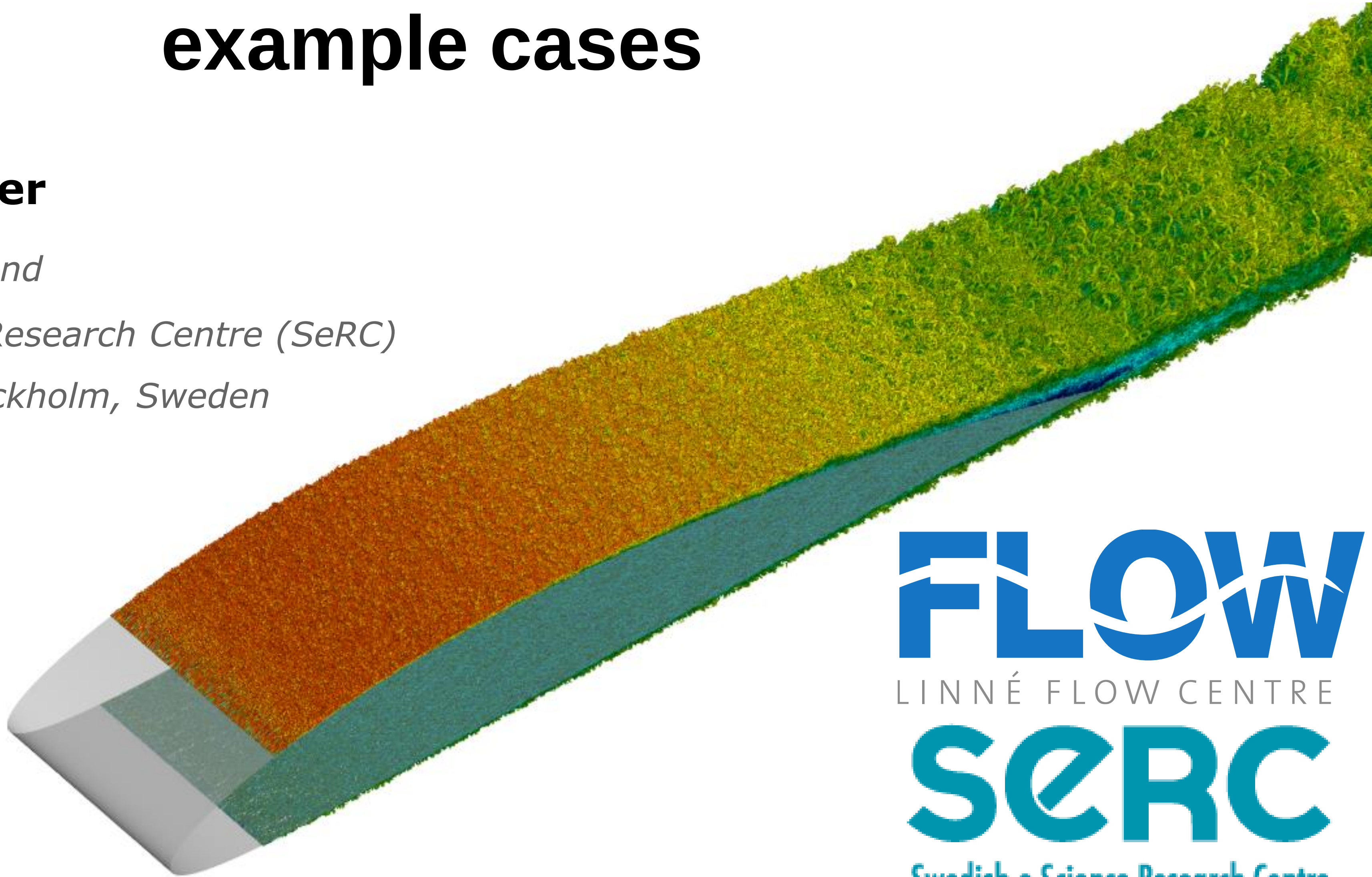
Overview of CFD and Nek5000, example cases

Philipp Schlatter

SimEx/FLOW *and*

Swedish e-Science Research Centre (SeRC)

KTH Mechanics, Stockholm, Sweden



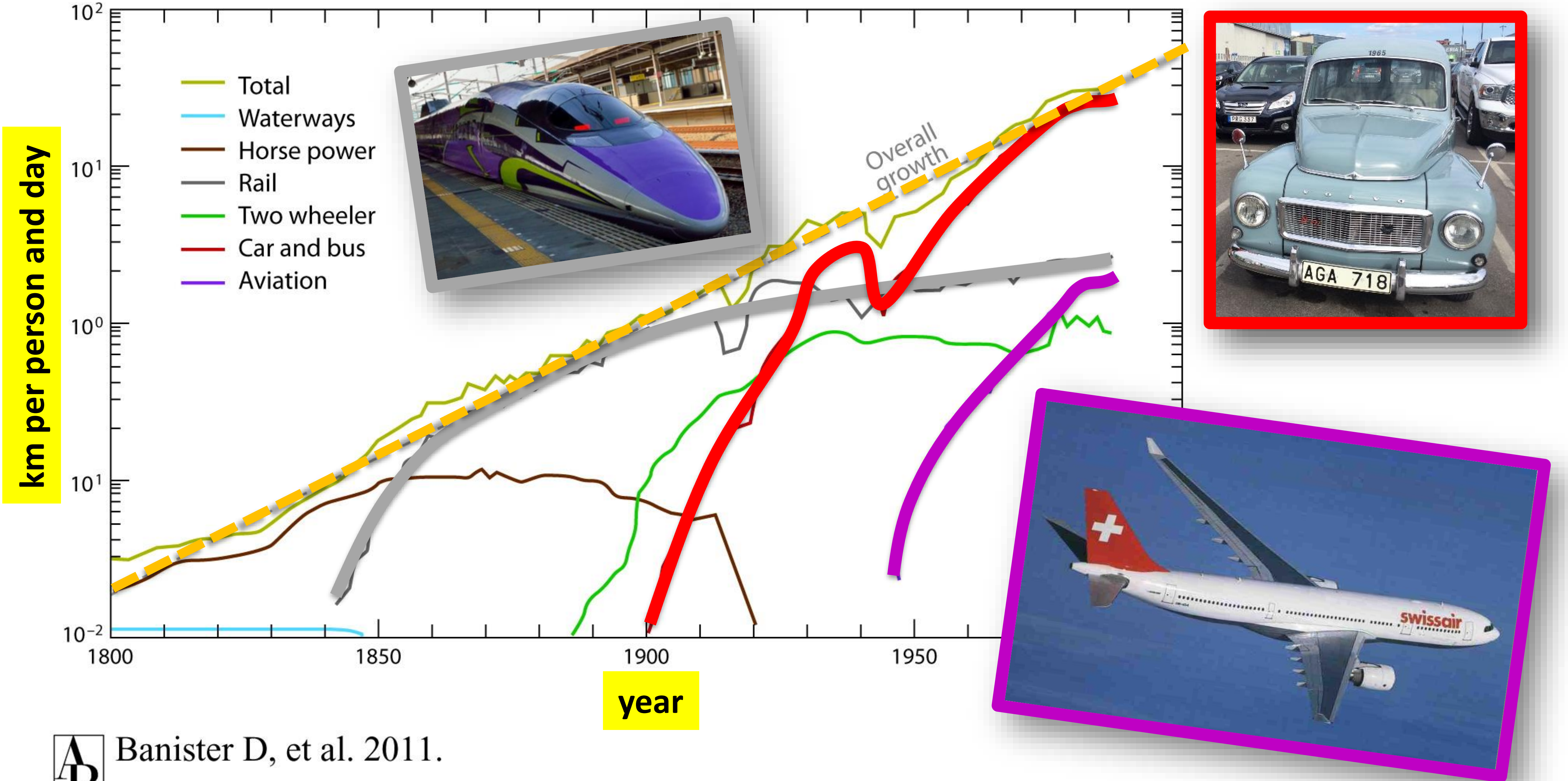
August 17, 2021

Numerical Simulations of Turbulence → CFD

- Motivation
- Brief History
- Numerical Methods
- Turbulence Modelling
- Some Examples
- Outlook

Why turbulence?

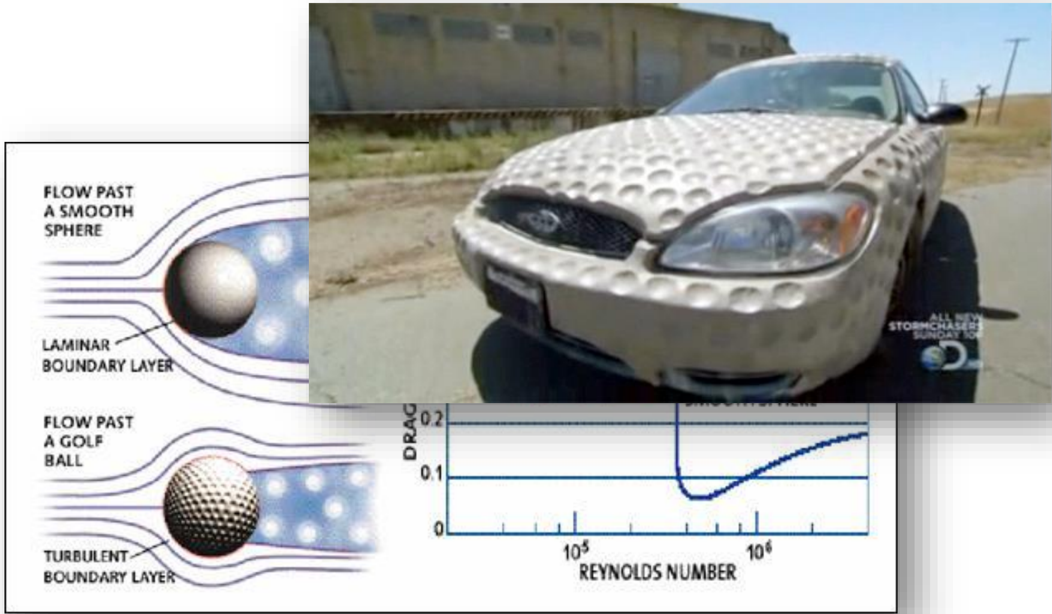
Skin friction/drag reduction is the key for economically and ecologically more efficient transport



Banister D, et al. 2011.
Annu Rev. Environ. Resour. 36:247–70

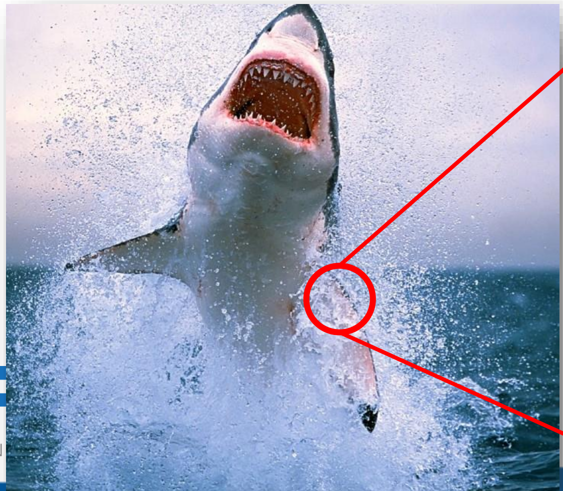
Why care about wall turbulence...

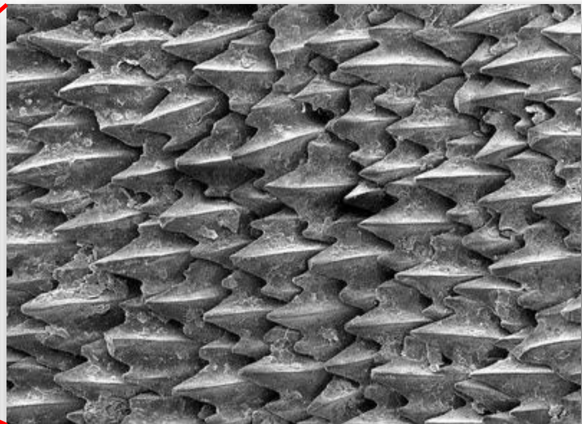
- Playing golf...

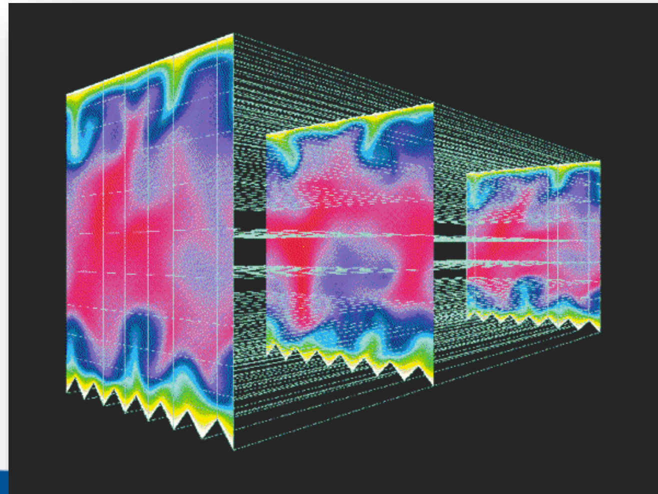


- Shark skin (riblets)...

10% drag reduction!







Why are we here…?

- “When a sufficiently **advanced computer** becomes available, we believe it will **replace the wind tunnel** as the principal facility for providing aerodynamic flow simulations”
- “If past trends continue, such computer performance should **be available in the mid-1980s**…”

Chapman, D. R., Mark, H., Pirtle, M. W., “Computers vs. wind tunnels for aerodynamic flow simulations”, Astronautics & Aeronautics **13**(4):22-30, 1975 (NASA Ames)

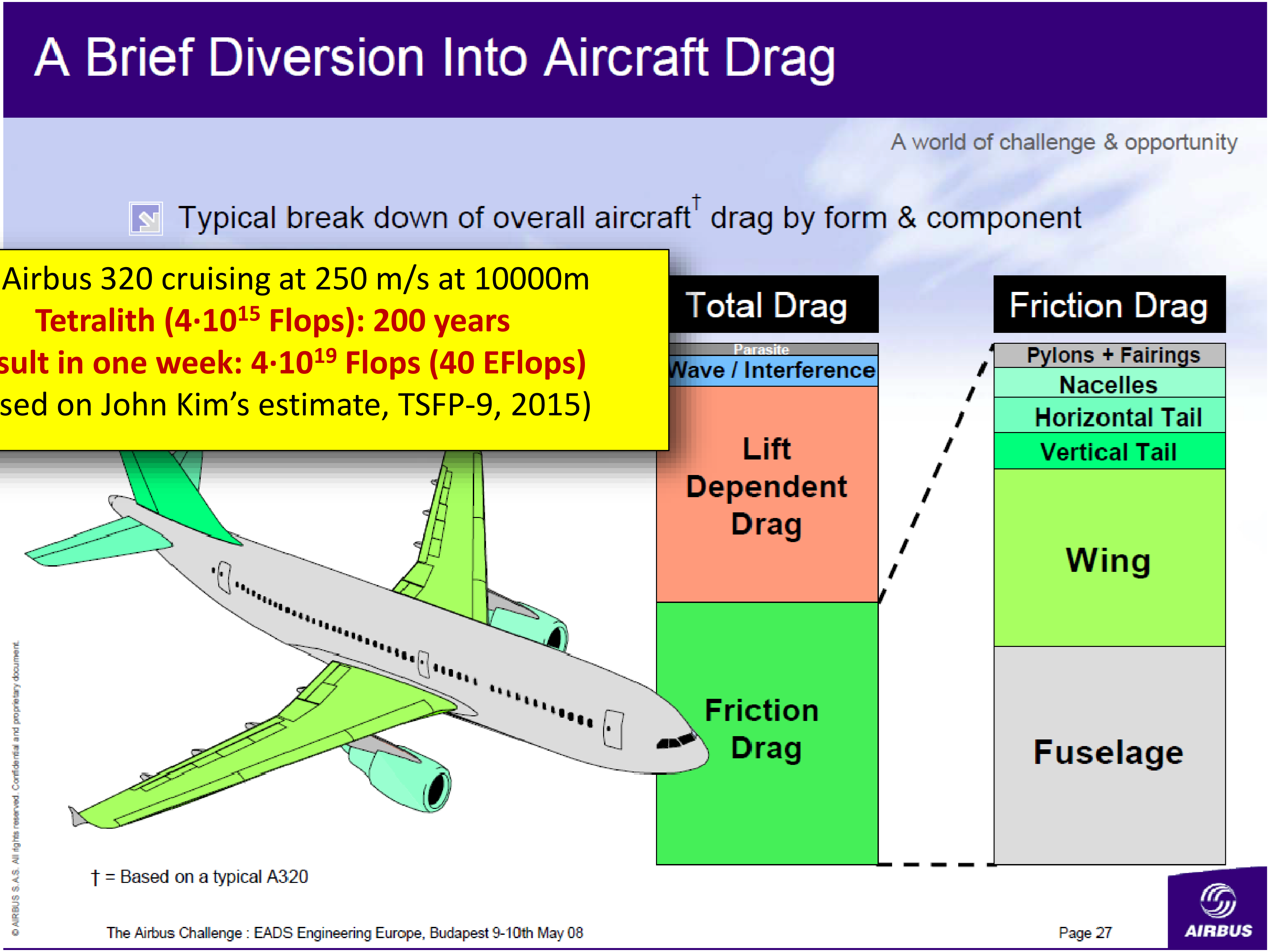
The Airbus Challenge, David Hills, 2008

An Airbus 320 cruising at 250 m/s at 10000m

Tetralith ($4\cdot10^{15}$ Flops): 200 years

Result in one week: $4\cdot10^{19}$ Flops (40 EFlops)

(based on John Kim's estimate, TSFP-9, 2015)



