Digital Math: constructive scientific framework unlocking grand challenges

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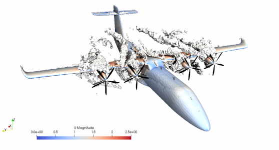
BCAM - Basque Center for Applied Mathematics, Bilbao [2]

Icarus Digital Math ("Red Hat" Open Source commercialization project) [3]

Docent lecture, KTH



Digital Math joint research environment BCAM-KTH

- Johan Jansson, Associate Professor KTH+BCAM
- Massimiliano Leoni, PhD student JJ, MSc Politecnico Milano
- Tamara Dancheva, PhD student JJ, MSc Strasbourg+KTH
- Måns Andersson, Research Engineer, MSc KTH
- Claes Johnson, Professor emeritus KTH+Chalmers
- Ridgway Scott, Professor emeritus Univ. of Chicago

Close collaborators:

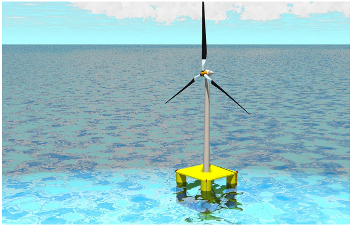
- David Kamaneksy, UCSD
- Alberto Paganini, Leicester
- Torbjörn Larsson, Creo Dynamics
- Philip Nysträmer, Nystromer Avionics

BCAM (Bilbao)

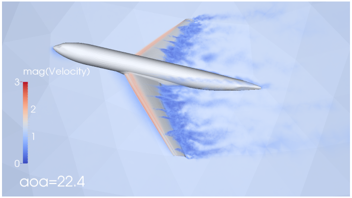
EXCELENCIA SEVERO OCHOA

KTH (Stockholm)

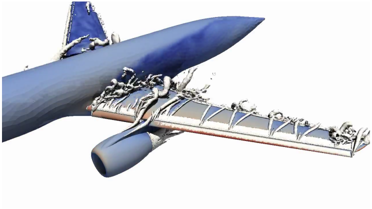
Focus application areas: aircraft, renewable energy, biomedicine



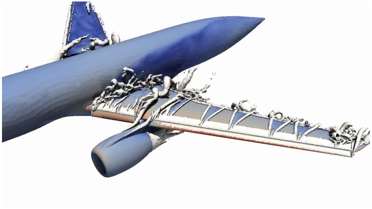
Digital Math: Marine



Digital Math: Human



Digital Math: F1



Digital Math: Aircraft

Need for **general simulation methodology**

Focus on 3 grand challenges in science, industry and education

1. Predictive aerodynamics - stall and behavior of a full aircraft
2. Reproducibility and replicability in science
3. Math and computer programming education

I will present the Digital Math program as a unified solution to all 3 challenges, with realization in Open Source FEniCS.

Problem 1

Established aircraft simulation does not predict reality ["NASA Vision 2030"]

$\Rightarrow$

Can lead to dangerous designs and errors (e.g. current aviation incidents), ineffective/costly process for design and certification

Main open question in CFD: NASA and Jameson

NASA Vision 2030 key finding:
"The use of CFD in the aerospace design process is severely limited by the inability to accurately and reliably predict turbulent flows with significant regions of separation [e.g. stall]."

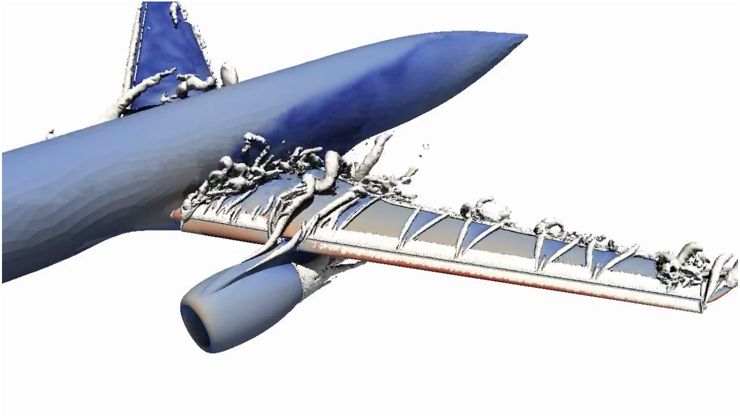
Stanford aero authority Jameson and Witherden, AIAA Future Visions 2017: "as a community we are still far away from [time-dependent simulation] LES of a complete air vehicle".

