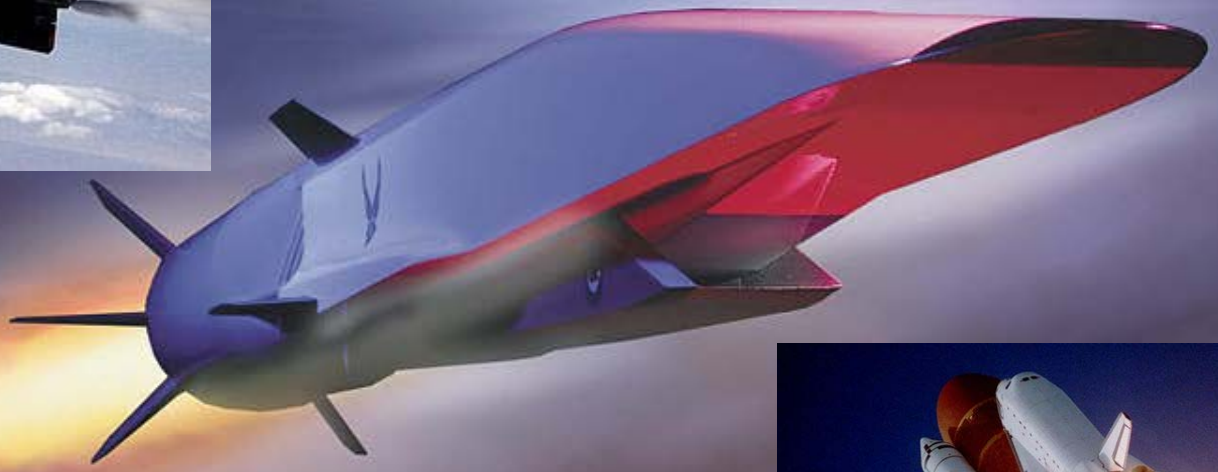
Towards aerospace design in the age of extreme-scale supercomputing

Qiqi Wang

Assistant Professor of Aero & Astro, MIT

with work by Patrick Blonigan and Chaitanya Talnikar

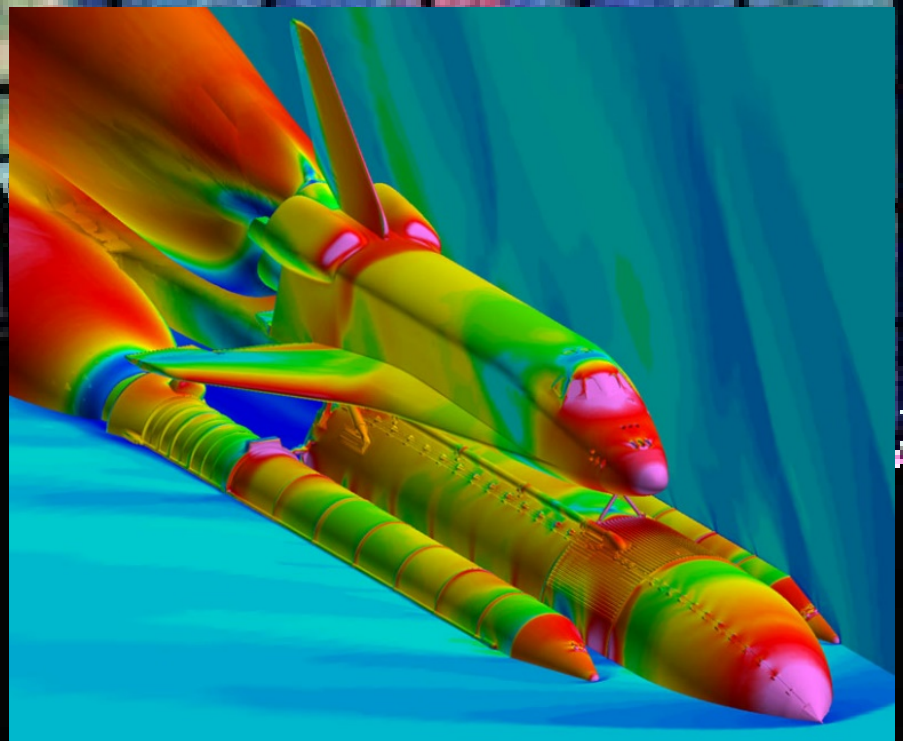


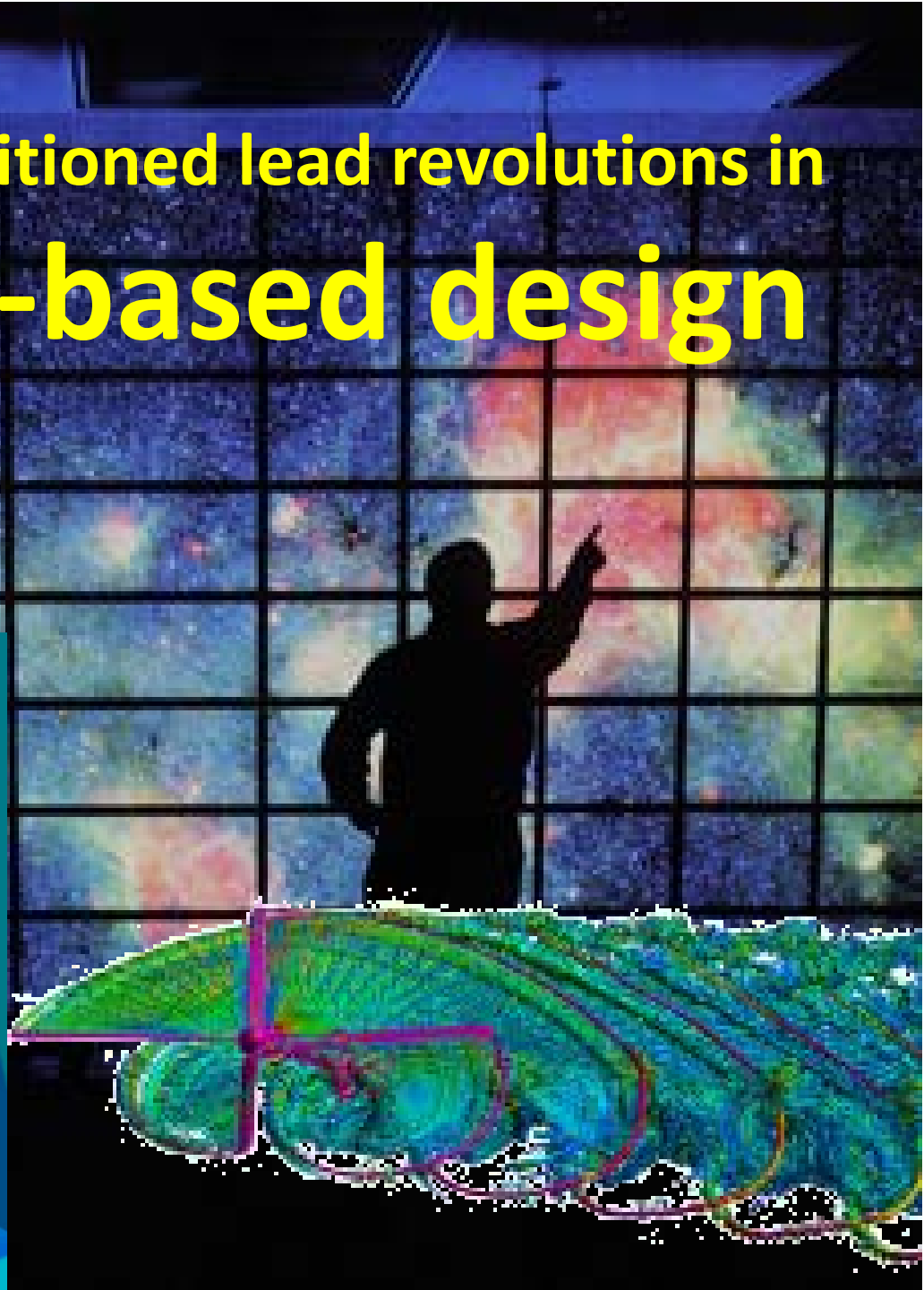
NASA has inspired the world with its

Aerospace Designs

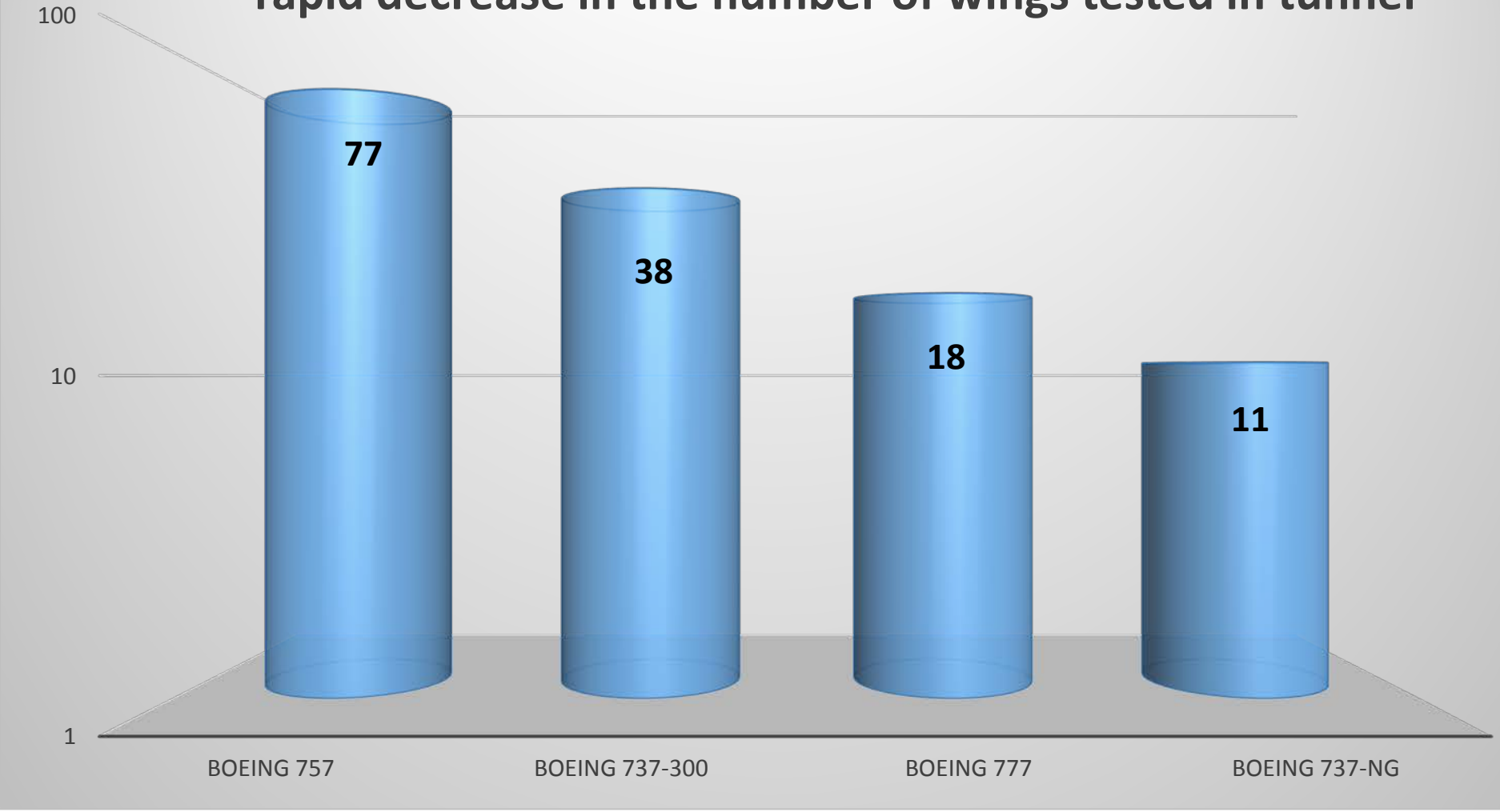
NASA is uniquely positioned lead revolutions in

simulation-based design





CFD methods developed during the ICASE period led to rapid decrease in the number of wings tested in tunnel



1980 from Jameson, 2012 **1995**

CFD has been on a **plateau for the last 15 years**.

– Jameson 2012

Plan and roadmap were created to help focus investments in technology development to help achieve the **CFD vision in 2030**

– Slotnick, Khodadoust, Alonso, Darmofal, Gropp, Lurie, Mavriplis, funded by **NASA** with Kleb and Malik

NASA/CR–2014-218178

CFD Vision 2030 Study: A Path to Revolutionary Computational Aerosciences

Jeffrey Slotnick and Abdollah Khodadoust
Boeing Research & Technology, Huntington Beach, California

Juan Alonso
Stanford University, Stanford, California

David Darmofal
Massachusetts Institute of Technology, Cambridge, Massachusetts

William Gropp
National Center for Supercomputing Applications, Urbana, Illinois

Elizabeth Lurie
Pratt & Whitney, United Technologies Corporation, East Hartford, Connecticut

Dimitri Mavriplis
University of Wyoming, Laramie, Wyoming

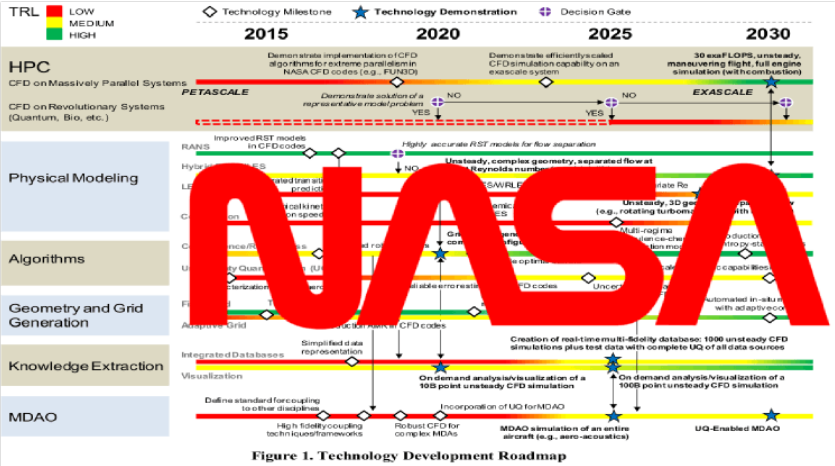
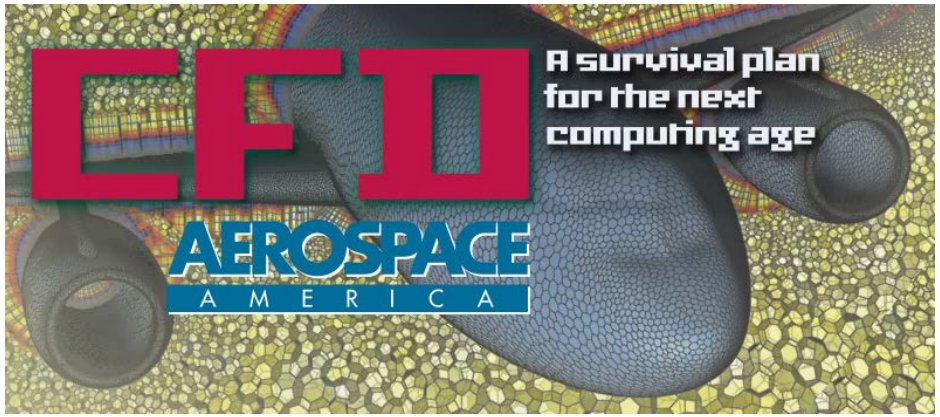


Figure 1. Technology Development Roadmap



http://goo.gl/FMHwTx

"Hybrid RANS/LES methods show perhaps the most promise in being able to capture more of the relevant flow physics for complex geometries at an increasingly reasonable computa- tional cost."

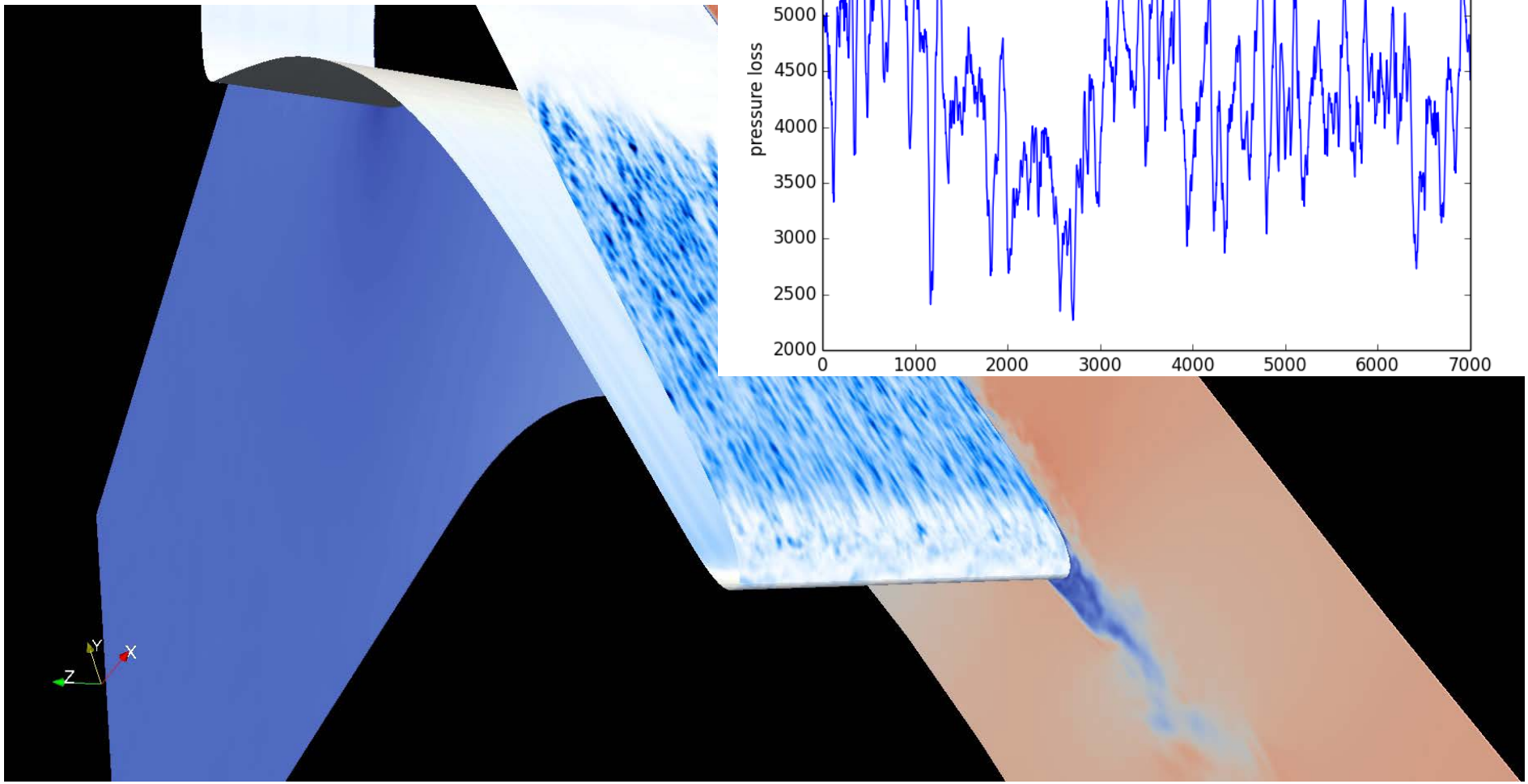
"WRLES is potentially feasible in 2030 for lower Reynolds numbers."