Pillars of Science & Uncertainties

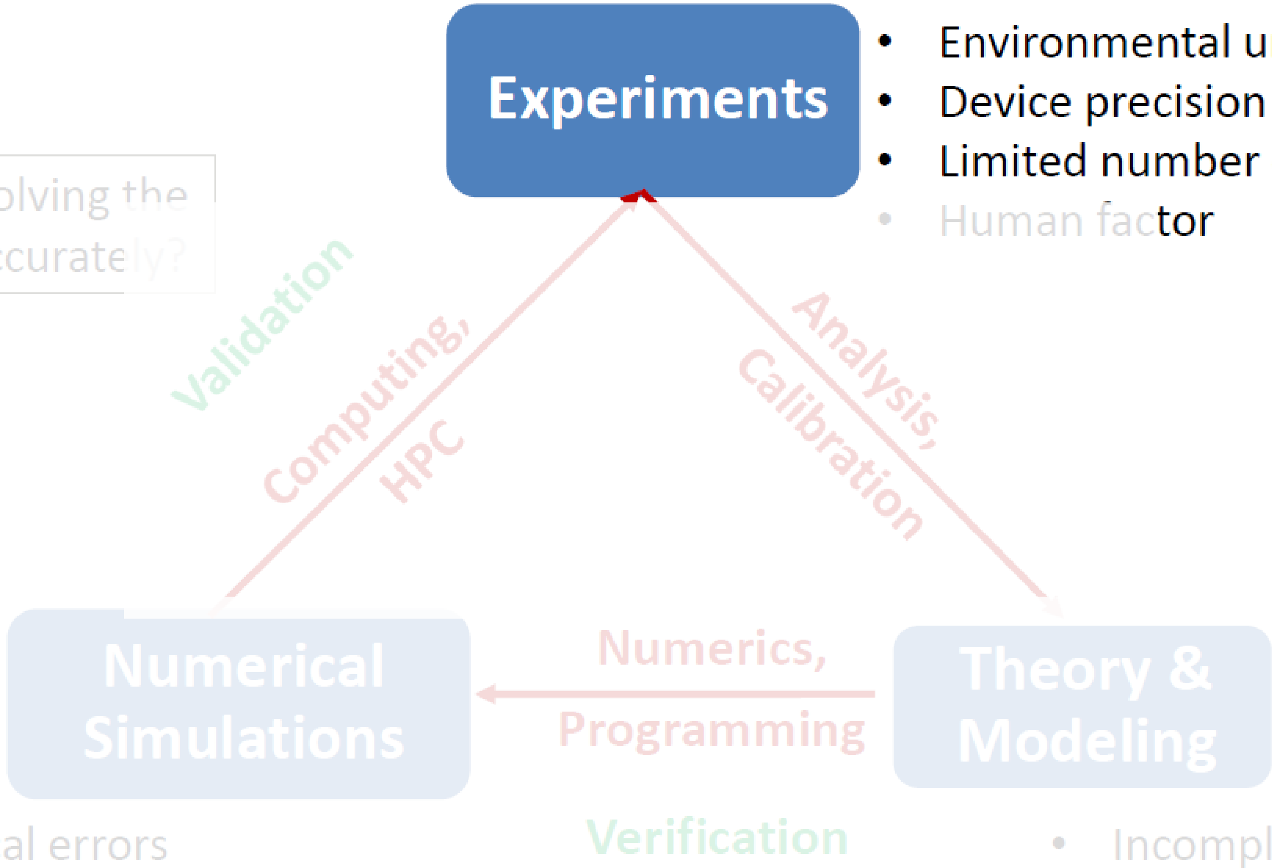
Experiments:
- Environmental uncertainties
- Device precision and bias
- Limited number of observations
- Human factor

Numerical Simulations:
- Numerical errors
- Programming bugs
- Domain uncertainties
- Computational mesh
- Initial and boundary conditions
- High-performance computing

Theory & Modeling:
- Incomplete knowledge
- Incomplete modeling
- Uncertain parameters

Oberkampf and Trucano, 2002. Roache, 1997

Pillars of Science & Uncertainties



- Environmental uncertainties
- Device precision and bias
- Limited number of observations
- Human factor

Are we solving the model accurately?

- Numerical errors
- Programming bugs
- Domain uncertainties
- Computational mesh
- Initial and boundary conditions
- High-performance computing

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Are we solving the model accurately?

Validation

Computing, HPC

Analysis, Calibration

Numerical Simulations

Numerics, Programming

Theory & Modeling

- Numerical errors
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Verification

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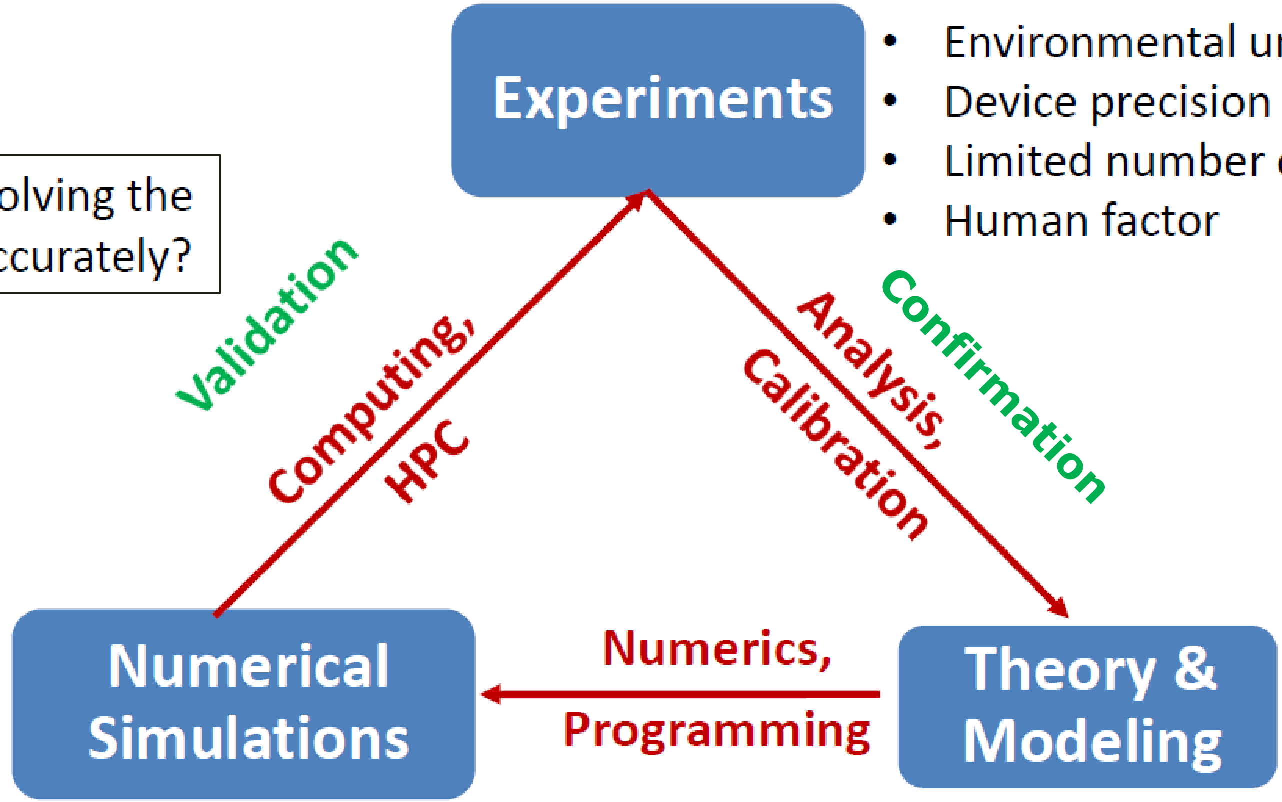
Pillars of Science & Uncertainties



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Oberkampf and Trucano, 2002. Roache, 1997

CFD – What is really the problem?

What is really the problem?

incompressible N.S. equations:

$$\underbrace{\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}}_{\frac{D}{Dt}} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} \qquad (1)$$

$u_j \frac{\partial u_i}{\partial x_j}$: non-linear; $-\frac{\partial p}{\partial x_i}$: pressure; $\frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j}$: viscous term

$$\frac{\partial u_i}{\partial x_i} = 0 \qquad (2)$$

incompressibility constraint

b.c. / i.c. (3)

Goal: $u_i(t)$, $p(t)$

What is really the problem?

- PDE second order (viscous term)
- strong nonlinearity, weak diffusivity ⇒ Turbulence
- no time derivative for p
    - no time integration possible
    - eq. (2) act as a constraint to eq. (1)

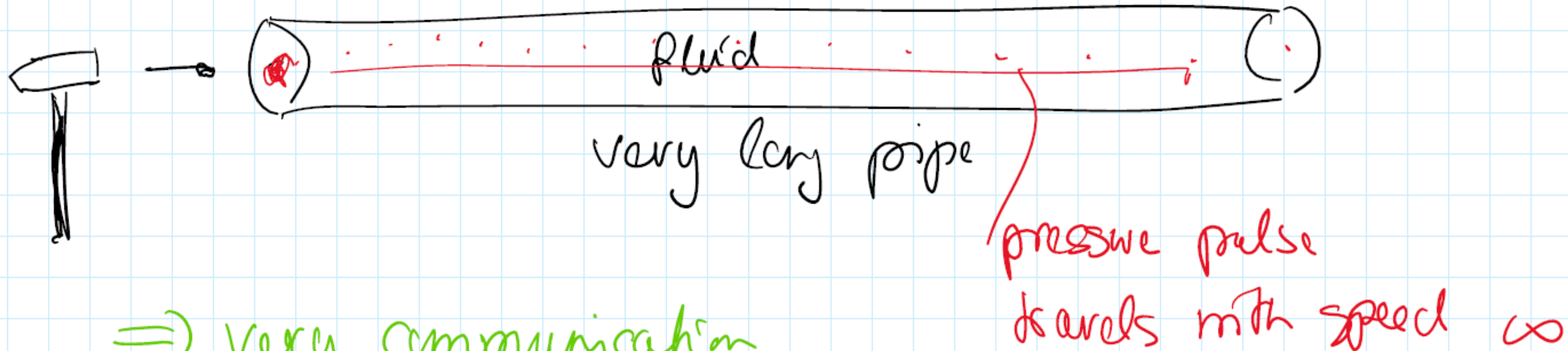
⇒ annoying solution schemes for N.S. equation.

↳ mixed type
  - elliptic pressure
  - parabolic viscosity
  - hypbolic convection

- specification of boundary & initial conditions (3) typically unknown

What is really the problem?

Example: elliptic behaviour of pressure:
Laplace, Poisson equation.

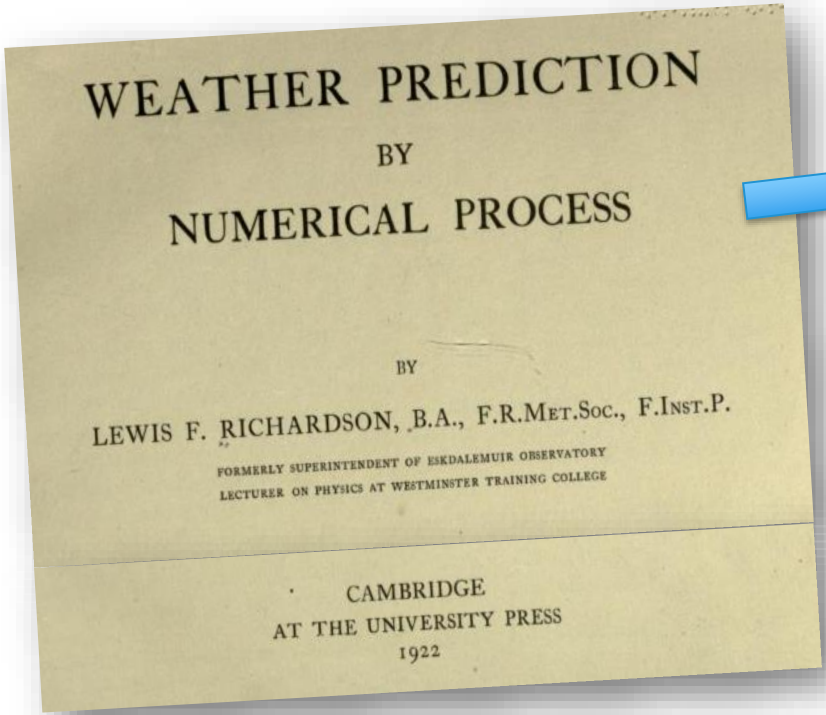


⇒ very communication
intensive!

Brief History

Humble beginnings 100 years ago…

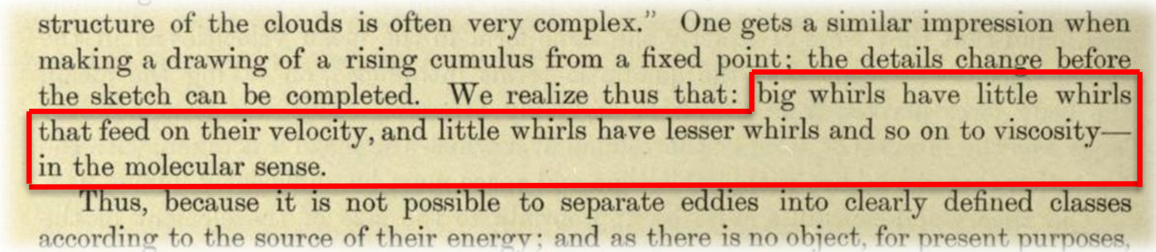
- Lewis Fry Richardson (1881-1953)


WEATHER PREDICTION
BY
NUMERICAL PROCESS

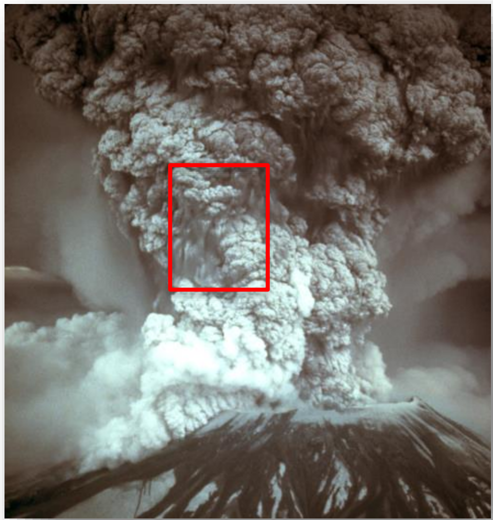
BY

LEWIS F. RICHARDSON, B.A., F.R.MET.SOC., F.INST.P.
FORMERLY SUPERINTENDENT OF ESKDALEMUIR OBSERVATORY
LECTURER ON PHYSICS AT WESTMINSTER TRAINING COLLEGE

CAMBRIDGE
AT THE UNIVERSITY PRESS
1922


structure of the clouds is often very complex." One gets a similar impression when making a drawing of a rising cumulus from a fixed point; the details change before the sketch can be completed. We realize thus that: big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to viscosity—in the molecular sense.

Thus, because it is not possible to separate eddies into clearly defined classes according to the source of their energy; and as there is no object, for present purposes,



play on Augustus de Morgan's famous paraphrasing[3] of Jonathan Swift

Humble beginnings 100 years ago…

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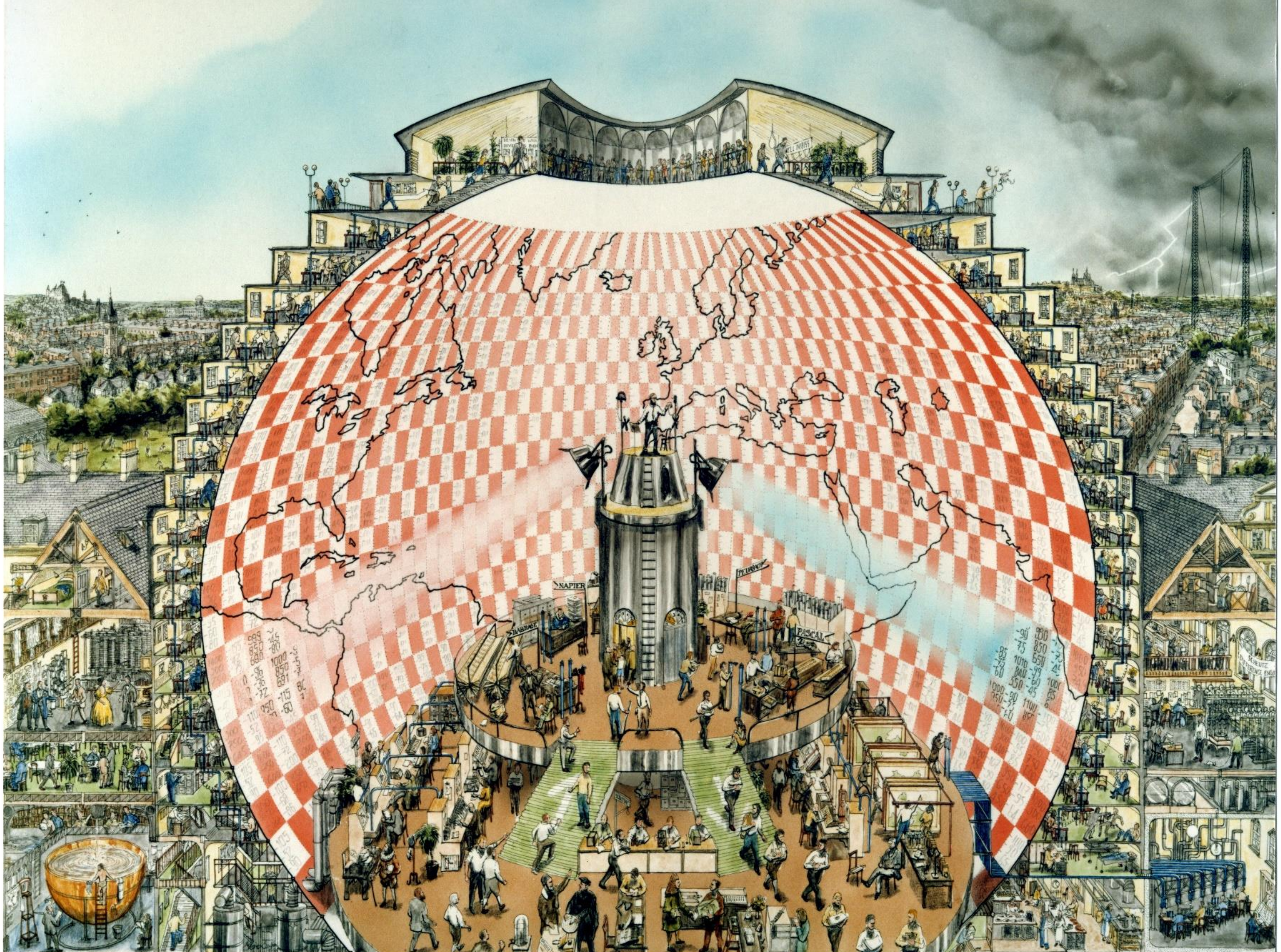
"First simulations" 1920: Eight hours weather prediction in 6 weeks, using **2000 *human* computers**

