

# High performance numerical simulation at ONERA

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Scientific director « Advanced numerical simulation »

EUCASS meeting, Lille

*Contribution to research and competitiveness*

*Grand challenge applications*

*ONERA strategy*

# Numerical simulation, third pillar of science

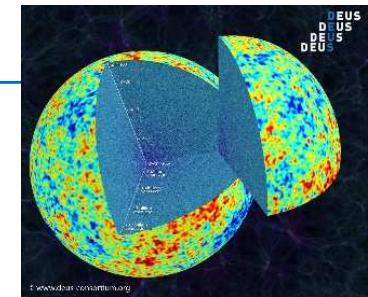
Integral part of science, added to theory and experimentation

- *Basic research* in astrophysics, climatology, biology...

DEUS Project  
CNRS

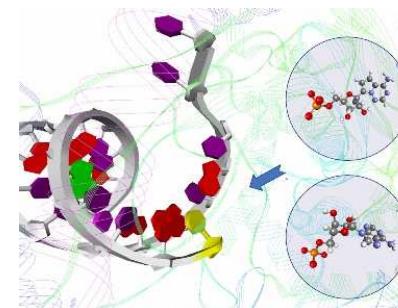
## Cosmology: Evolution of the Universe

- 1<sup>st</sup> full simulations in the evolution of the structuration of the whole observable Universe, from the Big Bang to nowadays
- 20 million core hours GENCI on Curie in 2012

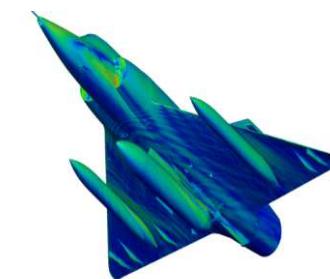
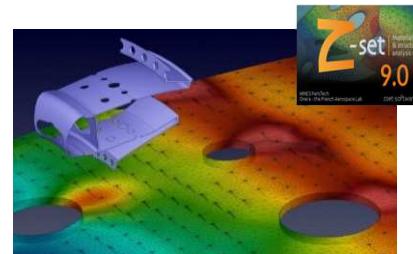
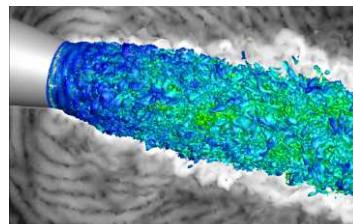


- Answer to *emergency situations* : earthquakes, tsunamis, epidemics...

The COVID-19 HPC consortium in USA  
(600 Petaflops, 7 million cores)



- *Engineering sciences* : fluid mechanics, acoustics, structural mechanics, materials, electromagnetism...



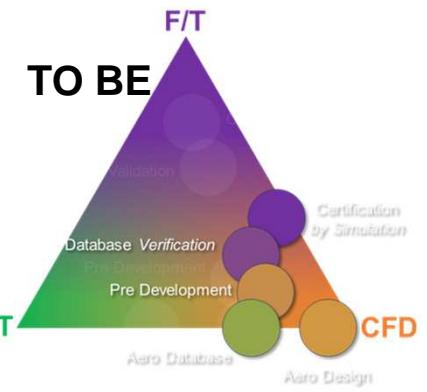
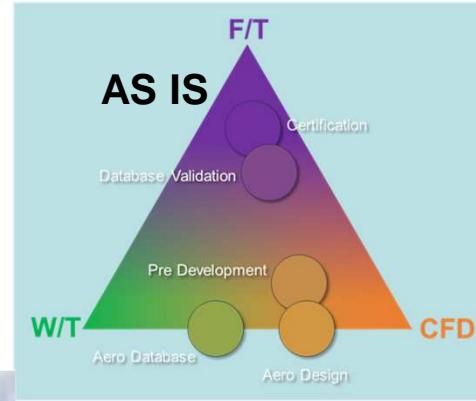
ONERA simulations

# Numerical simulation in aerospace

## For competitiveness

- Productivity gains in **design** of new aircraft
- Study of **breakthrough** configurations

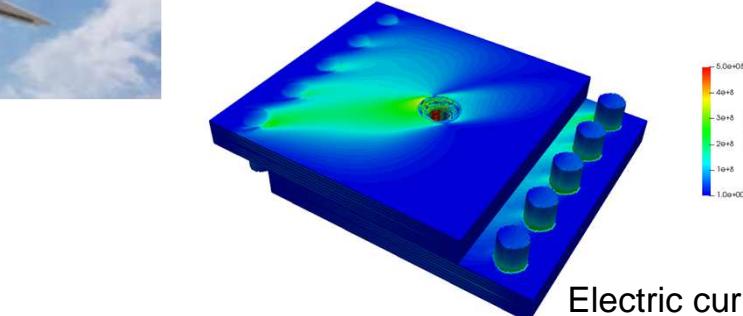
Configuration DRAGON  
@ONERA



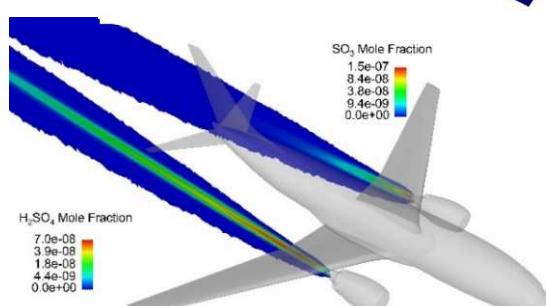
Airbus-Boeing talk (3AF 2019)

## For issues of general interest

- **Safety** : flight domain limits, icing problems, lightning effects...
- **Environment** : polluting emissions, climate impact, noise...



Electric current distribution  
In a structure struck by lightning  
Code TARANIS @ONERA



Contrail  
Code CEDRE @ONERA

# « Advanced Numerical Simulation » : a fifth scientific domain at ONERA since 2017

***Dealing with all (possibly coupled) disciplines of physics***

Aerodynamics	Materials
Aeroelasticity	Structural mechanics and dynamics
Aeroacoustics	Electromagnetism
Aerothermochemistry	Plasma
Conjugate heat transfer	Magnetohydrodynamics

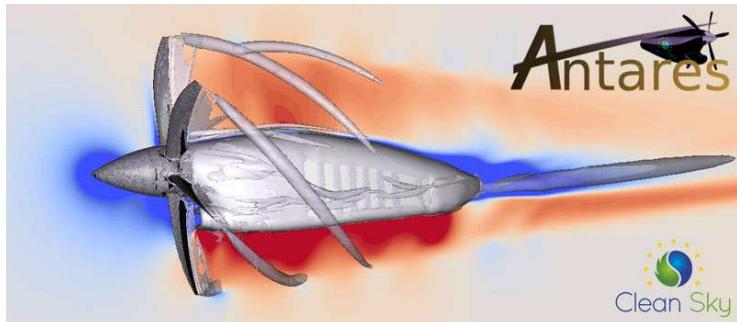
- For Aeronautics, Space and Defense
- Interacts with all ONERA research depts and the 4 other scientific domains
- Takes into account the important part of scientific and technical production corresponding to software
- Includes the whole range of involved research and development process

***Modelling, algorithmics and applied mathematics, HPC, coupling of physics, reduced modelling, uncertainty management, software policy, development partnerships...***

