AQTIVATE

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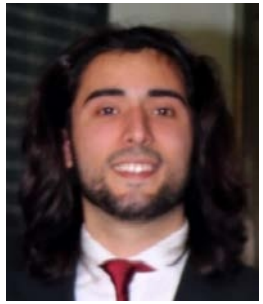
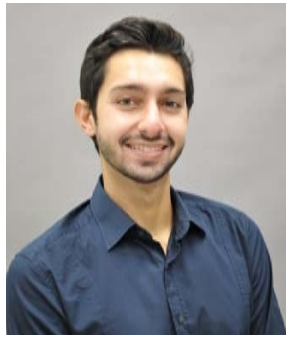


Damiano Capocci

Fabio Bonaccorso



Lorenzo Piro

Fabio Guglietta

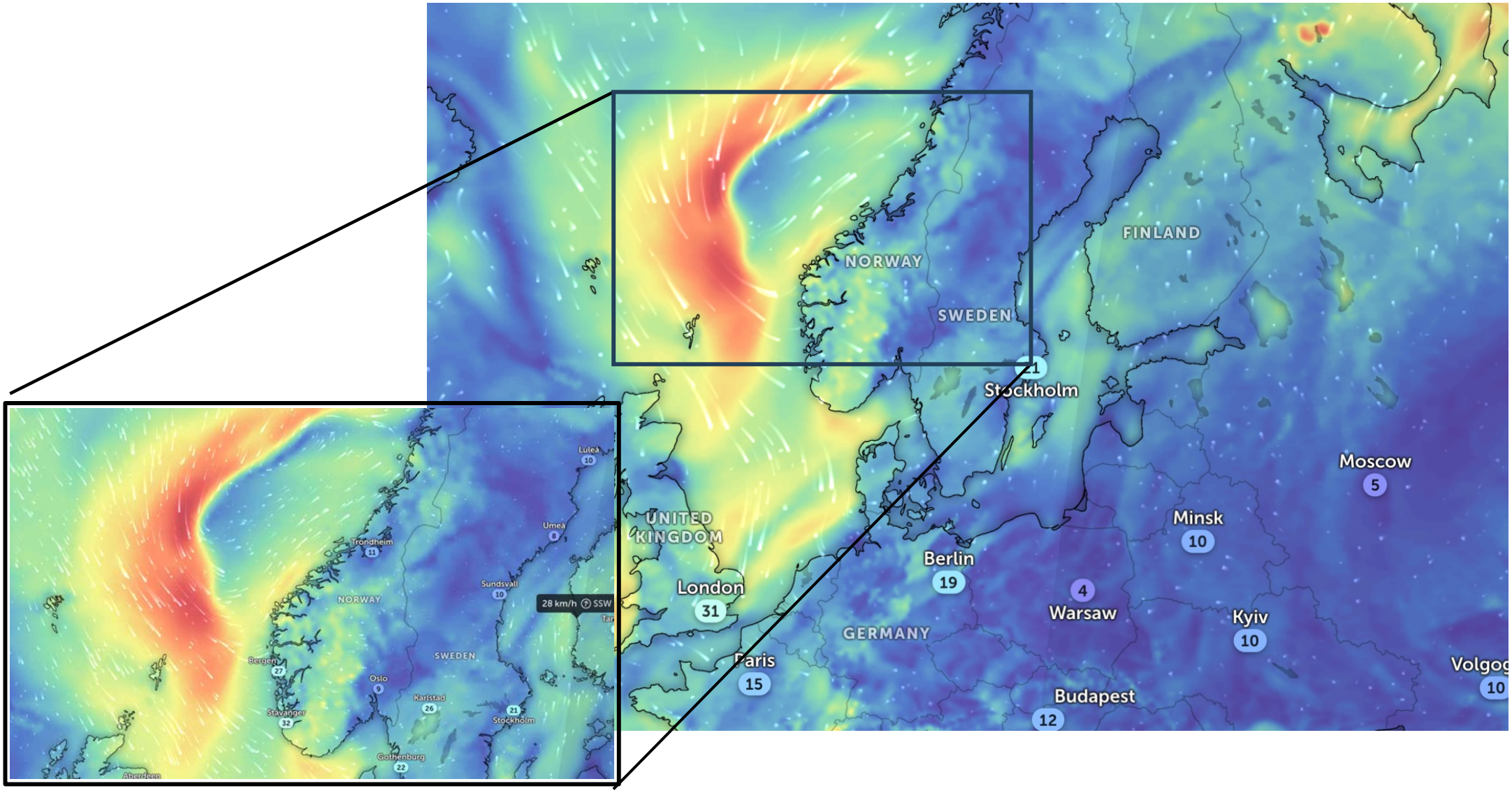
Francesco Fossella

Elisa Bellantoni

Andre Freitas

EARTH'S MAP

Carta Marina *et descriptio septemtrionalium terrarum ac mirabilium rerum in eis contentarum, diligentissime elaborata anno* ***1539*** *Veneciis.* **Olao Magno**


NORWAY
SWEDEN
FINLAND
Stockholm
UNITED KINGDOM
London
31
Berlin
19
Paris
15
GERMANY
Warsaw
4
Minsk
10
Moscow
5
Kyiv
10
Budapest
12
Volgog
10
Luleå
10
Umeå
6
Trondheim
11
Sundsvall
10
28 km/h SSW
Bergen
27
Oslo
9
Karlstad
26
Stavanger
32
Stockholm
21
Gothenburg
22

COMPLEX FLUIDS & COMPLEX FLOWS

$$\partial_t v + v \cdot \partial v = -\partial P + \nu \partial^2 v \; + F(B,B) \; + g\theta \; + \sum_i c_0(u_i, v)\delta(r - r_i) \; + f$$

$$\partial_t \theta + v \cdot \partial \theta = \chi \partial^2 \theta$$

$$\partial_t B + v \cdot \partial B = B \cdot \partial v + \chi \partial^2 B$$

$$\partial \cdot v = 0$$

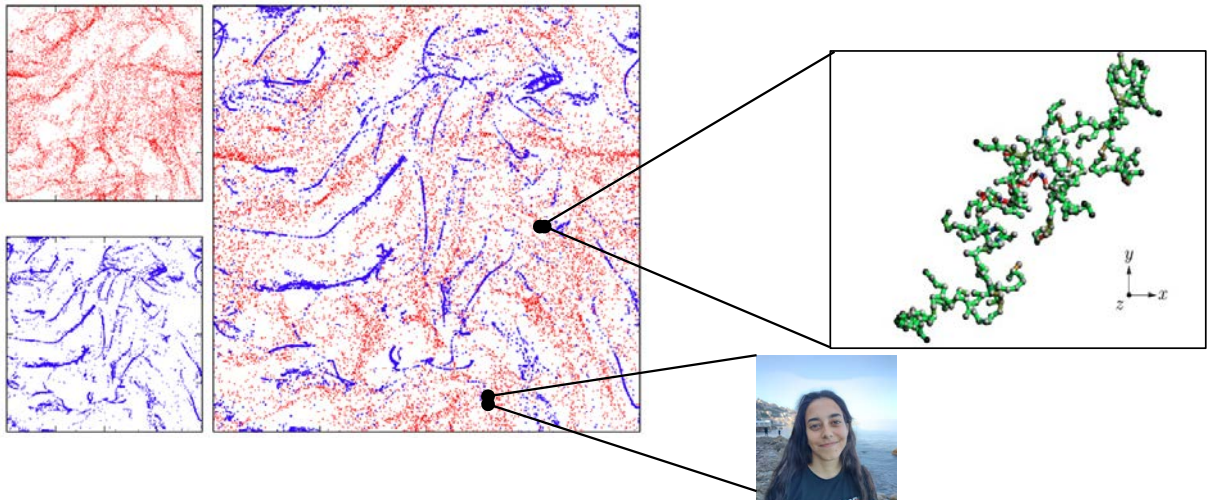
+ boundary conditions + initial conditions