'Design is "a huge carrot out there, in terms of what we'll be able to do in the future," Slotnick says. "In 20 years, engineers will not simply be doing CFD analysis," he predicts. "They'll be sitting and doing high-fidelity design using computational methods and incorporating CFD into the design, almost in real time."'

'The problem, Gropp says, is that today's well-understood CFD algorithms and software will have to be rewritten or overhauled to work on massively parallel computers or quantum computers. '

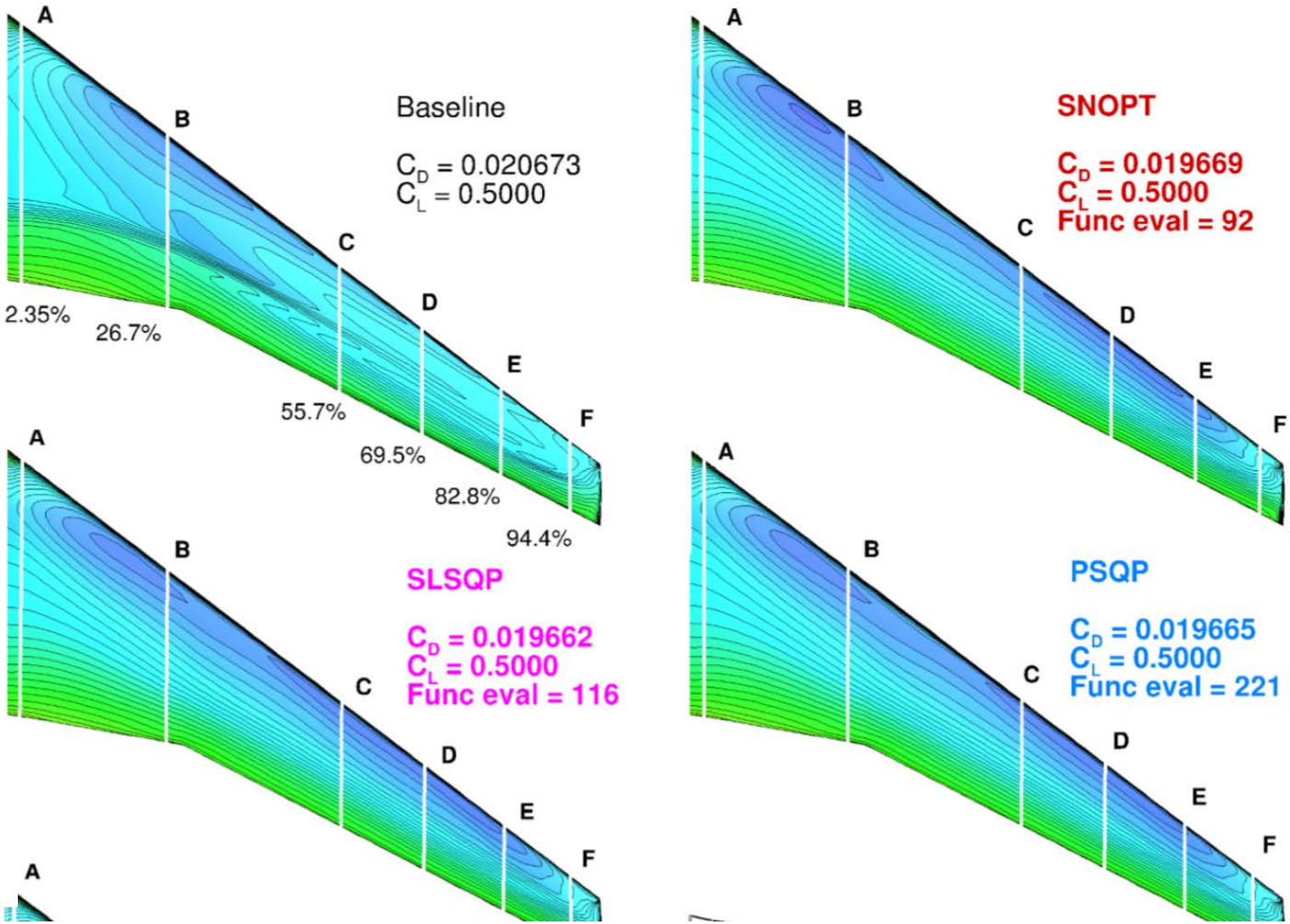
A typical high fidelity CFD requires **millions of time steps**

Talnikar, Blonigan, Bodart, Wang, 2014



The best optimization algorithm requires ~**100 simulations**

Lyu, Z, Xu, Z, Martins, JRRA, Benchmarking Optimization Algorithms for Wing, 2014

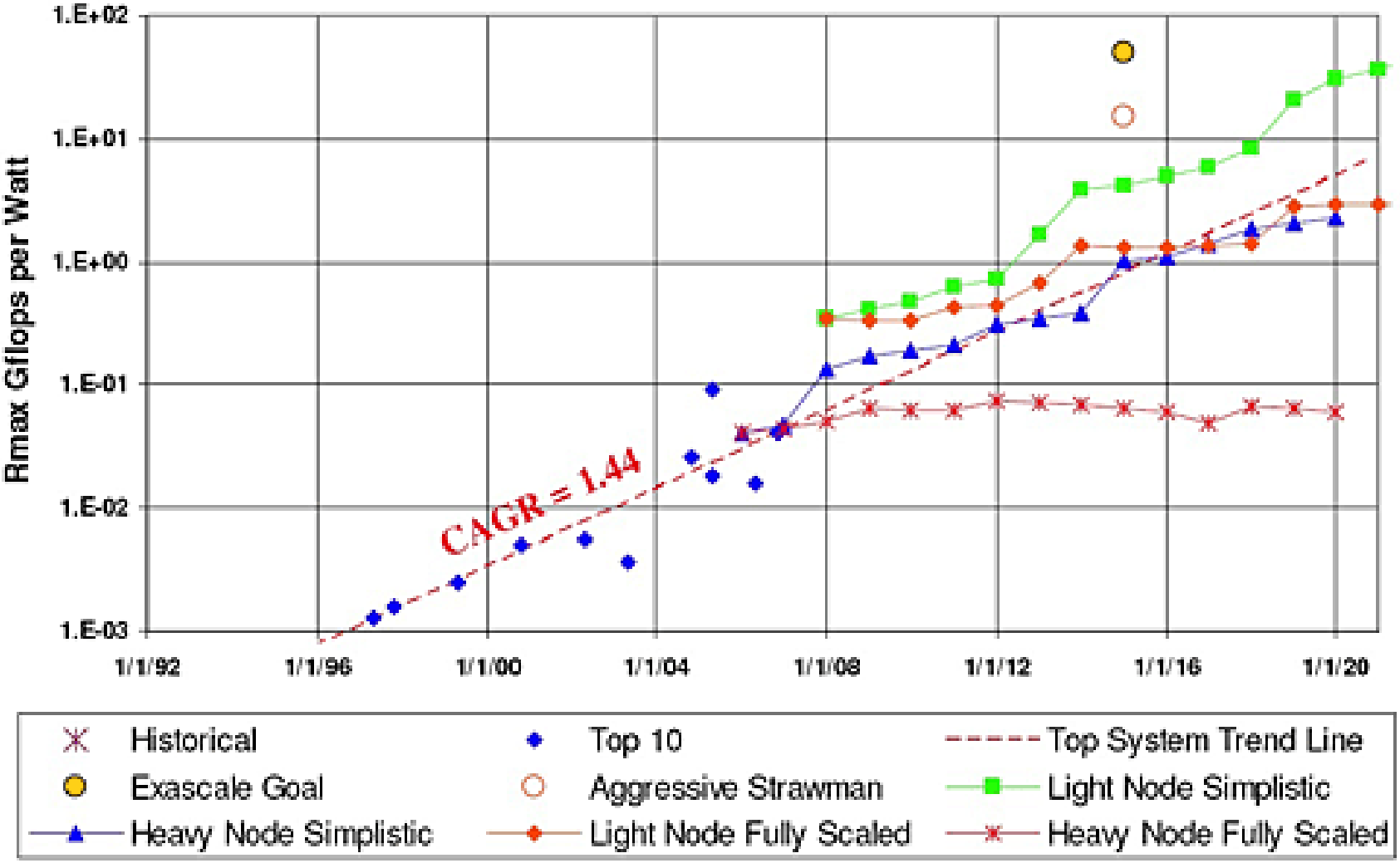


A typical high fidelity CFD requires **millions of time steps**. The best optimization algorithm requires ~**100 simulations.**

With today's methods, a high fidelity design optimization takes **weeks, if not months**.

Can we shorten a high fidelity design optimization to **minutes**?

Future supercomputer may be built with **“smartphone”s**



Bergman et al. ExaScale Computing Study: Technology Challenges in Achieving Exascale Systems (2008)

A typical high fidelity CFD requires **millions of time steps**. The best optimization algorithm requires ~**100 simulations.**

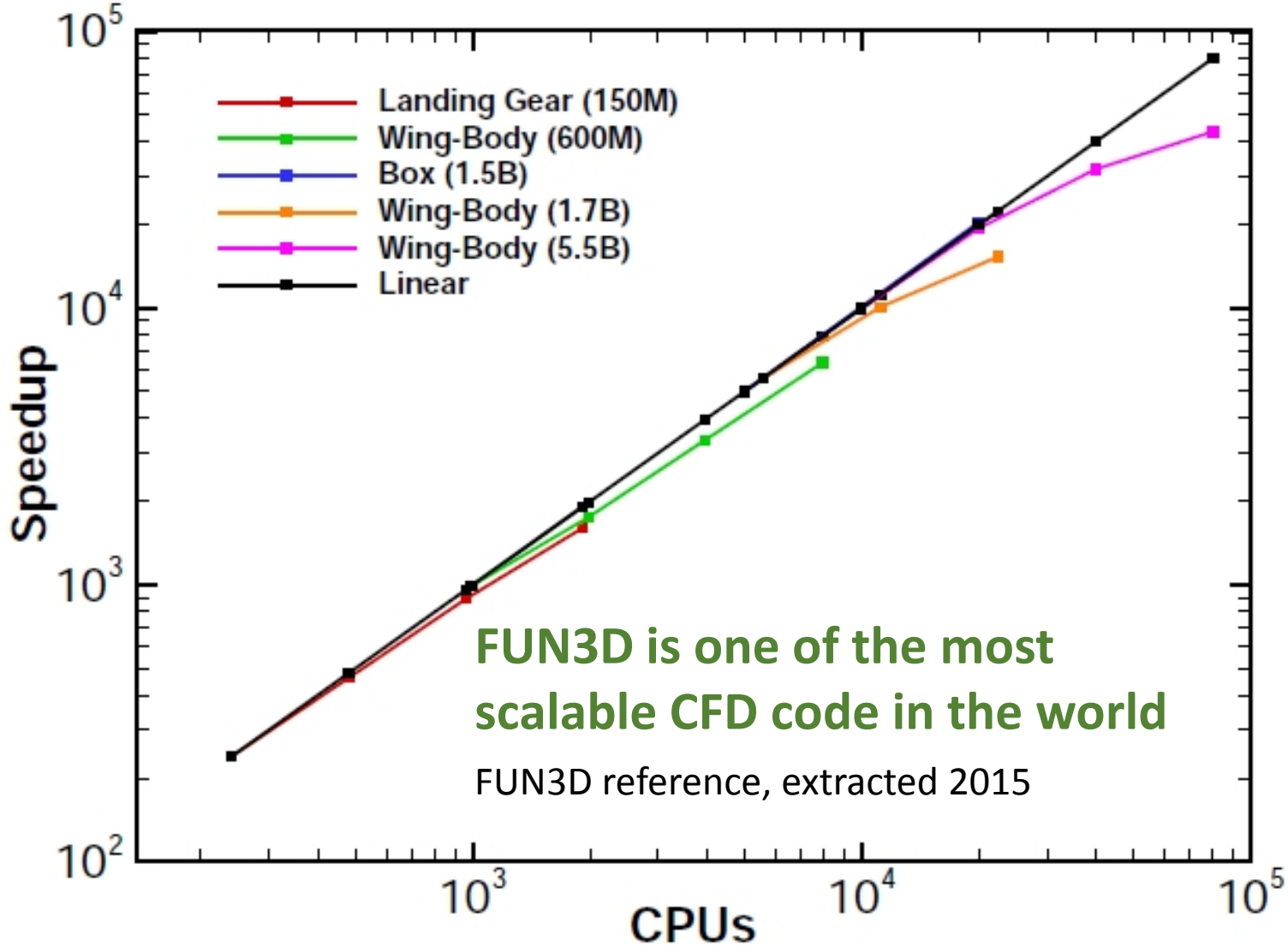
With today's methods, a high fidelity design optimization takes **weeks, if not months**.

Can we shorten a high fidelity design optimization to **minutes**, using billions of **"smartphone" nodes?**

Can we shorten a high fidelity design optimization to **minutes**, using billions of **"smartphone" nodes?**

- Can we shorten a high fidelity **simulation** to minutes?
- Can we shorten a high fidelity **optimization** to minutes?
- Can we shorten a high fidelity optimization with **many design parameters** to minutes?

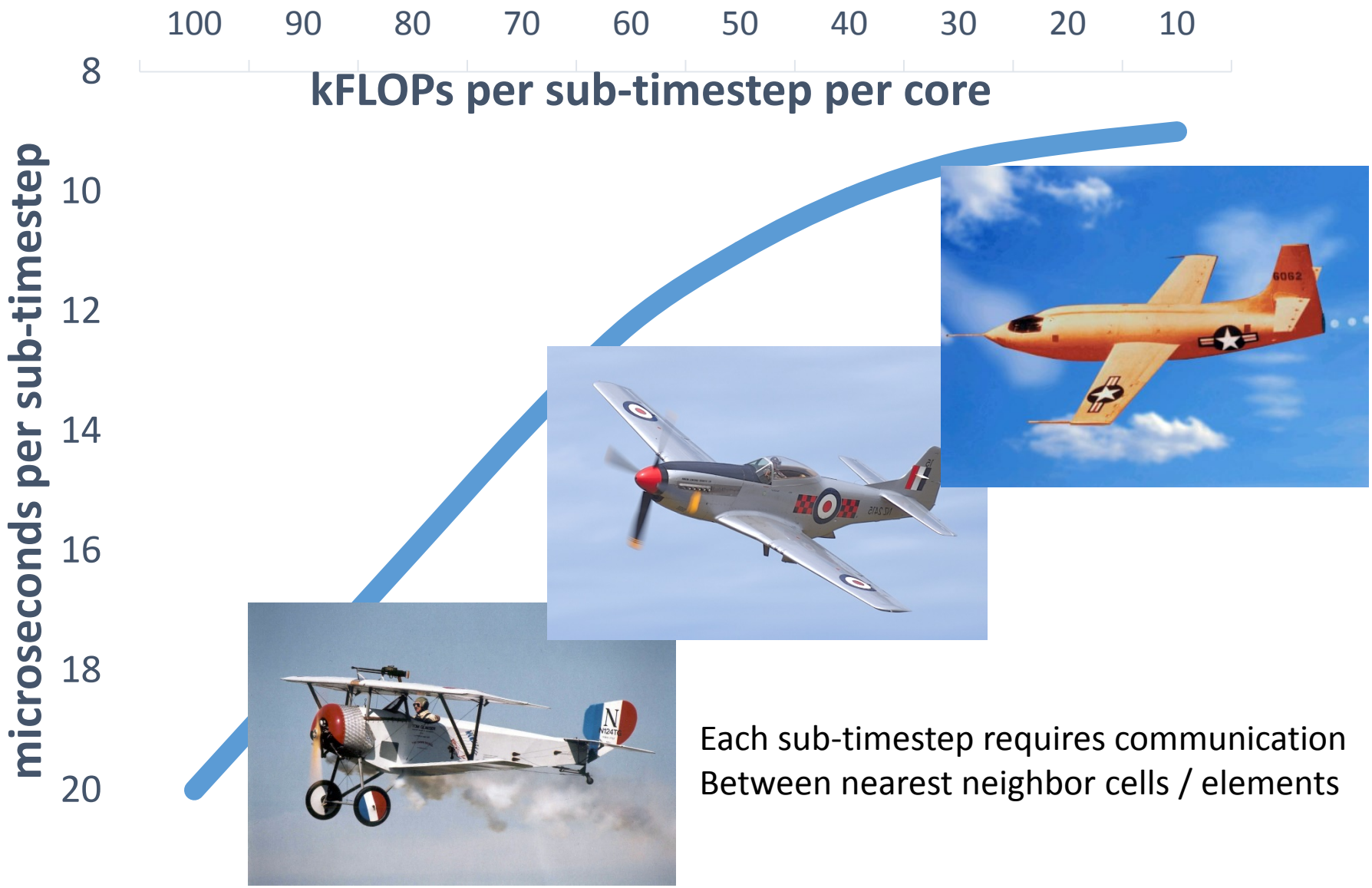
Accelerating high fidelity simulation with extreme scale parallelism