State-of-the-art in CFD: explicit turbulence modeling - add parametrized diffusive terms to conservation equations, wall functions, tuned to experiments, not predictive

Today CFD is not relied on in aerodynamics industry and science.

High Performance Finite Element Modeling

Breakthrough: Direct FEM Simulation solves NASA Vision 2030



Direct automated/parameter-free prediction of new configuration - best possible simulation at given cost

Extensively validated and compared against world-leading competition at HiLiftPW (NASA/Boeing) including stall, and now also in highest echelon of aero industry.

Direct FEM Simulation (DFS) methodology

Turbulent Euler model

Incompressible turbulent Euler as model for high Re flow:

$$
\begin{aligned}
R(\hat{u}) &= \begin{cases} \partial_t u + (u \cdot \nabla) u + \nabla p = 0 \\ \nabla \cdot u = 0 \end{cases} \\
u \cdot n &= 0, x \in \Gamma \quad \text{(Slip BC)} \\
\hat{u} &= (u, p)
\end{aligned}
$$

Weak residual $r(\hat{u}, \hat{v}) = (R(\hat{u}), \hat{v})$

General Galerkin (G2) method / Direct FEM Simulation (DFS)

Developed over a 20+ year period by Johnson, Hoffman, Jansson, etc.

Space-time FEM with Galerkin/least squares stabilization

$$(R(\hat{U}), \hat{v}) + (\delta R(\hat{U}), R(\hat{v})) = 0,\ \delta = h,\ \forall \hat{v} \in \hat{V}_h,\ \hat{U} \in \hat{V}_h$$

Adaptive error control and mesh refinement

$$|M(\hat{e})| = |(R(\hat{U}, \phi)| \leq \sum_{K \in T} \|hR(\hat{U})\|_K \|\nabla \hat{\phi}\|_K \leq TOL$$

or $\quad M(\hat{e}) = r(\hat{U}, \hat{\phi})$

Slip/friction boundary condition as boundary layer model $u \cdot n = 0$

Implicit parameter-free turbulence model based on stabilization

Dissipation: $D = \|\delta^{1/2} R(\hat{U})\|^2$

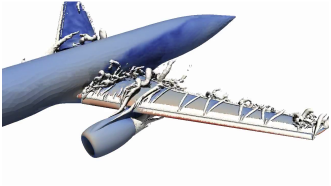
(similar approach to ILES, VMS)

Moving mesh, fluid-structure interaction, shock-capturing, etc.

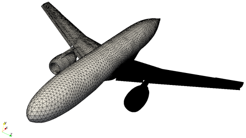
NEW methodology and possibilities

- No explicit turbulence model, no wall model: slip = small friction
- No parameters to fit
- First principles - solve purely conservation of momentum + incompressibility
- Direct stabilized FEM simulation, automated in Open Source Unicorn/FEniCS
- No manual mesh design - goal-oriented adaptive error control
- High performance - 10x faster and cheaper than Exa/RANS in HiLiftPW-3 - allows interactive simulation
- Compatible with current industrial CFD workflow - plug-in replacement for CFD solver

Fast and reliable prediction of turbulent separated flows for a full vehicle, identified as the main CFD challenge today [NASA, Jameson]



Validation: Time-resolved adaptive simulation of aircraft

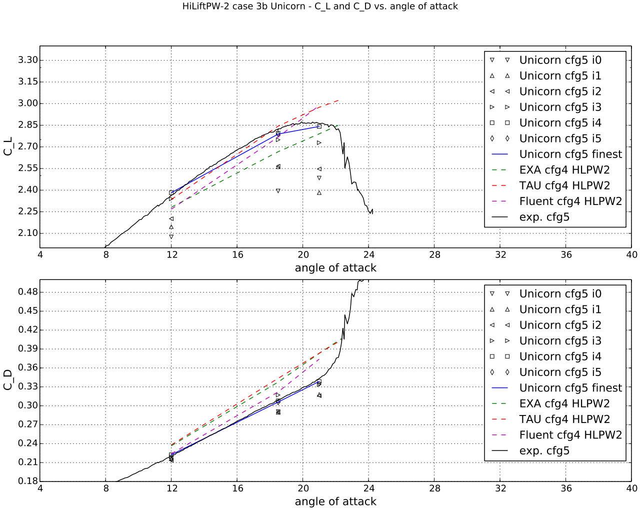


HiLiftPW 2 and 3 NASA/Boeing-organized “benchmark challenges”. Participated with good results, and our adaptive methodology was highlighted in summary. Invited to provide reference results for High Order CFD Workshop 2017 [Hoffman, Jansson, Johnson, JMFM, 2015] [Hoffman et. al., CMAME, 2015], [Jansson et. al., Hilift Springer brief, 2017]

Our computational results capture phenomena including the key stall mechanism well quantitatively at $Re \approx 10^6 - 10^7$.