temperature

magnetic field

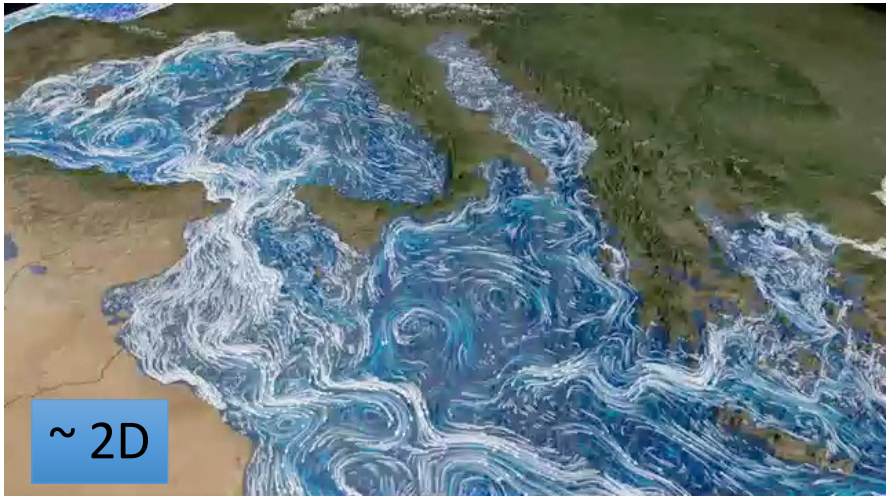
small particles/colloidal aggregates:
Stokes drag, added mass, lift force, etc...

$$\dot{u}_i(t) = -\frac{1}{\tau}(u_i - v) + \beta D_t v$$

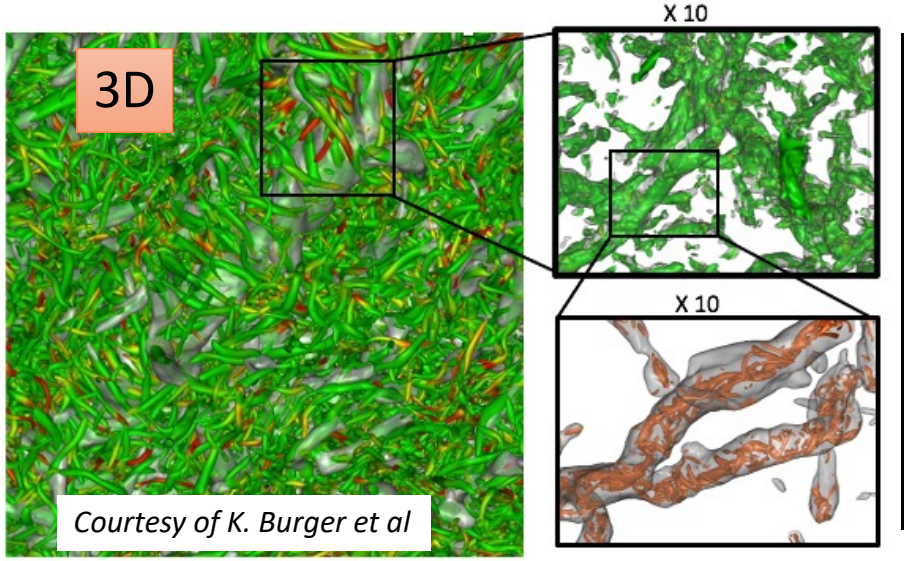


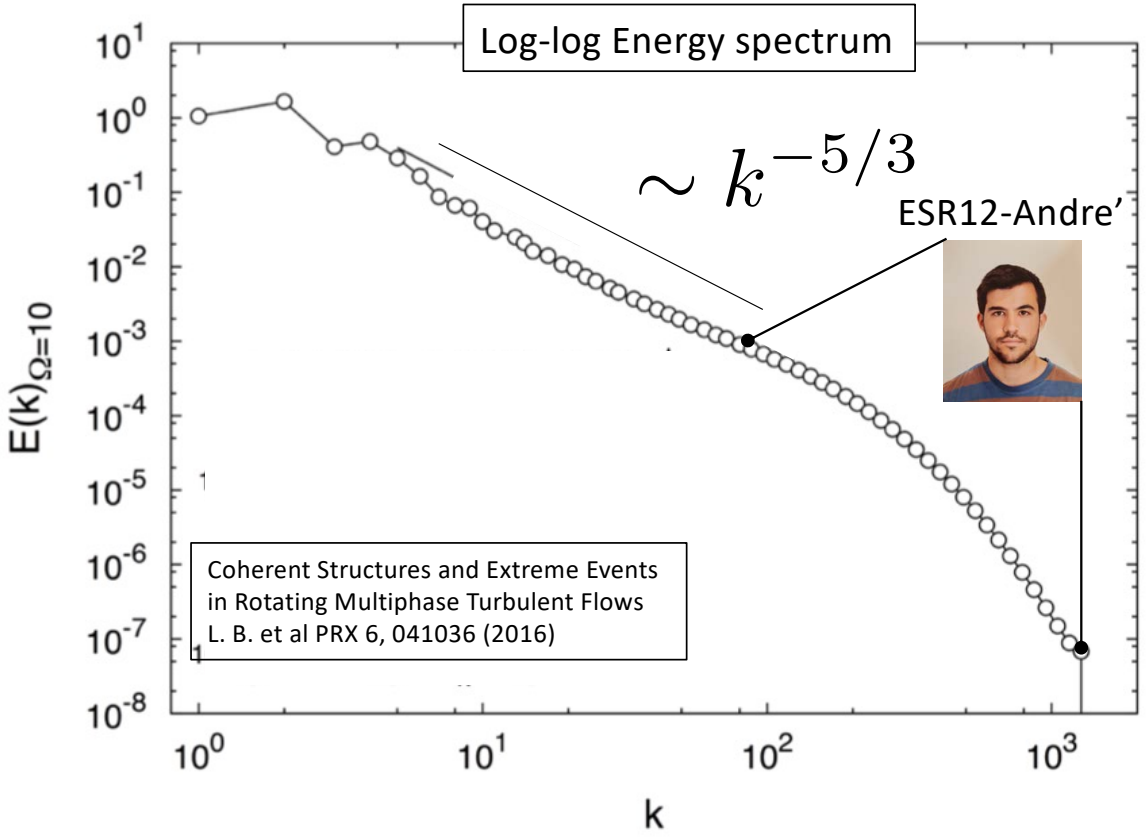
ESR13 - Elisa

SHORT VISUAL RECAP



(NASA/Goddard Space Flight Center Scientific Visualization Studio)