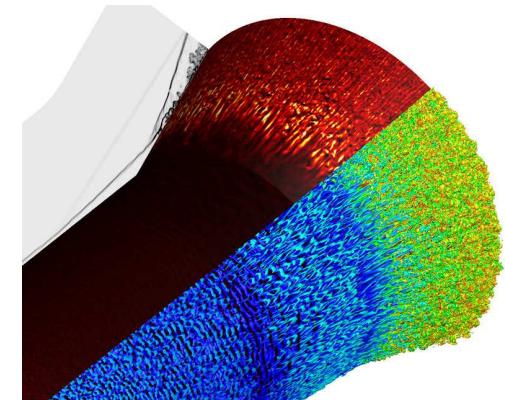
# Grand challenge simulations

## Many motivations

- « First of a kind » configurations
- Very high fidelity simulations to improve physical modeling
- Identification and solution of scientific issues
- Adaptation of methods and tools to new HPC hardware



e/lsA URANS simulation of a turboprop



FASTS QDNS simulation  
Hypersonic compression ramp

## Extension ONERA Sator supercomputer (autumn 2021)

- Offered to ONERA young researchers during 2 months for grand challenges
- NEC, 43600 cores (extension : Intel Xeon Cascade Lake)
- LINPACK performance : 1,8 PFlop/s
- 21 million CPU hours attributed to 14 challenges

→ big success !

# Grand challenge simulations : 4 examples from 4 different ONERA research departments

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## Electromagnetism

- Modeling of a scene of electromagnet. fields radiated by 4G/5G transmitters
- *Dept Electromagnetism and Radar* (R. Cranny & T. Volpert, DEMR)

## Aeroacoustics

- LBM simulations for the direct prediction of the noise of a grid turbulence impacting a blade cascade
- *Dept Aerodynamics, Aeroelasticity, Acoustics* (M. Buszyk & T. Le Garrec, DAAA)

## Energetics (CCRT)

- Fiber-regime atomization simulation for interfacial area quantification
- *Dept Multi-Physics for Energy* (J.C.Hoarau, L.H.Dorey, D.Zuzio, J.L.Estimalezes, DMPE)

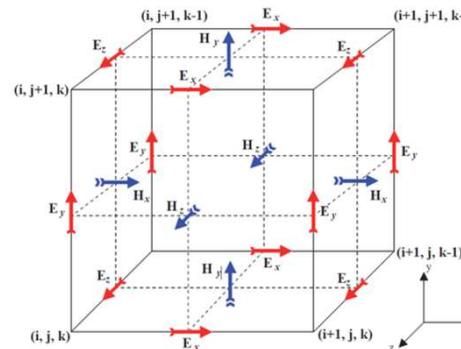
## MDO with uncertainties

- Uncertainty propagation study of performances of a reusable launcher
- *Dept Information Processing and Systems* (M. Balesdent & L. Brévault, DTIS)

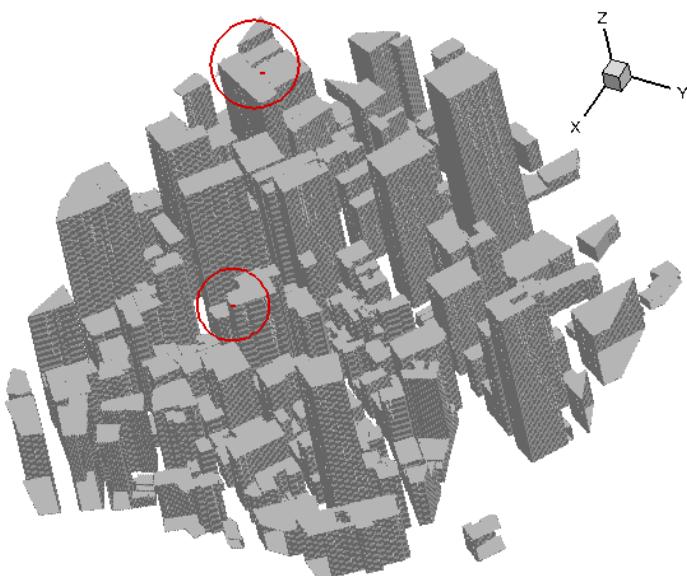
# ElectroMagneticCompatibility (EMC) simulation : calculation of EM fields radiated by 2 transmitters (1/2)

## Finite Difference Time Domain ALICE Code

- Developed by ONERA since the 90's initially for EMC applications
- Resolution of Maxwell's equations in time domain via the leap frog Yee' scheme
- Cartesian Grid
- Conductive and Dielectric materials
- Structured and unstructured wiring
- Plane wave and voltage/current generators
- MPI Parallel Code



$$\begin{aligned}\underline{\mu} \frac{\partial \mathbf{H}}{\partial t} + \nabla \wedge \mathbf{E} &= 0 , \\ \underline{\epsilon} \frac{\partial \mathbf{E}}{\partial t} - \nabla \wedge \mathbf{H} + \underline{\sigma} \mathbf{E} + \mathbf{J}_s &= 0 , \\ \nabla \cdot (\underline{\epsilon} \mathbf{E}) &= \rho , \\ \nabla \cdot (\underline{\mu} \mathbf{H}) &= 0 .\end{aligned}$$



### Model characteristics (Manhattan district) :

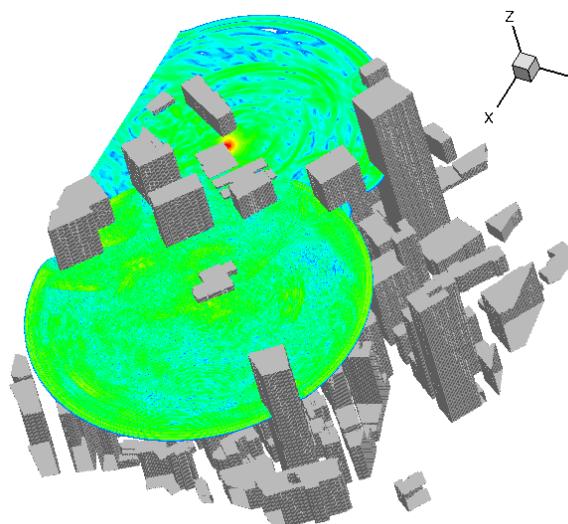
- Modelling area = 700m x 600m x 300m
- Cubic Cell size=10cm
- Frequency band of analysis=[10kHz – 500MHz]
- **126 billion cells**, 82000 time iterations.
- Conductive materials
- 2 transmitters (on building roofs)