FUN3D is one of the most scalable CFD code in the world

FUN3D reference, extracted 2015

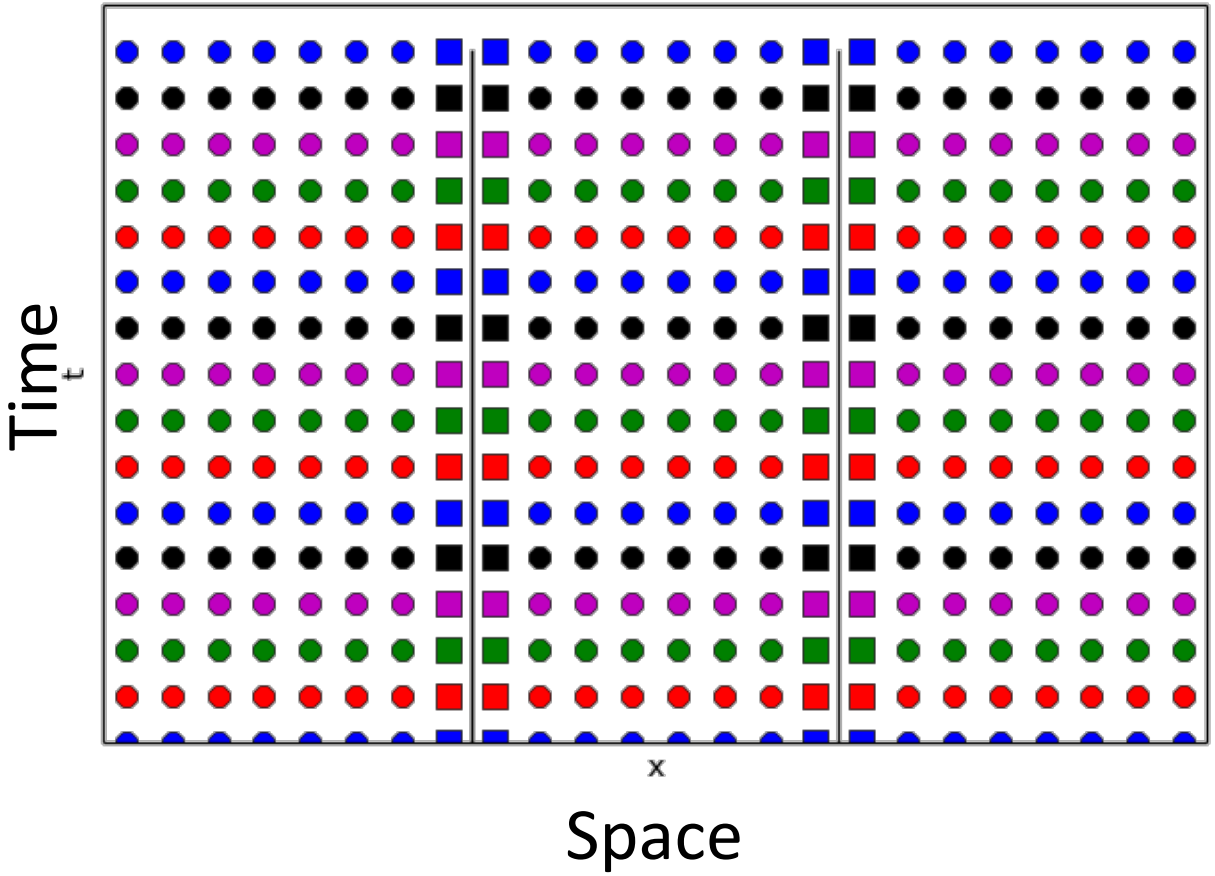
The latency barrier

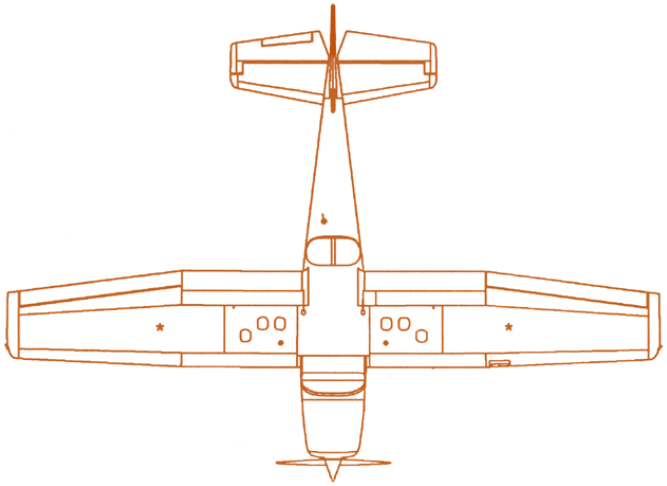


Each sub-timestep requires communication
Between nearest neighbor cells / elements

Breaking the latency barrier

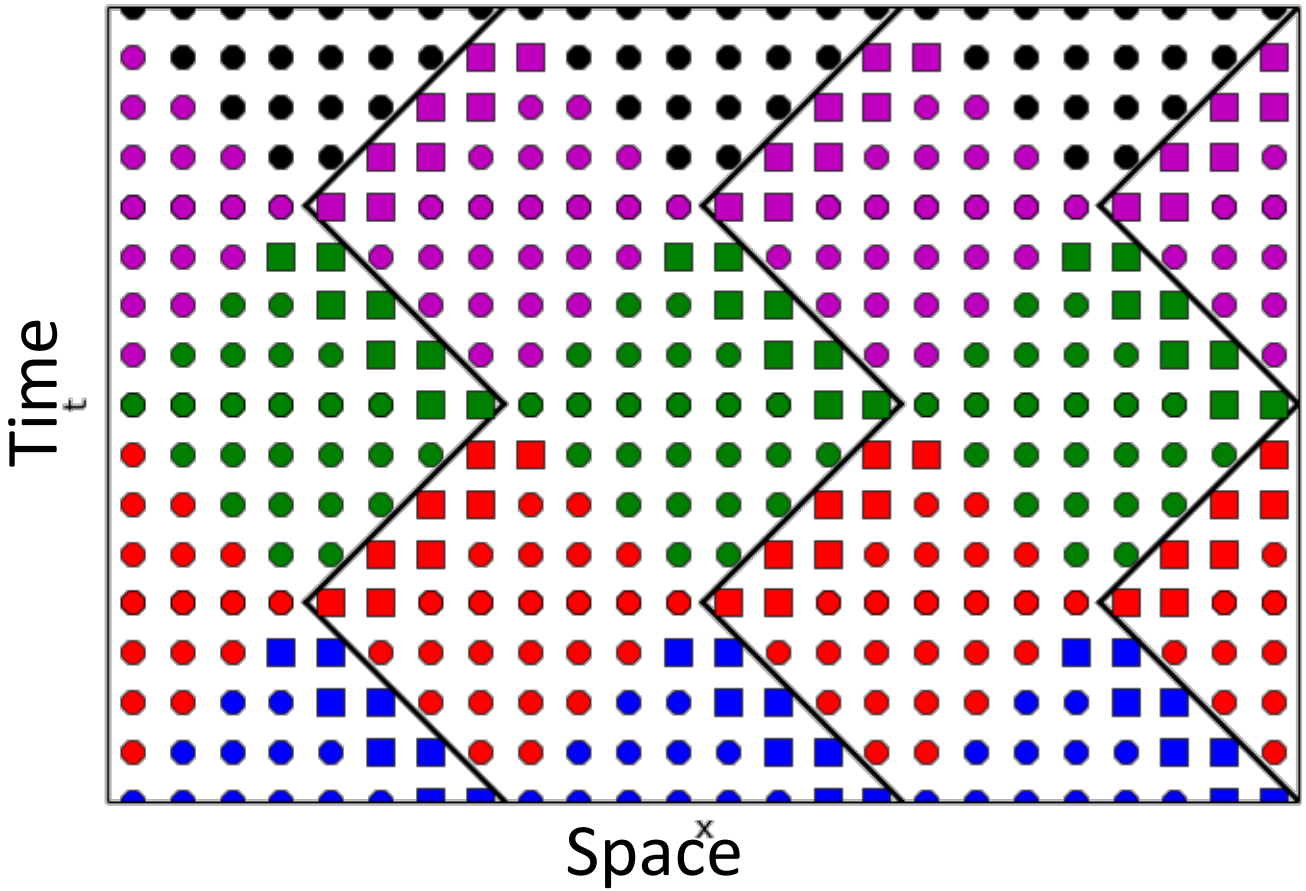
Classical “straight” domain decomposition