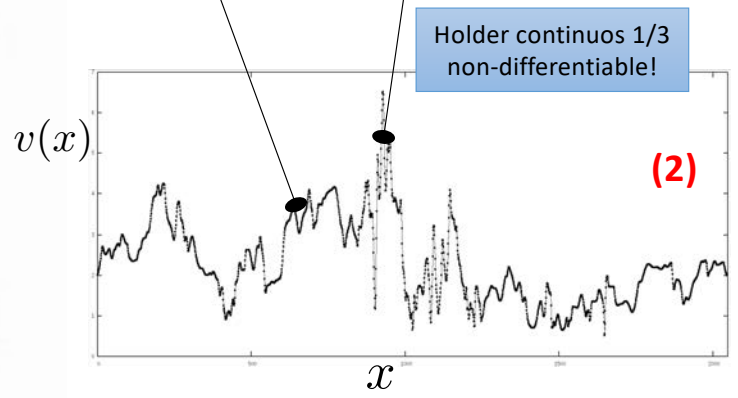


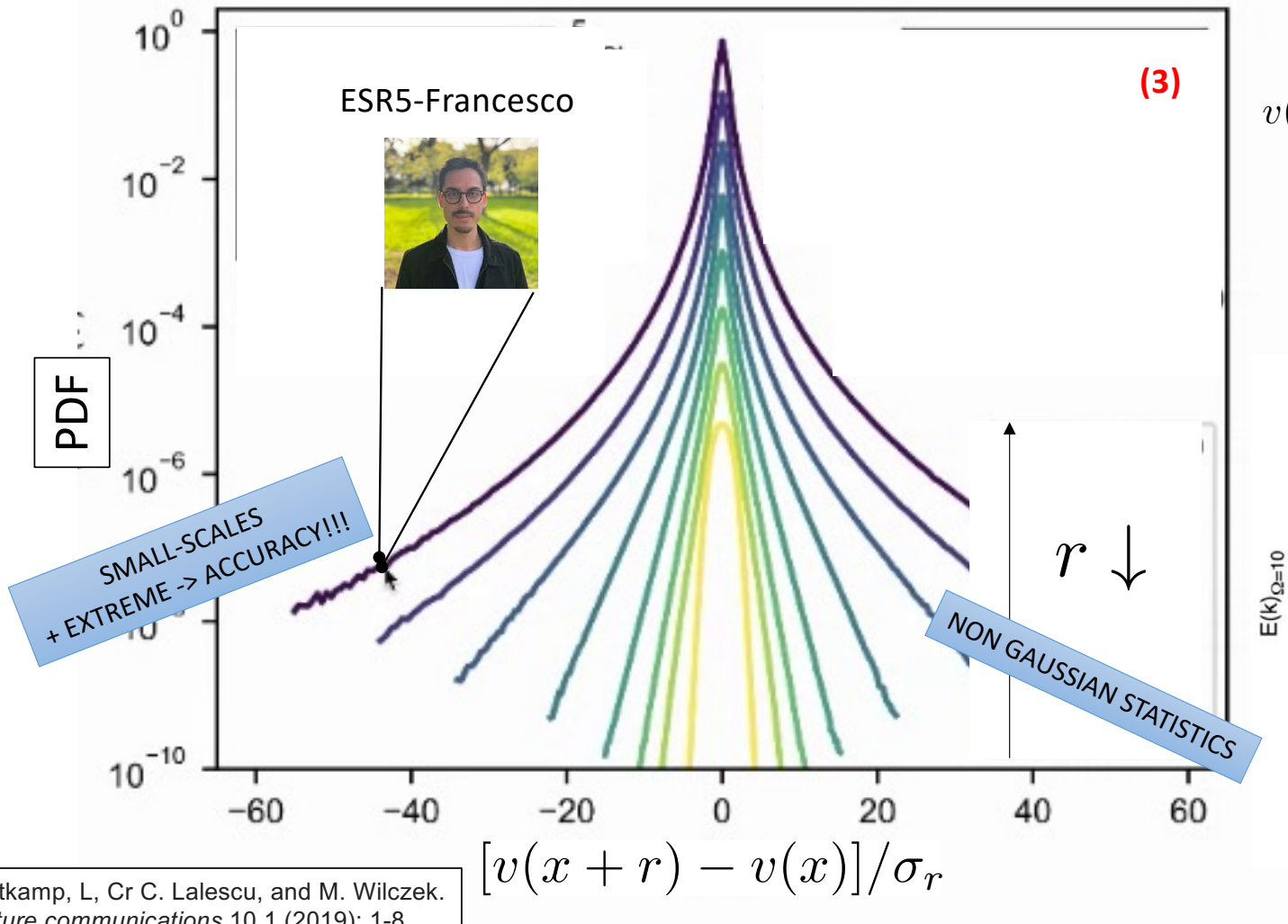


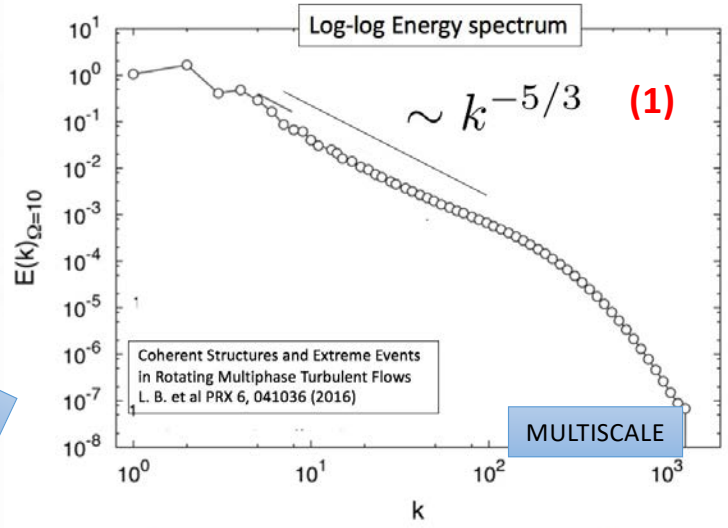
- MULTI-SCALE PHYSICS
- BILLIONS OF DEGREES OF FREEDOM
- ROUGH NON-DIFFERENTIABLE FIELDS (HOLDER CONTINUOS ONLY)
- NON-GAUSSIAN STATISTICS

1) MULTI-SCALE PHYSICS: BILLIONS OF DEGREES OF FREEDOM
2) ROUGH NON-DIFFERENTIABLE FIELDS
3) NON-GAUSSIAN STATISTICS

$$v(x+r) - v(x) \sim r^{1/3}$$



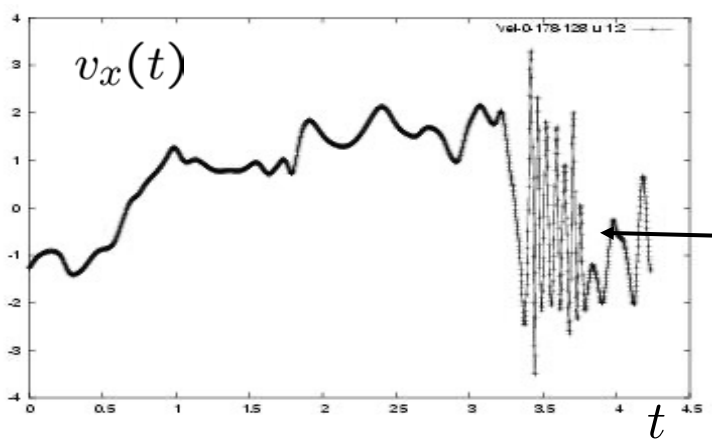


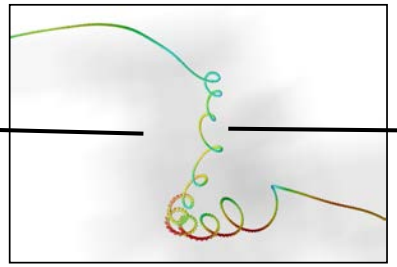


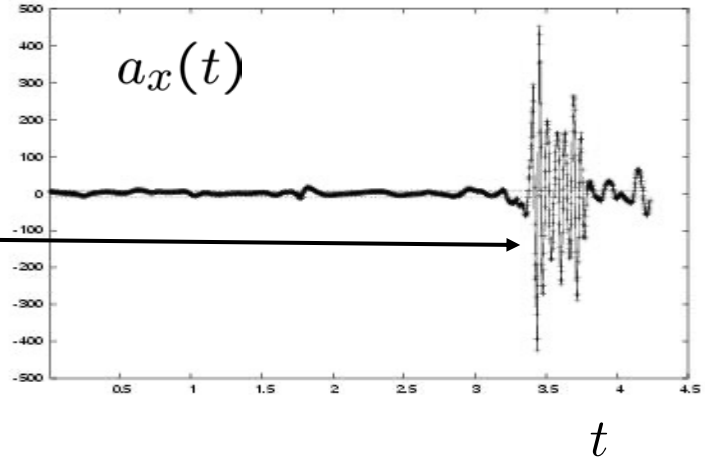
Bentkamp, L, Cr C. Lalescu, and M. Wilczek. "*Nature communications* 10.1 (2019): 1-8.