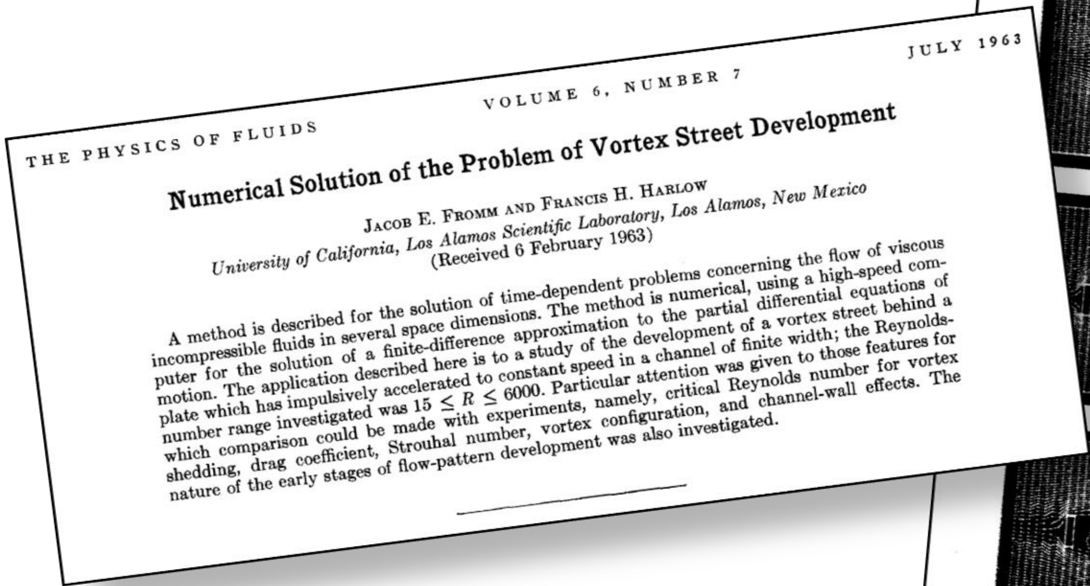
→ **"Forecast-Factory"**

The Weather Forecasting Factory by Stephen Conlin (1986)



Brief History (1/4): - 1960’s

- ”First simulations” (NWP) by Lewis Fry Richardson 1920: Eight hours weather prediction in 6 weeks, using **2000 ”human” computers**
- Low-*Re* cylinder wakes by Thom (1933), Kawaguti (1953) and Fromm & Harlow (1963), Los Alomos



THE PHYSICS OF FLUIDS VOLUME 6, NUMBER 7 JULY 1963

Numerical Solution of the Problem of Vortex Street Development

JACOB E. FROMM AND FRANCIS H. HARLOW
University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico

(Received 6 February 1963)

A method is described for the solution of time-dependent problems concerning the flow of viscous incompressible fluids in several space dimensions. The method is numerical, using a high-speed computer for the solution of a finite-difference approximation to the partial differential equations of motion. The application described here is to a study of the development of a vortex street behind a plate which has impulsively accelerated to constant speed in a channel of finite width; the Reynolds-number range investigated was $15 \leq R \leq 6000$. Particular attention was given to those features for which comparison could be made with experiments, namely, critical Reynolds number for vortex shedding, drag coefficient, Strouhal number, vortex configuration, and channel-wall effects. The nature of the early stages of flow-pattern development was also investigated.

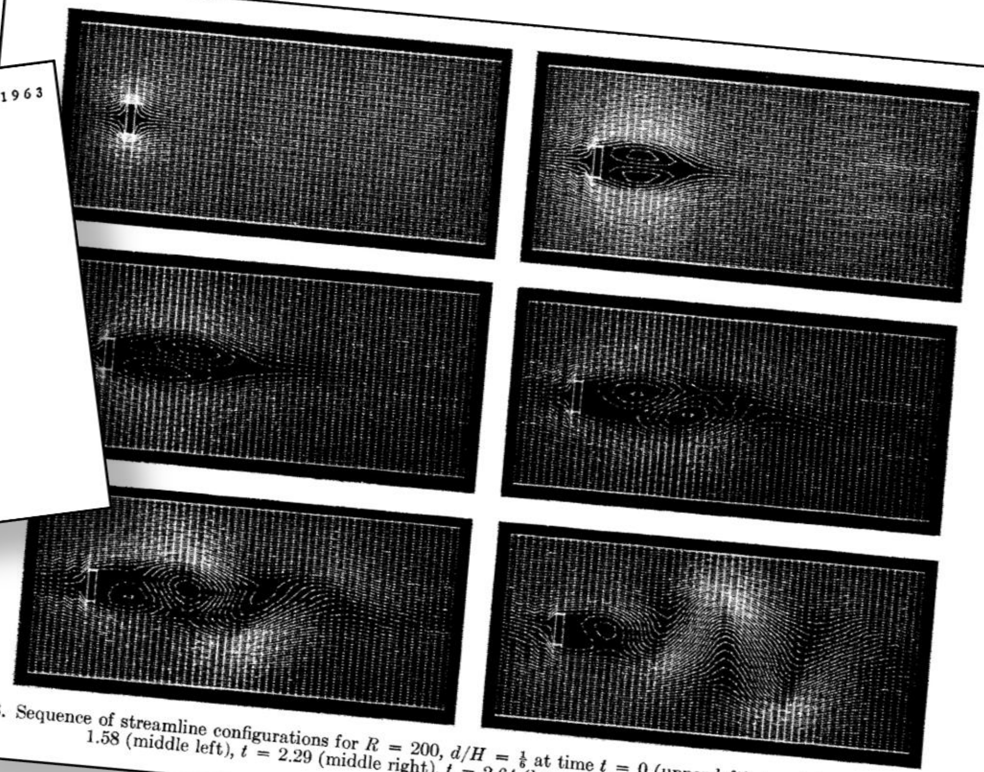


FIG. 3. Sequence of streamline configurations for $R = 200$, $d/H = \frac{1}{8}$ at time $t = 0$ (upper left), $t = 0.70$ (upper right), $t = 1.58$ (middle left), $t = 2.29$ (middle right), $t = 2.64$ (lower left), and $t = 3.16$ (lower right).

1440 grid points!

Brief History (2/4): 1960's

- 1965: **MAC** (Marker&Cell) method (Harlow&Welch): staggered grid
- 1966: Journal of Computational Physics founded
- 1968/1969: **Numerical methods for NS with pressure projection**: Chorin and Temam.

MATHEMATICS OF COMPUTATION
October, 1968, Vol. 22, No. 104
Pp. 745–762

Numerical Solution of the Navier-Stokes Equations*

By Alexandre Joel Chorin

Abstract. A finite-difference method for solving the time-dependent Navier-Stokes equations for an incompressible fluid is introduced. This method uses the primitive variables, i.e. the velocities and the pressure, and is equally applicable to problems in two and three space dimensions. Test problems are solved, and an application to a three-dimensional convection problem is presented.

Sur l'Approximation de la Solution des Équations de Navier-Stokes par la Méthode des Pas Fractionnaires (II)

R. Témam

Mémoire présenté par J. L. Lions

Introduction

Comme dans deux travaux précédents [8, 9], nous nous intéressons ici à l'approximation du problème de Navier-Stokes suivant: étant donné un ouvert borné Ω de R^2 et un nombre $T>0$, trouver les fonctions $u=\{u_1, u_2\}$ et p définies dans $\Omega\times[0,T]$ et qui vérifient les équations

$$\frac{\partial u}{\partial t}-\nu\Delta u+\sum_{i=1}^{2}u_i\frac{\partial u}{\partial x_i}+\operatorname{grad} p=f \quad (f \text{ donné}) \qquad (0.1)$$
$$\operatorname{div} u=0$$

et les conditions aux limites et initiales suivantes:

$$u(x,t)=0 \quad \text{si } x\in\Gamma \text{ (la frontière de } \Omega) \qquad (0.2)$$
$$u(x,0)=u_0(x) \quad (u_0 \text{ donné}).$$

La méthode que nous envisageons ici diffère des deux méthodes respectivement considérées en [8] et [9] en ce sens qu'elle ne repose pas sur une méthode de perturbation; par contre, comme en [9] la méthode considérée ici est encore une méthode discrète de pas fractionnaires [4, 6, 7].

Rappelons rapidement en quoi consiste la méthode des pas fractionnaires lorsqu'il s'agit d'approcher une équation d'évolution

$$\frac{\partial u}{\partial t}+Au=f \qquad (0.3)$$

Brief History (3/4): 1970's

- 1970: first channel-flow **large-eddy simulation**: Deardorff (6720 grid points), based on Smagorinsky model (1963)
- 1972: *k*-ε **turbulence model** (RANS): Spalding & Launder
- 1972: SIMPLE (semi-implicit method for pressure-linked equations): Patankar & Spalding
- 1972 (1967): The abbrevation **CFD** (**Computational Fluid Dynamics**, not "Colours for Directors"...) is coined


453

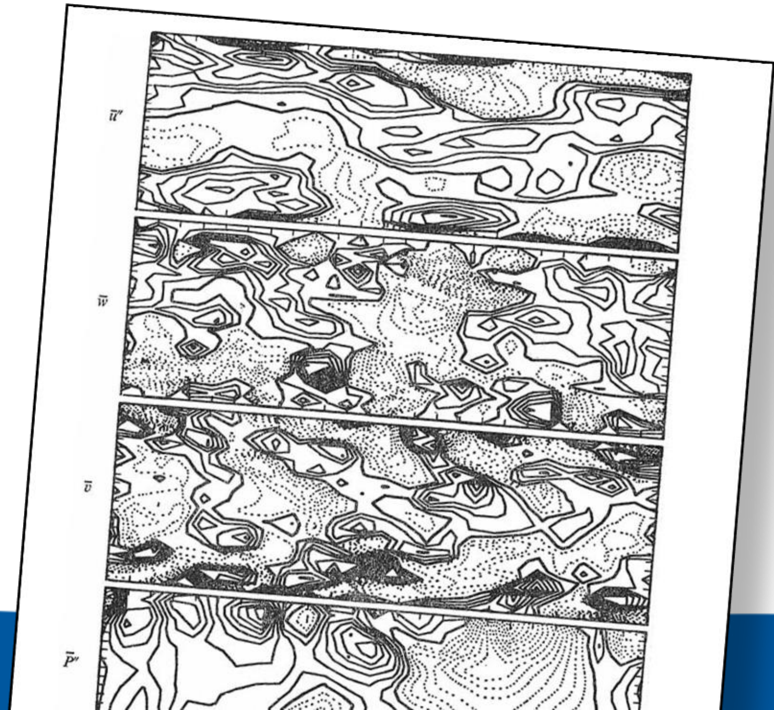
J. Fluid Mech. (1970), vol. 41, part 2, pp. 453–480
Boeing Symposium on Turbulence

A numerical study of three-dimensional turbulent channel flow at large Reynolds numbers

By JAMES W. DEARDORFF
National Center for Atmospheric Research, Boulder, Colorado 80302

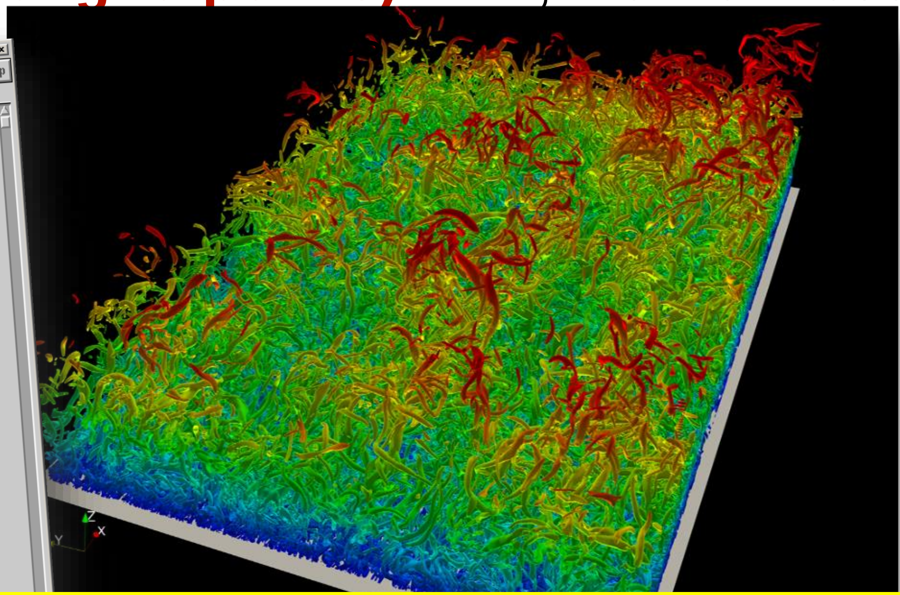
(Received 9 May 1969)

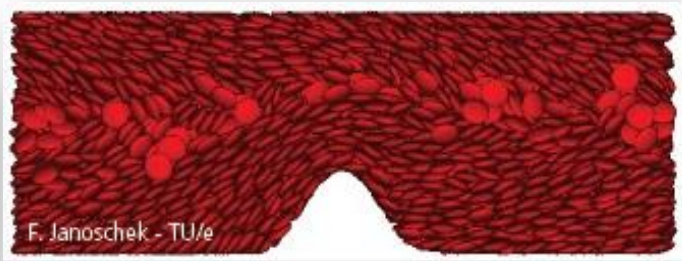
The three-dimensional, primitive equations of motion have been integrated numerically in time for the case of turbulent, plane Poiseuille flow at very large Reynolds numbers. A total of 6720 uniform grid intervals were used, with sub-grid scale effects simulated with eddy coefficients proportional to the local velocity deformation. The agreement of calculated statistics against those measured by Laufer ranges from good to marginal. The eddy shapes are examined, and only the *u*-component, longitudinal eddies are found to be elongated in the downstream direction. However, the lateral *v* eddies have distinct down-stream tilts. The turbulence energy balance is examined, including the separate effects of vertical diffusion of pressure and local kinetic energy.
It is concluded that the numerical approach to the problem of turbulence at large Reynolds numbers is already profitable, with increased accuracy to be expected with modest increase of numerical resolution.



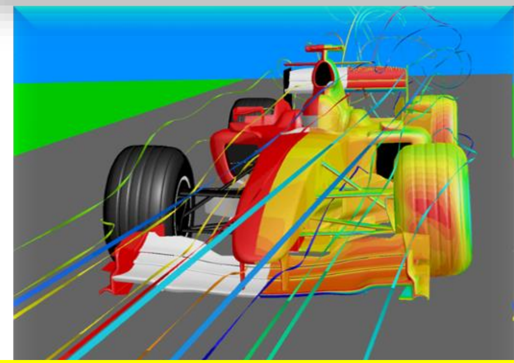
Brief History (4/4): 1980's -

- 1980 - : CFD codes used in engineering (e.g. Fluent, ANSYS, *etc.*); first for aircrafts, then also automotive *etc.*
- 1987: **First fully resolved DNS of channel flow ($4x10^6$ grid points):** Kim, Moin & Moser





TU Eindhoven

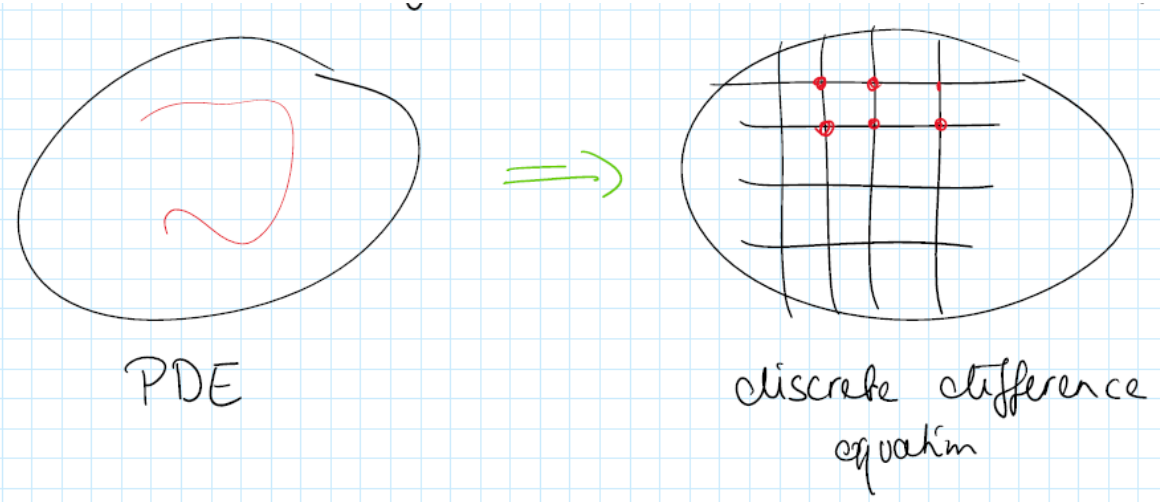


Fluent

today:
- Computational fluid dynamics is integral part of both engineering and research, calculations up to **$50x10^9$ grid points** and **1'000'000 cores** "easily" possible
- Data post processing! Storage! Visualisation!