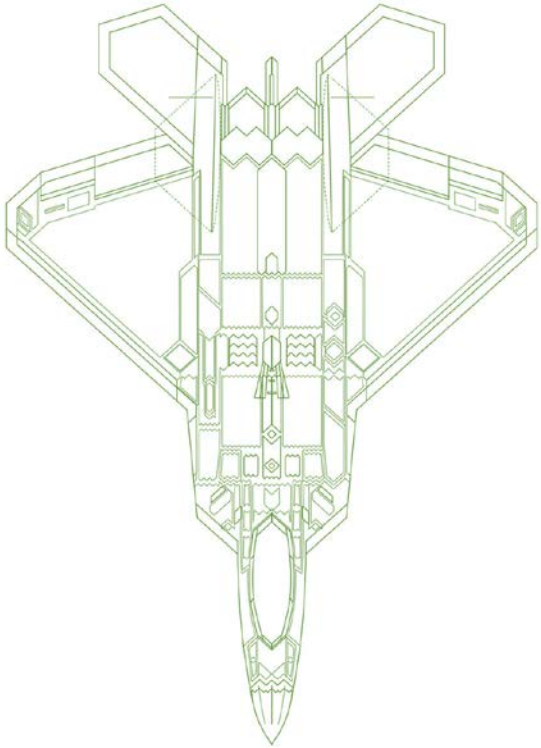




Breaking the latency barrier

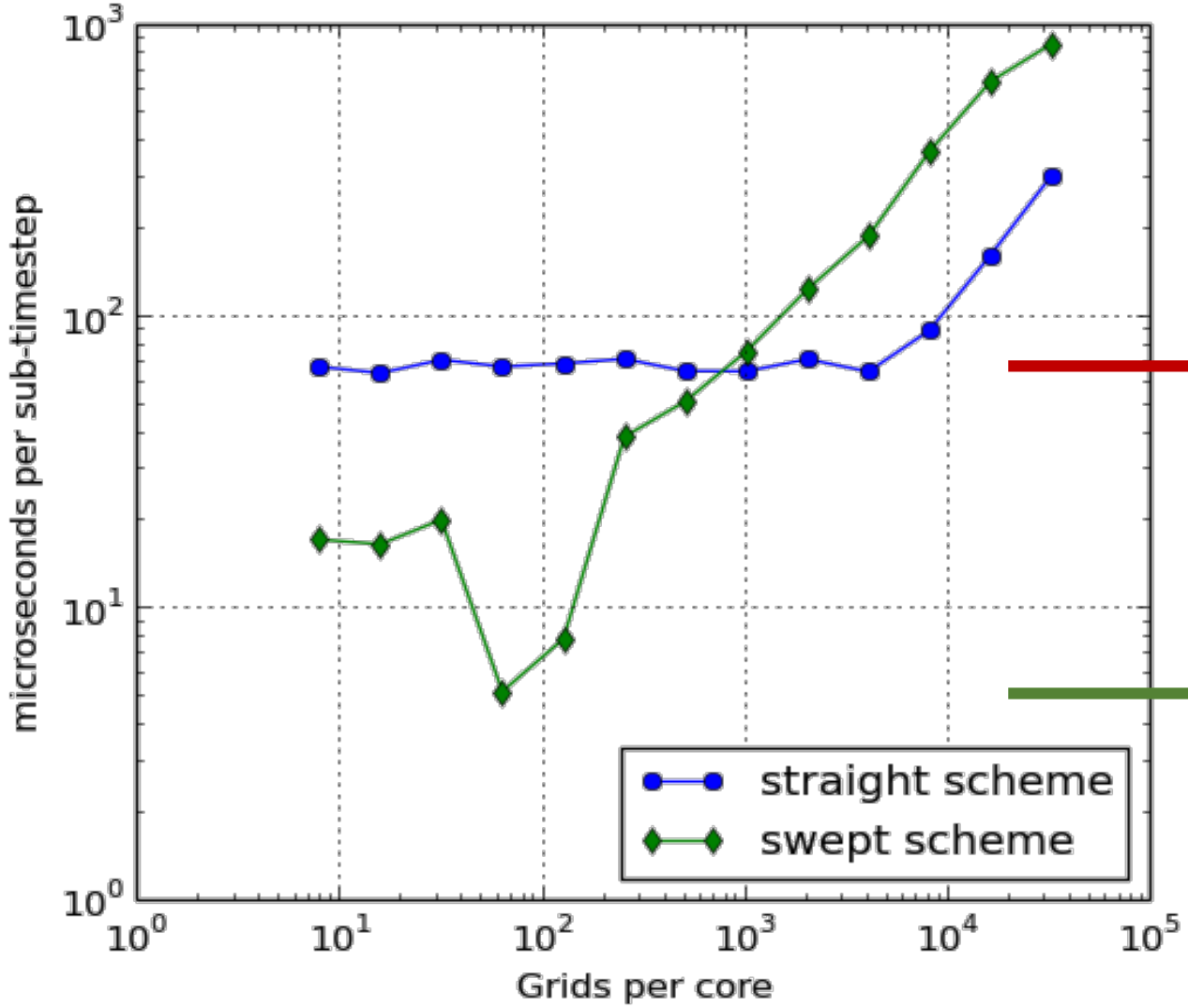
"Swept" domain decomposition





Breaking the latency barrier

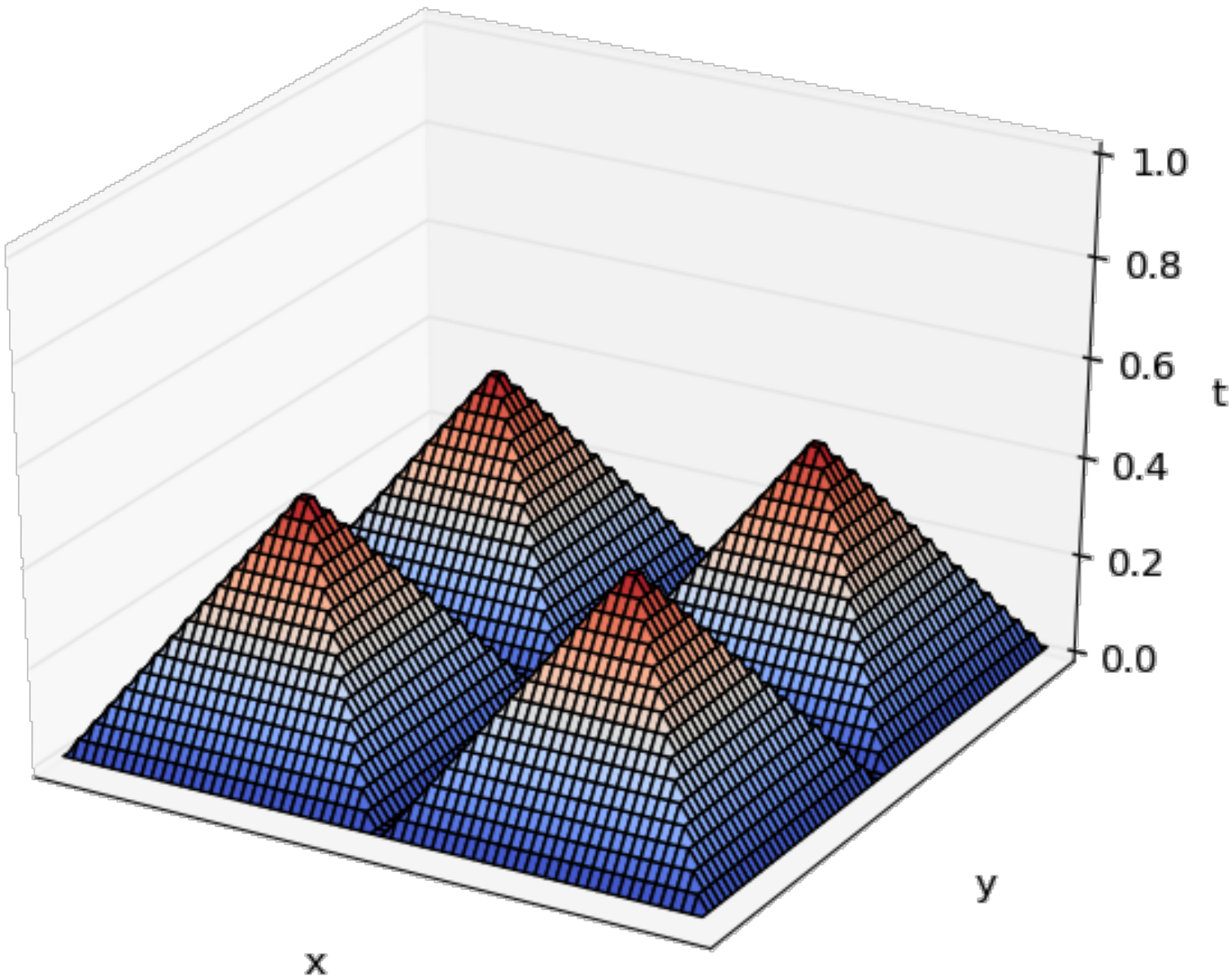
for the Kuramoto-Sivashinsky equation



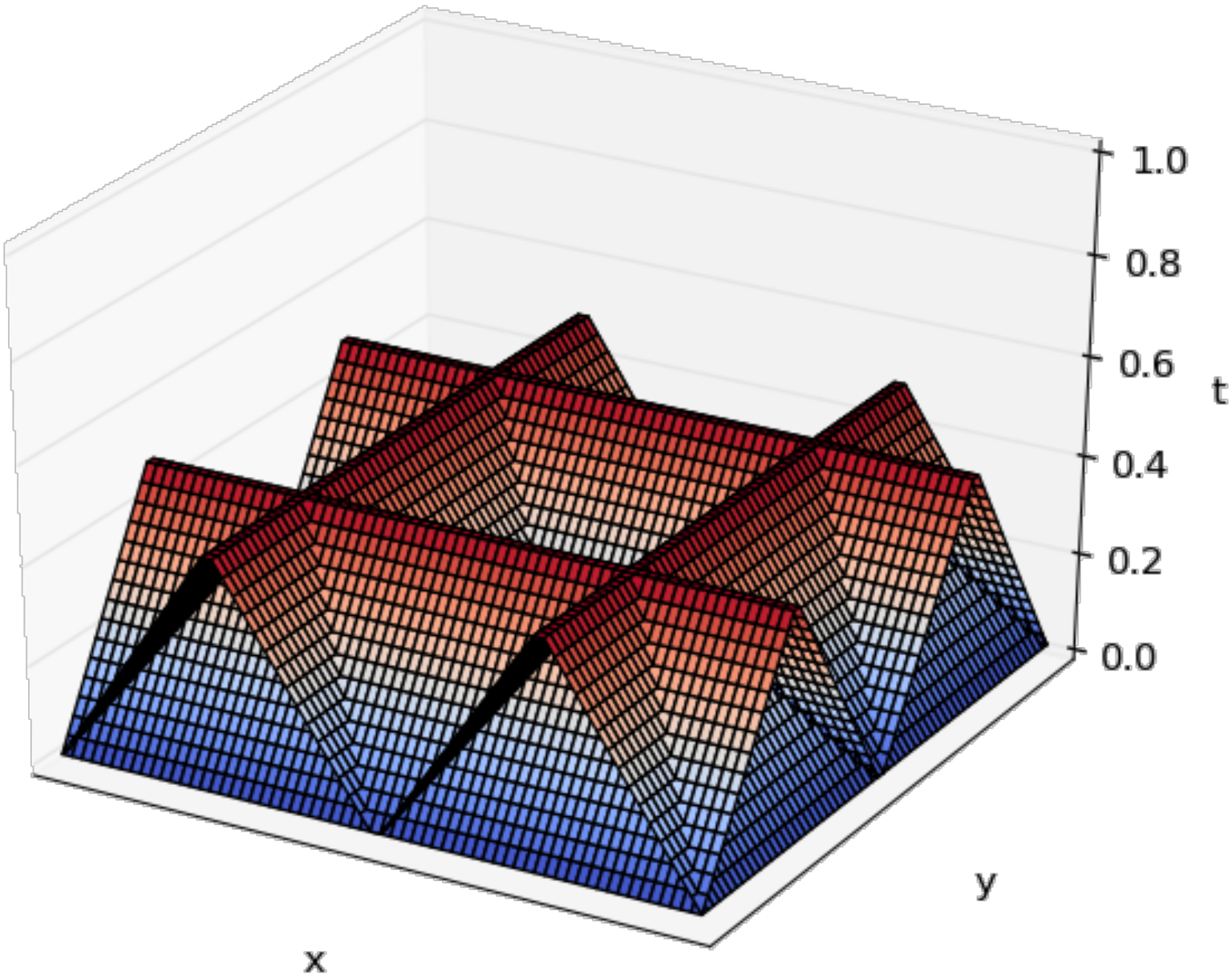
Latency barrier

broken by a factor of 10

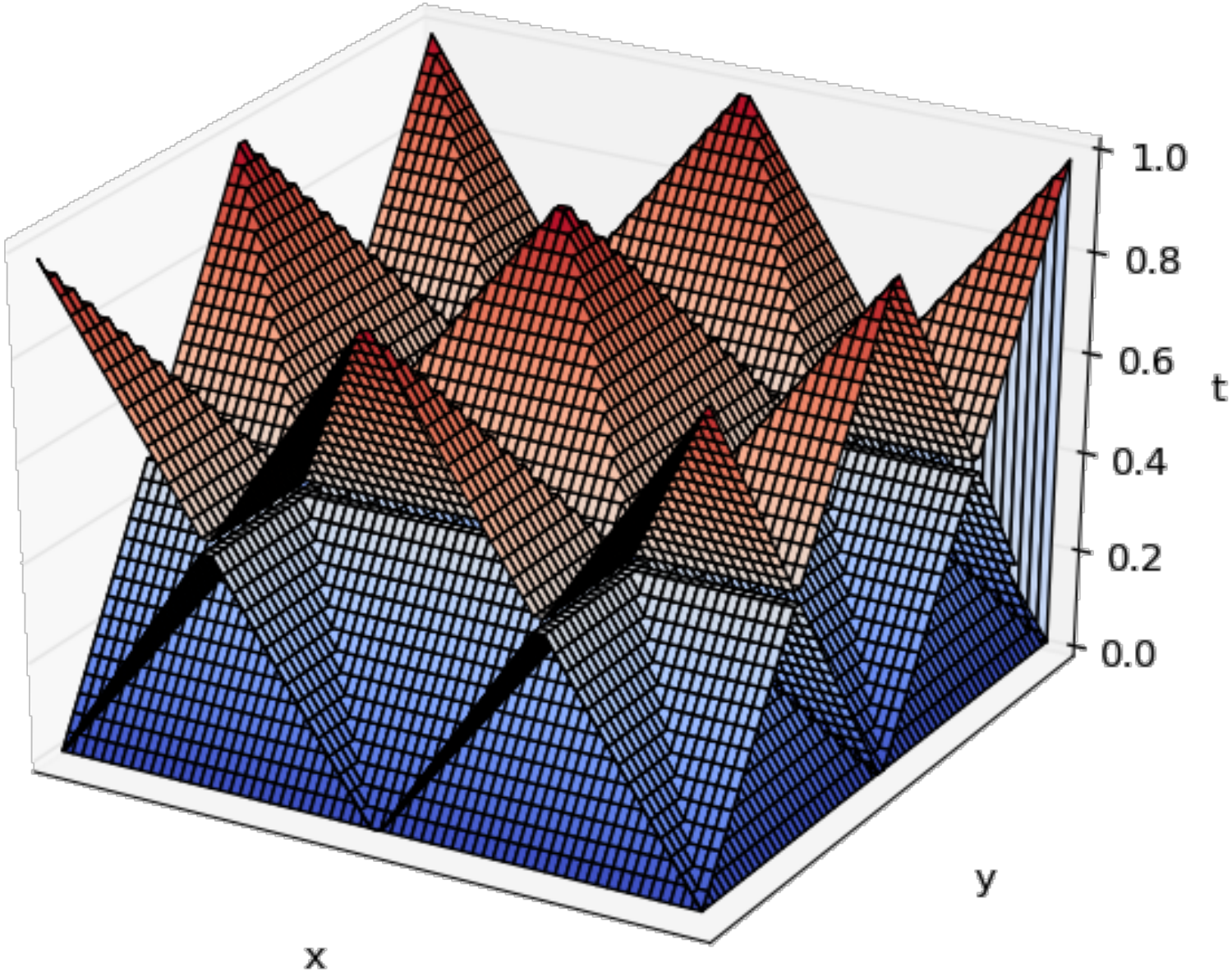
“Swept” decomposition in 2D (1)



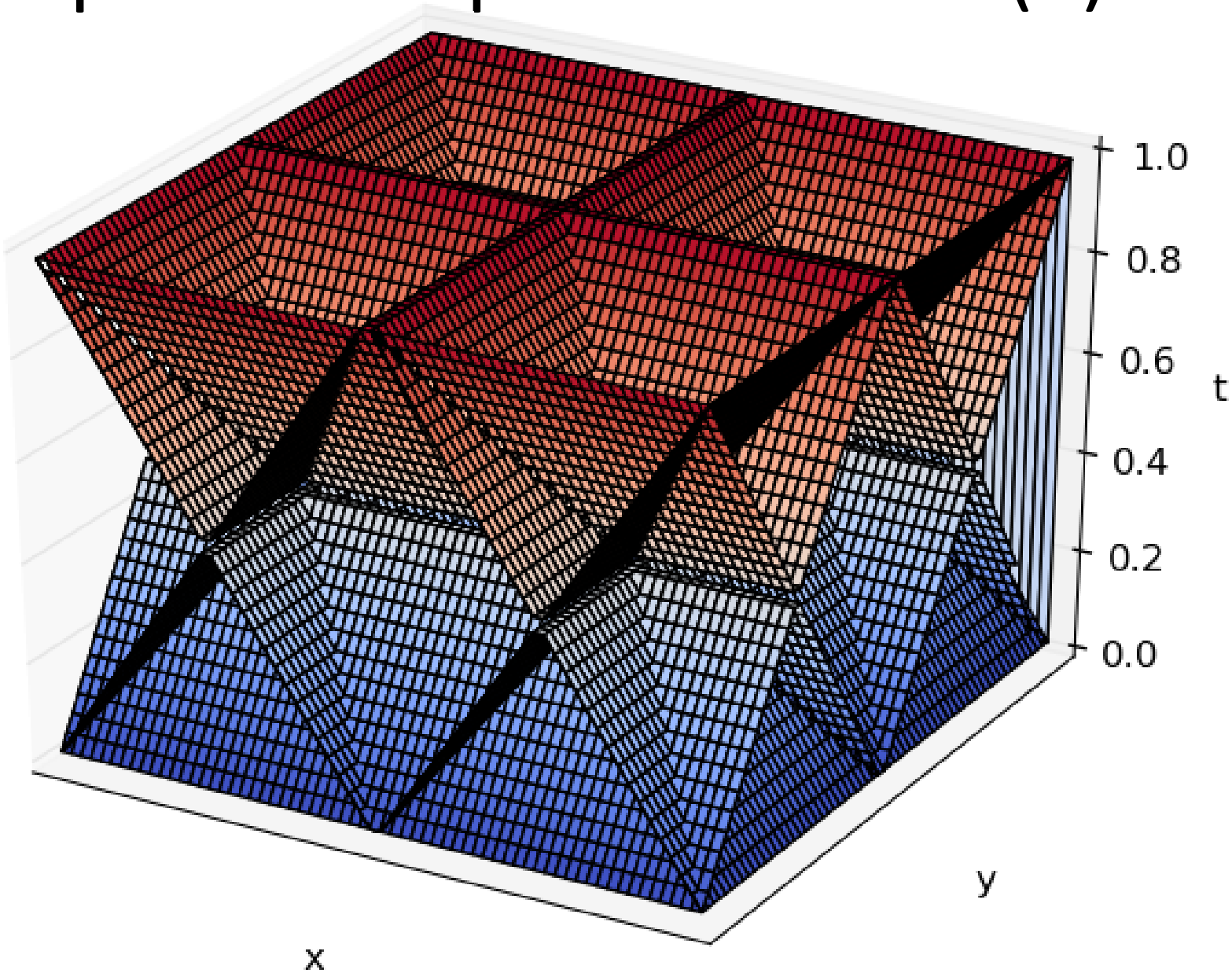
“Swept” decomposition in 2D (2)



“Swept” decomposition in 2D (3)



“Swept” decomposition in 2D (4)



Accelerating high fidelity simulation with extreme scale parallelism

First attempt broke the latency barrier by a factor of 10

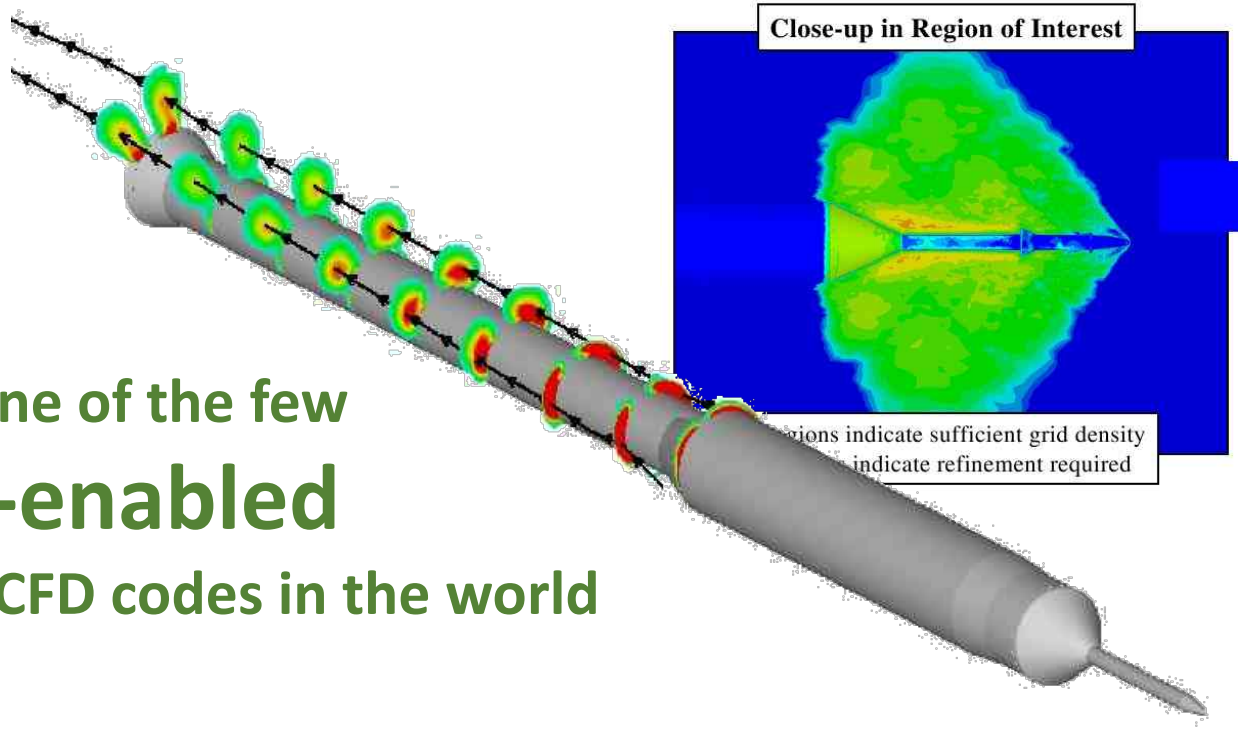
Can be improved a lot by a **talented programmer**

Can be extended to **2D and 3D**, and **unstructured** mesh

Further acceleration through **hierarchical** decomposition

Huge potential

Accelerating high fidelity **optimization** with extreme scale parallelism



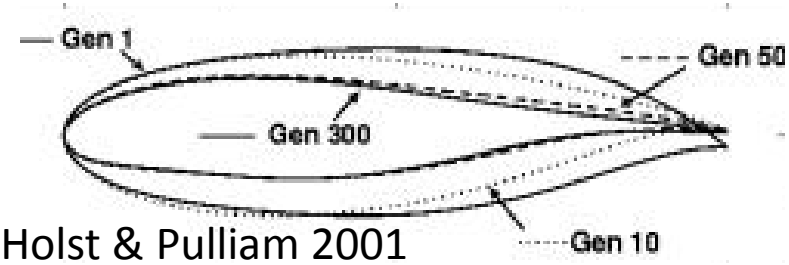
FUN3D is one of the few

adjoint-enabled

full-blown CFD codes in the world

How can extreme scale parallelism benefit **optimization?**

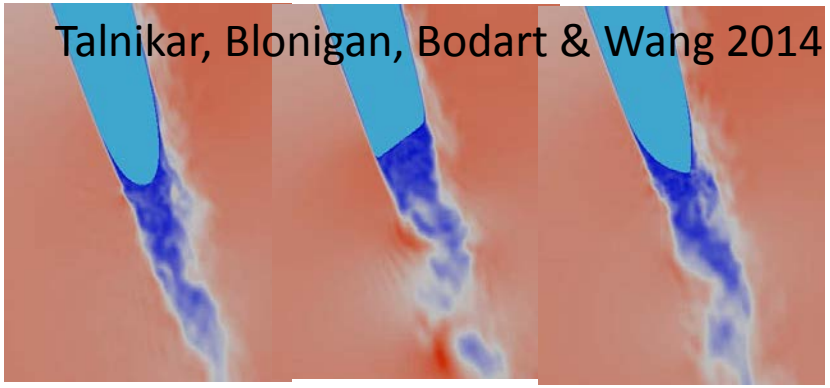
Classic optimization



Holst & Pulliam 2001

- **One** simulation at a time
- Each costs the **same**
- A good scheme minimizes the **number of simulations**

High fidelity CFD optimization



Talnikar, Blonigan, Bodart & Wang 2014

- **Concurrent** simulations
- Simulations run **indefinitely**
- A good scheme minimizes the **time-to-design**

The **design** of **experiments**.

RA **Fisher** - 1935 - psycnet.apa.org

Abstract 1. Different types of experimentation are considered with reference to their logical structure, to show that valid conclusions may be drawn from them without using the disputed theory of inductive inferences, ie, of arguing from observation to explanatory theory. This is ...

