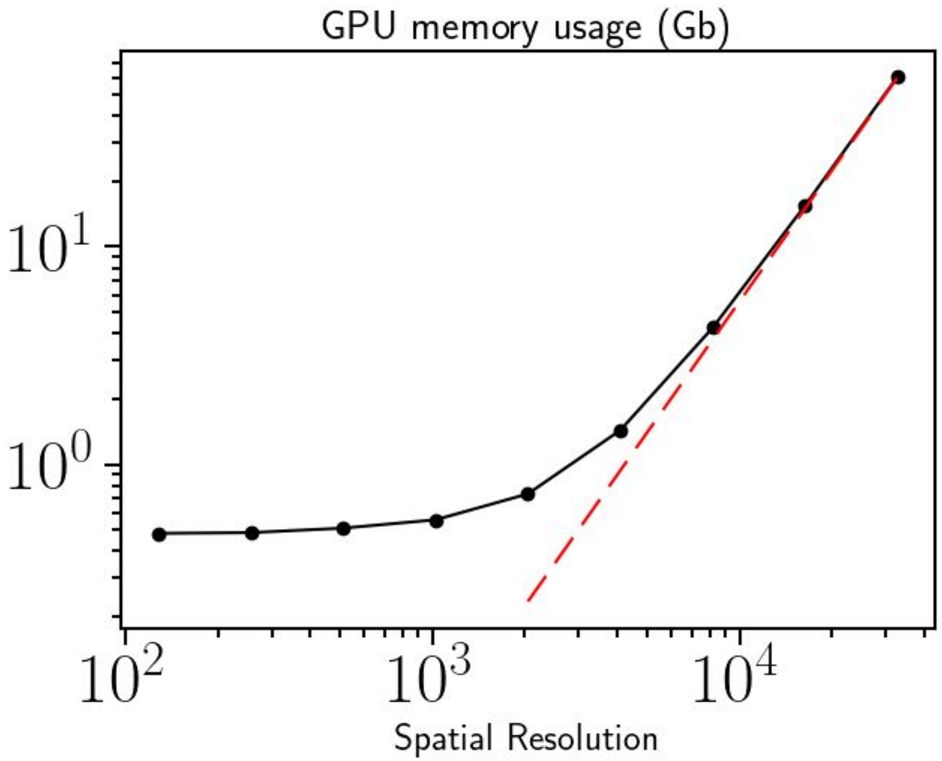

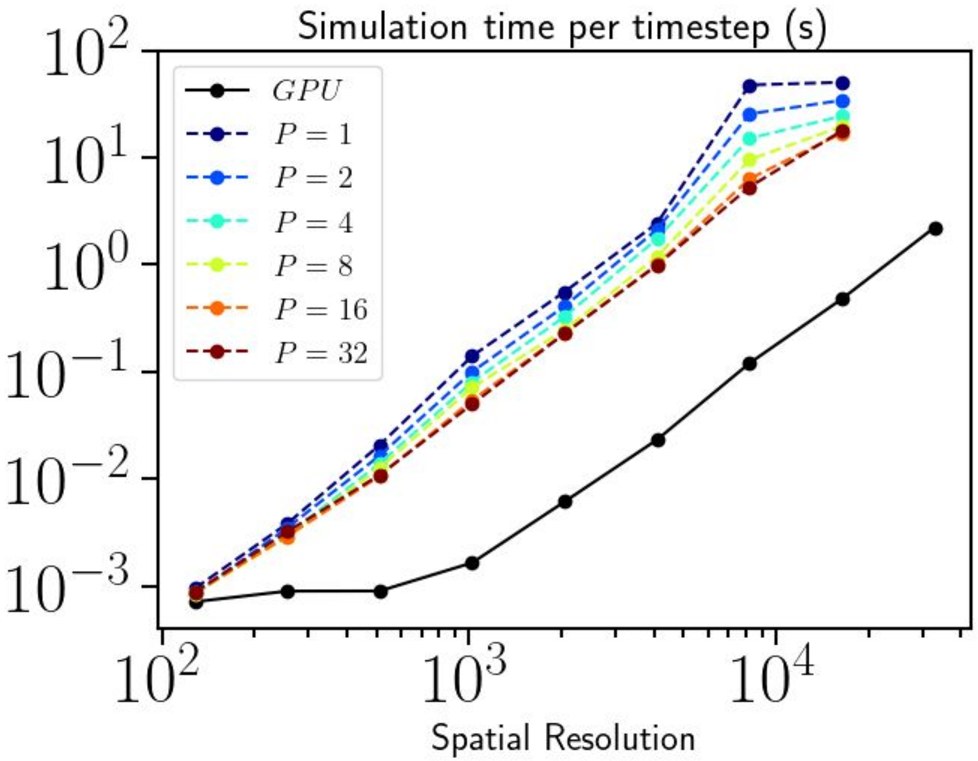

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