Discretisation:

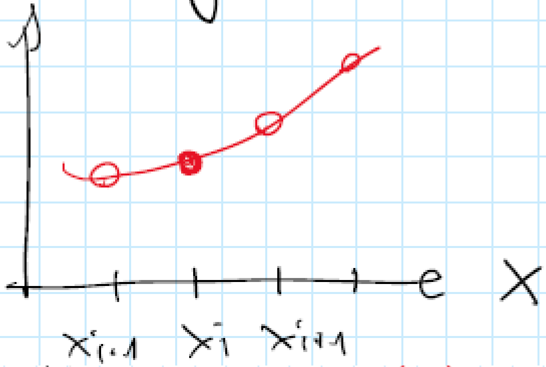
Find a numerical solution $u_j^n = u_N(x_j, t^n)$ at discrete points in space & time with idea it converges to the exact solution $u(x_j, t^n)$



Numerical Methods

Finite difference scheme

Basic idea: Taylor series



$$u(x+\Delta x) = u(x) + \Delta x \left.\frac{\partial u}{\partial x}\right|_x + \frac{1}{2}\Delta x^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_x + \frac{1}{6}\Delta x^3 \left.\frac{\partial^3 u}{\partial x^3}\right| + \dots$$

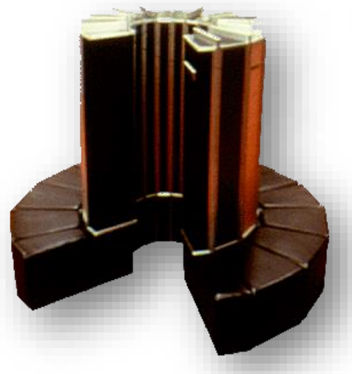
$$\left.\frac{\partial u}{\partial x}\right|_x = \frac{u(x+\Delta x) - u(x)}{\Delta x} + \frac{1}{2}\Delta x \frac{\partial^2 u}{\partial x^2} + \frac{1}{6}\Delta x^2 \frac{\partial^3 u}{\partial x^3} + \dots$$

$$\frac{\partial u}{\partial x} \approx \frac{u(x+\Delta x) - u(x)}{\Delta x} + \mathcal{O}(\Delta x)$$

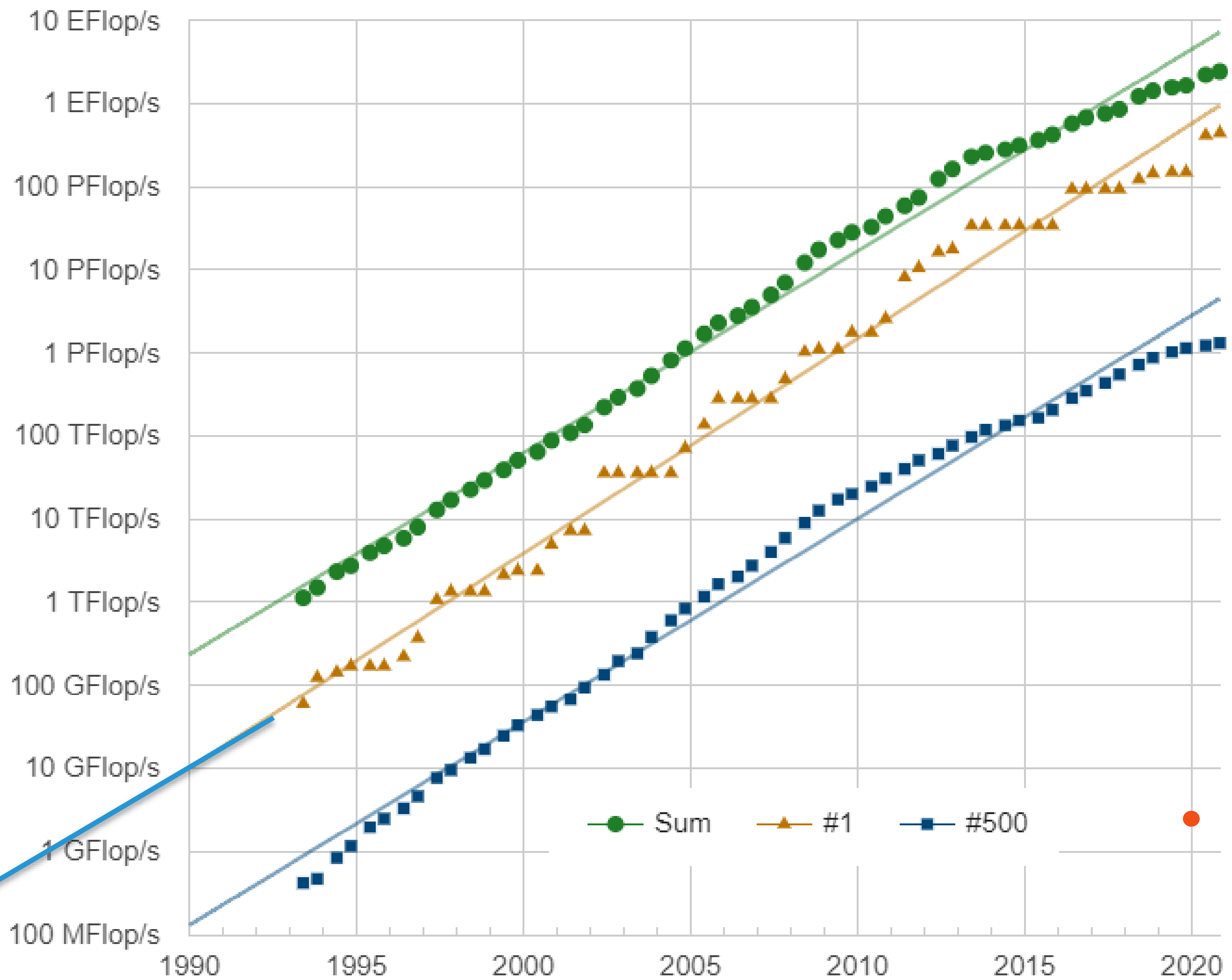
finite difference approximation of first order

Top500 list (www.top500.org)

- How fast are big computers?



Cray-1 (1976)
100 MFlops
1 core



iPhone11

Navier-Stokes equations…

Data from Mira (ANL, 2013), million core hours

• Engineering/CFD	525	19%
• Subsurface flow & reactive transport	80	3%
• Combustion	100	4%
• Climate	280	10%
• Astrophysics	133	5%
	1118	**40%**

(fraction of Navier-Stokes based simulations on current supercomputers)

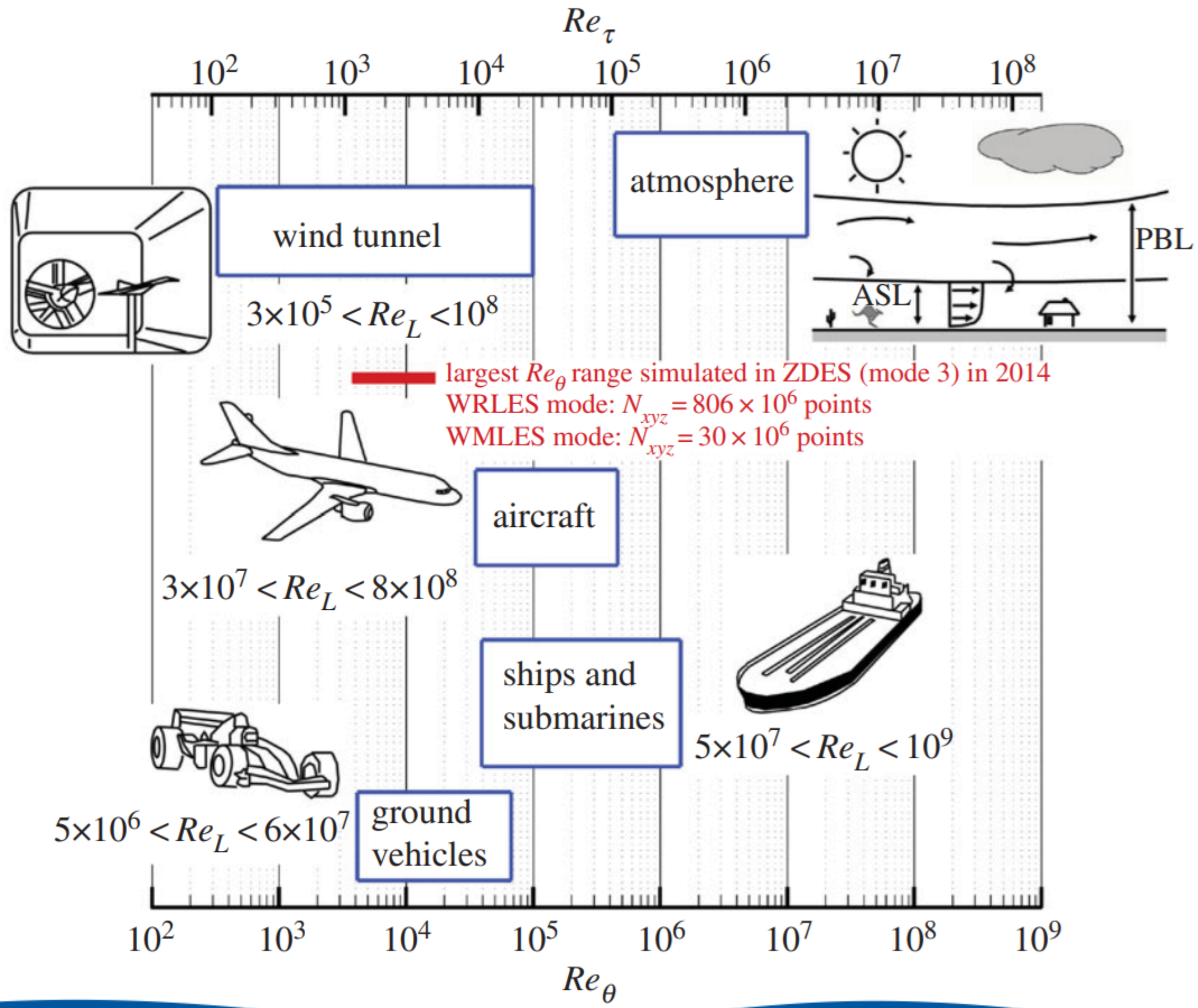
Physical Models

Numerical Experiment!

- Orszag and Patterson (1972), homogeneous isotropic turbulence, 32x32x32 points
- “Directly” from Navier Stokes, i.e. no turbulence model (Orszag 1970)
- May be very (very!) expensive (several months of computations on thousands of processors).

Numerical Simulation

- High computational cost
- Unknown influence of uncertainties



Deck et al. 2014

Numerical Simulation

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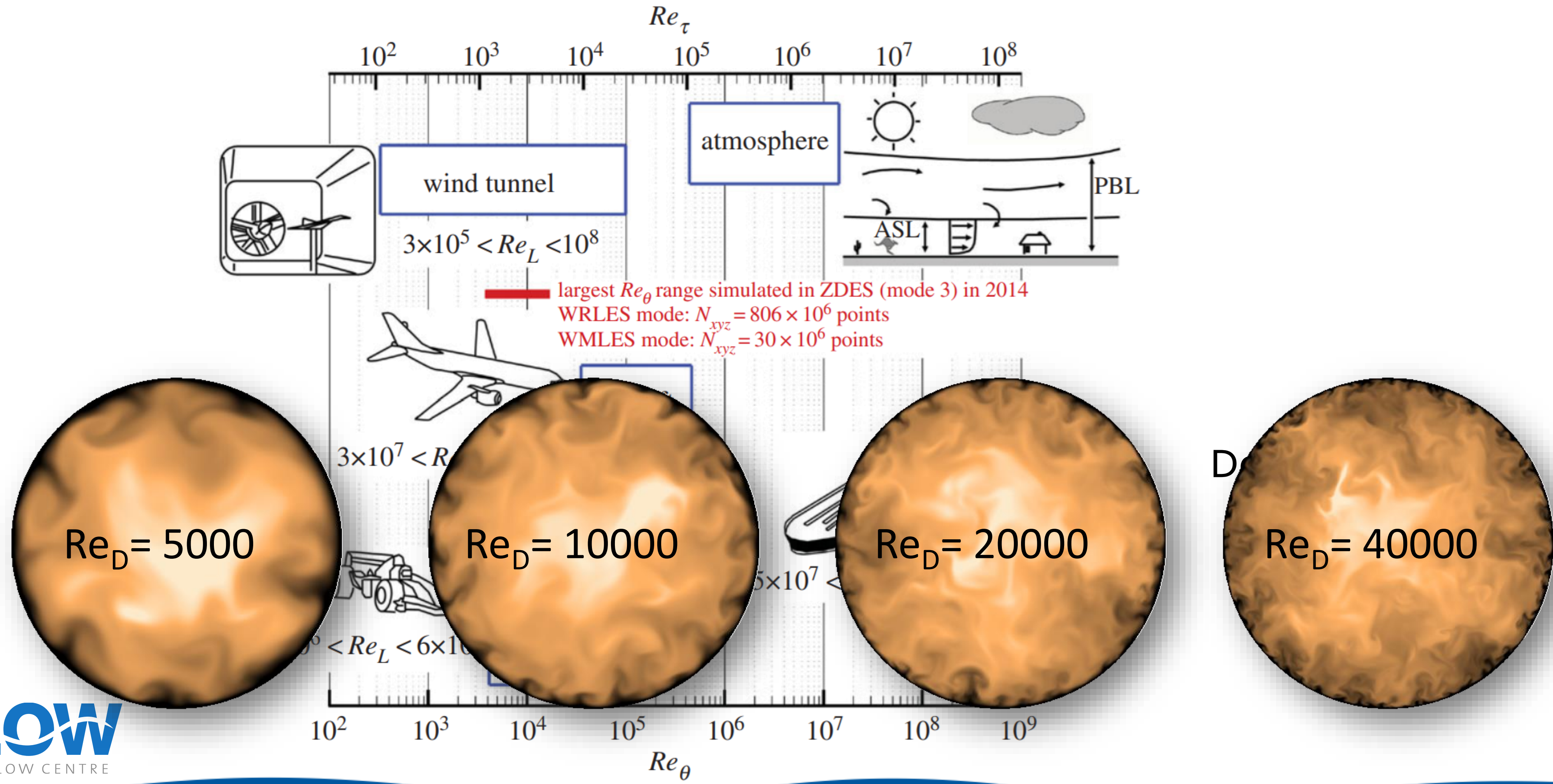


Numerical Simulation

- High comp
- Unknown i

Meaning of the **Reynolds number**:

$Re_D < 2500$ laminar

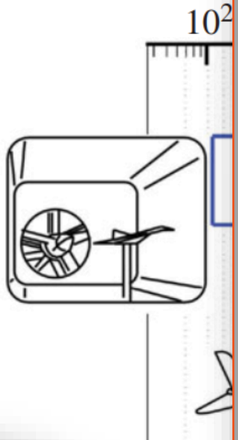
$Re_D = 1000$ blood in veins

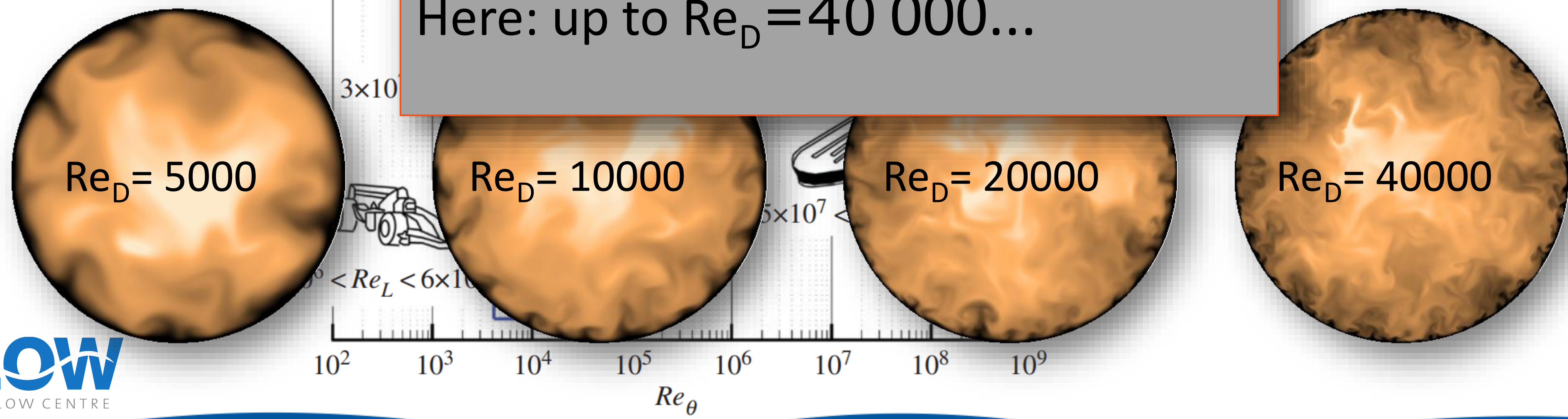
$Re_D = 3000$ soda with a straw

$Re_D = 100\,000$ oil pipelines

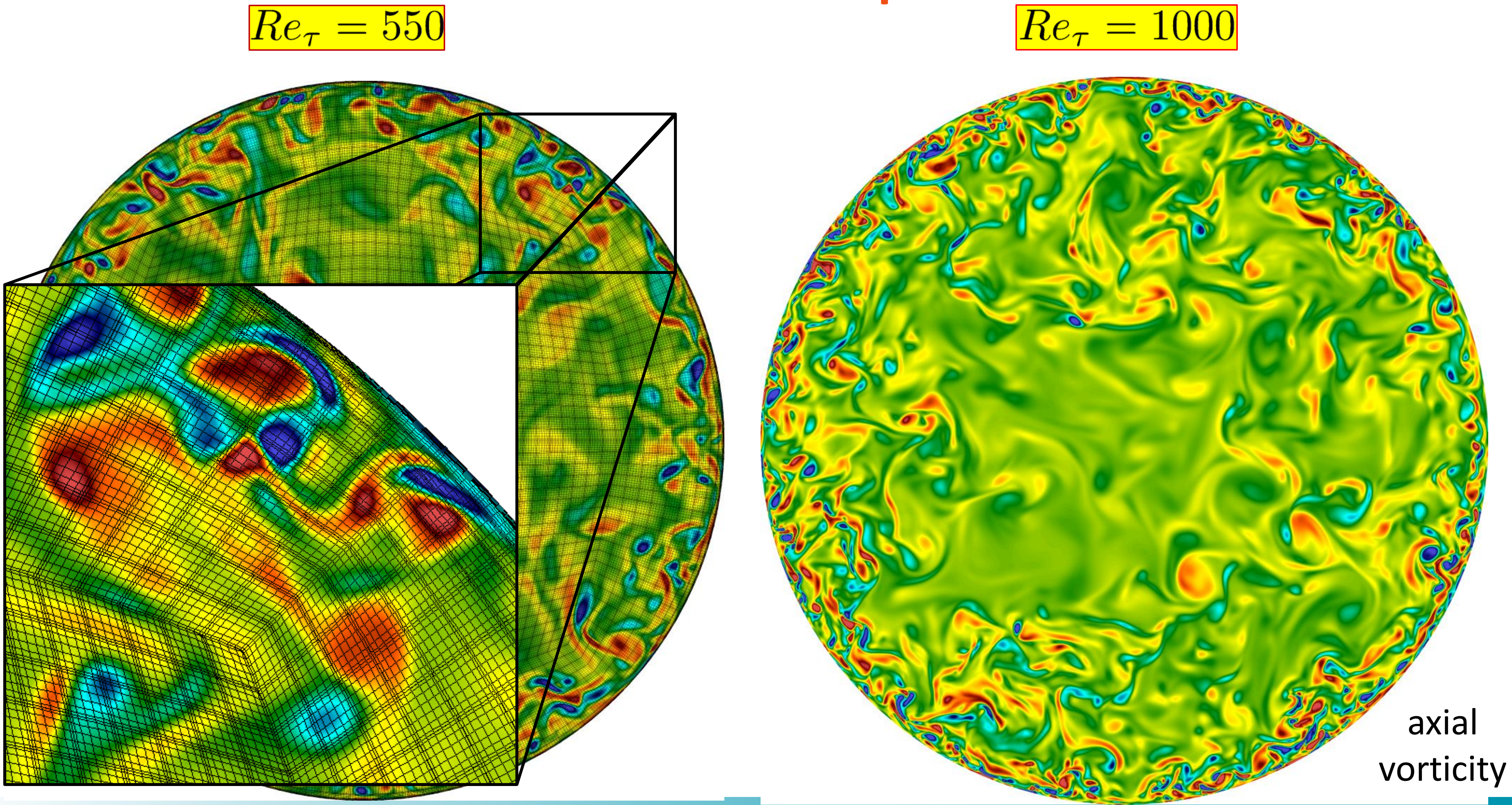
$Re_D = 10^7$ gas pipelines

Here: up to $Re_D = 40\,000$...