### Run parameters (on ONERA HPC SATOR):

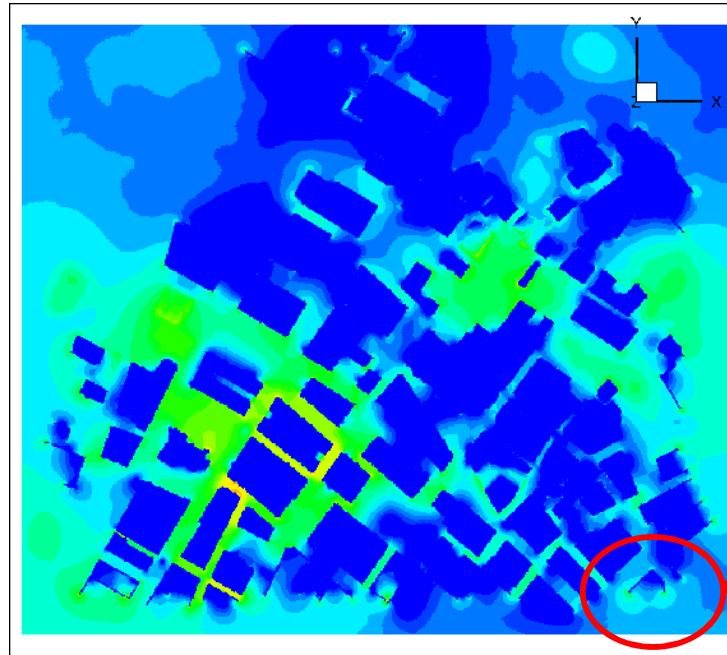
- 22 CPU hours on 11264 processors

# ElectroMagneticCompatibility (EMC) simulation : calculation of EM fields radiated by 2 transmitters (2/2)

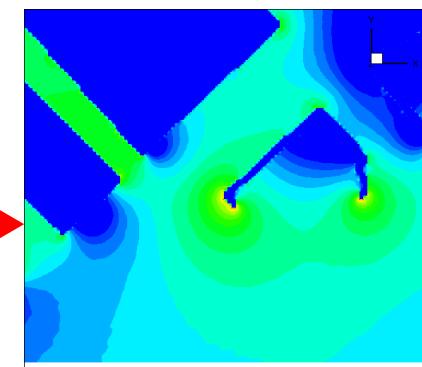
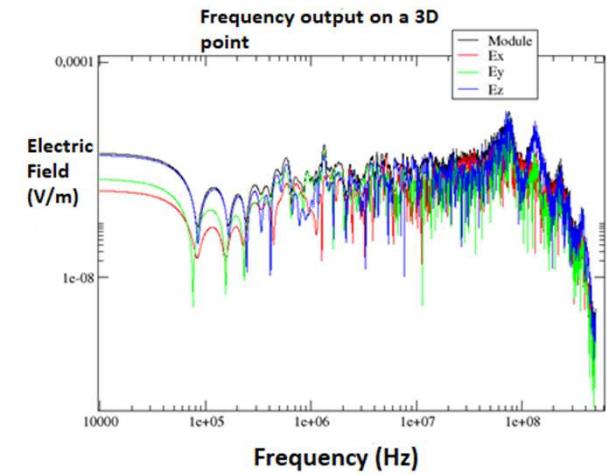
Time domain E-fields  
Height=150m  
Time=0.75  $\mu$ s



E-fields at 500MHz  
Height=50m



Large band frequency output



Lessons learned :

- Dealing with very large meshes
- Post-processing of large amount of data
- Scalability tests > 10 000 procs

First of a kind simulation → application perspectives, such as :

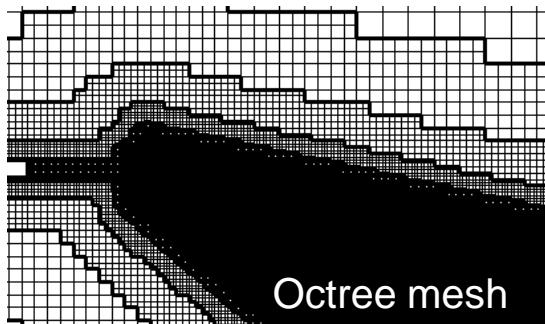
**Resistance of UAV to electromagnetic environments in urban operation**

# 2 billion points LBM simulations for turbulence-airfoil interaction noise reduction

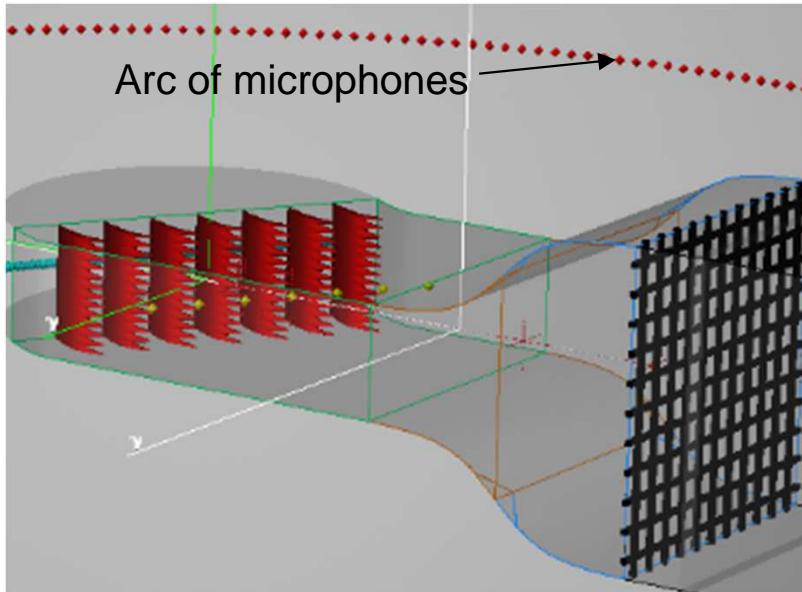
InnoSTAT – Innovative STATOR  
EU project to design low-noise stators



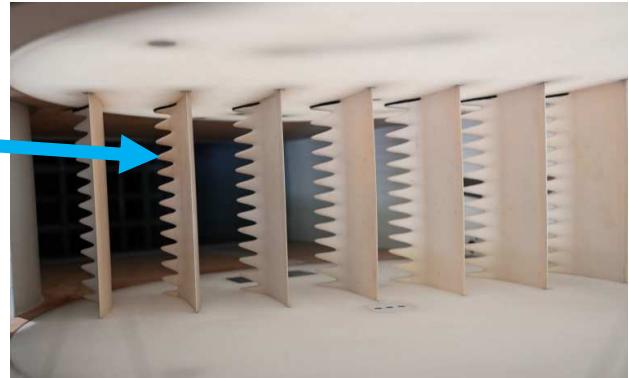
ONERA : - low-noise designs: **leading edge serrations**  
- **lattice Boltzmann Method (LBM) simulations**  
with ProLB (developed by a French consortium)



- Immersed boundary cond.
- Full **setup** with **full span airfoils, wind tunnel walls and inlet turbulence grid generator**