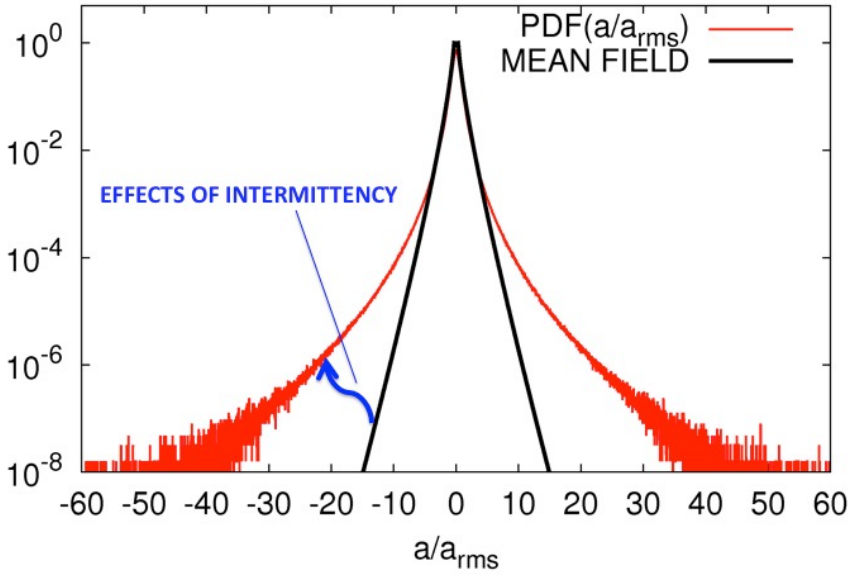
EXTREME EVENTS

L.B. et al Particle trapping in three-dimensional fully developed turbulence
Physics of Fluids 17 (2), 021701 (2005)



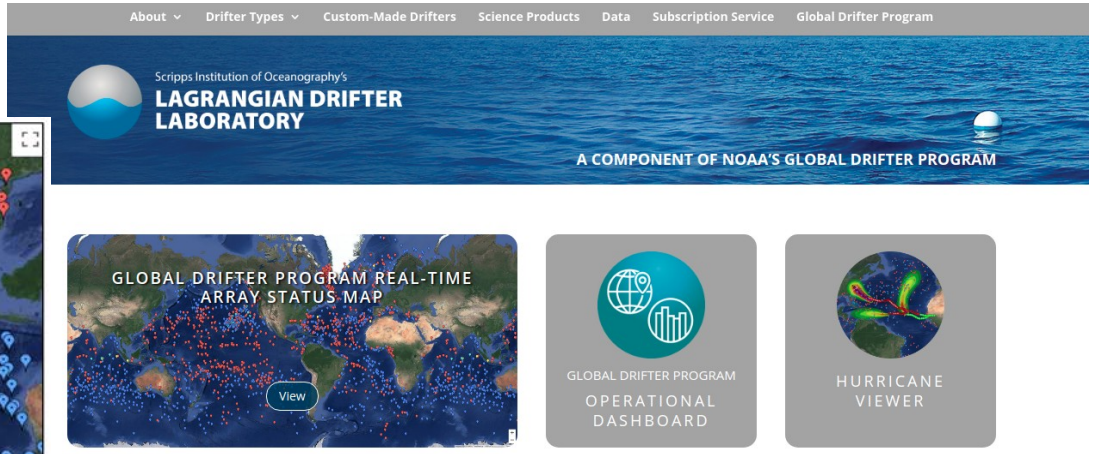






ACCELERATION PROBABILITY DISTRIBUTION FUNCTION (PDF) AT RE ~ 10^5 [Bi04]
COMPARED WITH THE PREDICTION FROM MEAN FIELD (KOLMOGOROV THEORY)

https://gdp.ucsd.edu/ldl/



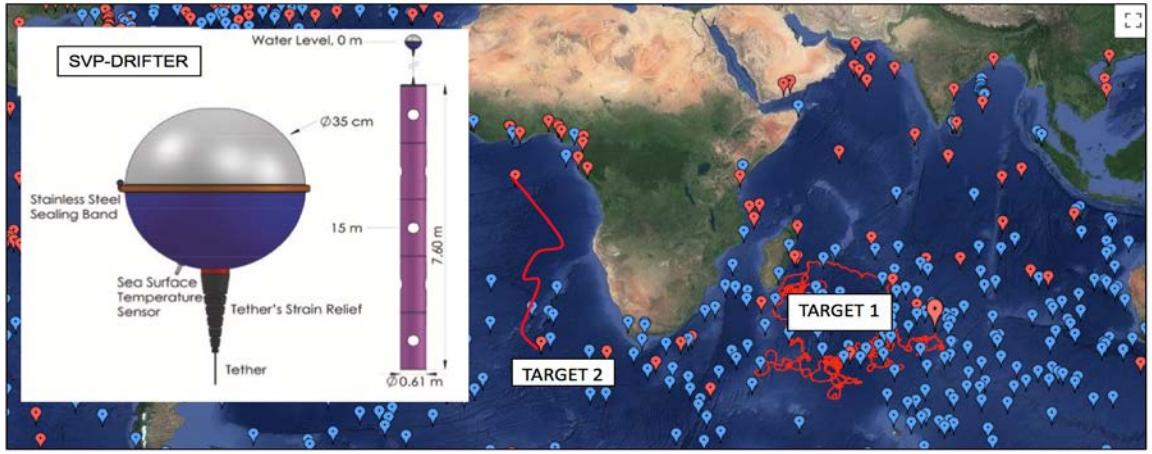


FIG. 1: INSTANTANEOS WORLDWIDE DISTRIBUTION OF DRIFTERS FROM THE GLOBAL DRIFTER MAP PROGRAM [www0]. WE HIGHLIGTHED IN RED TWO POTENTIAL TARGETS: (1) KEEP THE PROBES INSIDE A GIVEN REGION OR (2) MINIMISING THE NAVIGATION TIME AMONG TWO END-POINTS (ZERMELO PROBLEM). INSET: A SKETCH OF THE DRIFTER WITH THE LONG DROUGE AT 15M DEPTH.

GLOBAL DRIFTER PROGRAM
ARGO PROGRAM

D. Roemmich, G.C. Johnson, S. Riser, R. Davis et al.
The Argo Program: Observing the global ocean with profiling floats.
Oceanography 22, 34 (2009)

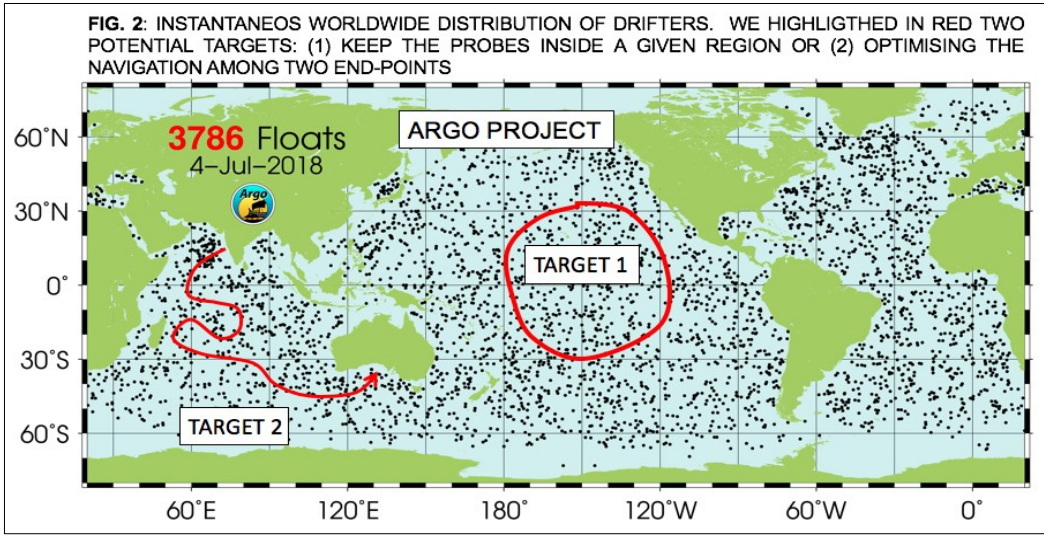


FIG. 2: INSTANTANEOS WORLDWIDE DISTRIBUTION OF DRIFTERS. WE HIGHLIGTHED IN RED TWO POTENTIAL TARGETS: (1) KEEP THE PROBES INSIDE A GIVEN REGION OR (2) OPTIMISING THE NAVIGATION AMONG TWO END-POINTS