Our adaptive results were specifically highlighted in the summary by the NASA organizers (we were only participant out of 30 with adaptivity).

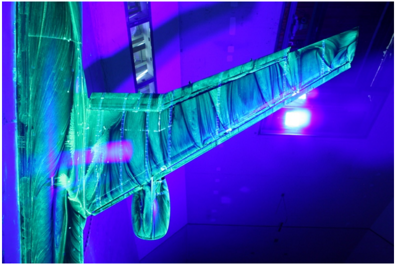
HiLiftPW-2: our results

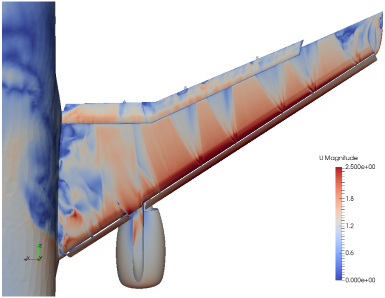


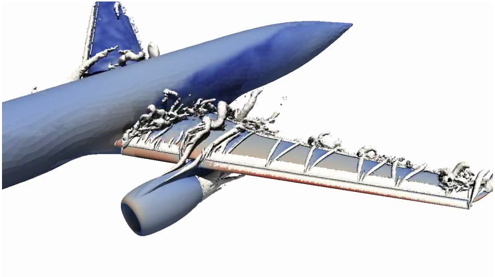
DFS/Unicorn/FEniCS consistently $\sim$ 2% error and reliable prediction of separation. For new config. we expect low predictive capability of Exa/RANS, $\sim$ 10% error and no separation prediction.

HiLiftPW-3: Surface velocity pylon-on

Stall: $\alpha = 21.57$ and $\alpha = 22.56$



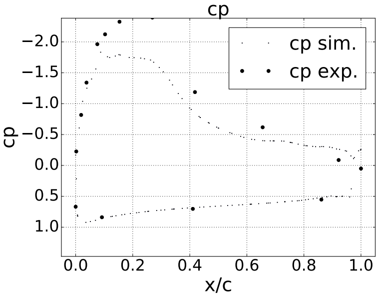




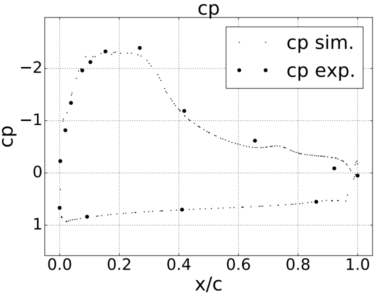
HiLiftPW-3: Illustrative cp ex.: adaptivity

JSM pylon-on, $\alpha = 4.36$, flap D-D
NB: Adaptivity targets mean quantity, not pointwise pressure

Adaptive iter. 0 (starting mesh)

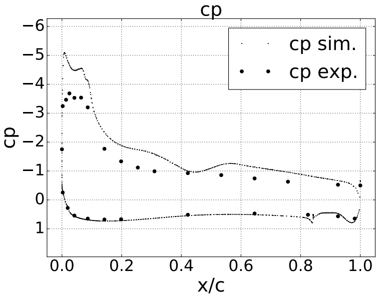


Adaptive iter. 3

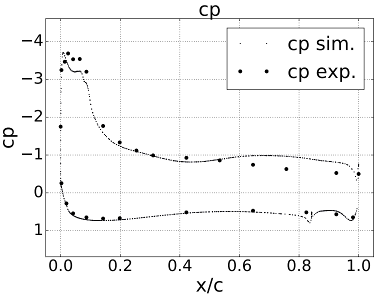


HiLiftPW-3: Illustrative cp ex.: stall

JSM pylon-on, $\alpha = 22.56$, wing B-B



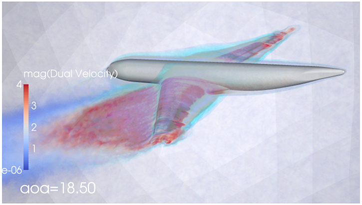
No trip-force



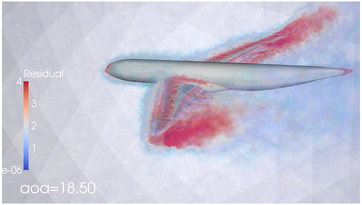
With trip-force

Adaptive mesh refinement - adjoint velocity

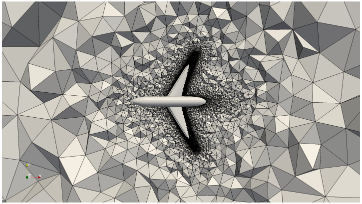
Goal quantity: drag and lift
Recall: $M(\hat{e}) = (-R(\hat{U}), \hat{\phi})$