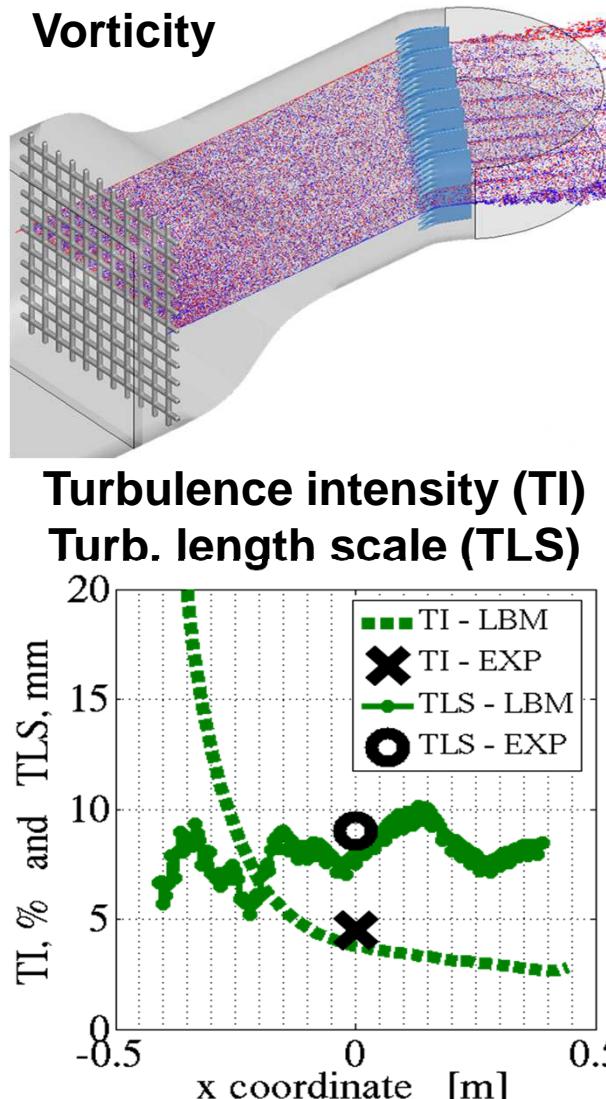
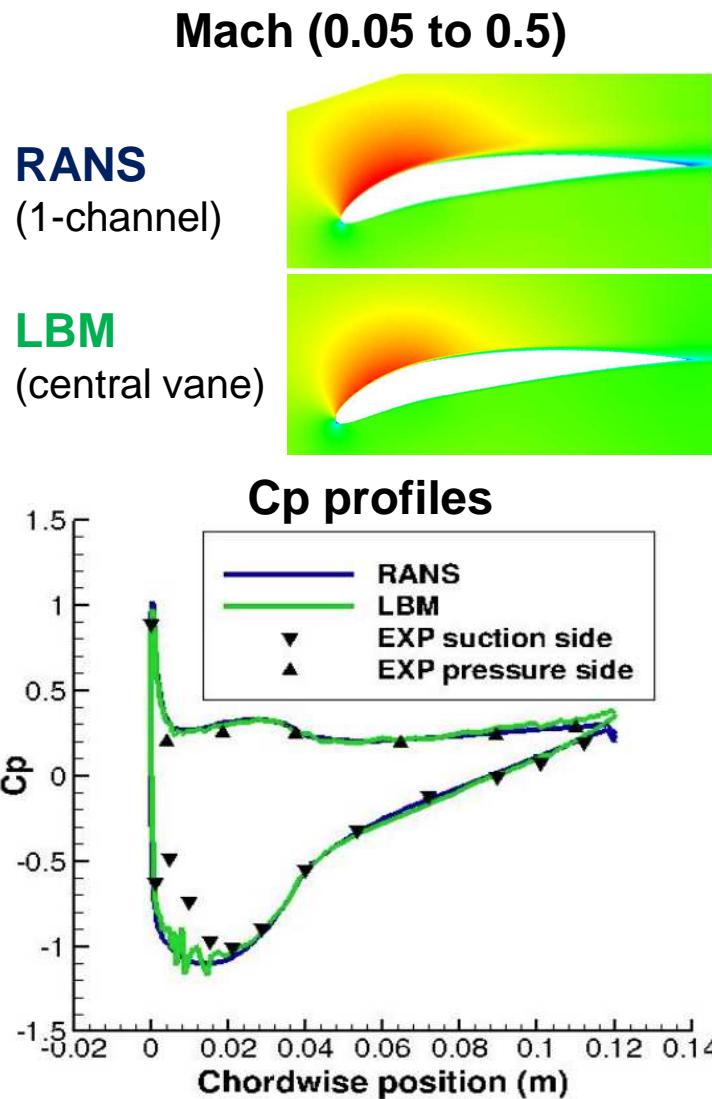
Exp. (Ecole Centrale Lyon)



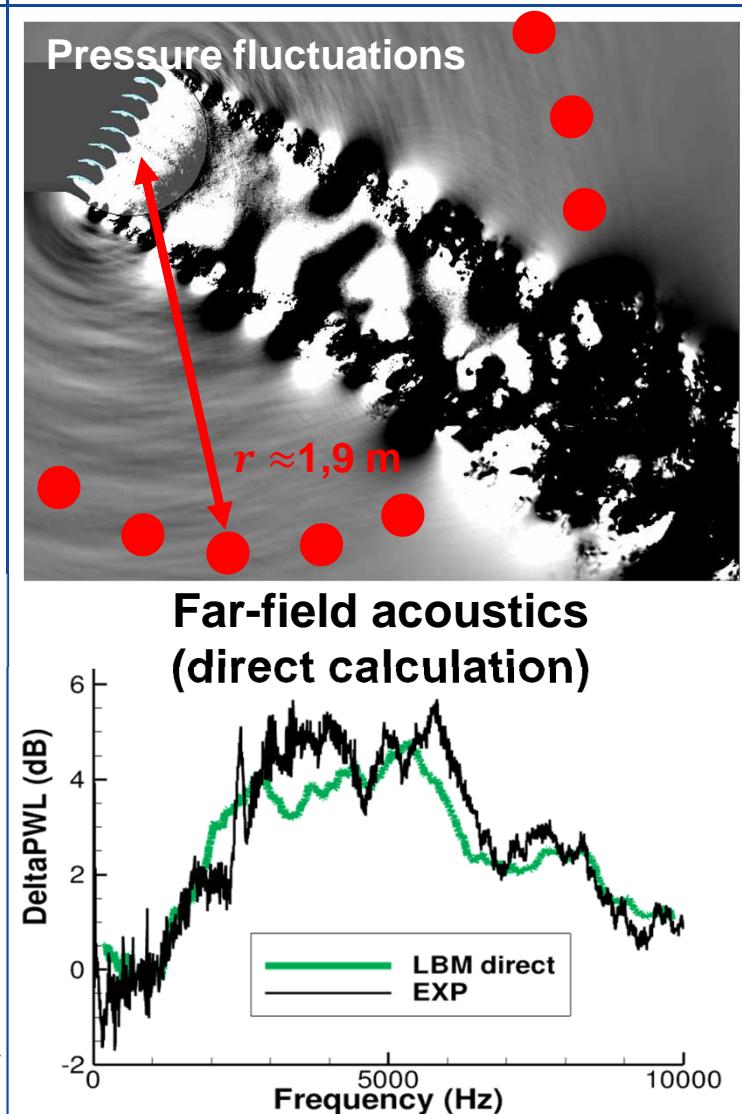
Cores	4000 / 8000
Restitution Time	≈ 2 / 4 days
CPU time	320 / 400 kh
Points	<b>2 billion</b>
Physical Time / Without transient	≈ 0.4 s / ≈ 0.2 s
0.2 s ≈ 192 chord/U	

Very fine mesh (better mesh transitions in wake, points around blades X 2) → Improved physics description

# Aerodynamics performance



# Prediction of broadband noise reduction



Aerodynamics and Acoustics match very well with RANS and EXP !