Direct Numerical Simulation – DNS
→ numerical experiment

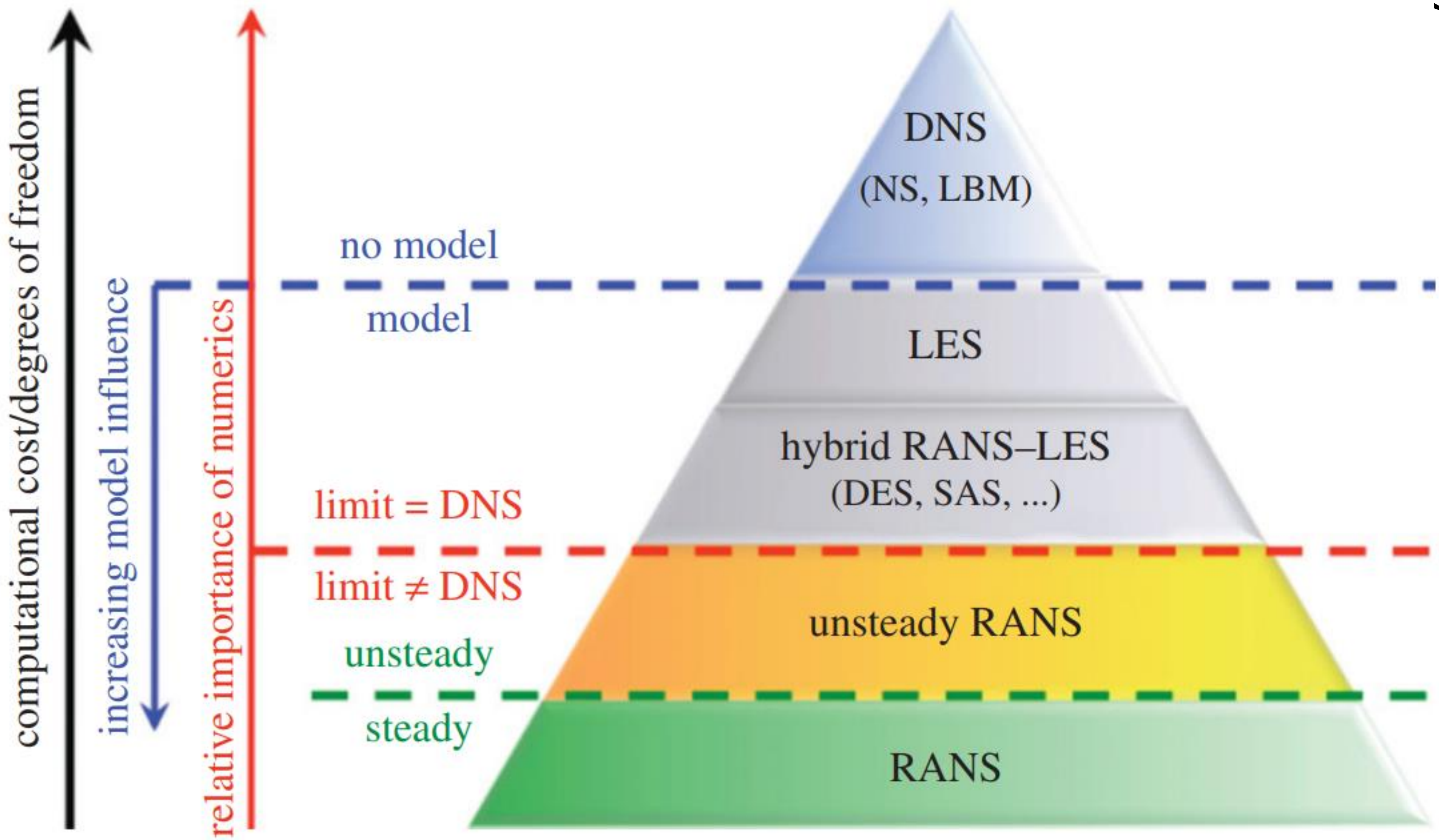


Very high resolution close to walls needed!

Numerical Simulation

- High computational cost
- Unknown influence of uncertainties

Sagaut et al. 2013

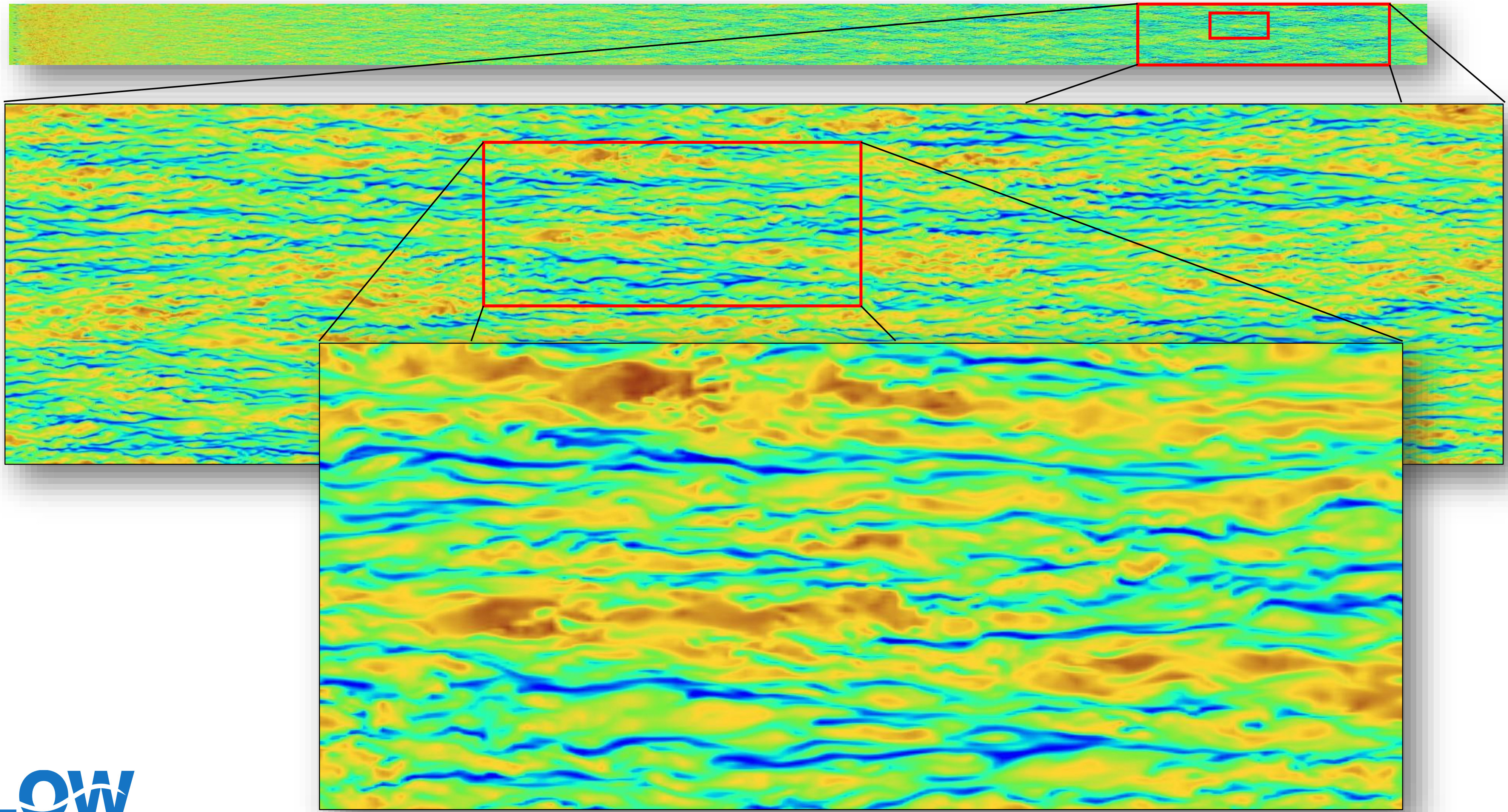


Turbulent flow close to solid walls...

Schlatter and Örlü (2010…)

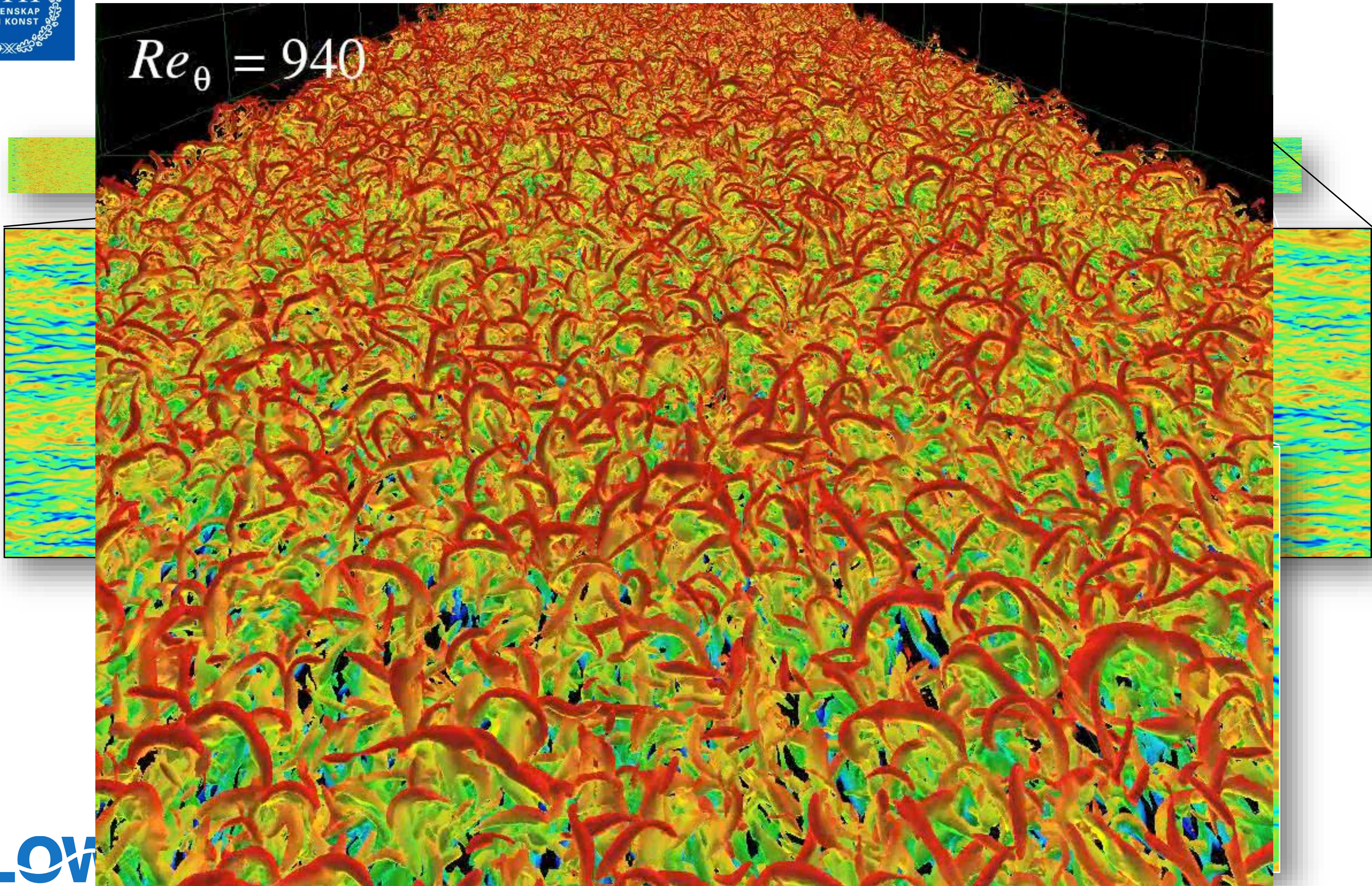
Turbulent flow close to solid walls...

simulation result



Schlatter and Örlü (2010…)

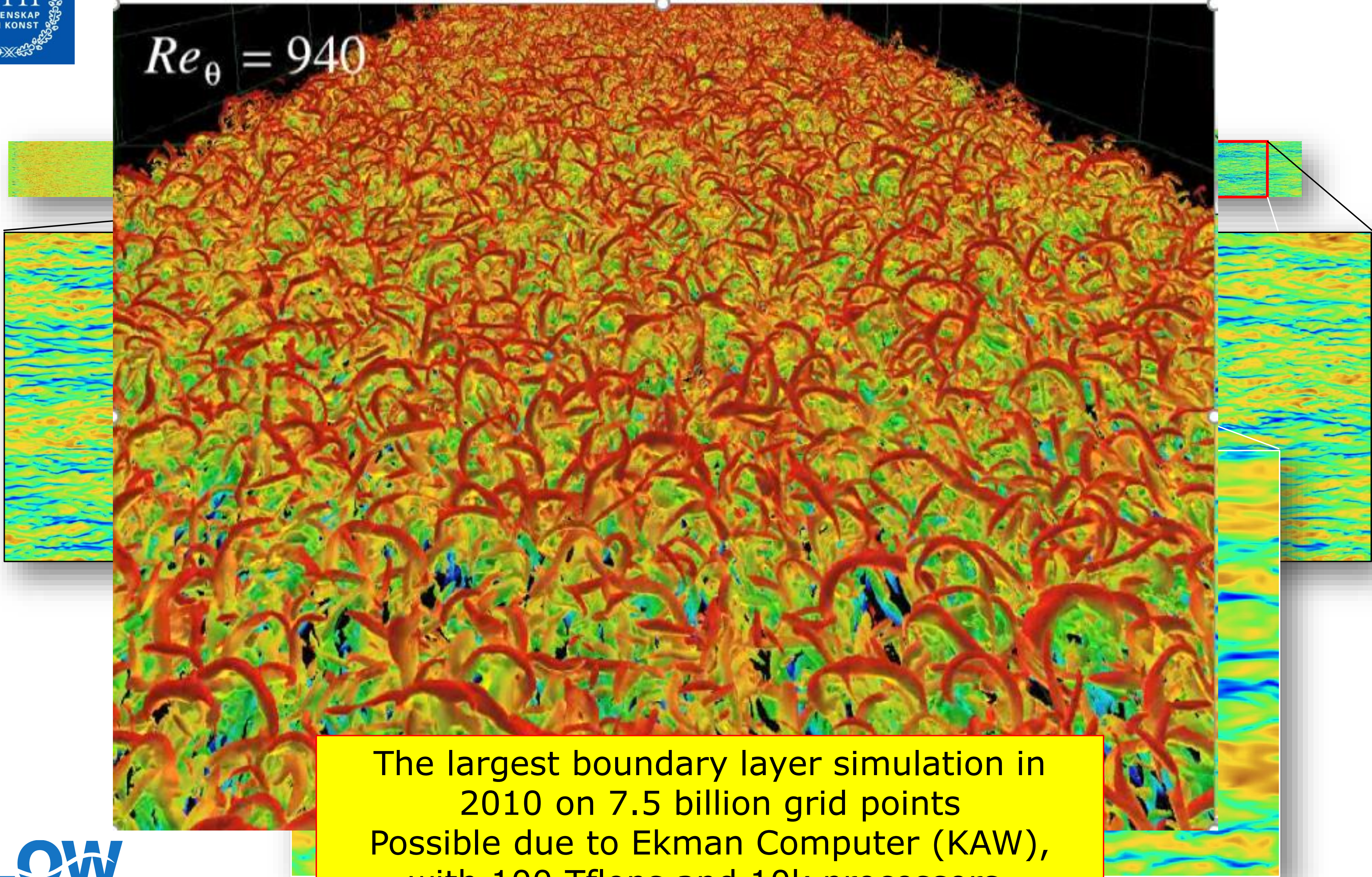
Turbulent flow close to solid walls...