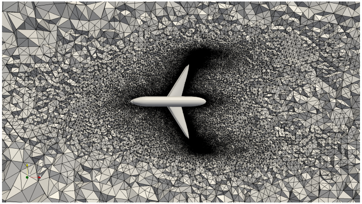
Dual velocity $\hat{\phi}$



Residual $R(\hat{U})$



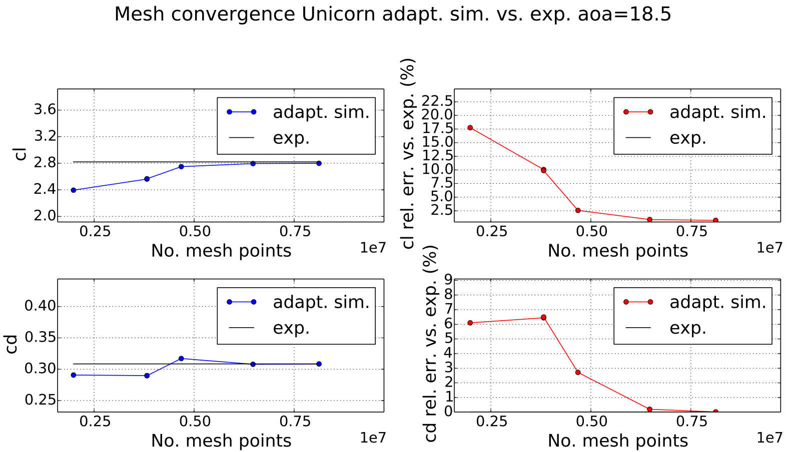
Coarse starting mesh



Refined mesh 5 adapt. it.

Aerodynamic forces $\alpha = 18.5^\circ$

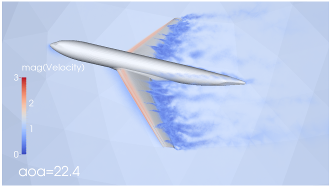
Lift and drag within 1.5% of exp.
Use 1280 cores on SuperMUC supercomputer



NEW Possibilities

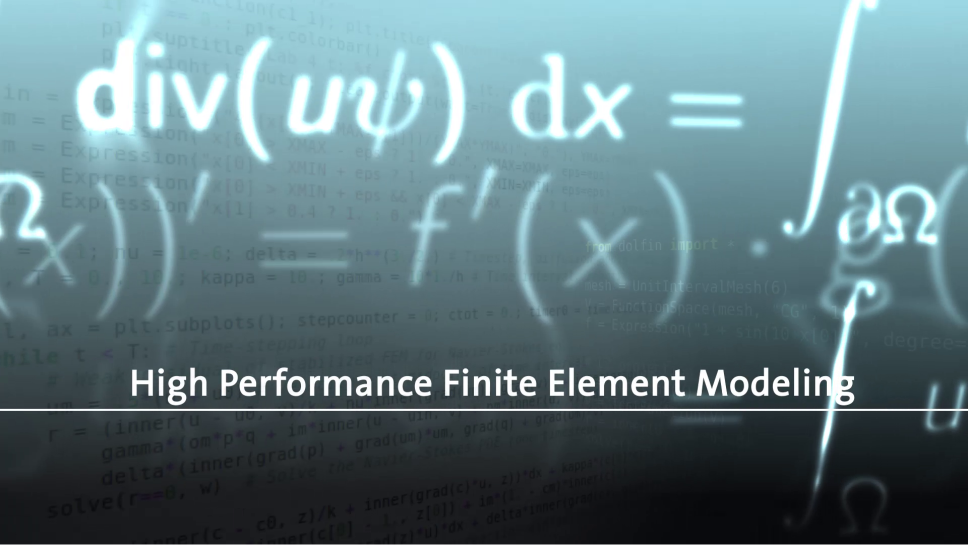
Predictive fast+cheap transient general simulation offers new possibilities

- Potential for pseudo-real-time simulation with 0.1s/large timestep, enormous efficiency possibilities with slip+adaptivity: coarse mesh, coarse geometry, etc.
- Interactive design/parameter studies: geometry, maneuvering, stability, transient adjoint-based design.
- Multi-physics: Fluid-structure interaction (FSI) already established for no-slip, preliminary good results for slip. Moving mesh/geometry possible.