$$\partial_t v + v \cdot \partial v = -\partial P + \nu \partial^2 v \; + F(B,B) \; + g\theta \; + \sum_i c_0(u_i, v)\delta(r - r_i) \; + f$$

$$\partial_t \theta + \boldsymbol{v} \cdot \boldsymbol{\partial} \theta = \chi \partial^2 \theta$$

$$\partial_t \boldsymbol{B} + \boldsymbol{v} \cdot \boldsymbol{\partial} \boldsymbol{B} = \boldsymbol{B} \cdot \boldsymbol{\partial} \boldsymbol{v} + \chi \partial^2 \boldsymbol{B}$$

$$\partial \cdot v = 0$$

+ boundary conditions + initial conditions

temperature

magnetic field

$$\frac{d\boldsymbol{u}_i(\boldsymbol{r}_i, t)}{dt} = -\rho_f |\boldsymbol{u}_i - \boldsymbol{v}|(\boldsymbol{u}_i - \boldsymbol{v})$$

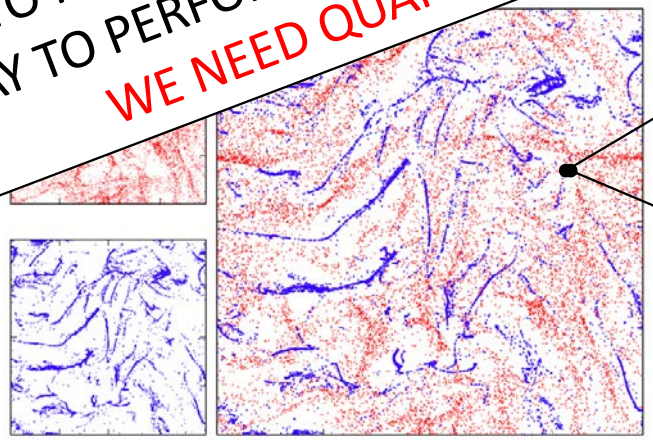
$$+\rho_f \left(\frac{D\mathbf{v}}{Dt} - \frac{D\boldsymbol{u}_i}{}\right)$$

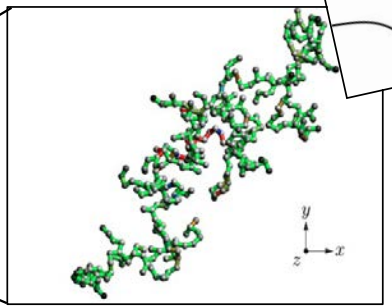
gates:

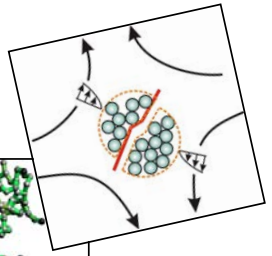
lass, lift force, etc...

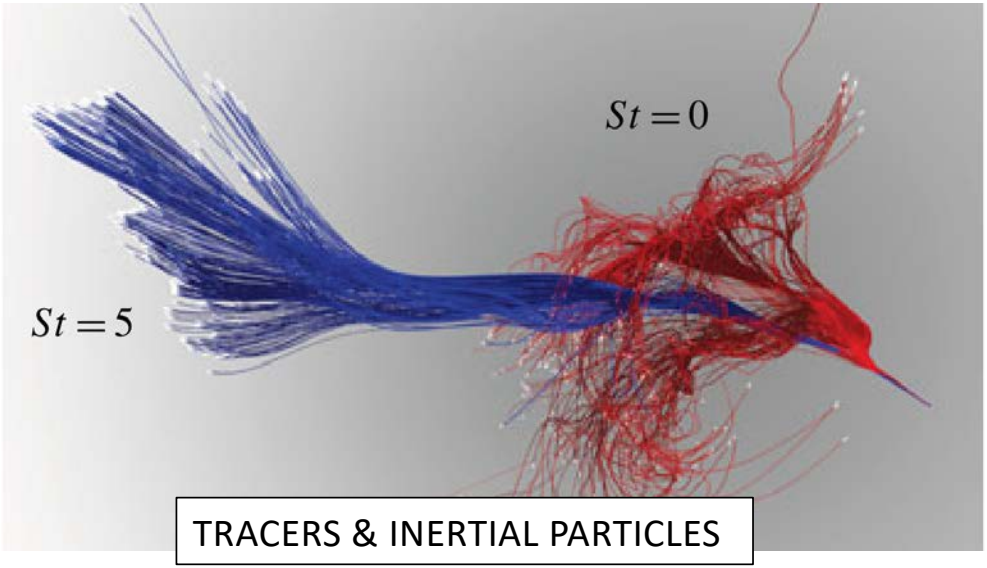
1. NO WAY TO PREDICT STATISTICS FOR MEAN PROFILES OR EXTREME EVENTS FROM EoM
2. NO WAY TO PERFORM DIRECT NUMERICAL SIMULATIONS FOR REALISTIC PROBLEMS

WE NEED QUANTITATIVE MODELS AND TOOLS TO MODEL!