# Direct numerical simulation (DNS) of coaxial atomization

## Fiber regime atomization in liquid rocket engine injection

### Objectives of the DNS simulation

- Validation base for atomization modeling
- Visualization of the formation mechanism of droplets and their repartition



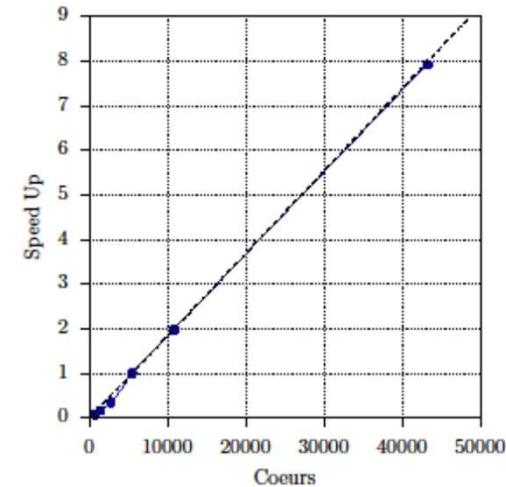
J. C. Hoarau, F. Granger, L. H. Dorey, D. Zuzio, J. L. Estivalezes

### Two-phase simulation (DYJEAT research software)

- Incompressible Navier-Stokes
- Sharp interface reconstruction (CLSVOF)
- Regular Cartesian mesh

### Numerical setup

- 3 billion mesh points
- CCRT TOPAZE : 110 592 cores
- Use of 43200 / 86 400 cores
- 45 million CPU hours

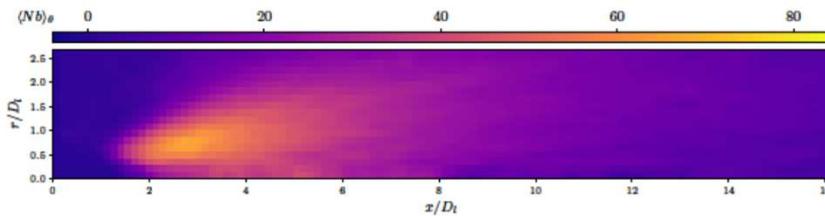


# Direct numerical simulation (DNS) of coaxial atomization

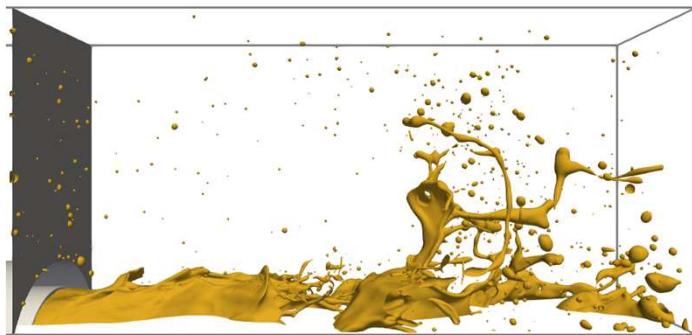
## Fiber regime atomisation in liquid rocket engine injection

New results not available in experiments :

- Averaged number of droplets



- Precise visualization of the atomisation process

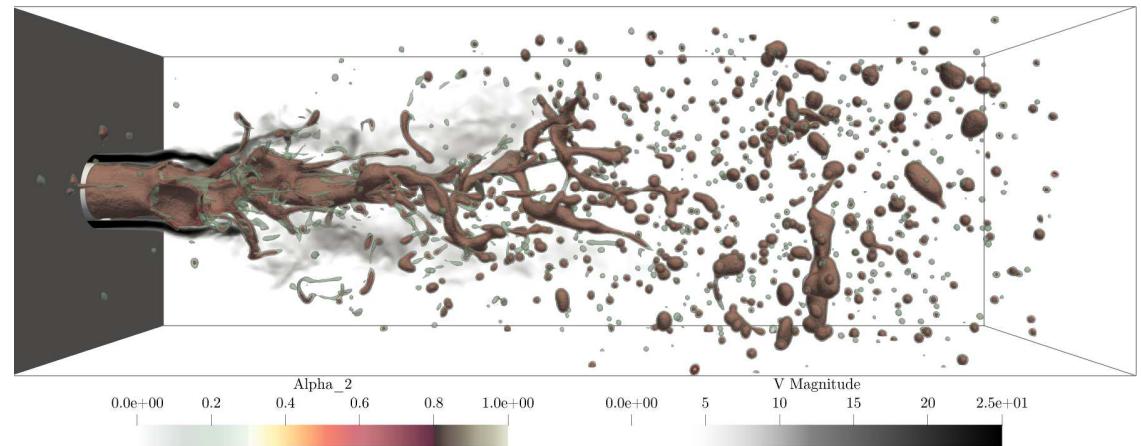


Validation database for LES simulation :

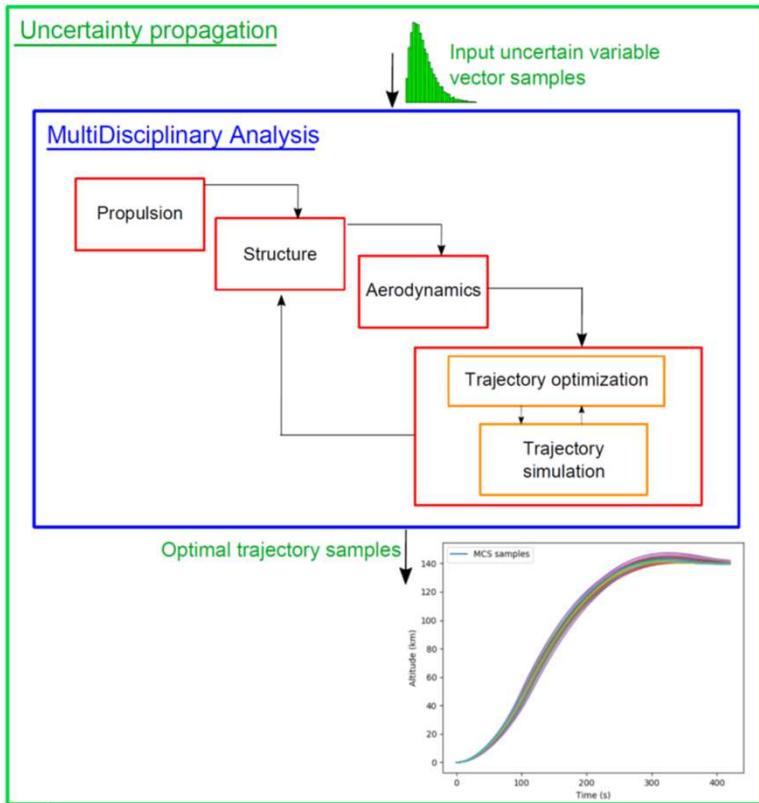
- Sub-grid modeling of the interface density transport
- Dynamic and repartition of the droplet creation