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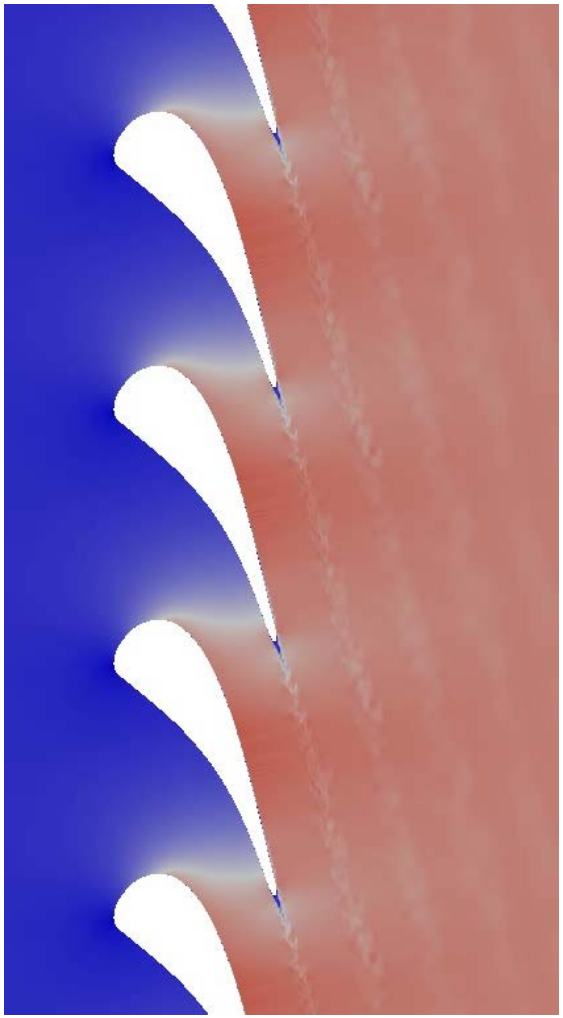
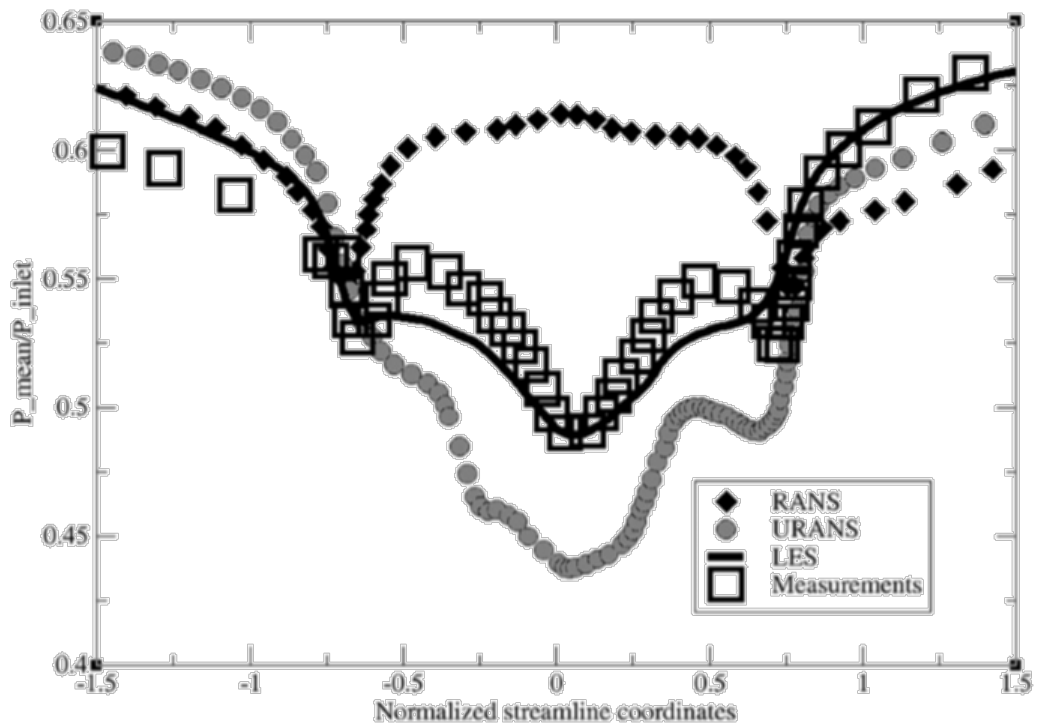
We found the **Bayesian framework** suitable for high fidelity CFD optimization

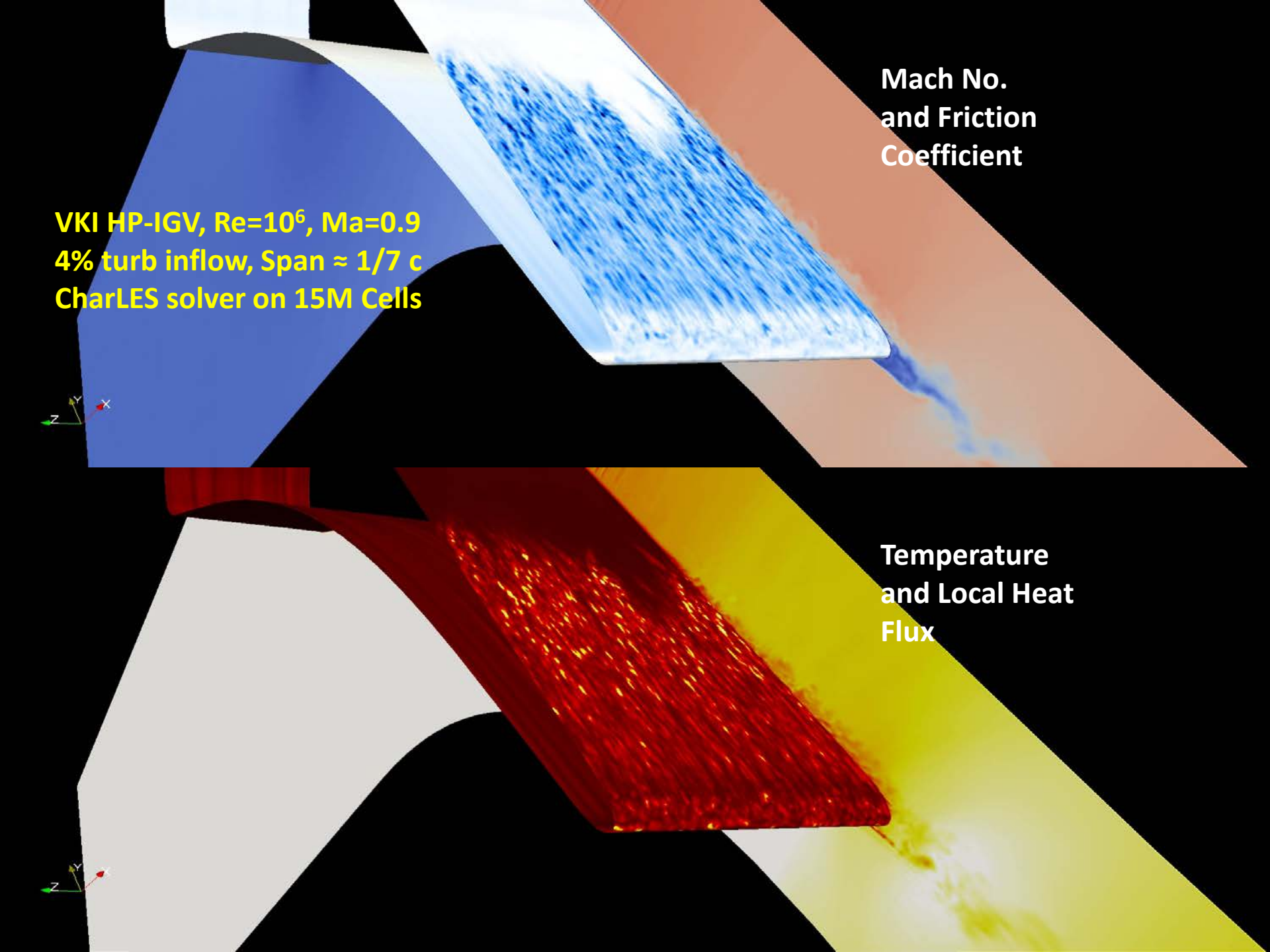


Design **rounded trailing edge** to minimize Pressure Loss and Heat Transfer.

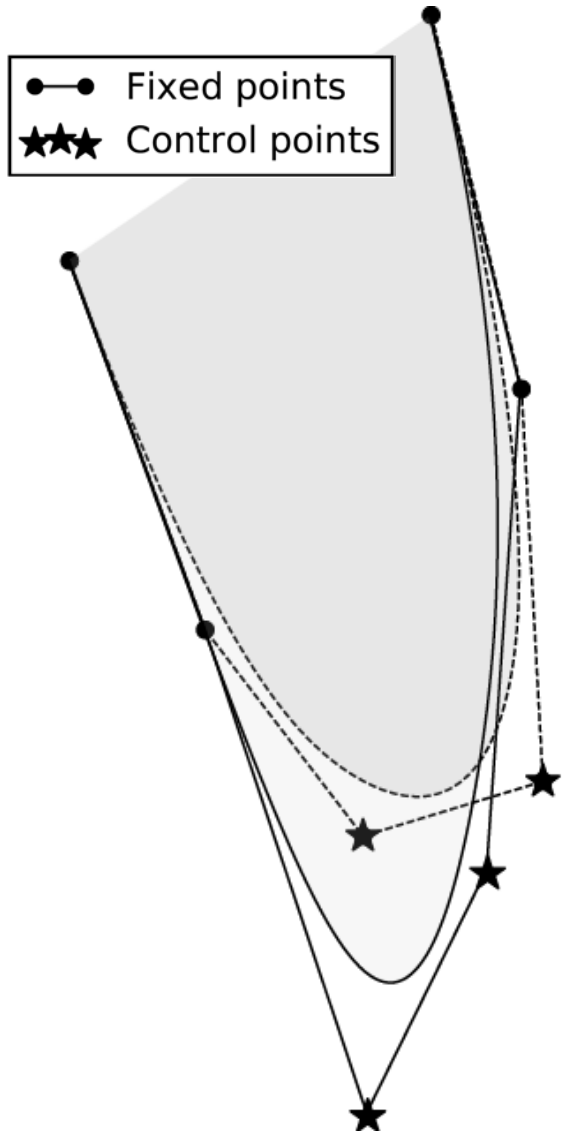
Requires high fidelity simulation



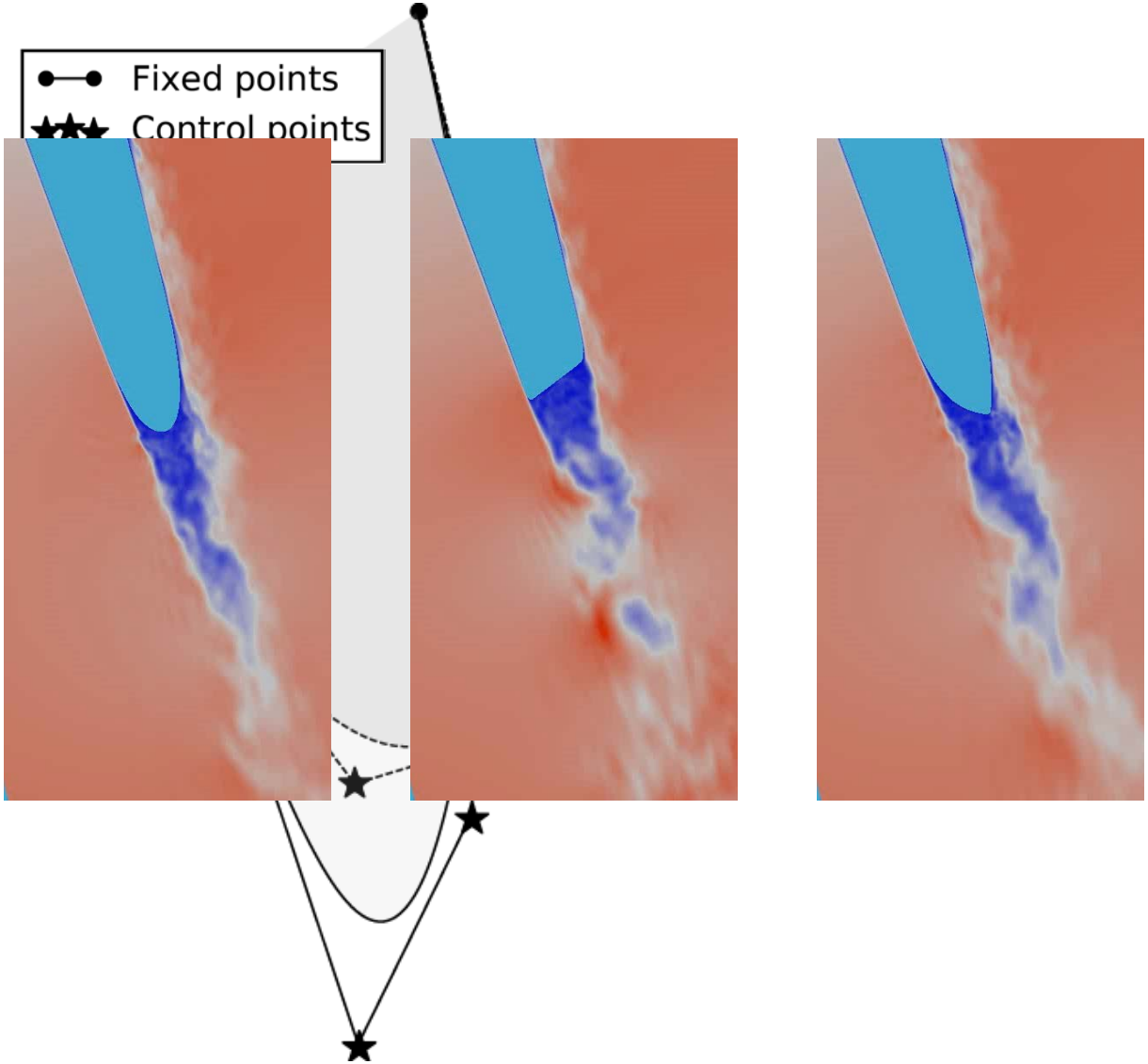
Léonard, Gicquel, Gourdain & Duchaine 2014


Mach No.
and Friction
Coefficient
VKI HP-IGV, Re=10^6, Ma=0.9
4% turb inflow, Span ≈ 1/7 c
CharLES solver on 15M Cells
Temperature
and Local Heat
Flux