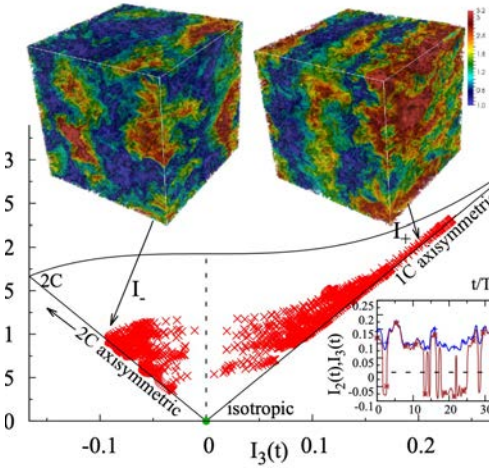




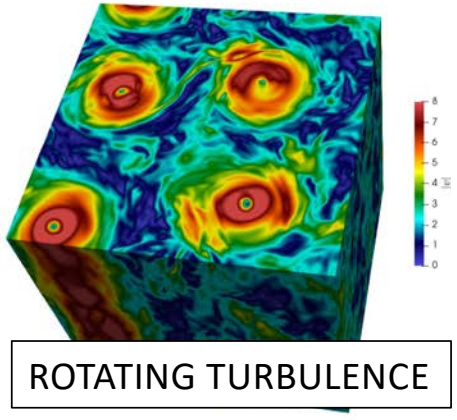




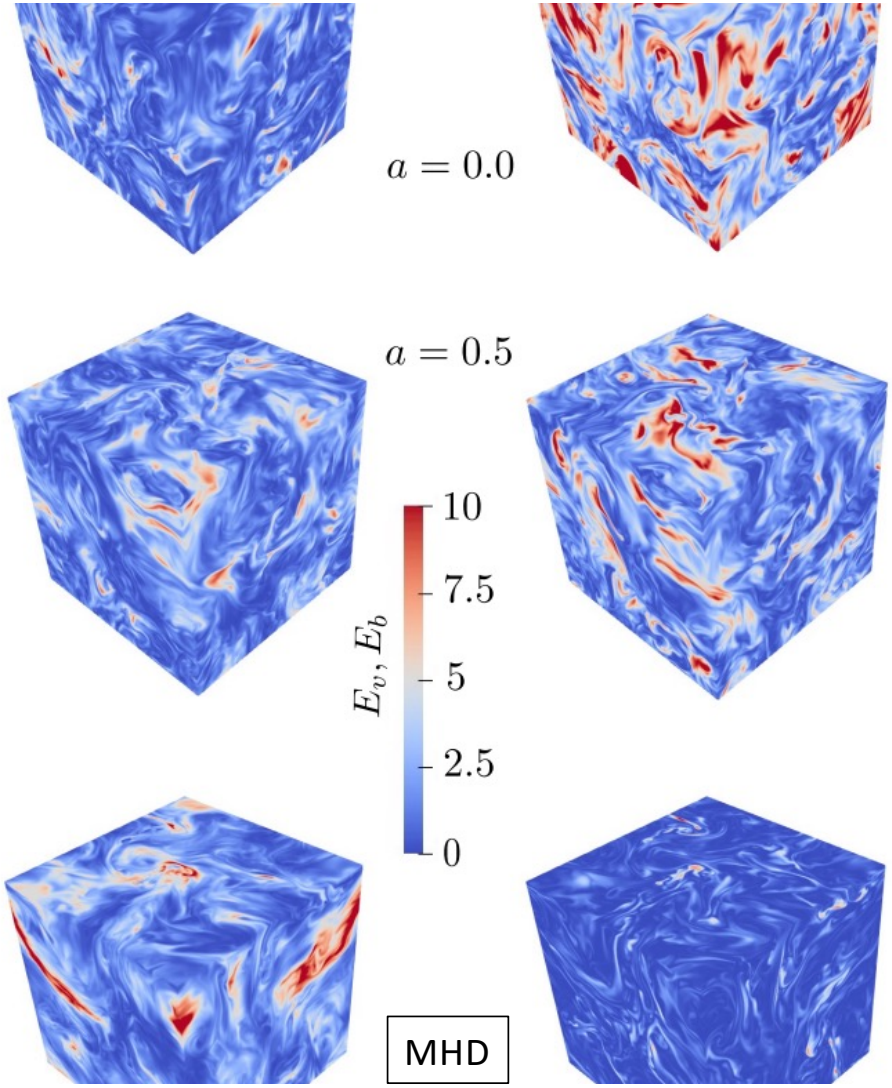
TRACERS & INERTIAL PARTICLES



SHEARED TURBULENCE



ROTATING TURBULENCE



MHD

WP number	4	Start Month	6	End Month	48
WP title	Applications				
Lead Beneficiary	UTOV				

Objectives: Adapt and implement novel HPC algorithms and ML approaches to address challenges in LQCD, CFD and CBio applications and produce groundbreaking scientific results.

Description of Work and Role of Specific Beneficiaries / Associated partners:

Task T4.1: Lattice QCD - Lead UCY/Co-Lead BUW (M6-M48). Four gauge ensembles simulated with physical values of the quark masses by ETMC will be employed to compute key hadron quantities to high accuracy. Specifically, we will target the hadronic vacuum polarization for $g_\mu - 2$, and GPDs enabling us, for the first time, to take the continuum limit. Multi-grid and improved trace estimation algorithms developed in WP1 will be incorporated as being developed to speed up the computations.

Task T4.2: CFD - Lead UTOV/Co-Lead TP-IMT (M6-M48). ML-based approaches for a-posteriori training of optimal sub-grid modeling for large eddy simulations of strongly turbulent flows will be implemented and validated on 2D models for natural convection flows and, then apply in state-of-the-art simulations of realistic 3D Rayleigh-Bénard convection cells. Furthermore, neural network architectures will be employed to improve low-fidelity models and/or simulations, by complementing them with a data-driven component so that the new model accurately and efficiently captures the outputs of high-fidelity simulations to expedite parametric studies for uncovering optimal droplet transport mechanisms.

Task T4.3: CBio - Lead FZJ/Co-Lead KTH (M6-M48). Deep generative flows will be implemented to speed up free energy calculations, by extending the present QM/MM interface in GROMACS to include ML/MM support. A novel method which is based on metadynamics and path probability distribution will address the key issues of code scalability and the timescale problem in free energy computations.

Description of Deliverables:

D4.1 Initial benchmarks of new algorithms for LQCD - UCY (M24). Report on new algorithms providing performance input for WP1.

D4.2 Results on $g_\mu - 2$ and GPDs - UCY (M40). Report on results for $g_\mu - 2$ and the three isovector GPDs in the continuum limit.

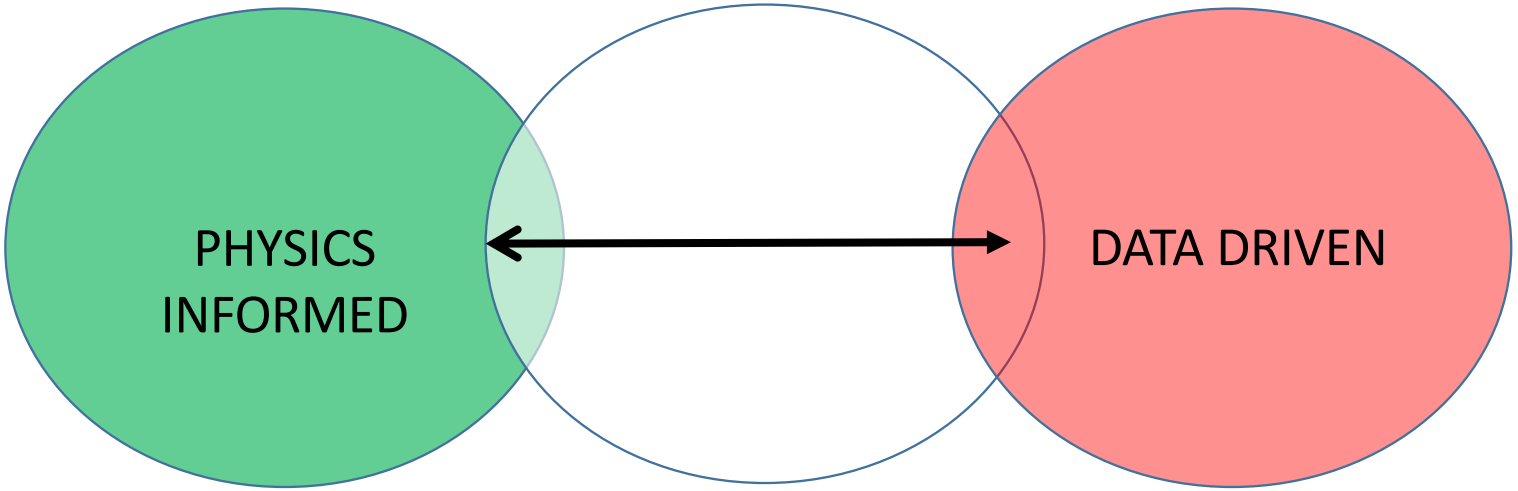
D4.3 Performance of new data-driven tools applied to CFD simulations - UTOV (M36). Report on AI and data-driven methods in CFD simulations for turbulent flows and complex wetting phenomena.

D4.4 Free energy evaluation using improved QM/MM GROMACS interface - FZJ (M40). Report on the efficiency of the QM/MM GROMACS interface and results on free energy calculations.

ESR5: Deep-data assimilation and deep-feature-based metric for turbulent flows

ESR12: Large eddy simulation models in a deep machine learning loop

ESR13: Complex wetting problems using neural networks



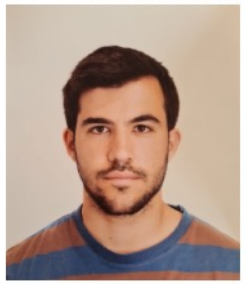
NEED FOR QUANTITATIVE BENCHMARKS, CHALLENGES, BASELINES:
MOVING AI FROM CHERRY PICKING (PROOFS-OF-CONCEPT) TO ROBUST QUANTITATIVE USEFUL TOOLS (SUPREMACY?)