Time: 0.137335

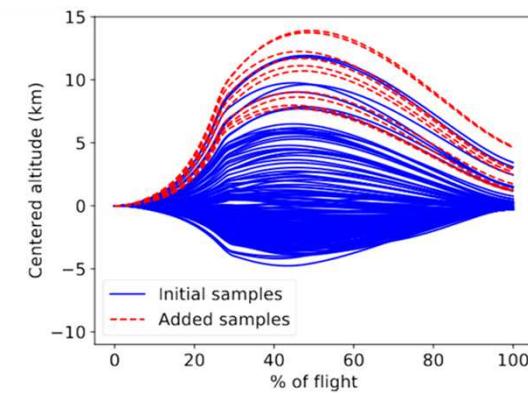
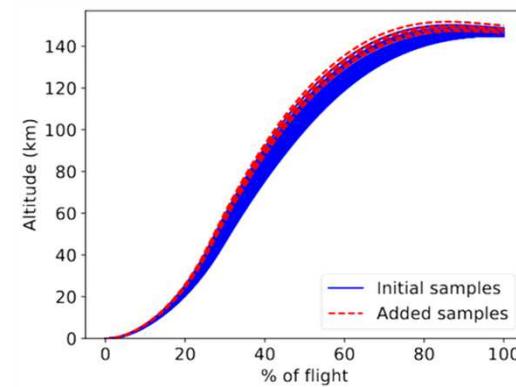
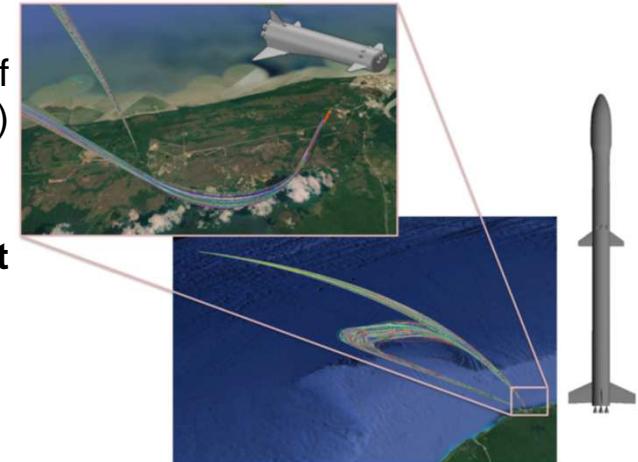
ONERA CEDRE



# MDO under uncertainties : Estimation of flight envelopes of launch vehicles



- Characterization of flight envelopes of launchers under uncertainties by estimation of quantiles
- Methodology based on combination of model reduction (Karhunen-Loève) and Gaussian process
- Devel. of an **adaptive enrichment strategy**  
→ adaptive selection of CPU-costly multidisciplinary simulations to improve the accuracy of the estimation of quantiles



« ONERA HPC SATOR Grand challenges for young scientists » (November 2021)  
→  $6 \times 10^5$  h CPU on 4500 cores, use of OpenMDAO and OpenTURNS

# ONERA strategy to deal with the major challenges of numerical simulation

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## Modeling, simulation & methodologies

1. Multi-physics high fidelity and multi-fidelity
2. *Integration of the input of applied maths*
3. Exploitation of large mass of data
4. Reduction of models for MDA and MDO
5. Uncertainty quantification

## HPC & software engineering

6. *HPC efficiency, minimal dependency to computer evolution*
7. *Exploitation of innovations for scientific software*
8. *Interoperability and perennity of a set of evolutive scientific computer codes*

2. Applied maths laboratory
8. Multiphysics simulation platform
- 6.-7. New CFD software project

# ONERA Applied Maths lab (LMA2S)

<https://w3.onera.fr/lma2s>

- Recently created at ONERA to promote links and improve synergy between applied maths scientists belonging to « disciplinary departments » (lab « without walls »)

- 8 scientific axes

Waves

HPC (Linear algebra)

Multi-scales

Meshes and visualization

Optimization, control, identification

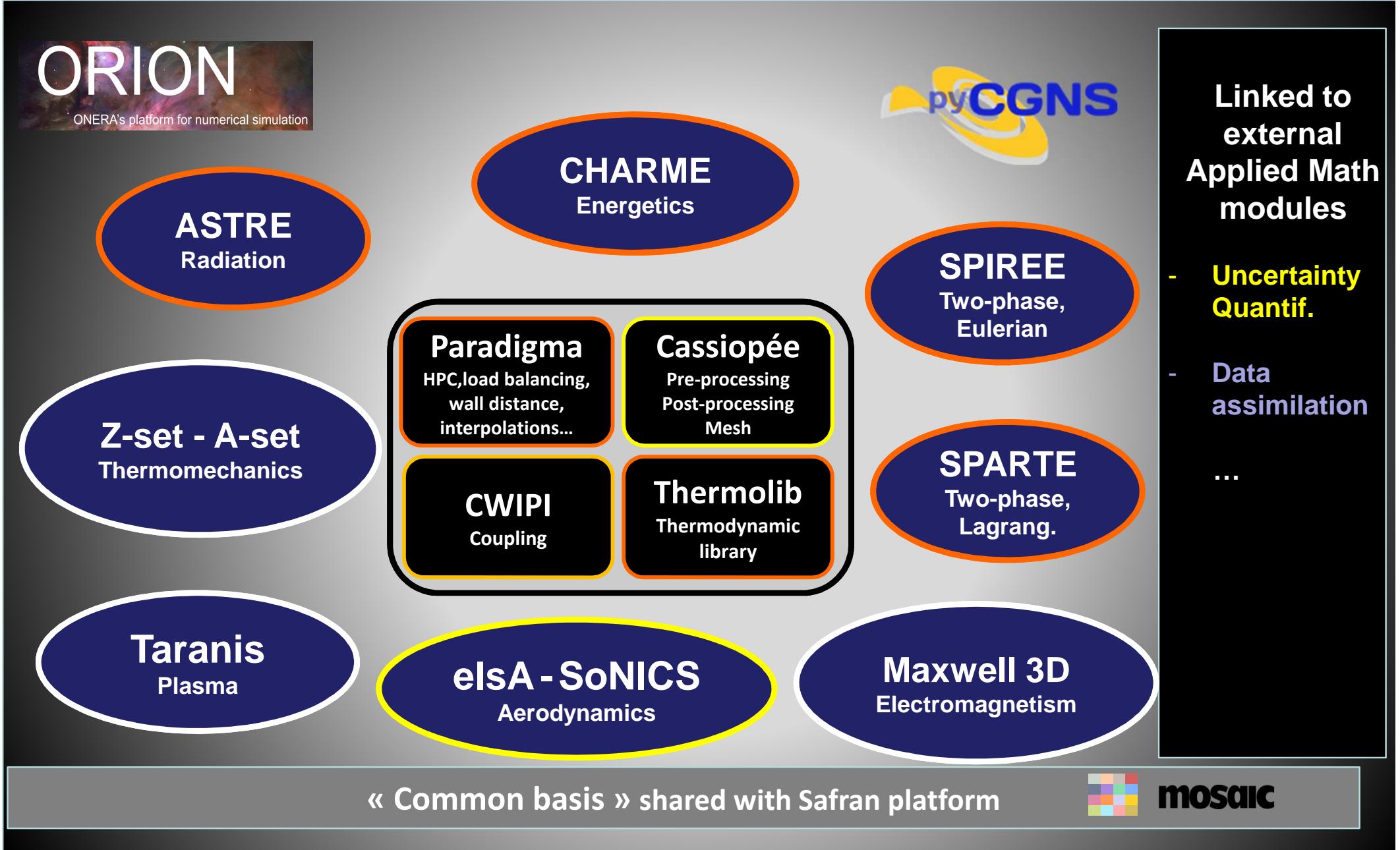
Uncertainty Quantification

CFD schemes

“White” axis (data based numerical simulation...)