Trailing Edge Parameterization

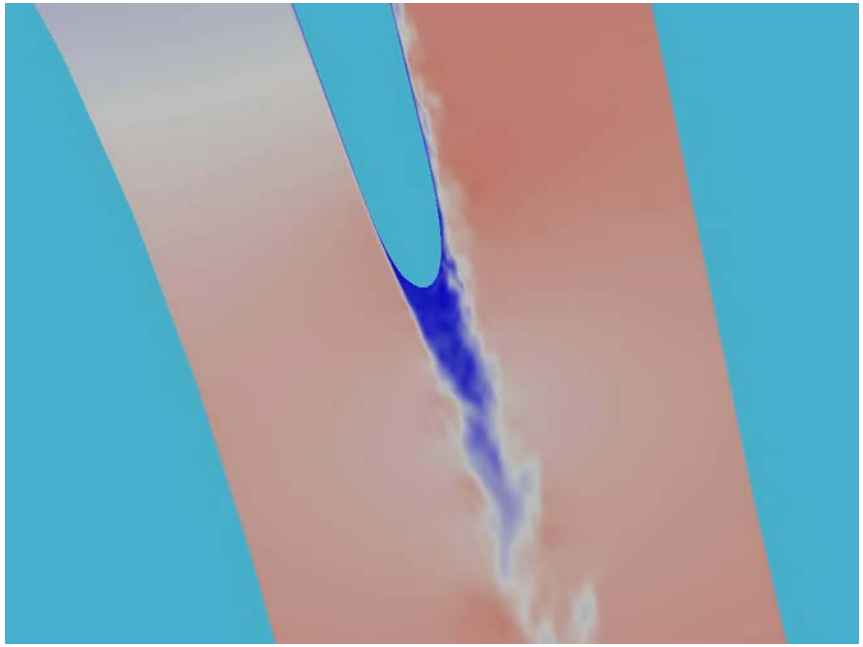


Trailing Edge Parameterization

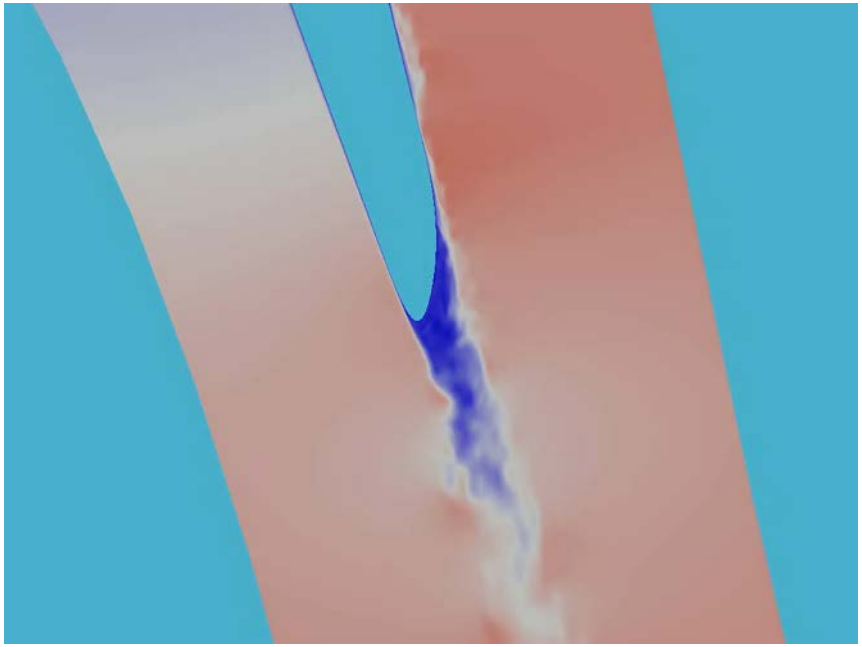


Optimization and Results

Baseline Design



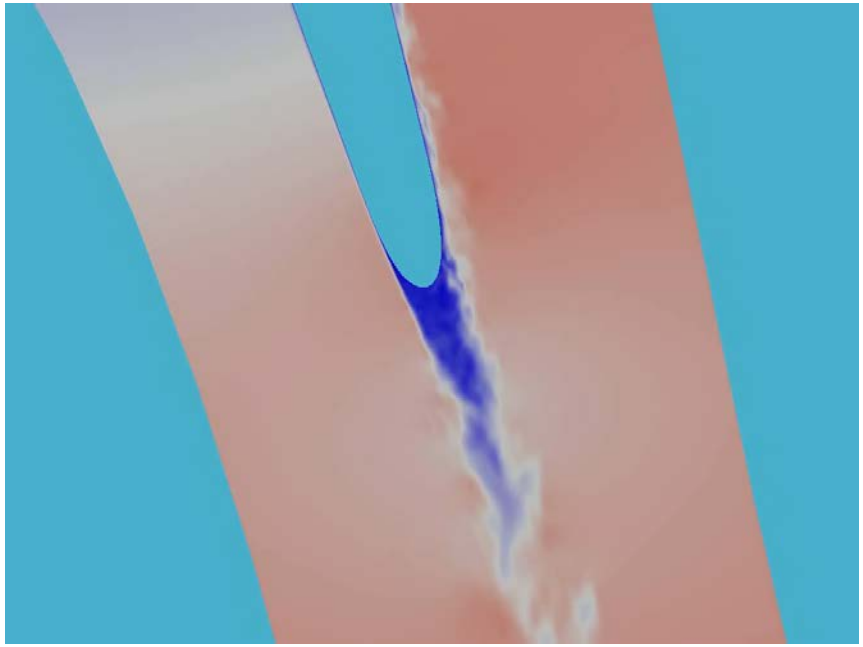
Optimized Design



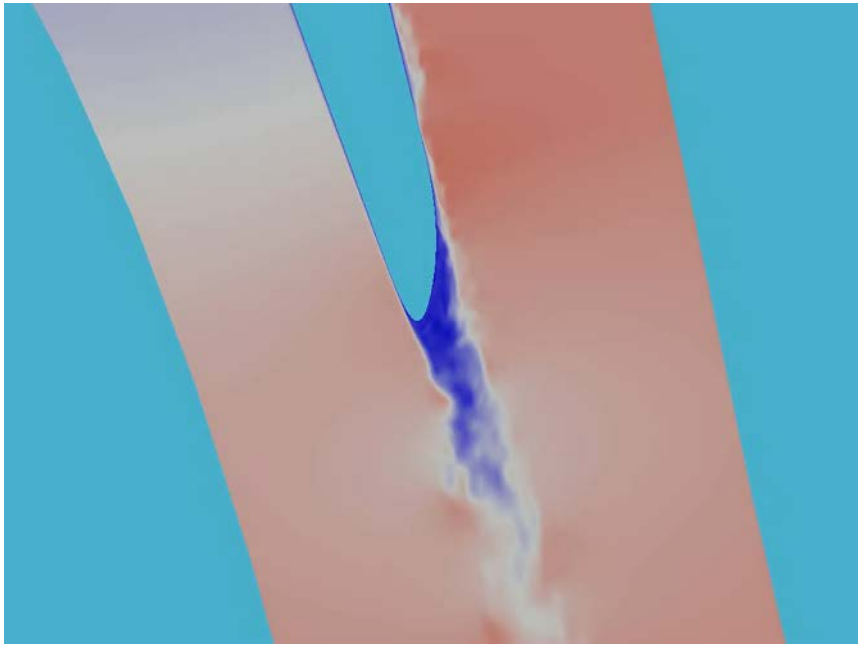
- 4 design variables, Single objective
- 4 concurrent simulations, each running for at least 12 hours, sometimes much longer.
- Optimization completed in one week.

Optimization and Results

Baseline Design



Optimized Design



- **<u>21 % reduction</u>** in pressure loss
- **<u>17 % reduction</u>** in heat transfer

Accelerating high fidelity **optimization** with extreme scale parallelism

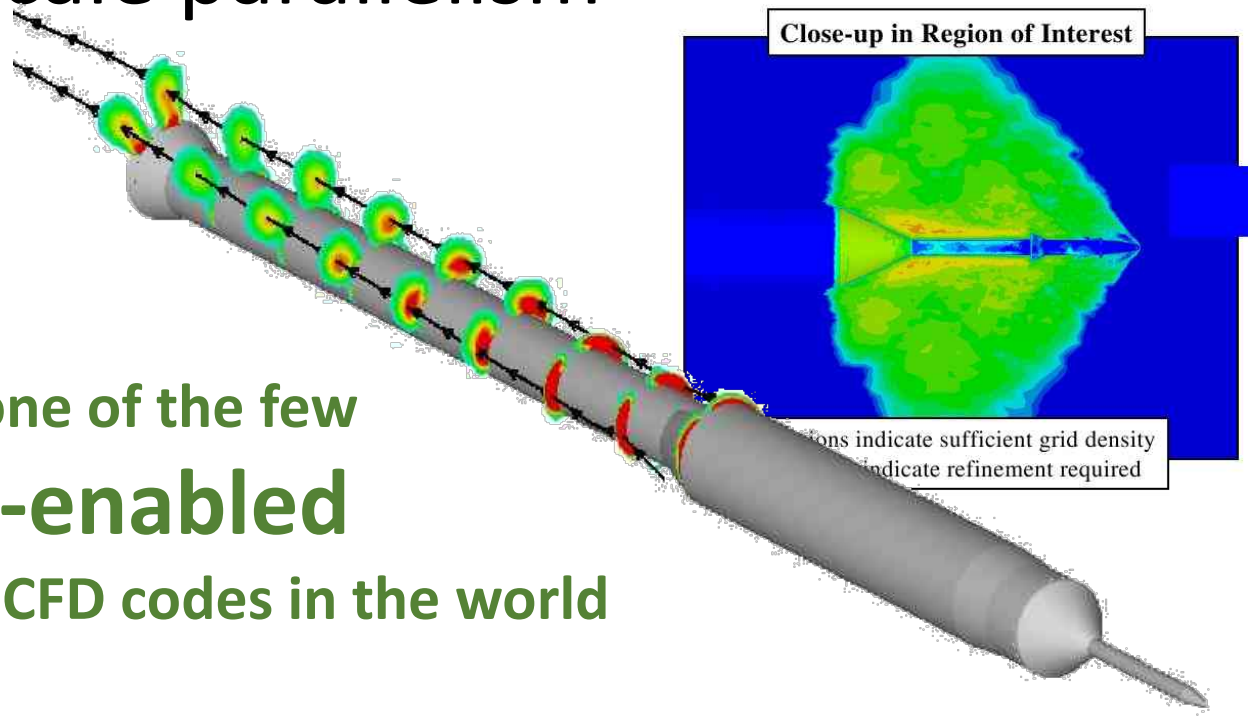
Talnikar and Blonigan did it in their **spare time**

Can **benefit a lot from better algorithm** deciding when to pause and resume simulations

Tested only on 4 design variables. Extension to more design variables likely need the **adjoint**

The algorithm is still **primitive**; further improvements can multiply its **benefit** to application engineers.

Accelerating high fidelity optimization with **many design parameters** with extreme scale parallelism



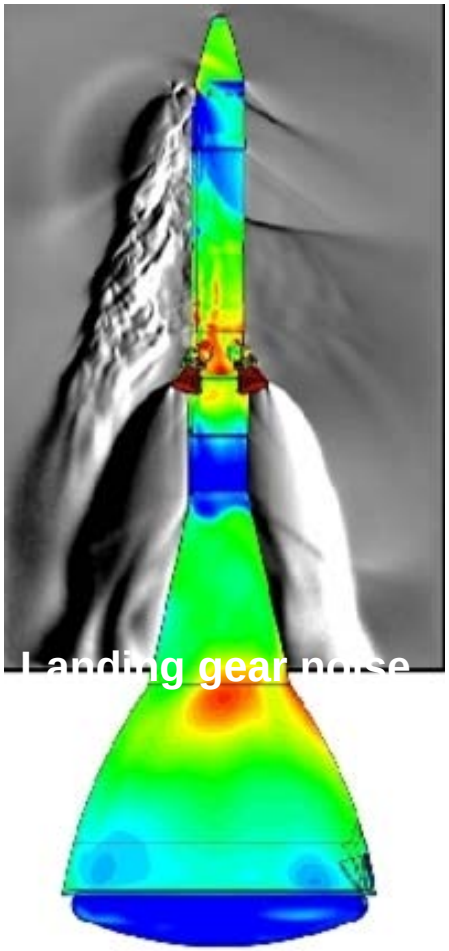
FUN3D is one of the few

adjoint-enabled

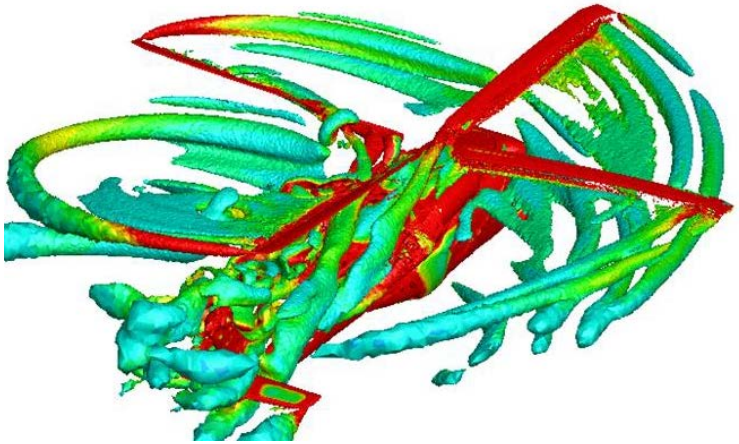
full-blown CFD codes in the world

Adjoint alleviates the “curse of dimensionality”, thus is often essential in optimization with many (>10) design parameters.

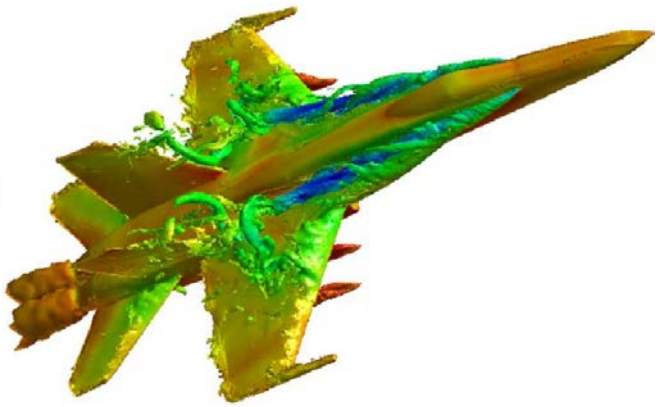
Many high fidelity simulations in important aerospace applications are unsteady and chaotic



Launch abort system (NASA)



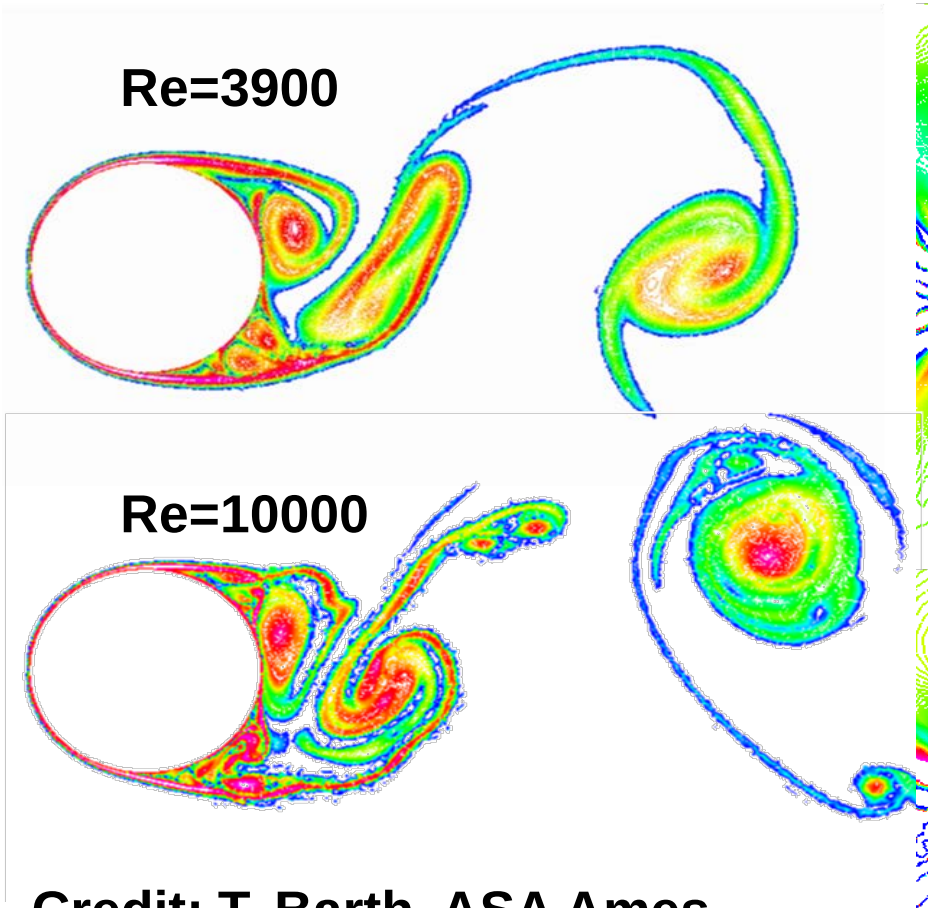
Rotorcraft (NASA)

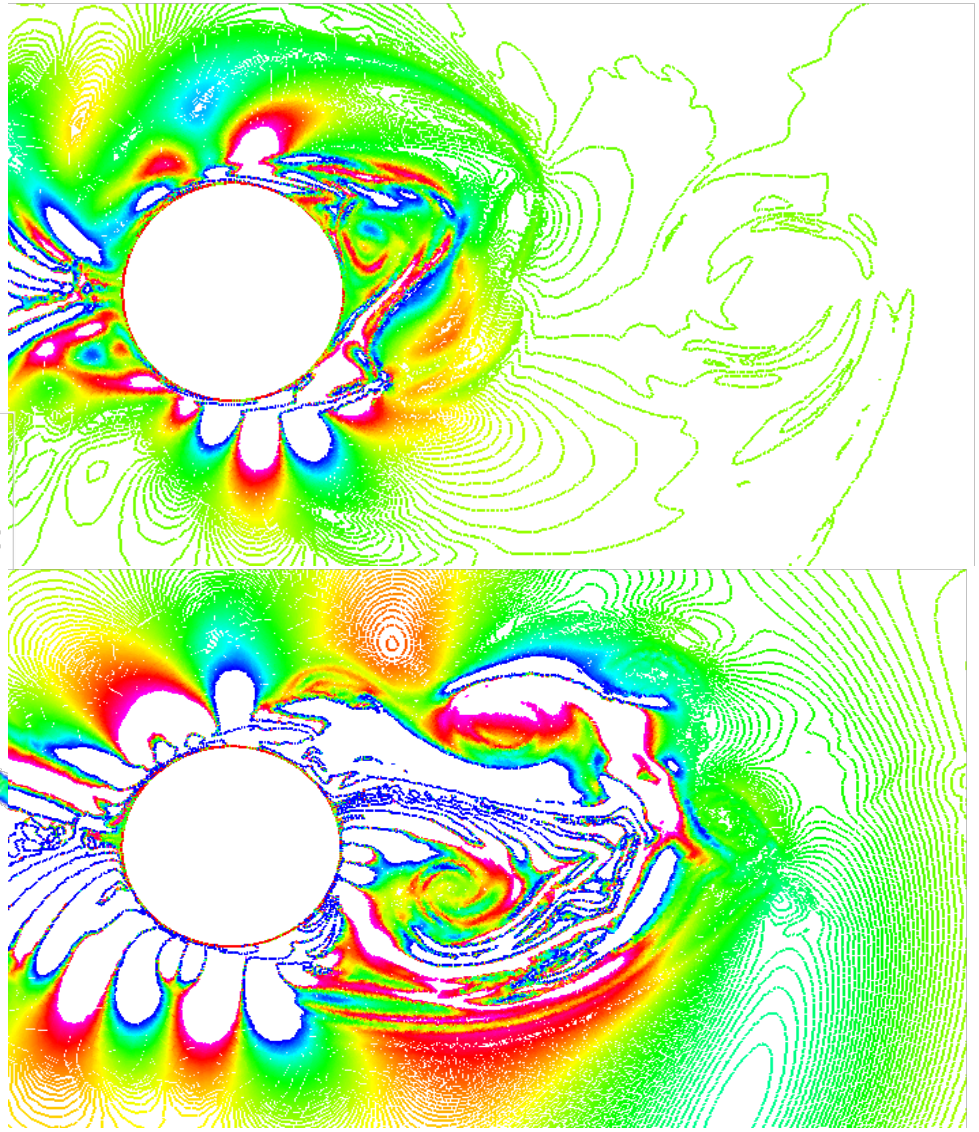


Maneuvering vehicle (Airforce)

High fidelity optimization with many design parameters requires **adjoining chaos.**