Schlatter and Örlü (2010…)

Turbulent flow close to solid walls...

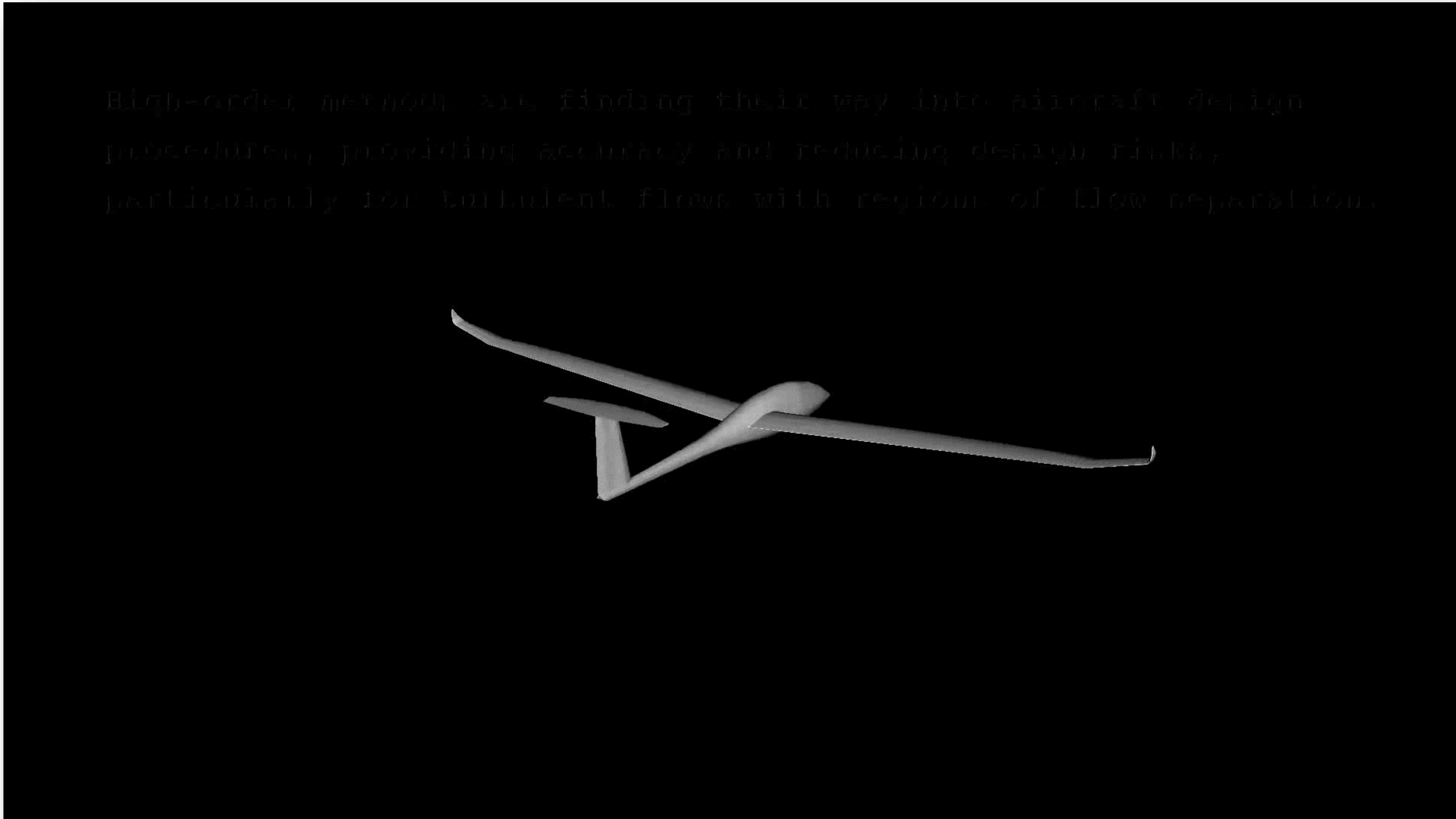
2010



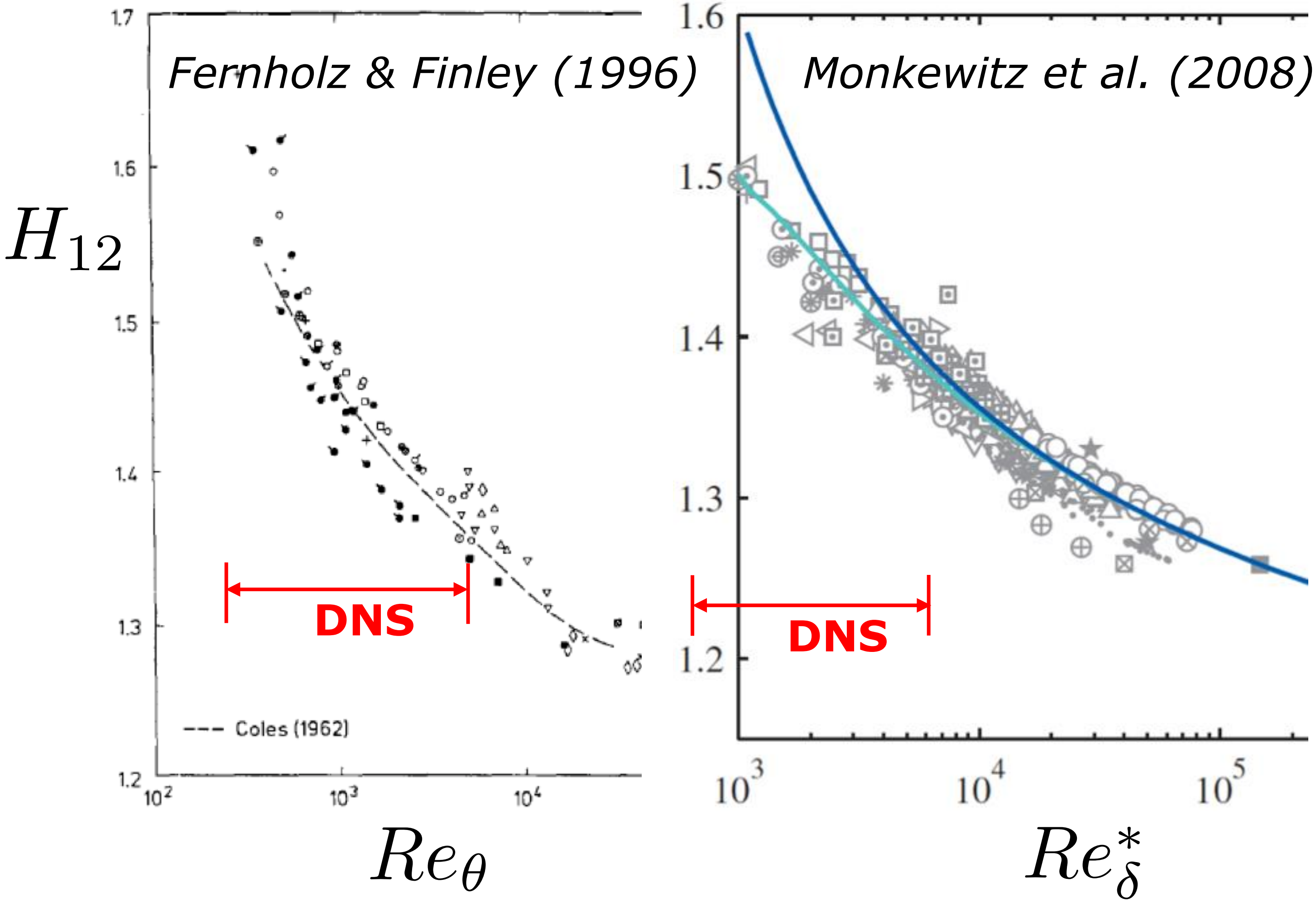
The largest boundary layer simulation in
2010 on 7.5 billion grid points
Possible due to Ekman Computer (KAW),
with 100 Tflops and 10k processors.

DNS of flow around a NACA4412 wing section; Re_c=400 000 and AoA=5°

2016



What we are used/expect to see …



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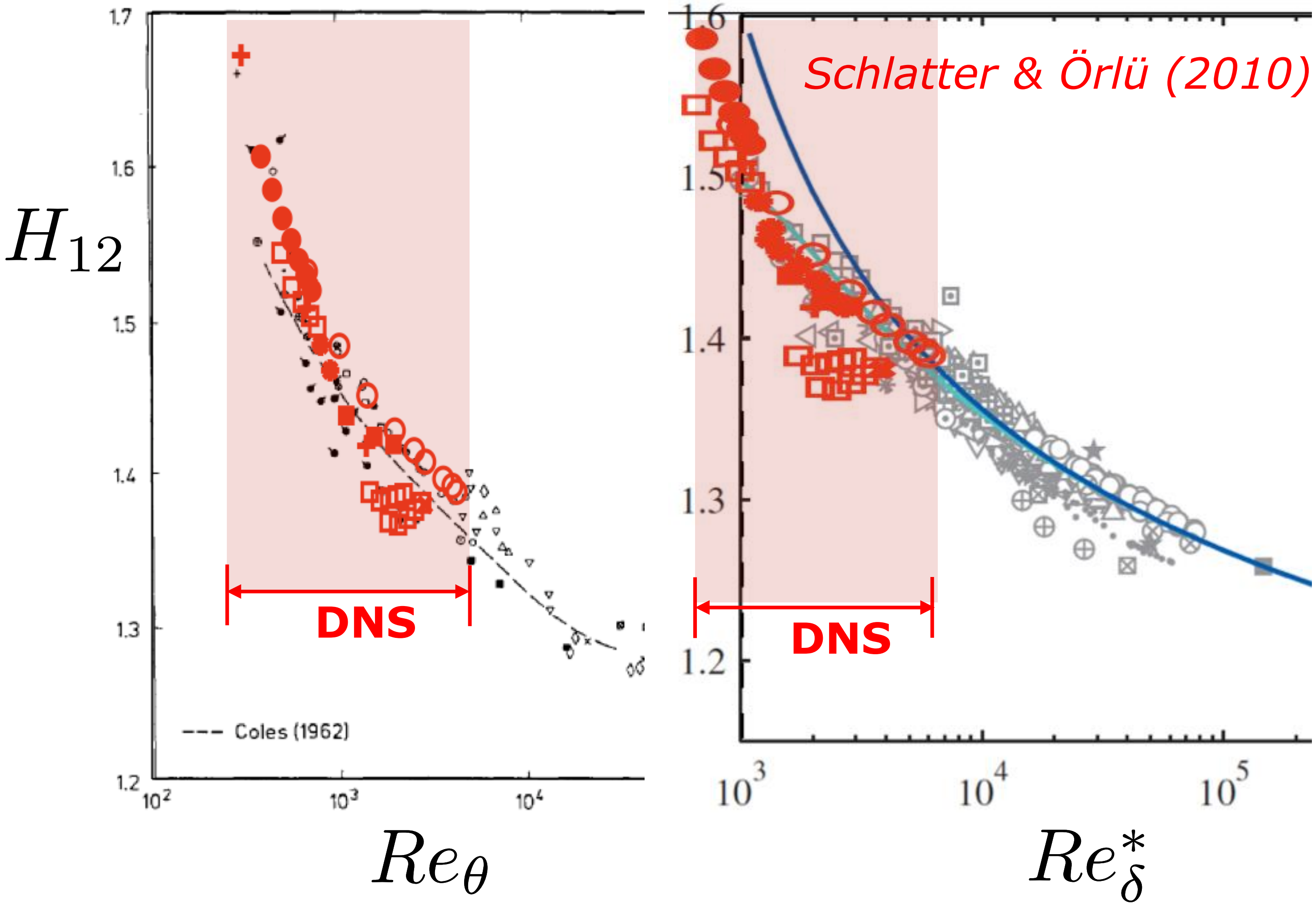
Compilation/
Assessment of
experimental data
from ZPG TBL flows

Physical experiments are commonly scrutinised before they are employed to calibrate, test, or validate other experiments, scaling laws or theories

… and what "we" are not so used to see



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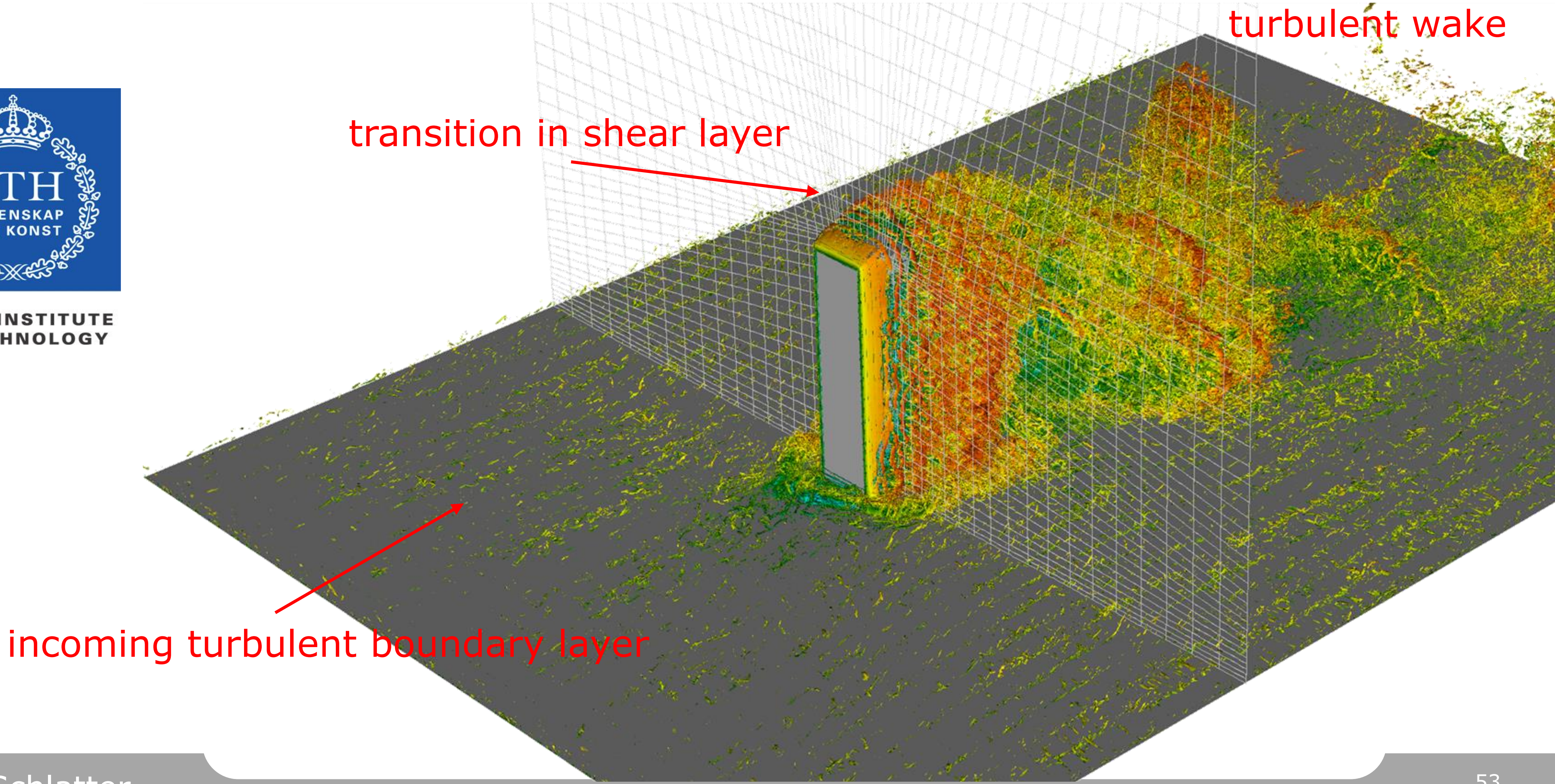
Red symbols are data from 7 independent DNS from ZPG TBL flows

Simulation data are hardly scrutinised, when it comes to basic (integral) quantities

TBL with ”obstacles”

- ”Skyscraper” reference case: Canadian CFD Challenge (2014)