- An additional objective : providing disciplinary software with Maths apps software components of general interest

# ONERA project of multiphysics simulation platform (ORION) : synergy, mutualization, coupling



# Software evolution with respect to hardware

- Development time of large scientific software > Evolution time of hardware  
→ *Develop abstraction for agnosticity with respect to hardware evolution*
- Do not let the gap widen between peak performances and real performances
- Promote openness to data science



From the HPDA platform Jean Zay of GENCI  
to the near-coming exaflopic platform

One example of new generation scientific software in development at ONERA :  
CFD - from e/sA to SoNICS (DGAC support, Safran partnership)



Operator graph  
generator



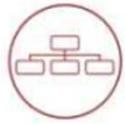
Code generator



Automatic graph  
differentiation



HPC layer



Operator graph



Operators



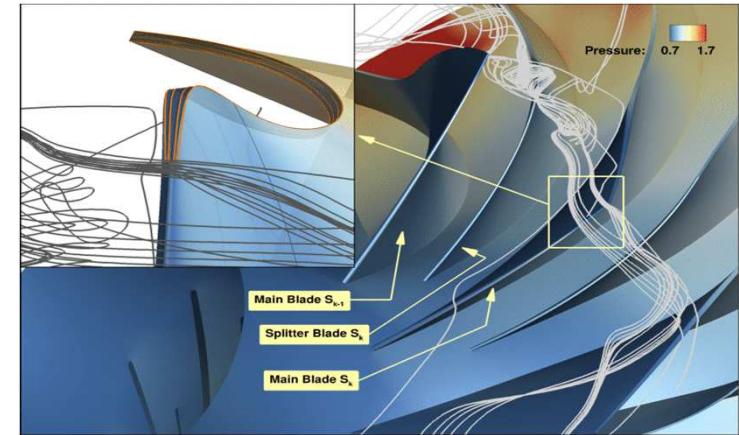
Data base  
for coupling



HPC scheduler

# Some perspectives for high performance simulation

- Still tremendous progress to be done in representativity of the reality : need of **more multi-physics**
- Exaflopic **HPDA** architectures
  - Transition of « legacy » scientific software
  - HPC efficiency
  - Rely on data science without forgetting physics
- Better **validate and qualify** simulation results (certification)
- Need to associate a **large variety of skills** : physical modeling, applied maths, numerical algorithms, data science, computer science, software development, aerospace engineering...
- Rely on **partnerships** :  
ONERA entered the OpenTURNS consortium for UQ in 2019



Aeroelastic simulation of a centrifugal compressor

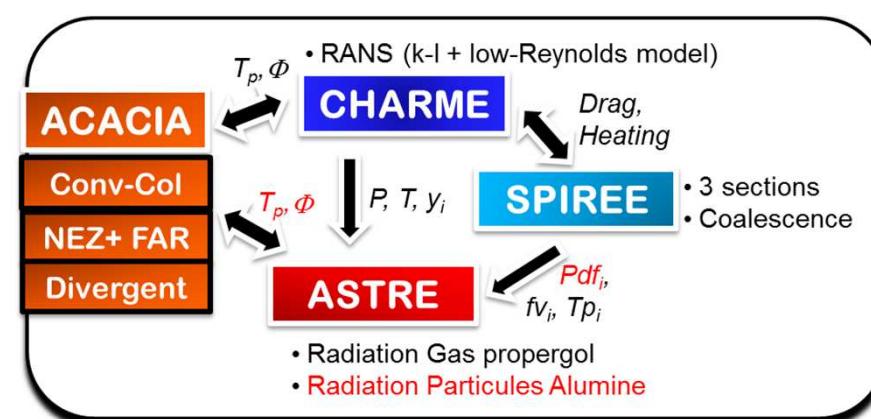
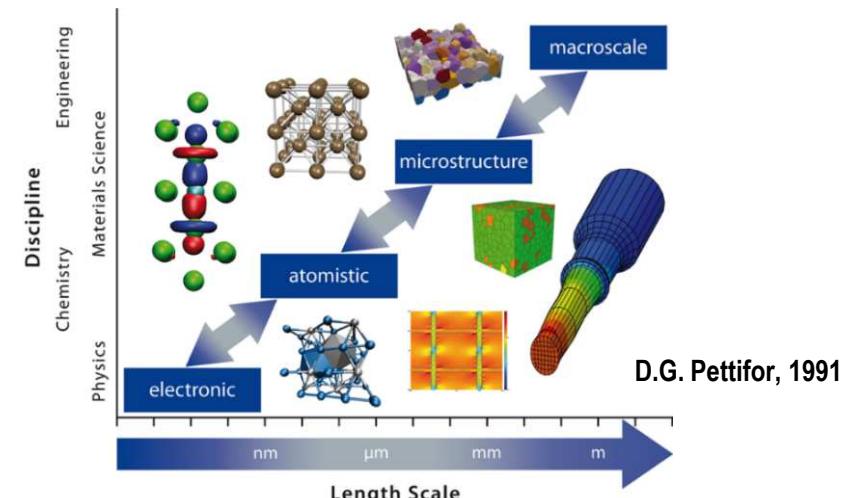


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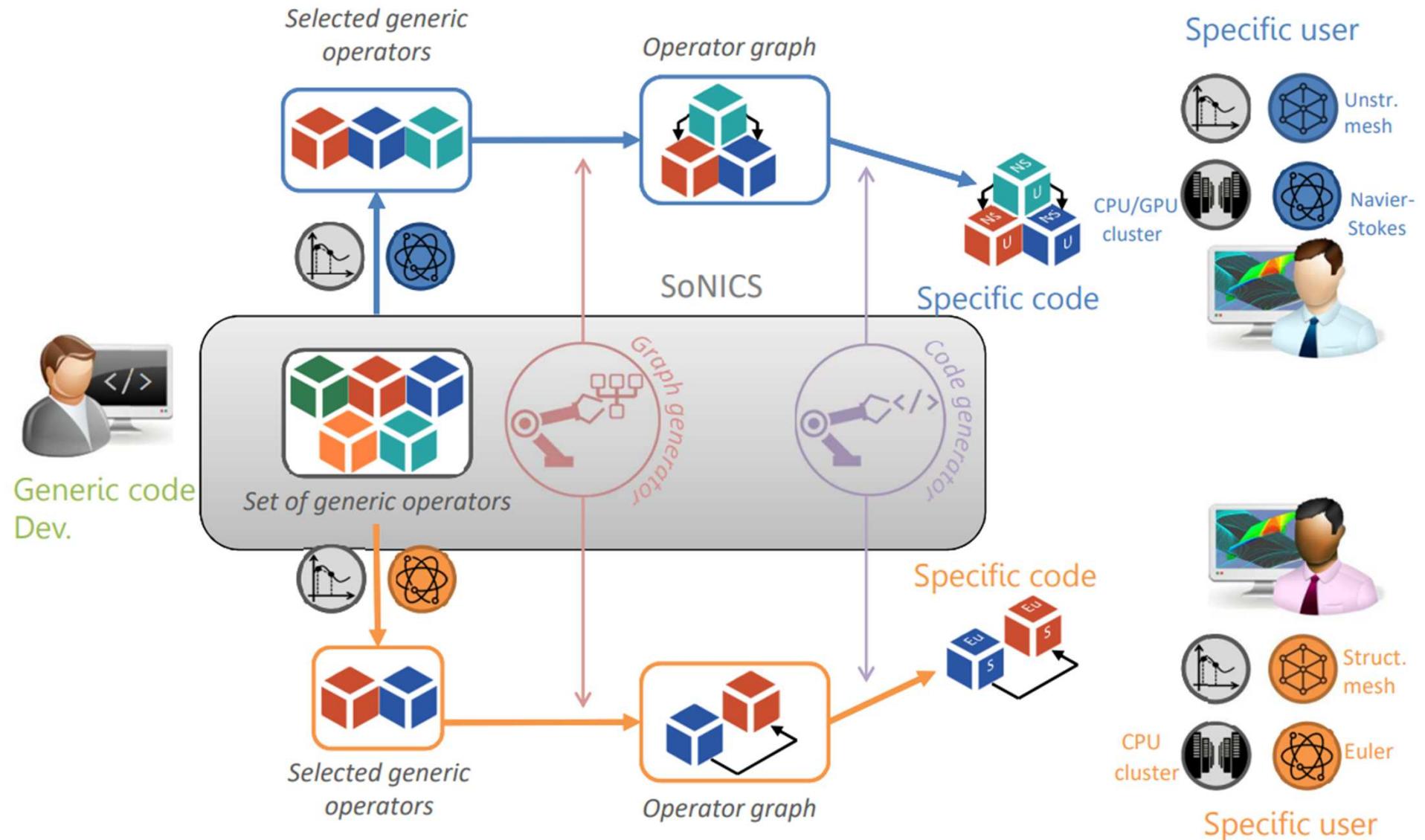
# BACK UP