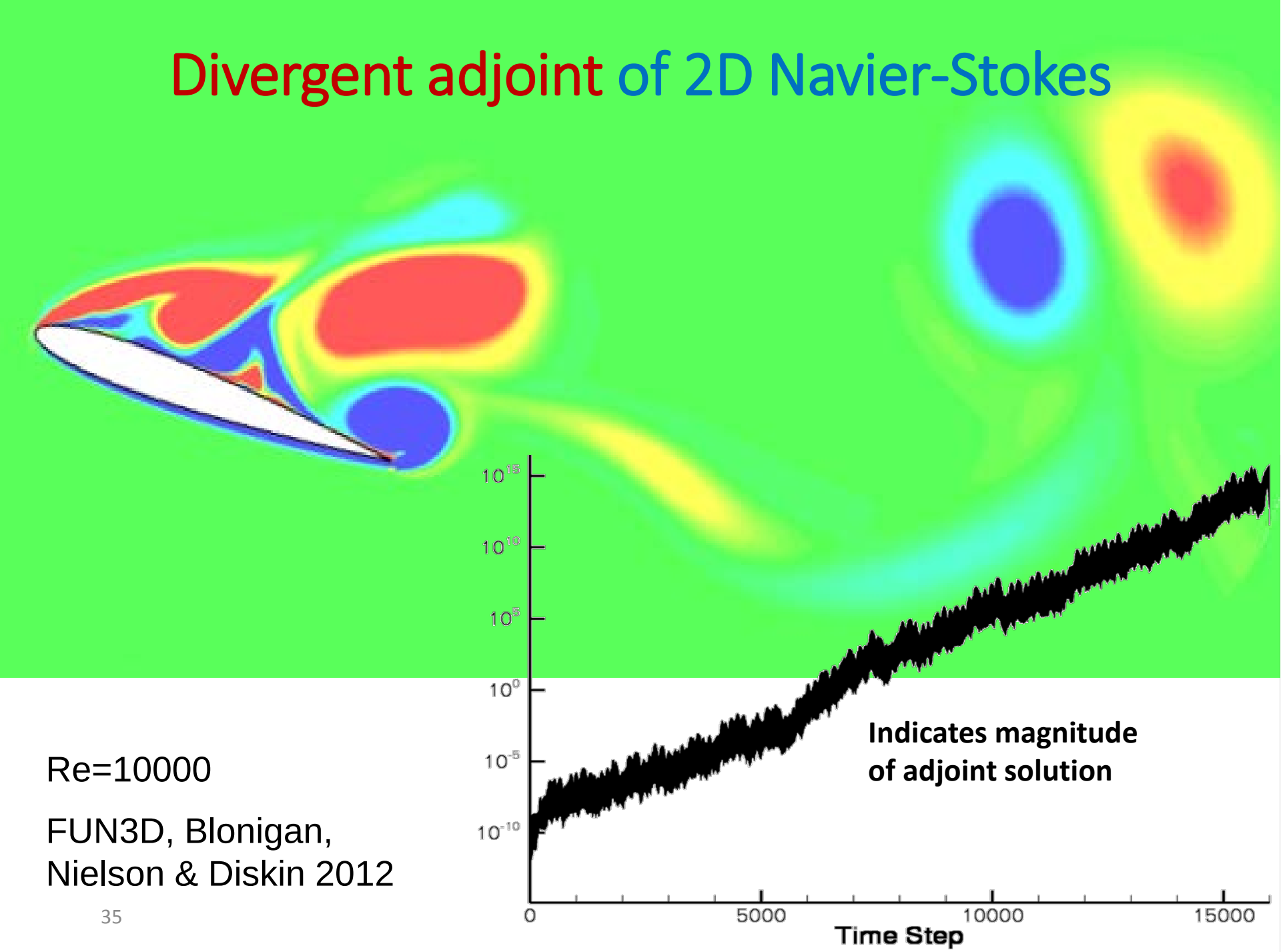
Divergent adjoint of 2D Navier-Stokes





Credit: T. Barth, ASA Ames.

Divergent adjoint of 2D Navier-Stokes



Re=10000

FUN3D, Blonigan, Nielson & Diskin 2012

For a "uniformly hyperbolic" dynamical systems

$$\frac{du}{dt} = f(u, s)$$

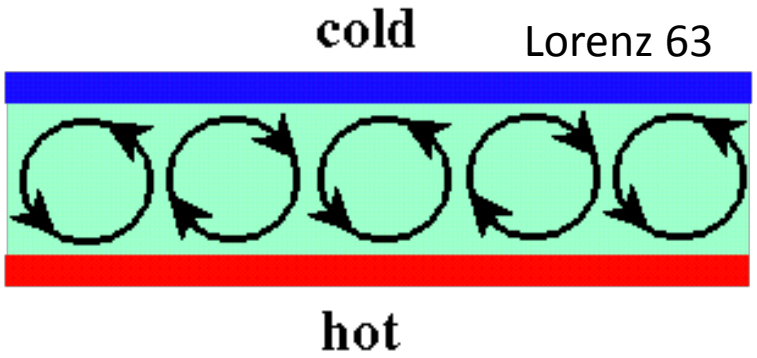
and its ergodic time average

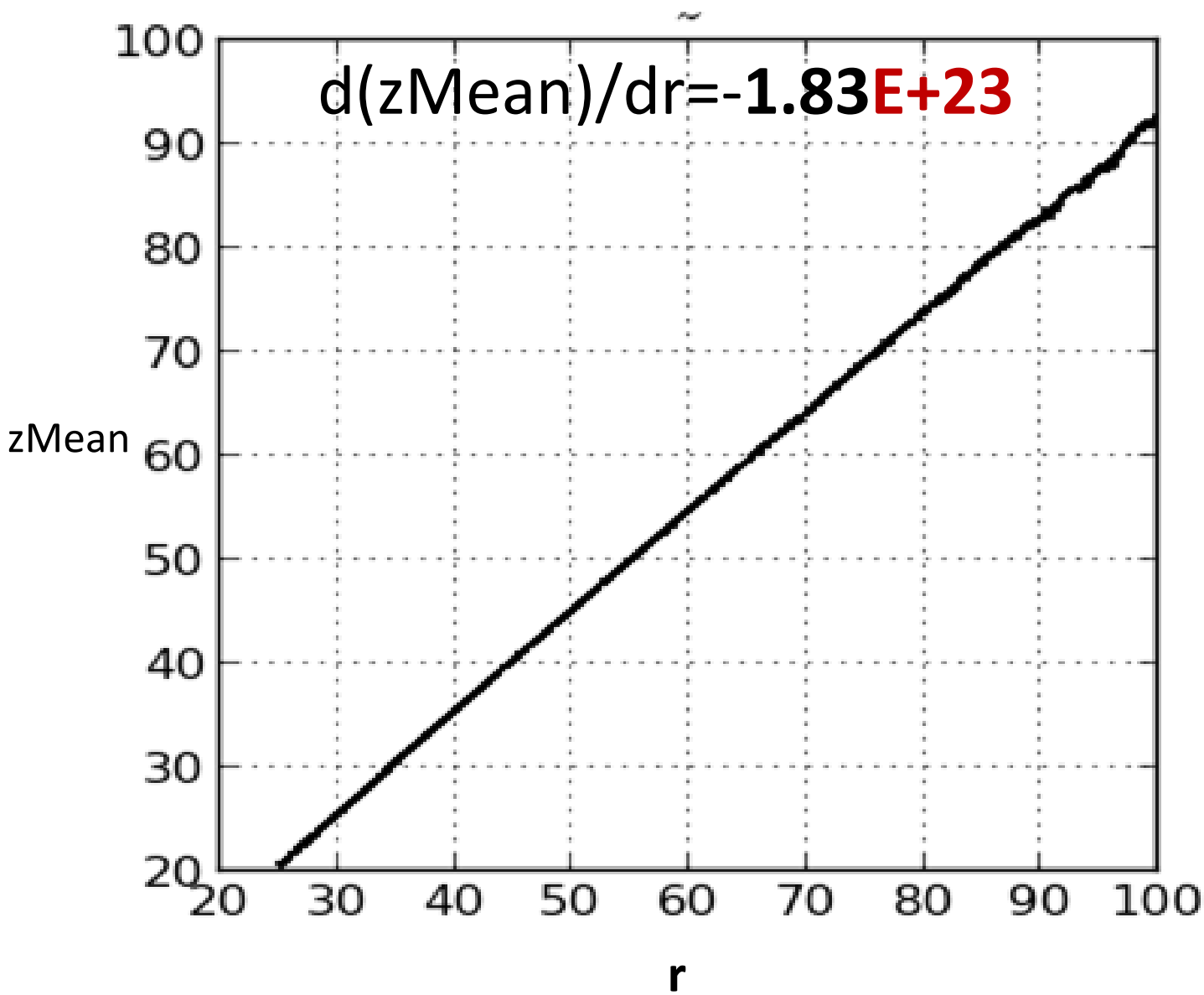
$$\langle J \rangle := \lim_{T \to \infty} \left(\frac{1}{T} \int_0^T J(u) dt \right)$$

$$\frac{d\langle J \rangle}{ds}$$ **exists, but**

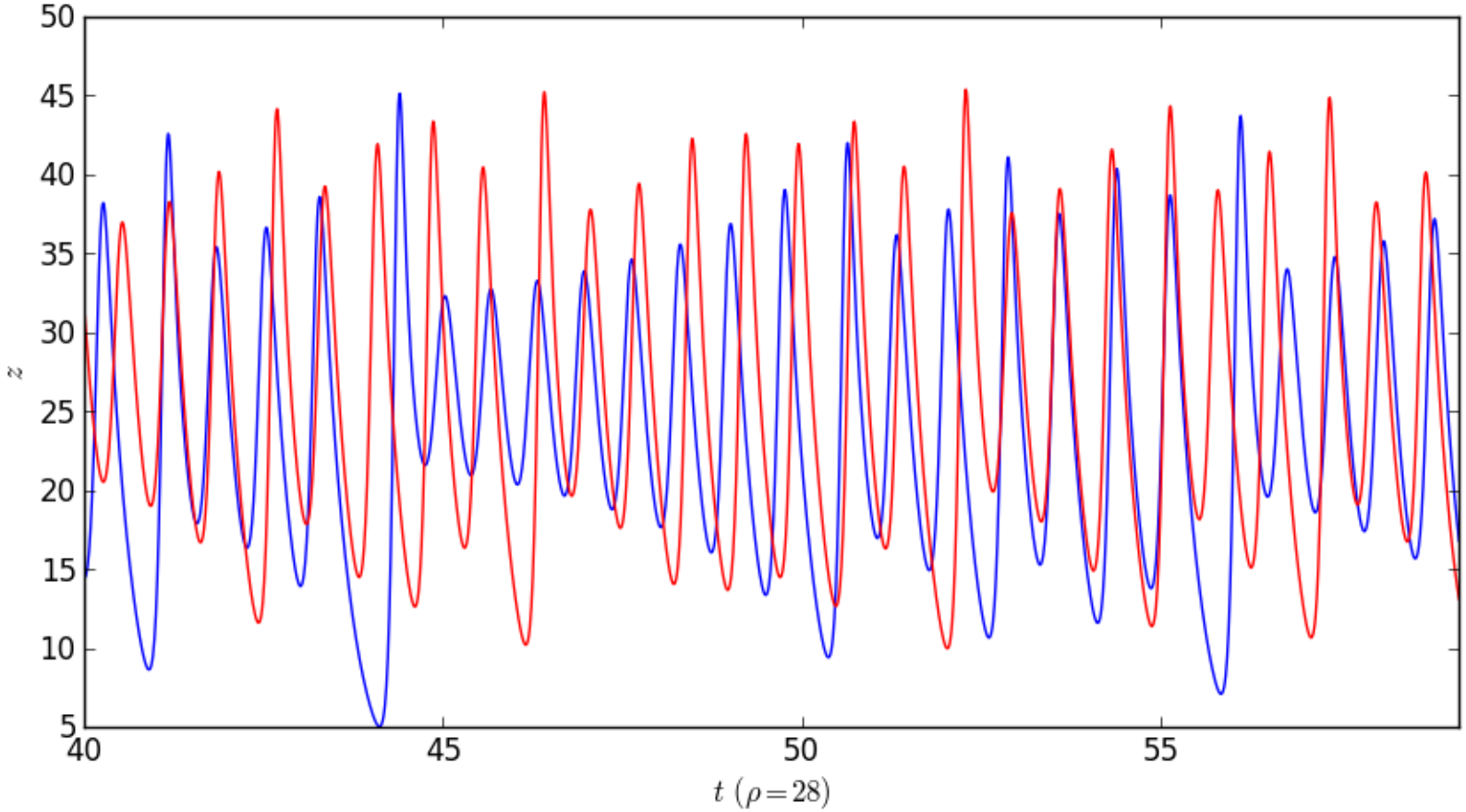
$$\frac{d\langle J \rangle}{ds} \neq \lim_{T \to \infty} \frac{d}{ds} \left(\frac{1}{T} \int_0^T J(u) dt \right)$$

```
double lorenz(r)
{
    double b = 8./3., s = 10.;
    double T = 100., dt = 0.01;
    double x = 1., y = 1., z = 1., zMean = 0.;
    for (double t = 0; t < T; t += dt) {
        double dx = s * (y - x);
        double dy = x * (r - z) - y;
        double dz = x * y - b * z;
        x += dt * dx;
        y += dt * dy;
        z += dt * dz;
        zMean += dt * z / T;
    }
    return zMean;
}
```



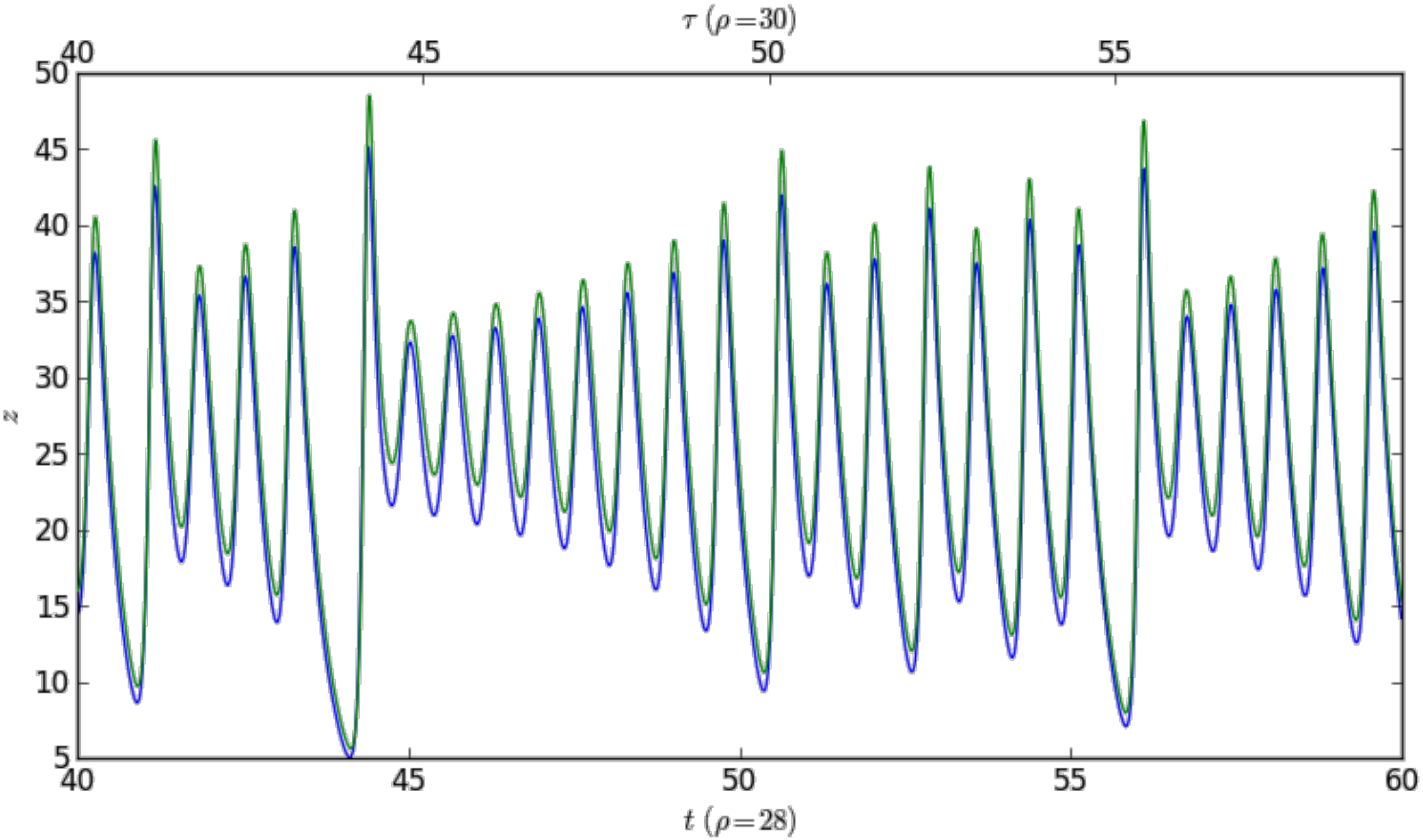

d(zMean)/dr=-1.83E+23
zMean
r
100
90
80
70
60
50
40
30
20
20
30
40
50
60
70
80
90
100