Vinuesa *et al.* 2015

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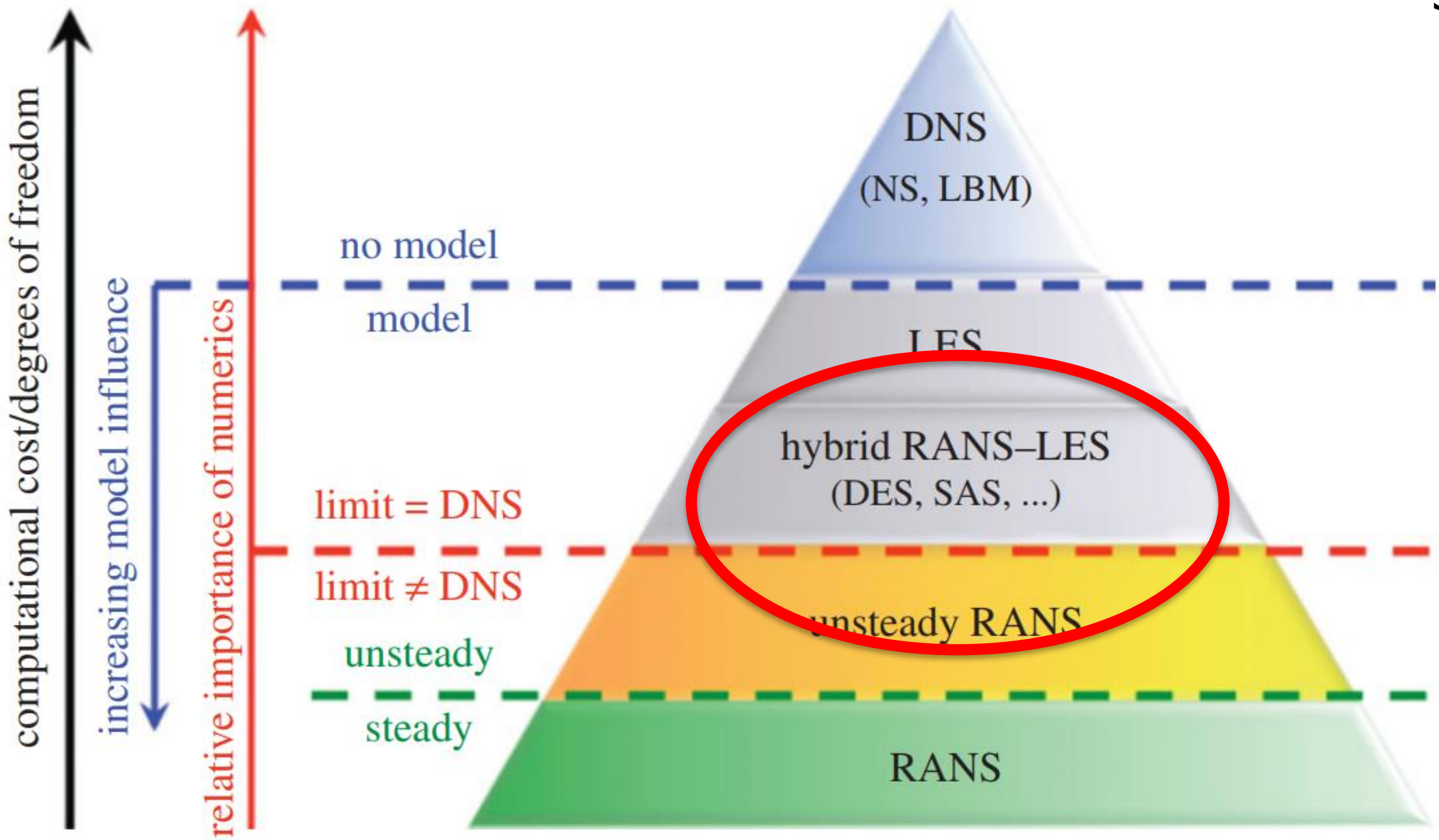
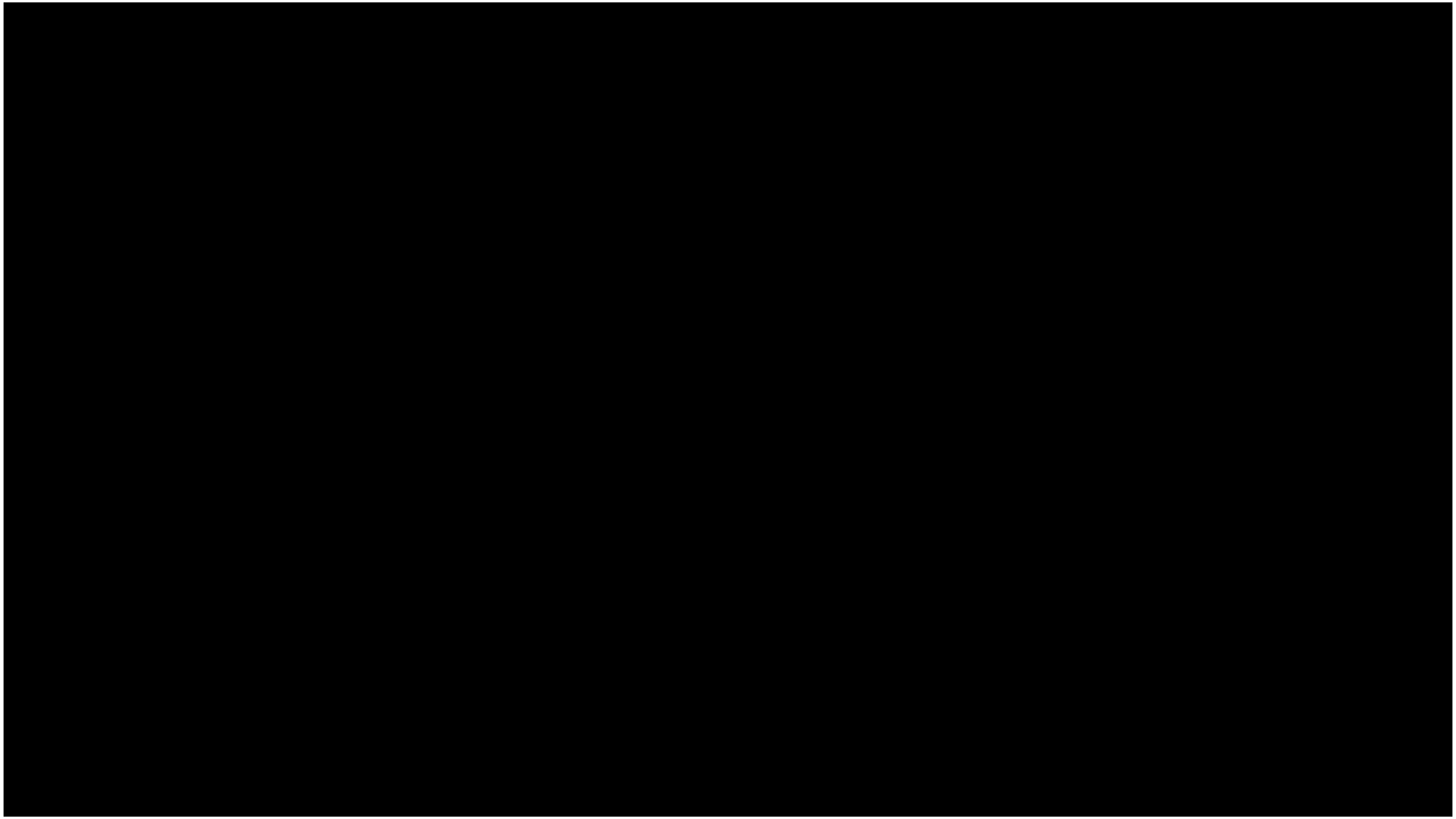
Numerical Simulation

- High computational cost
- Unknown influence of uncertainties

Sagaut et al. 2013



CFD – Scale resolving using OpenFOAM



Ville Vuorinen, Aalto University, Finland

Numerical Simulation

- High computational cost
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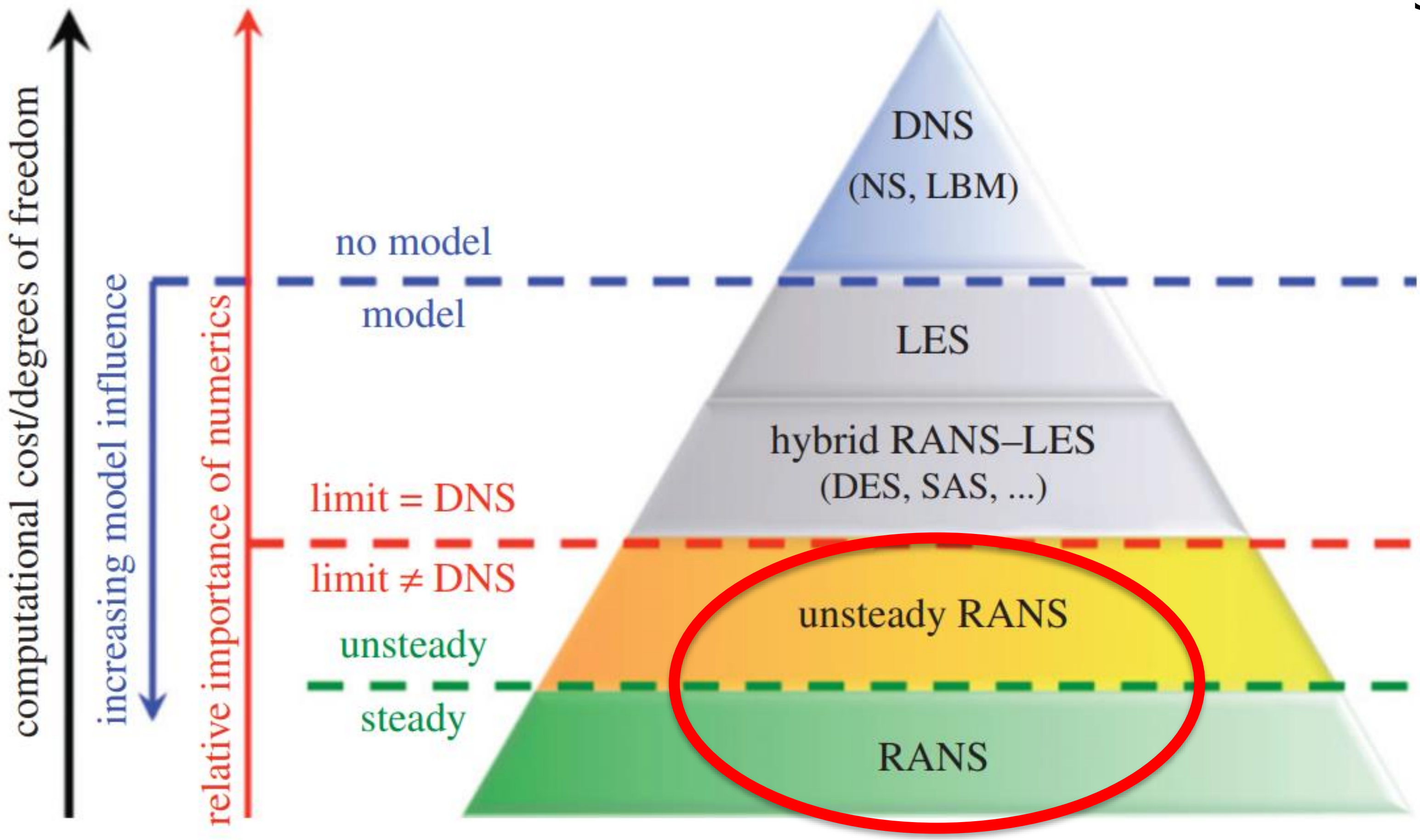
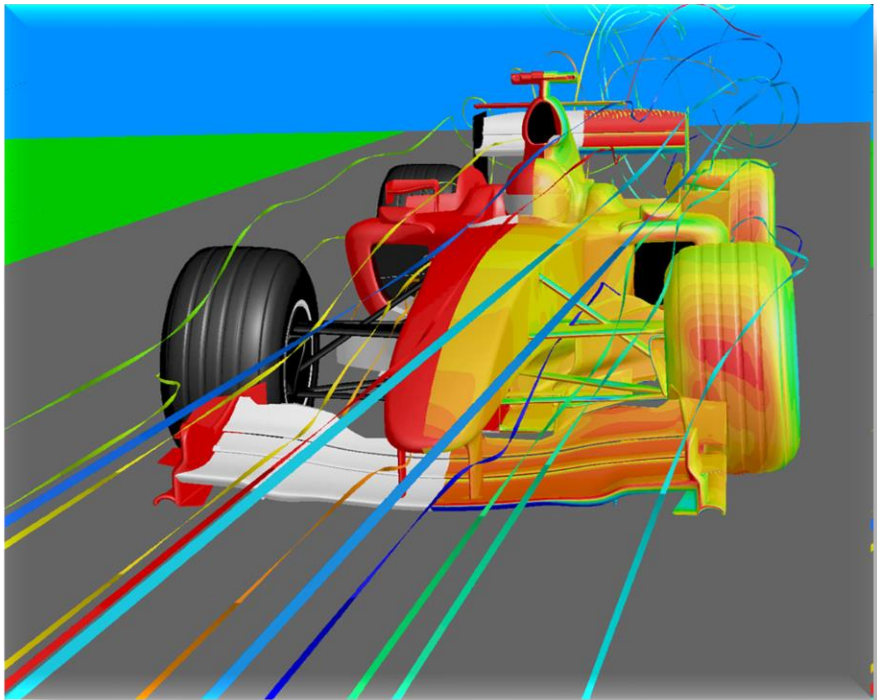
Sagaut et al. 2013



RANS – Reynolds-averaged Navier-Stokes

- “traditional” turbulence modelling using e.g. k-epsilon models
- Original meaning of CFD
- Typically steady-state solutions
- Limited accuracy and fidelity, however trends can be captured



From NASA CFD Vision 2030 (Slotnick et al. 2014)

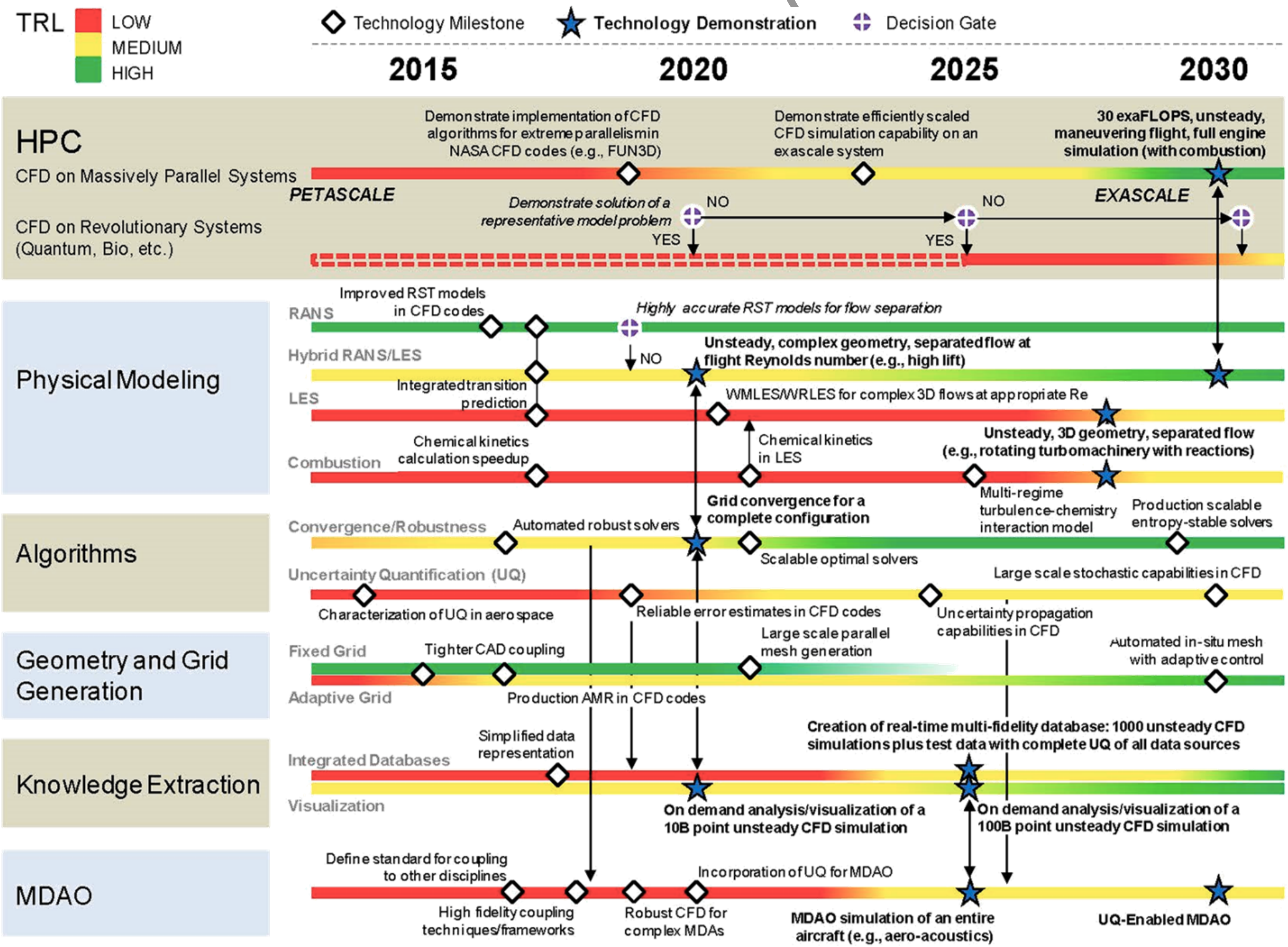


Figure 1. Technology Development Roadmap

Summary and Outlook

- CFD extremely valuable tool for R&D in fluid mechanics
- May be very expensive, or “very” relying on turbulence models
- Verification and validation
- Research both on methods, tools and physics
- CFD at intersection of engineering, physics, mathematics and computer science
- My professor called it an “art”…

Multiscale modelling

Advanced modelling means getting **at the reasonable cost the right answer**, i.e. capturing all flow features in a range of scales and preserving conservation laws.

Problems:

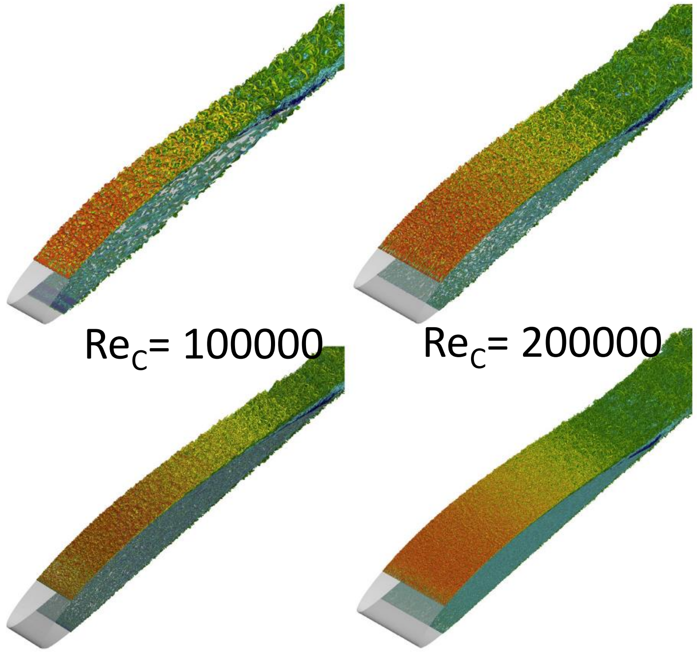
- Nonlinearity → turbulence, small scales
- Incompressibility → global coupling
- Small viscosity (but NON-ZERO) → thin boundary layers

Multiscale simulation hierarchy involving:

Increased Costs ↑

1. Experiments
2. DNS (direct numerical simulation of turbulence)
3. LES (large eddy simulation)
4. RANS (Reynolds-averaged Navier-Stokes)
5. Subchannel or lumped-parameter models

Increased Modeling ↓



Re_C= 100000 Re_C= 200000

Re_C= 400000 Re_C= 1000000

Multiscale modelling

Advanced modelling means getting **at the reasonable cost the right answer**, i.e. capturing all flow features in a range of scales and preserving conservation laws.

