

WP3 “Compute-Driven Use-Cases at Exascale”

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Partners and Tasks of WP3

Partner	FZJ	UOI	Cyl	RWTH	BSC	CERFACS	BULL	RTU	SAFRAN
PM	12	6	18	24	30	38	23	7	26

Task	Title	Lead	Duration	Status
3.1	AI for turbulent boundary layers	RWTH	M1-M36	
3.2	AI for wind farm layout optimization	BSC	M1-M36	
3.3	AI for data-driven models in reacting flows	CERFACS	M1-M36	
3.4	Smart models for next-generation aircraft engine design	SAFRAN	M1-M36	
3.5	AI for wetting hydrodynamics	Cyl	M1-M36	

Deliverables and Milestones of WP3

Deliverable	Title	Due	Lead	Status
D3.1	Report on outcomes of WP3 use-cases (1)	M12	RWTH	Accepted
D3.2	Report on outcomes of WP3 use-cases (2)	M24	CERFACS	Submitted
D3.3	Report on outcomes of WP3 use-cases (3)	M42	CERFACS	Not started

Milestone	Title	Due	Lead	Status
MS1	Project kick-off	M1	FZJ	Done
MS4	Use-cases / technical developments	M24	UOI	Done
MS6	All final reports	M42	FZJ	Not yet achieved

Compute-Driven Use-Cases at Exascale

Several physics problems spanning a variety of domains, with common ground

Challenging

Relevant to
the industry

Computationally
intensive

AI tools are applied on these problems to:

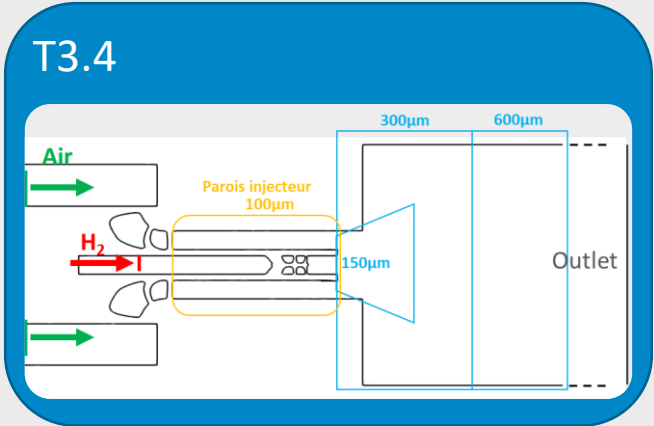
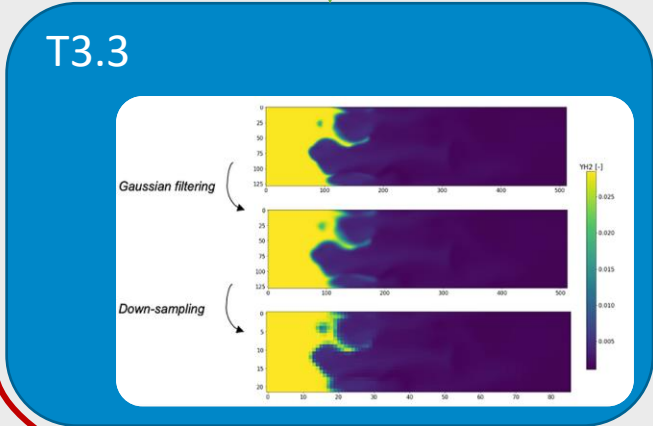
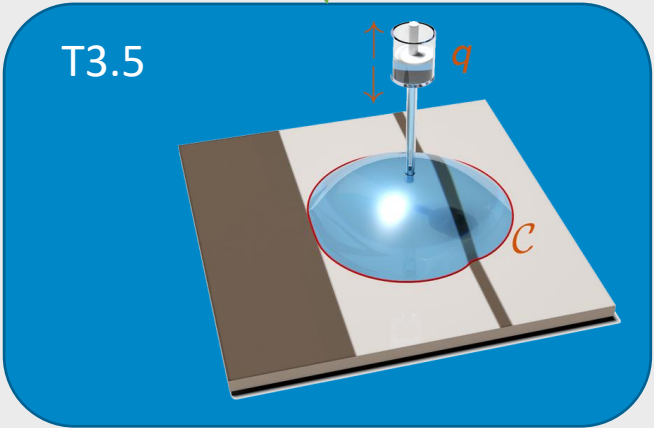
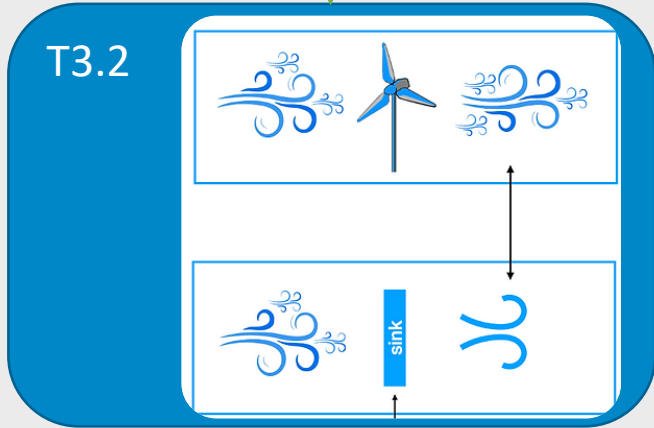
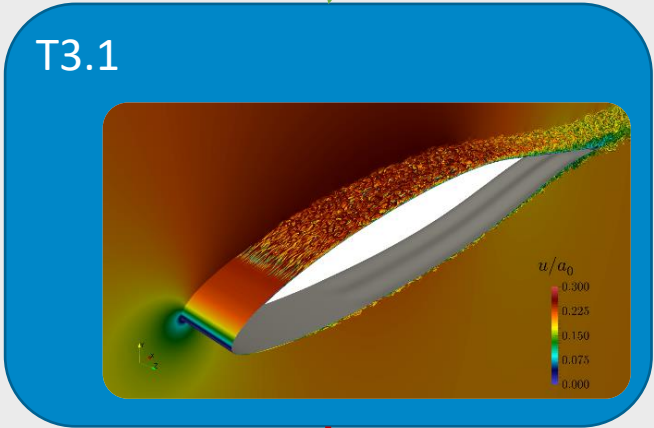
Accelerate existing
workflows
(lower cost, lower
time to solution)