# High performance computing needs in aerospace

- Increase in configuration size (for ex., from one blade to a full engine)
- Increase in geometrical fidelity
- Better representation of physics and range of scales
  - Turbulence in fluid mechanics
  - **Science of materials**
  - Electromagnetism
- Unsteady phenomena
- **Multi-physics coupling**
- Optimization processes



# Software evolution with respect to hardware



# Software evolution with respect to hardware

## Building key components and achieving first milestones with SoNICS

- Key SoNICS software components



Operator graph generator



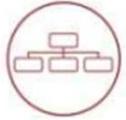
Code generator



Automatic graph differentiation



HPC layer



Operator graph



Operators



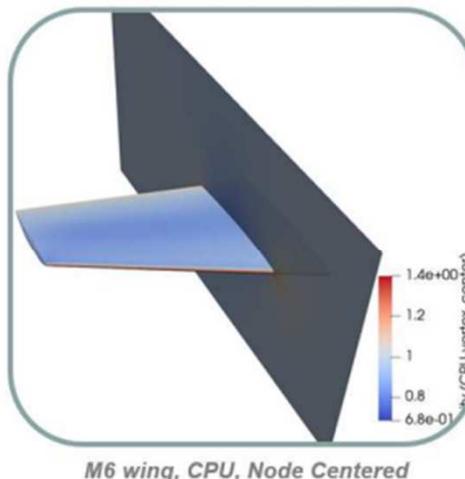
Data base for coupling



HPC scheduler

- Achieved milestones

- Cell centered on CPU
- Node centered on CPU
- Cell centered on GPU
- Notable performance speedups compared with elsA
  - **CPU X 14 speedup/ elsA**
  - **GPU X 100 speedup/ CPU (mono-proc)**



- Next milestone

- Rotor 37 use case / distributed parallel CPU+GPU
- TRL 2 → TRL 3 @Safran

# Concluding remarks

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**Calcul et données. Nouvelles perspectives pour la simulation à haute performance. (2021, 58 p.)** Voir également 46<sup>ème</sup> forum ORAP : **Calcul haute performance : vers une hybridation avec l'IA**

## 6 recommandations :

- renforcer le développement de **méthodes hybrides**, associant physique de base et apprentissage
- s'appuyer sur des **infrastructures matérielles convergées** permettant à la fois le calcul scientifique et le traitement des données
- mieux **valider, qualifier et expliquer** les résultats des simulations
- organiser un meilleur **partage des données** entre utilisateurs potentiels
- promouvoir une **formation hybride** adaptée et bien reconnaître les métiers associés
- aider à la **transition des grands codes de calcul scientifique** déjà développés

# La simulation numérique dans le secteur aérospatial : les défis à venir

Défis en termes de réduction de la consommation d'énergie, d'émission de polluants, de nuisances sonores

Objectif d'une aviation civile neutre en carbone en 2050

- La simple évolution incrémentale des configurations ne suffira pas !
- Concepts en forte rupture : abandon du « tube and wing », recours à l'hydrogène, avion plus/tout électrique...
- ⇒ Tirer parti de la révolution numérique et des progrès en science des données

Digitalisation croissante de l'ensemble des activités

Mise en place d'une forte continuité numérique

- Tout au long du cycle de vie d'un produit (notion de jumeau numérique)
- Entre sociétés contributrices (co-conception entre industriels partenaires)
- Entre les différentes disciplines de la physique

Progrès requis dans le domaine de la quantification des incertitudes (certification)

Importance croissante du *big data*

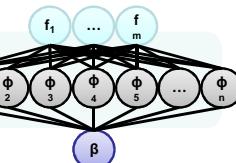
# « Data driven modelling »

Apprentissage d'un modèle de type moyenne-fidélité RANS à partir de données de référence numériques :

Données haute fidélité (DNS, EXP)

Assimilation de données

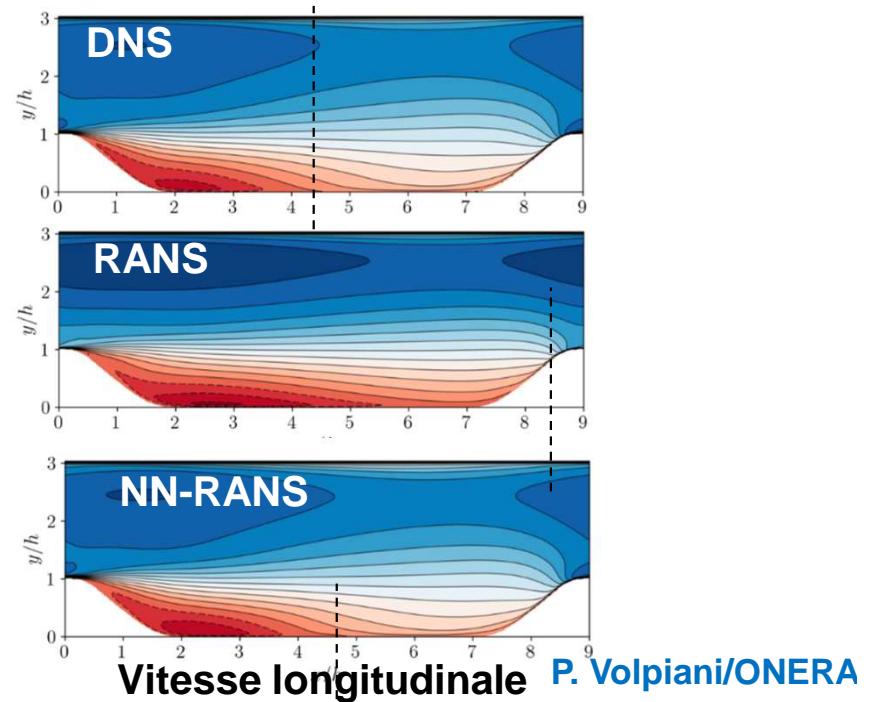
Apprentissage profond



Test du modèle RANS corrigé

NN-RANS testé sur d'autres configurations

Colline périodique ( $Re=5600$ )



*Sciences de l'ingénieur : besoin de données en quantité et de qualité pour l'apprentissage des modèles (**small data**)  
Cf. Base de données ImageNet : 14 millions d'images annotées manuellement avec 20000 étiquettes (**big data**)*