Trajectories with similar parameters



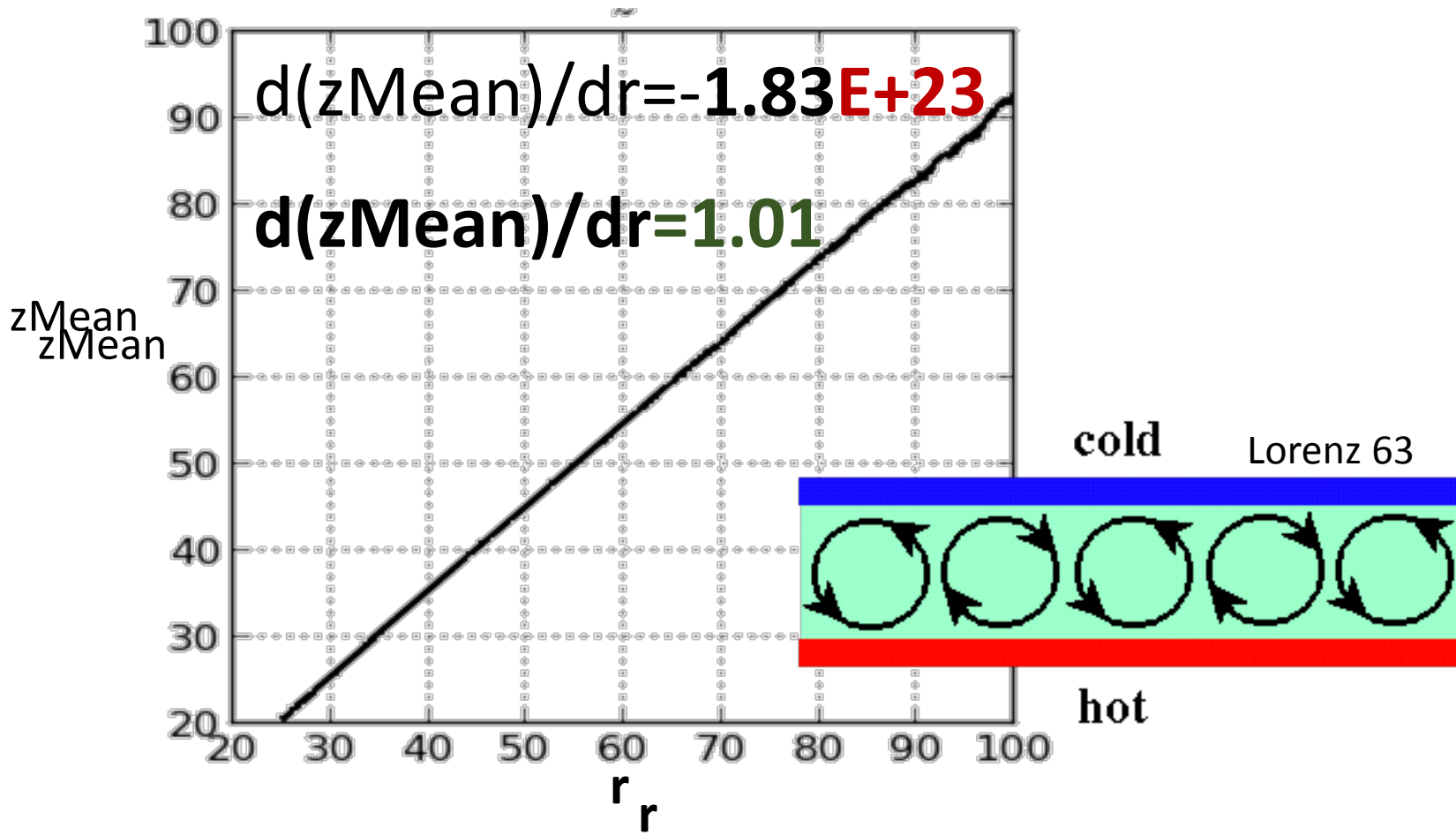
- **u(t) (ρ=30) and u_r(t) (ρ=28) are very different after some time!**

Trajectories with similar parameters



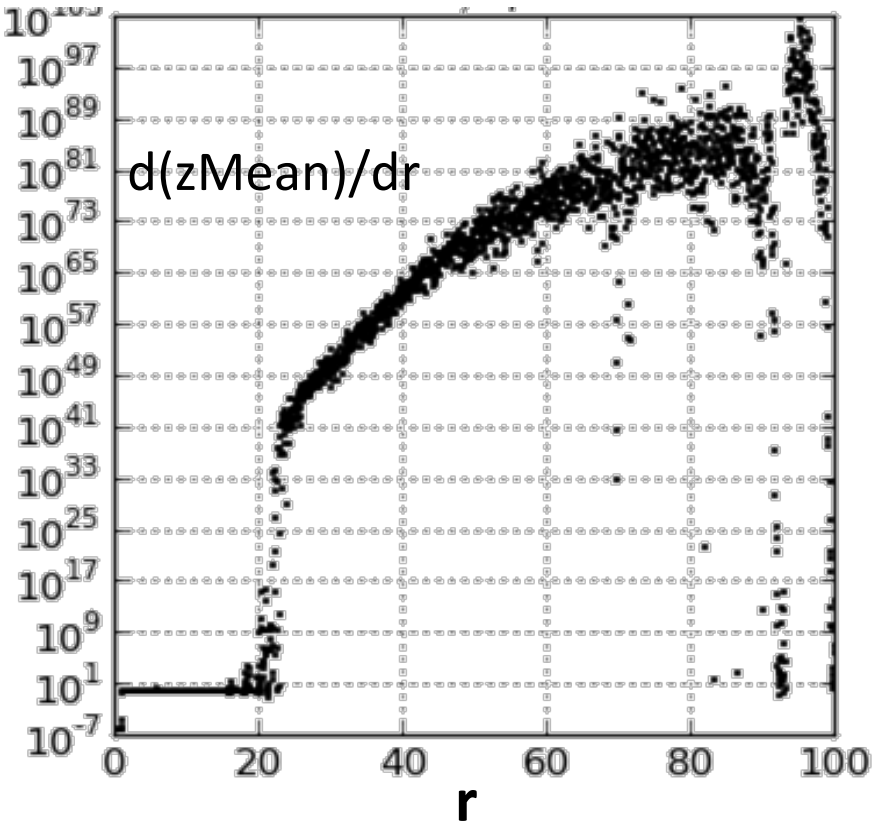
- **u(τ) (ρ=30) shadows u_r(t) (ρ=28)!**

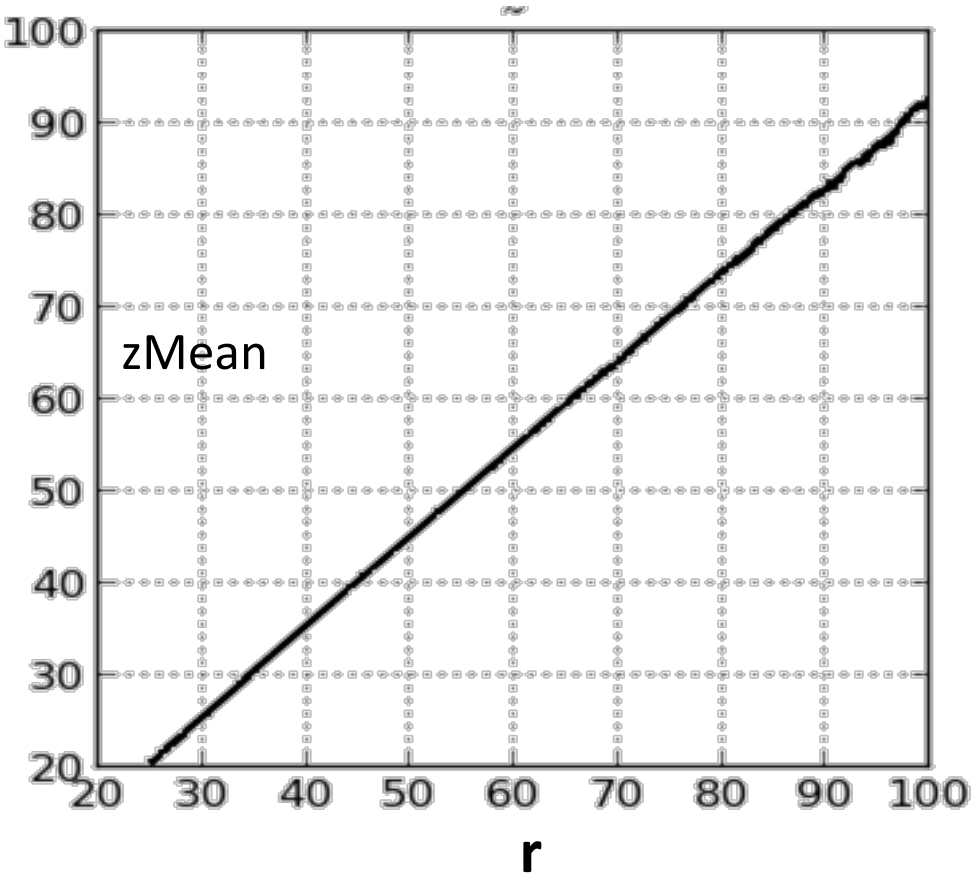
“Least Squares Shadowing” Works



before **after**

“Least Squares Shadowing” Works

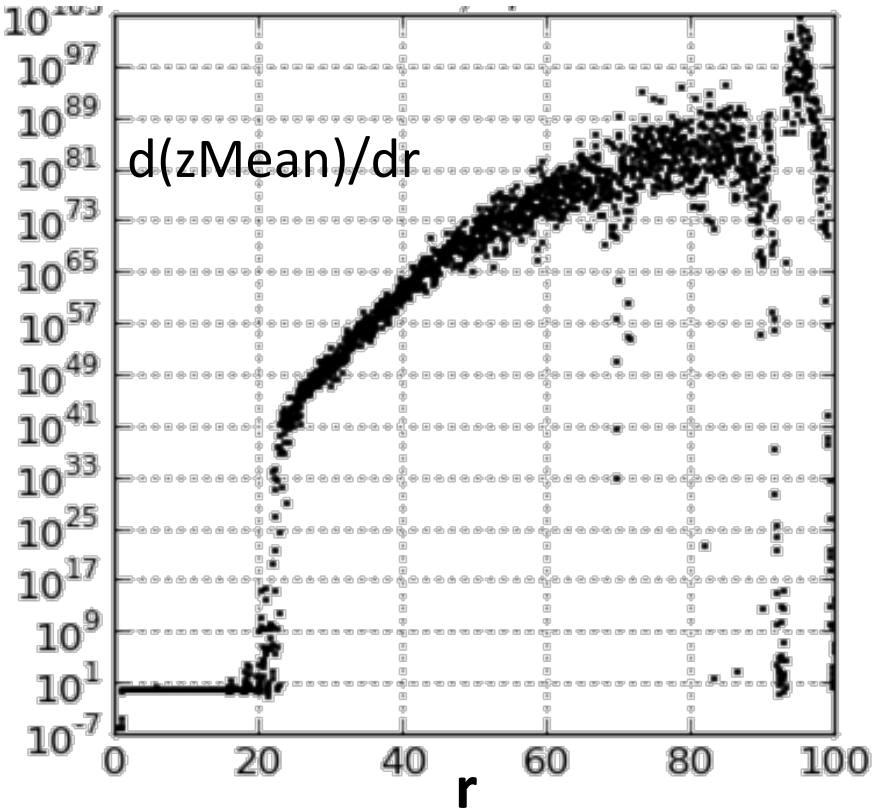


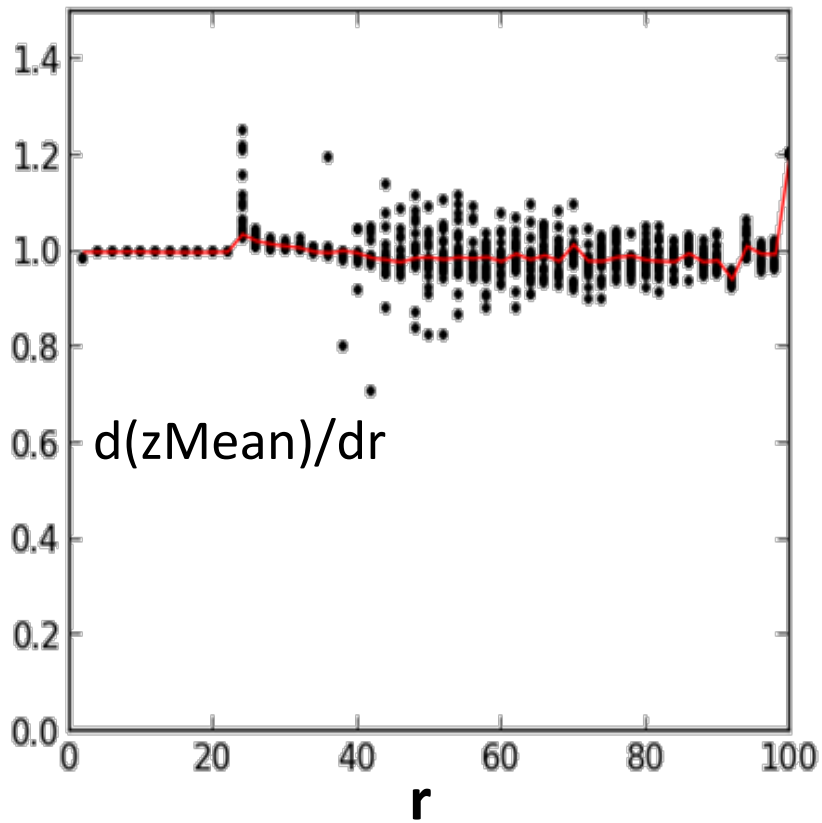


Computed derivative from Initial value problem

before

“Least Squares Shadowing” Works





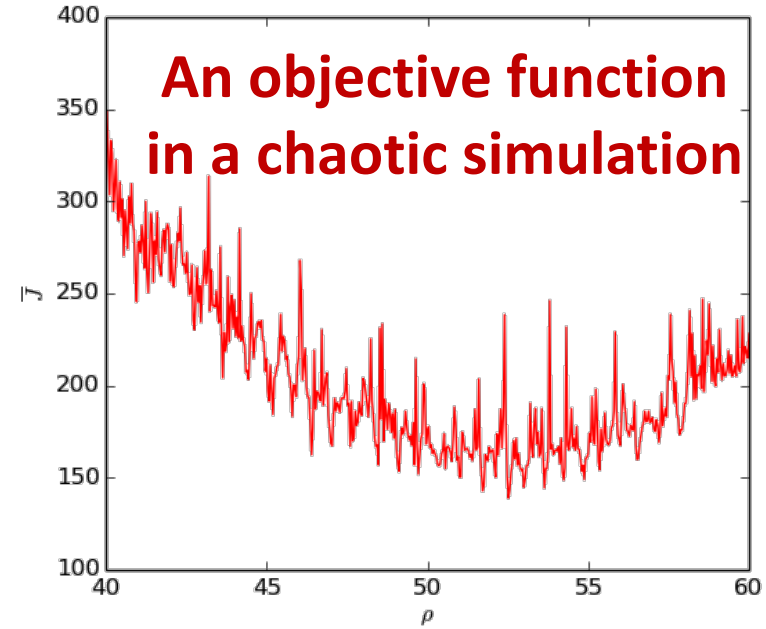
Computed derivative from Initial value problem

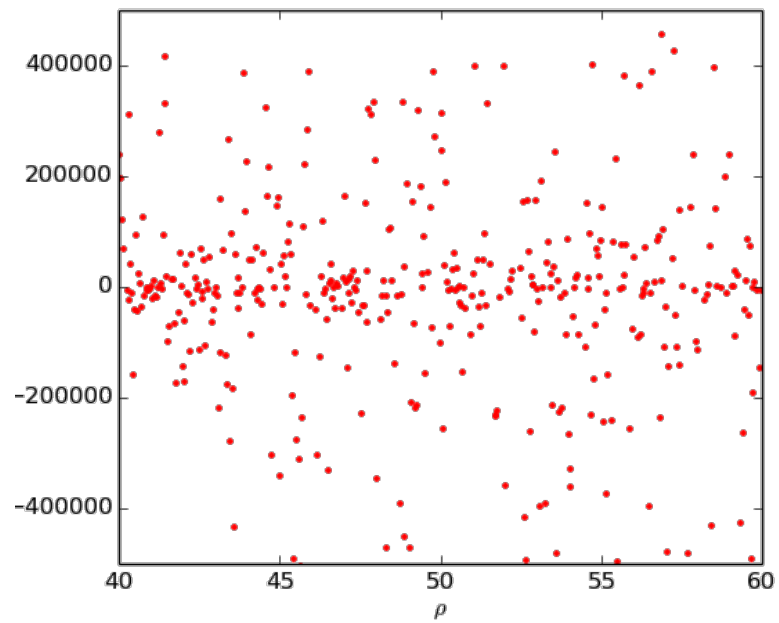
before

Computed derivative from Least squares problem

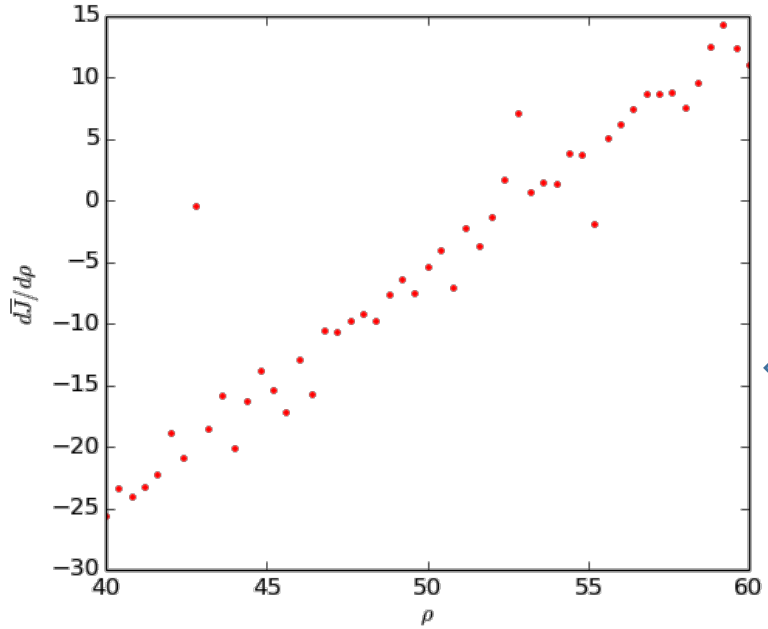
after

“Least Squares Shadowing” Works





Before



After

Accelerating high fidelity optimization with **many design parameters** with extreme scale parallelism

Much of this work is done by **Patrick Blonigan**

Extending to full CFD applications with

Boris Diskin and Eric Nielson

Combined with faster simulations and parallel optimization, we aim to accelerate high fidelity optimization with many design variables to **minutes**.

Towards aerospace design in the age of extreme-scale supercomputing

We can break the “latency barrier”. Performing **high fidelity CFD in minutes, even seconds, is not a dream**. Let’s do it.

Optimization can concurrently run many simulations. Let’s improve the method so that it **finds optimal designs in just a few batches** of high fidelity simulation.

Adjoint works on chaotic simulations. Let’s devise an efficiently implementation, so that **optimization with many design variables will be as fast** as that with a few design variables

Let’s do these, so that high fidelity optimization can **be the next slide rule** for every aerospace engineer.