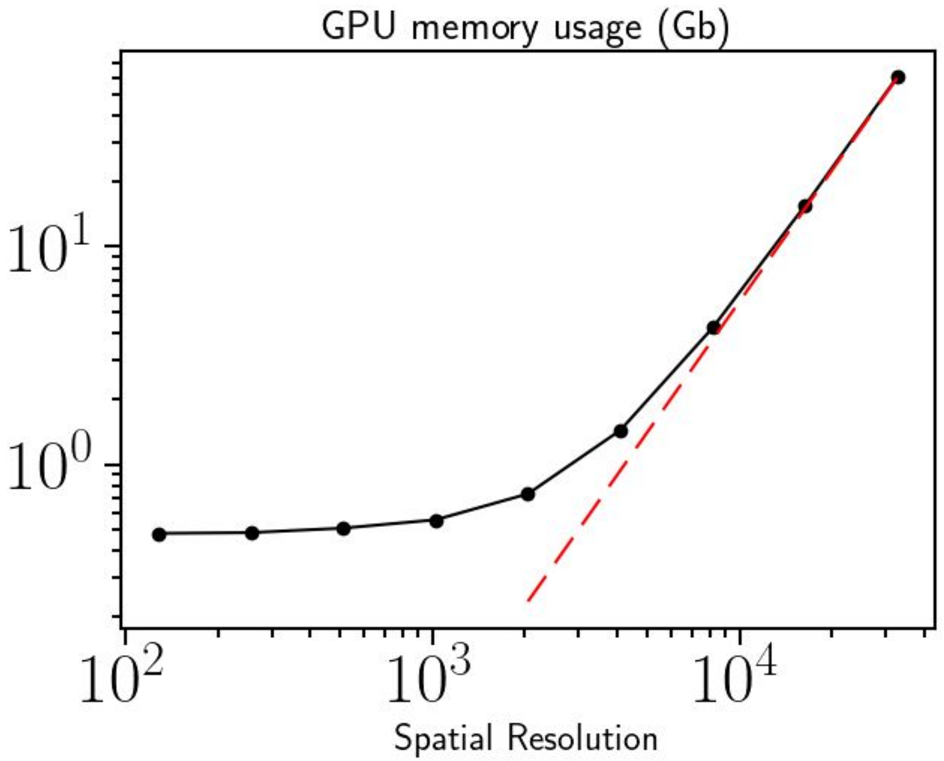
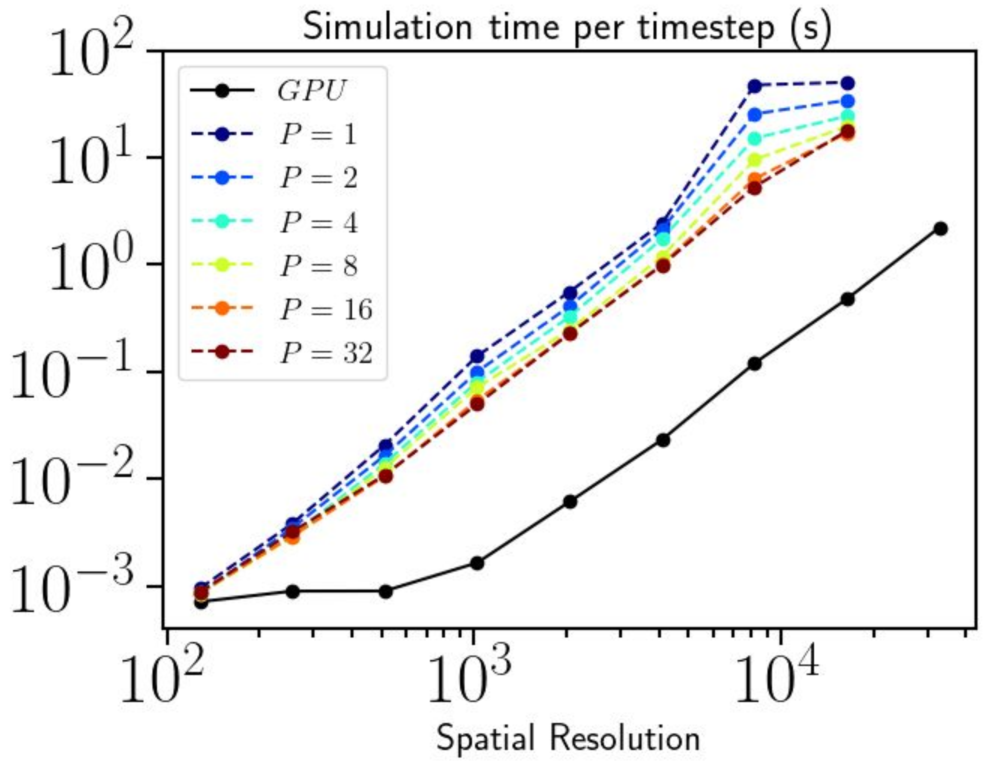
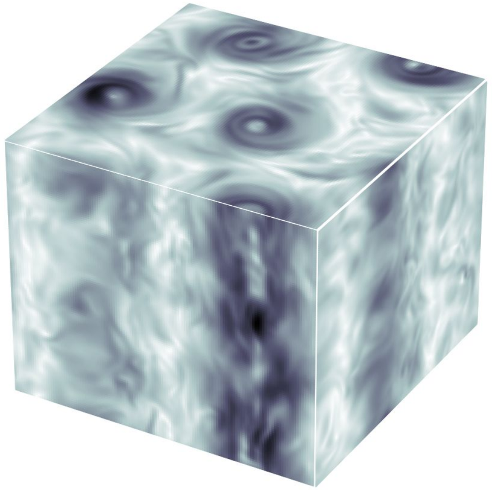