Nek5000:

- CFD solver covering **2, 3** and **4**.
- High order; based on **Spectral Element Method**
- **Highly scalable** (up to 1 million MPI ranks)

Multiscale simulation hierarchy involving:

Increased Costs ↑

1. Experiments
2. DNS (direct numerical simulation of turbulence)
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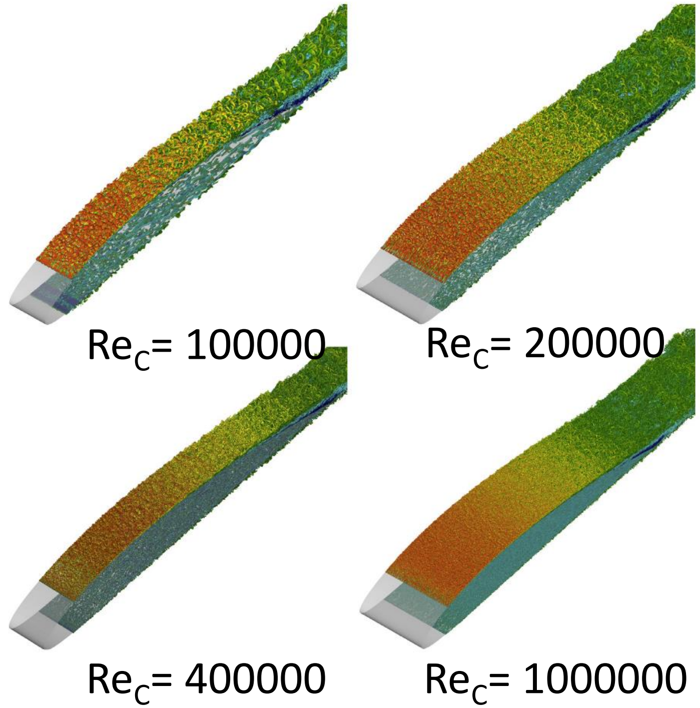
Increased Modeling ↓



General overview

- Open source code by **Paul F. Fischer**, Argonne National Lab, USA
- First commercially-available code for distributed memory computers (marketed by Fluent as Nekton into the mid 90s)
- **Gordon Bell Prize 1999 in HPC** for algorithmic quality and performance on 4096 processors

  (Tufo & Fischer '99)
- **R&D 100 Award 2016**
- General purpose CFD solver
- Fortran 77 & C code with MPI parallelization
- "Keep it simple" – world's most powerful computers have very weak operating systems

Nek5000 Users Meeting, Tampa 2018

General overview

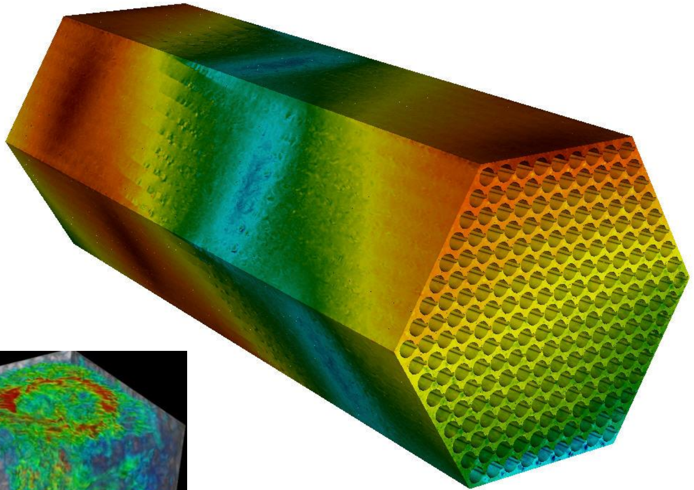
EXCELLERAT

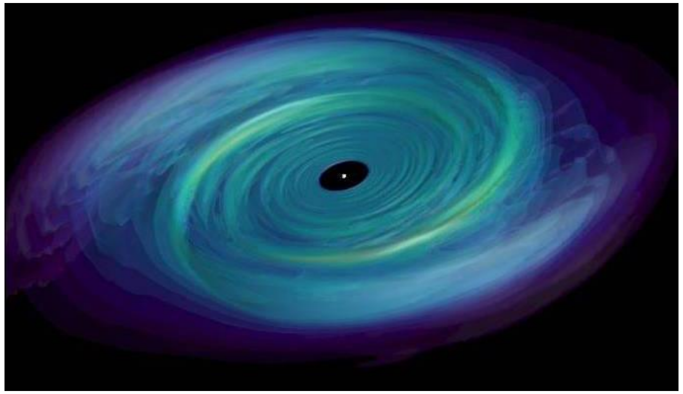
Selected features:

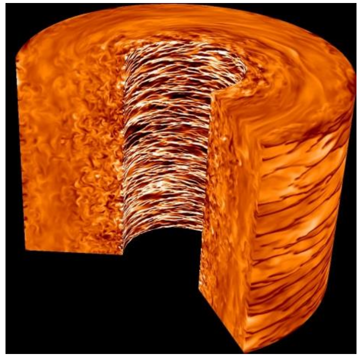
- Incompressible and Low-Mach.
- Species Transport (passive scalars and reactive scalars).
- MHD.
- Conjugate heat transfer.
- Moving meshes, FSI (with structural codes).
- Combustion.
- Multiphase (Eulerian-Eulerian, Eulerian-Lagrangian).
- Free surface.
- Various turbulence models (RANS).
- Ensemble Averaging.
- Multimesh on unstructured grids.

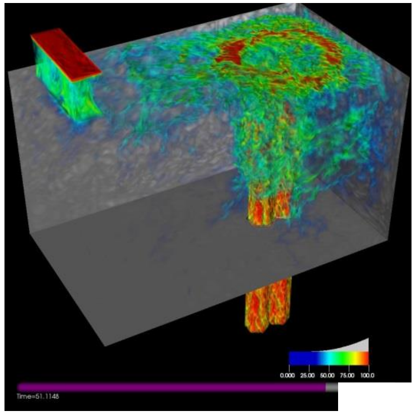
Nek5000 Users Meeting, Tampa 2018

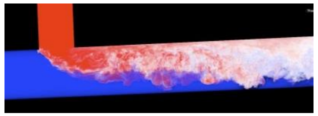
Applications





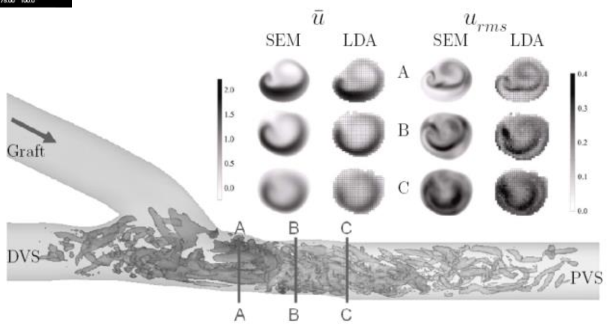


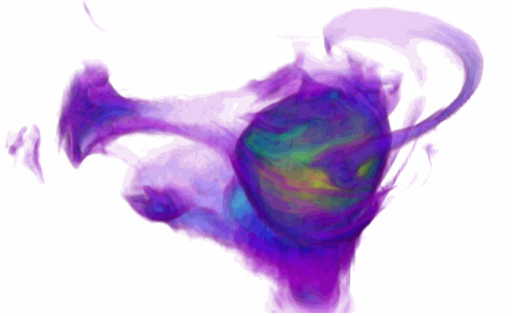


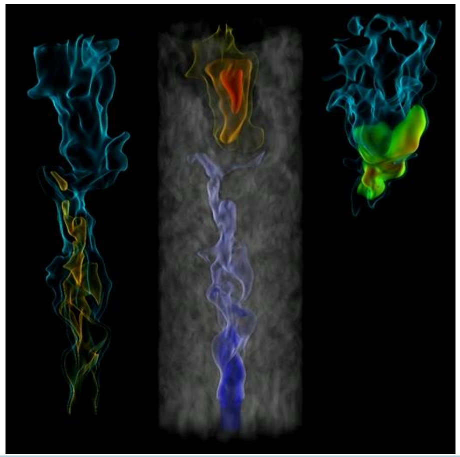


Clockwise from upper left:

- *Reactor thermal-hydraulics*
- *Astrophysics*
- *Combustion*
- *Oceanography*
- *Vascular flow modeling*

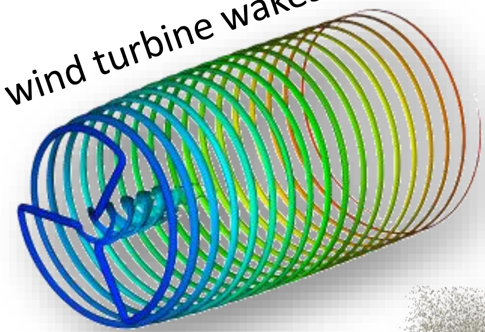




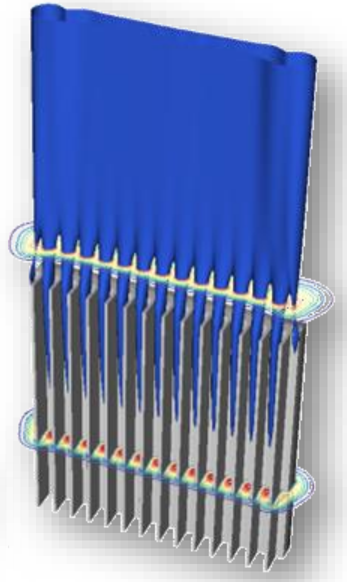


Applications (KTH)

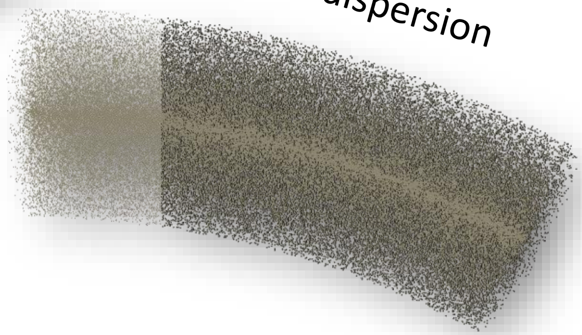
stability tools for jet in crossflow



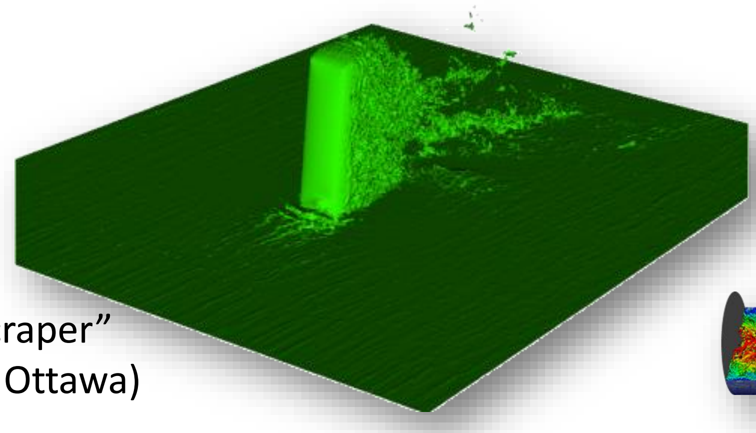
wind turbine wakes



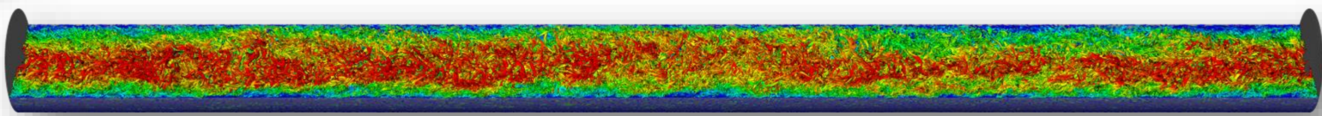
optimisation of heat sinks



particle dispersion



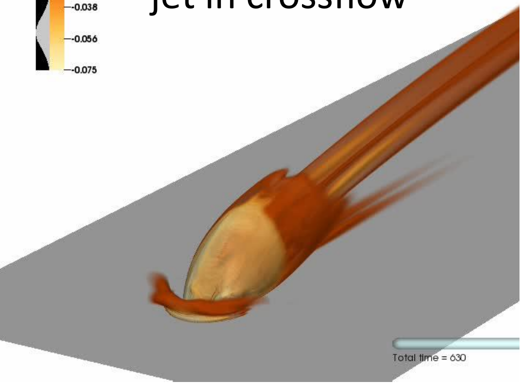
"skyscraper" (with U Ottawa)

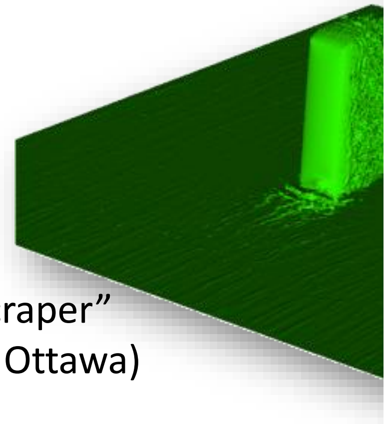


turbulent pipe flow

Applications (KTH)

stability tools for
jet in crossflow





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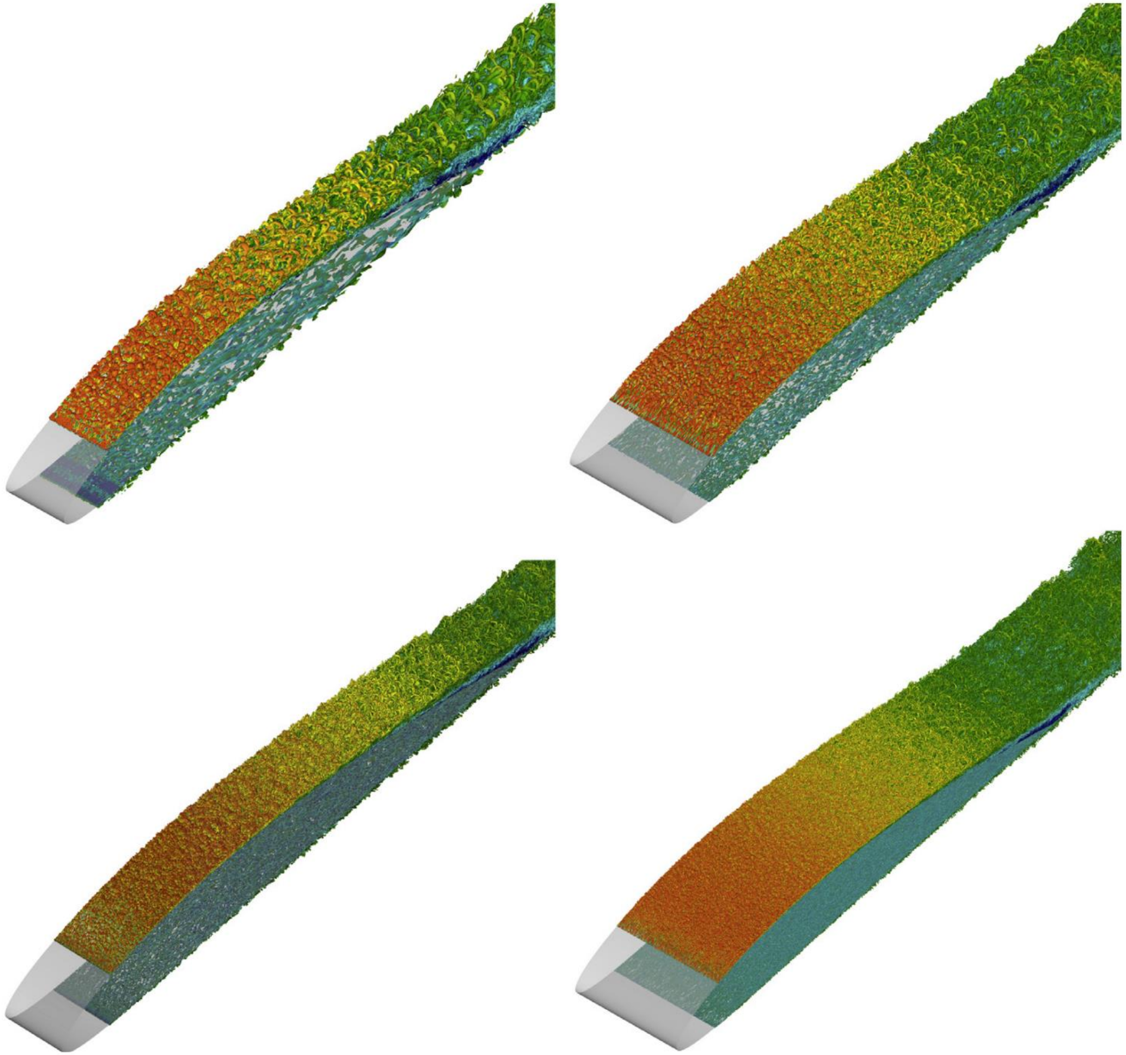

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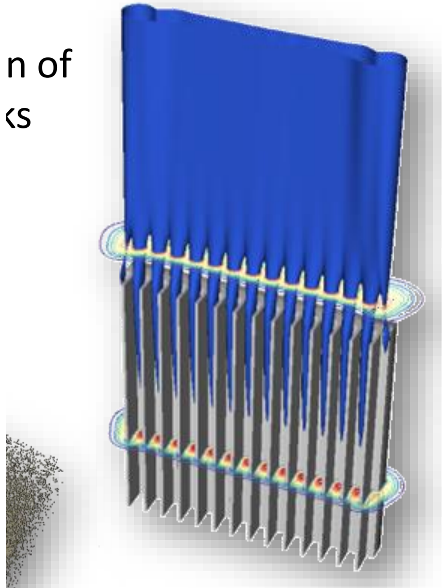

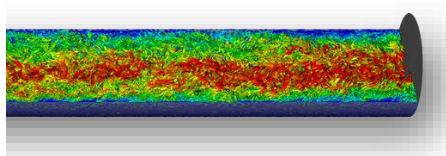

Applications (KTH)