ESR5: DATA ASSIMILATION

GROUND TRUTH

Francesco Fossella

Elisa Bellantoni

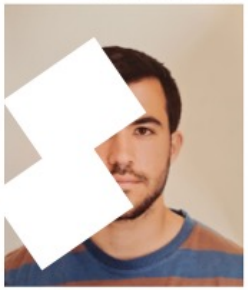


Andre Freitas

CORRUPTED IMAGE

Francesco Fossella

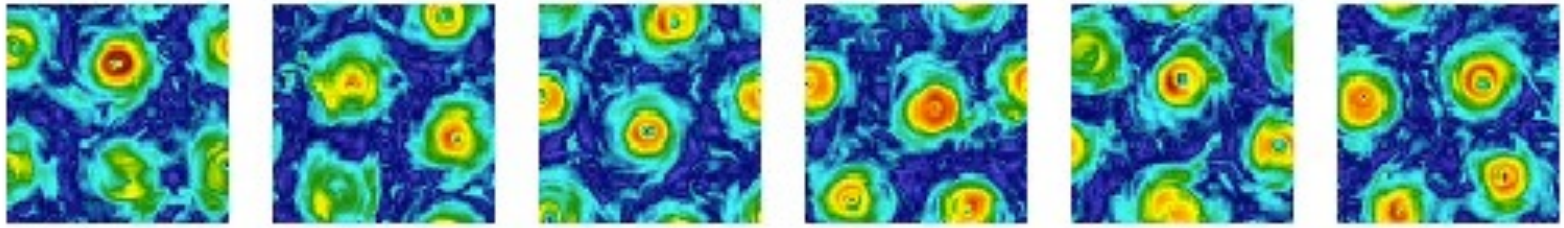
El :oni



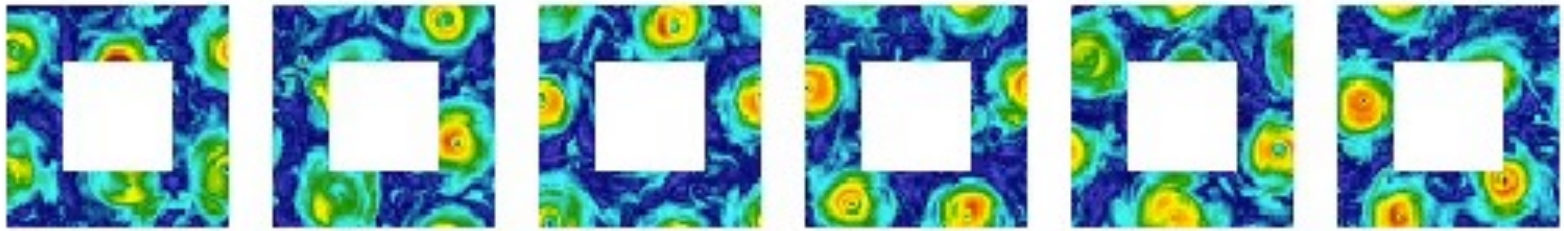
Andre Freitas

ESR5: DATA ASSIMILATION

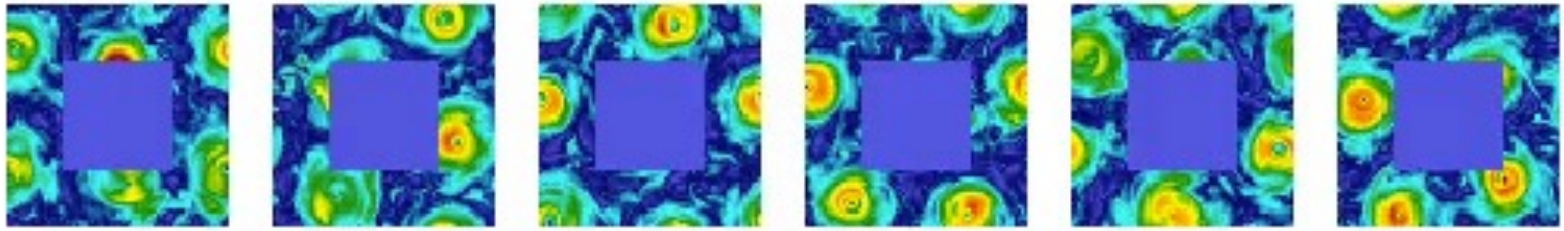
GROUND TRUTH VELOCITY MAGNITUDE



CORRUPTED IMAGE

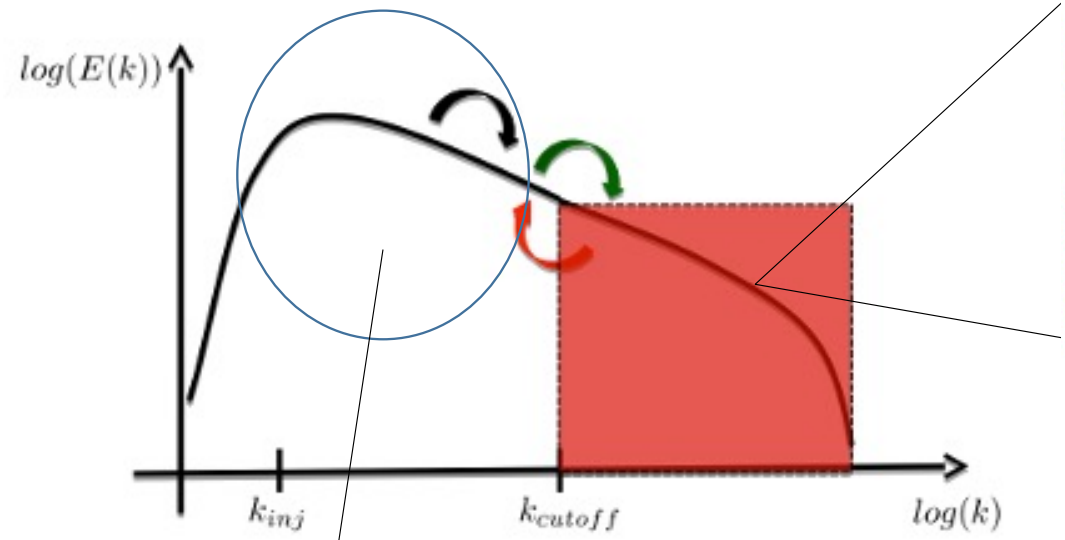


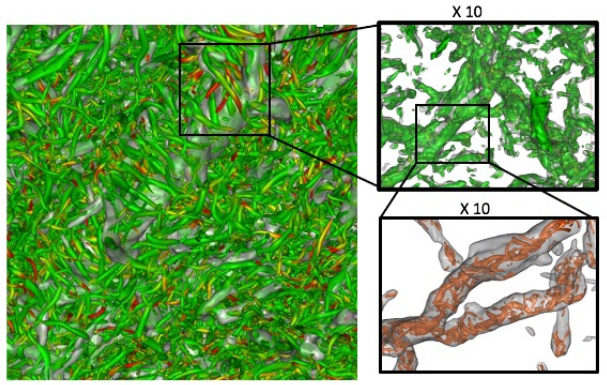
FILLED



ESR12: TURBULENCE MODELING

$$\overline{\boldsymbol{v}}(\boldsymbol{x},t) \equiv \int_{\Omega} d\boldsymbol{y}\; G(|\boldsymbol{x}-\boldsymbol{y}|)\; \boldsymbol{v}(\boldsymbol{y},t) = \sum_{\boldsymbol{k}\in\mathbb{Z}^3} G(\boldsymbol{k})\; \hat{\boldsymbol{v}}(\boldsymbol{k},t) e^{i\boldsymbol{k}\boldsymbol{x}}$$