Increase scale /
accuracy of
adressable problems

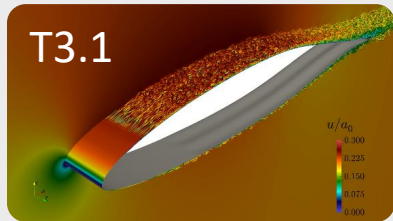
Produce new
workflows relisient to
evolving hardware

WP3 Structure

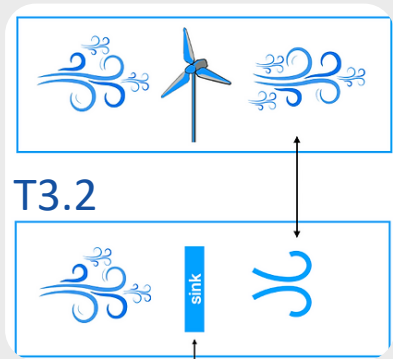
WP2 Algorithms



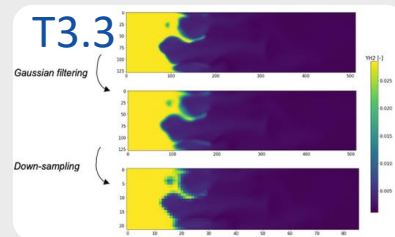
WP3 CFD software



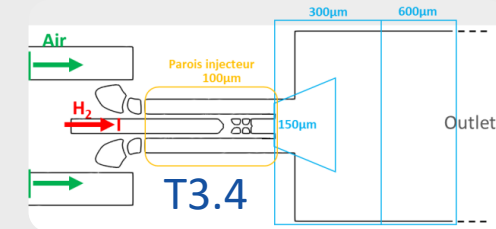
m-AIA



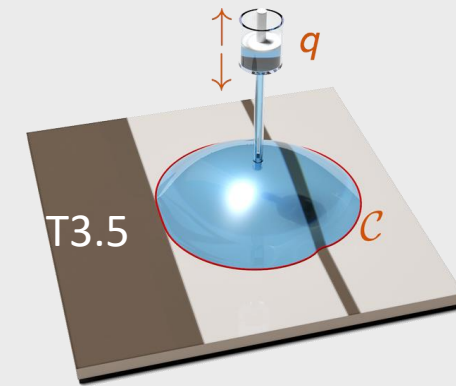
Alya



PhyDLL



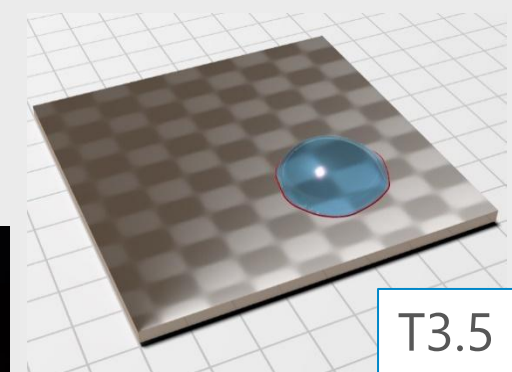
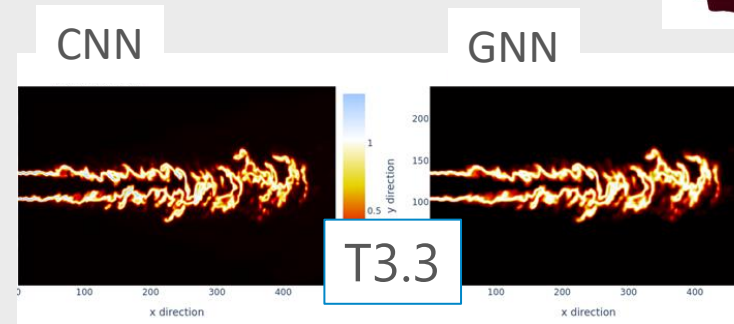
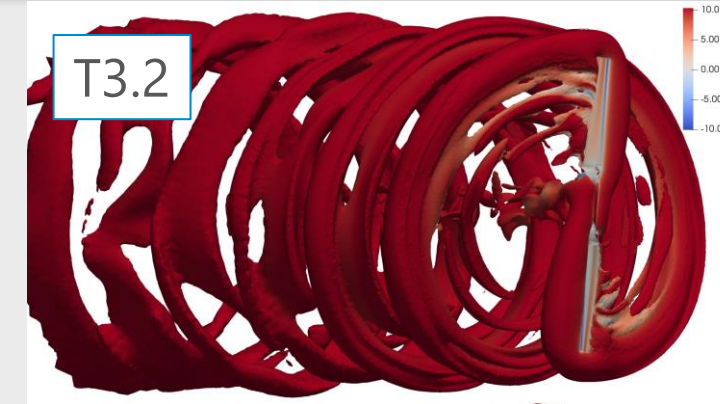
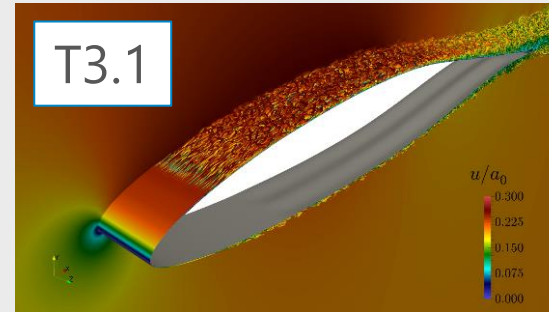
AVBP-DL



Basilisk

Deliverable 3.2 Highlights

- Common objectives
 - Explore methodologies for AI-CFD hybrids
 - Accelerate simulation workflows manyfold
 - Enable larger-scale simulations
- Synergies
 - Similar data between problems (CFD data) means similar handling and training issues. Commonalities in tooling.
 - Discovery and sharing of learning algorithms well suited to fluid flow (physics-informed, fourier, native fluid mesh...)
 - Development of new, generic tools for hybrid simulation (e.g. PhyDLL).



Some Notable Next Steps

- T3.1: Extend method to new physics (incompressibility and pressure gradient effects, flow separation, higher Reynolds) and explore Physics-Constrained learning
- T3.2: Scale-up training data with large variety of simulations and expand methods
- T3.3: develop the PhyDLL open-source library, explore domain decomposition training and inference for GNNs
- T3.4: demonstrate T3.3 developments on an industrial scale engine simulation
- T3.5: improve distributed learning through libraries(Horovod, Ray-Tune...), developments (parallel-io, GPU...), and optimizations

drive. enable. innovate.



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