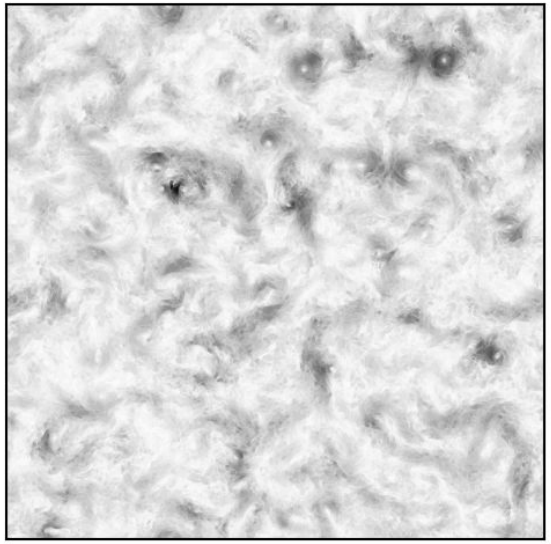
- About 40x speed up respect to 32 cores serial code;
- 24 hour use: 9.6 kWh (GPU) vs 6.0 kWh (CPU);
- It consumes 25 times more energy to run the same simulation time in the CPU;
- Budget consuming reduced by 4 times because 1 GPU = 8 CPU cores at Leonardo;

Is it worth doing the same for 3D homogeneous turbulence?

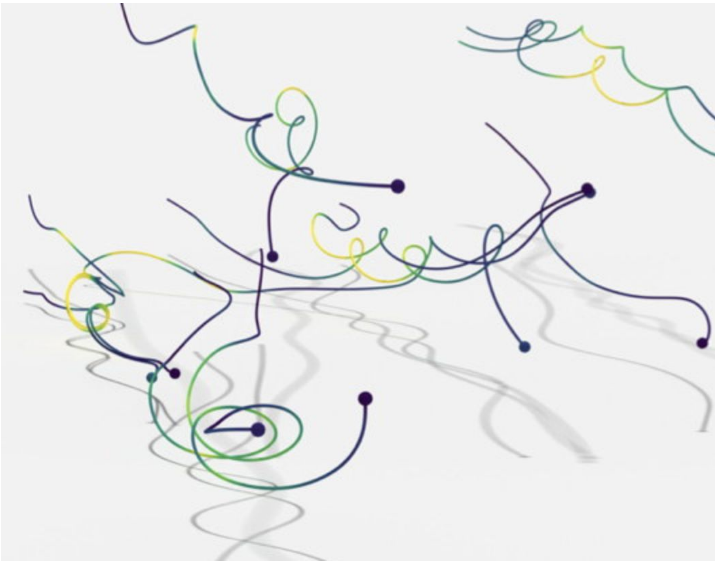
YES



Rotating Turbulence



3D thin layer



Lagrangian statistics

Timetable and Next Steps

Milestone 7

- Nov 23 - TURBO project was officially started by mid M7;
- Jan 24 - We successfully ported the pseudospectral code for a class of 2D turbulence models to run in single GPUs with significant improvement with respect to the serial version;
- Feb 24 - Solutions for second and fourth order Runge-Kutta integrators were presented;
- Feb 24 - The code was adapted to include passive scalar turbulence code, but it is still separated of the main 2D TURBO solver;

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Next Steps

- It has still some work to do regarding the asynchrony of computation of online diagnostics on all codes 2D and 3D;
- Scalability to multi-GPU;
- Lagrangian statistics online;
- A detail documentation of the 2D solver is under preparation;

In collaboration with:


Stefano Musacchio


Marco Crialesi-Esposito


Andrea Mignone


Filippo De Lillo


Guido Boffetta

Thank you for your attention!