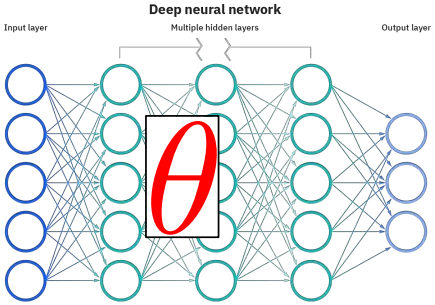
NEED TO MODEL NON-GAUSSIAN & MULTI-SCALE PHYSICS !!!

$$\partial_t \overline{\boldsymbol{v}} + \nabla \cdot (\overline{\boldsymbol{v}} \otimes \overline{\boldsymbol{v}}) = -\nabla \overline{p} + \nabla \cdot \tau^{\Delta}(\boldsymbol{v},\boldsymbol{v}) + \nu \Delta \overline{\boldsymbol{v}}$$

$$\tau_{ij}^{\Delta}(\boldsymbol{v},\boldsymbol{v}) = \overline{v_i v_j} - \overline{v}_i \overline{v}_j \xrightarrow{??????} \tau(\overline{v},\overline{v})$$

ESR12: TURBULENCE MODELING

PDE SOLVERS IN THE LOOP



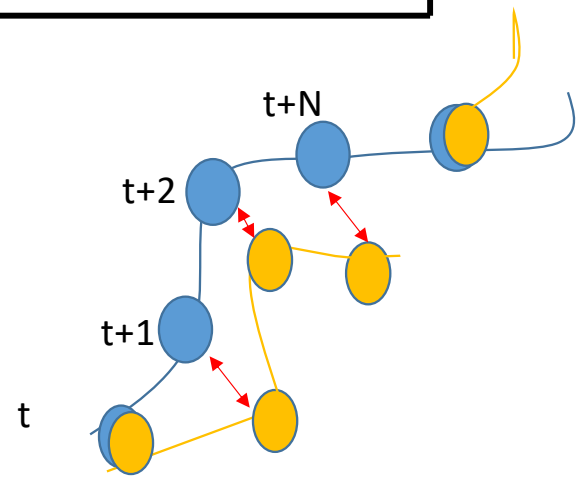
$$[\bar{v}_\theta(t)] \quad \tau(\bar{v}_\theta(t),\theta) \quad \text{NAVIER-STOKES SOLVER} \quad [\bar{v}_\theta(t+\delta t)]$$

REPEAT N-TIMES

$$L(\theta) = D[v(\cdot), \bar{v}_\theta(\cdot)] = \int dx \int_0^T dt ||v(t) - \bar{v}_\theta(t)||_2$$

$$\theta_{k+1} = \theta_k - \alpha \partial_\theta L(\theta_k) \longrightarrow \partial_\theta L = \partial_{\bar{v}} L \, \partial_\theta \bar{v}$$

PROBLEM !!!!!!

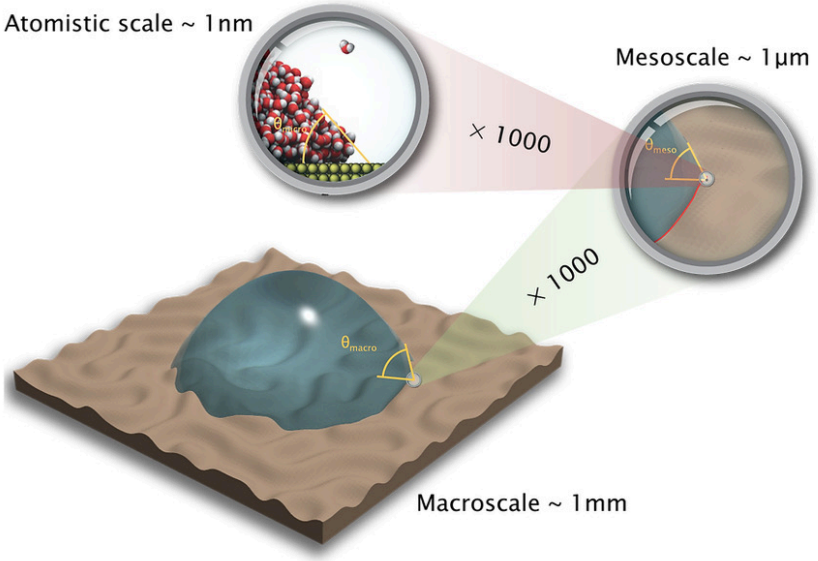


$$\partial_t \bar{v}_\theta + \nabla(\bar{v}_\theta \otimes \bar{v}_\theta) = -\nabla \bar{p}_\theta + \nabla \tau(\bar{v}, \theta) + \nu \Delta \bar{v}_\theta$$

ESR13: COMPLEX PHYSICS INFERRING

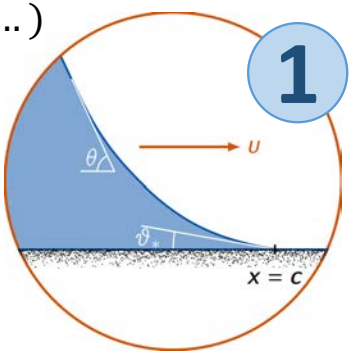
Wetting hydrodynamics

an inherently multiscale phenomenon

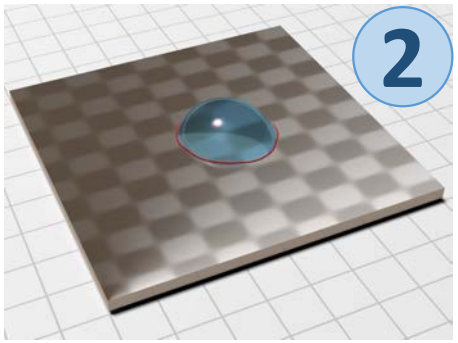


Reduced-order models

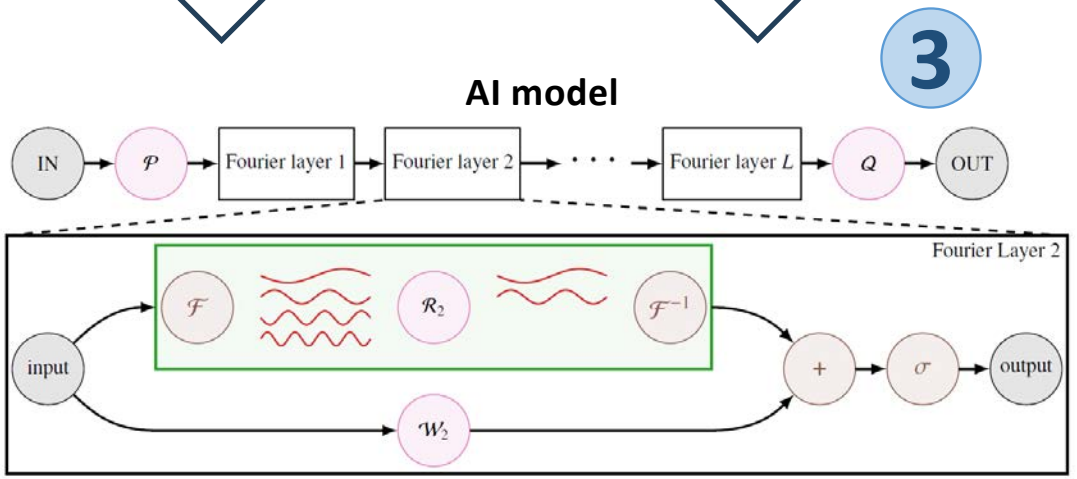
$u = \mathrm{F}(\theta, \vartheta_*, \dots)$



Lattice-Boltzmann Simulations



AI model



Expected results

- Accelerated CFD simulations
- Novel workflows for droplet transport