Recognition at highest level of academia and industry

- Predictive aerodynamics validated at highest level in High Lift Prediction Workshop (NASA/Boeing)
- Adaptivity highlighted by NASA
- Elected to IVA Royal Swedish Academy of Engineering Sciences 100-list
- Fields medalist
- Now highlighted and presented by AIAA Chief Engineer at Columbia University
- Global online course MOOC-HPFEM, 10000+ students, KTHs largest MOOC, join the fun!



High Performance Finite Element Modeling

Commercialization: Icarus Digital Math

Vinnova verification for growth VFT-1 DigiMat project (coached by KTH Innovation)

Collaboration projects with highest echelon of aerodynamics industry.

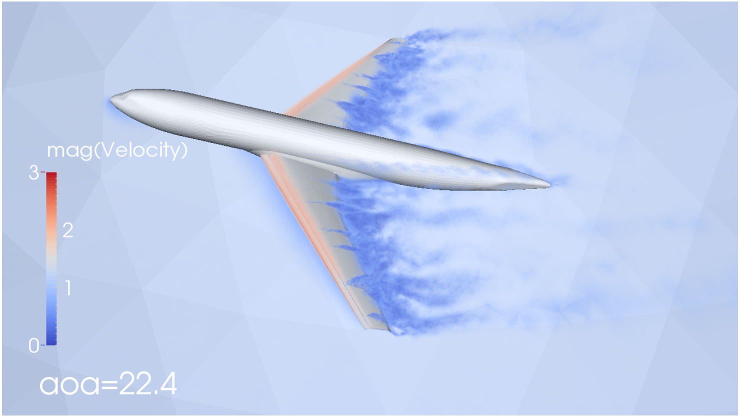
- Pilot project top Formula 1 team
- Pilot project airline
- Pilot project aircraft manufacturer
- ELISE Vinnova project and Heart Aerospace transforming Sweden to electric aviation.
- Commercialization of Digital Math education
- Largest supercomputer in the world - Amazon HPC - with Heart Aerospace

Open Source - “Red Hat Linux” of computational math

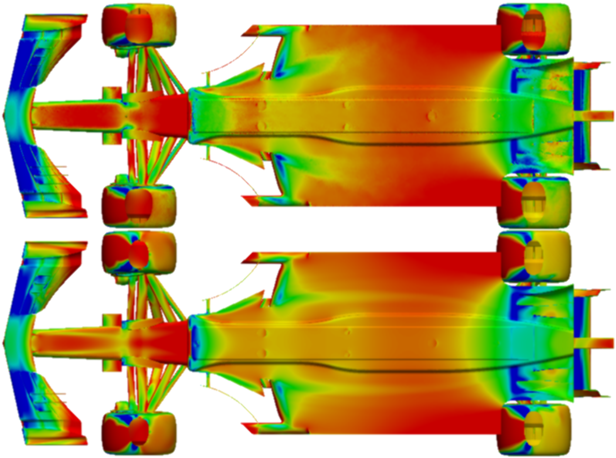
Excellent team KTH+BCAM - spin-off Icarus Digital Math:

- Johan Jansson, Associate Professor KTH+BCAM, CEO+Chair Icarus
- Rahul Kumar, Post-doc JJ, PhD Houston (Glowinski)
- Ezhilmathi Krishnasamy, PhD student JJ, MSc LTH
- Massimiliano Leoni, PhD student JJ, MSc Politecnico Milano
- Tamara Dancheva, PhD student JJ, MSc Strasbourg+KTH
- Claes Johnson, Professor emeritus KTH+Chalmers
- Ridgway Scott, Professor emeritus Univ. of Chicago

Vorticity (Q-criterion) Perrinn F1 benchmark DFS/Unicorn/FEniCS



CP Perrinn F1 DFS/Unicorn/FEniCS (top) vs. Fluent (bottom)



CD and CL within 4% . 20x more cells in Fluent mesh.

In collaboration with Torbjörn Larsson (previous head of CFD in F1), Creo Dynamics.

Problem 2

Many research publications are not reproducible and replicable - not based on the scientific method! [National Academies of Sciences, Engineering, and Medicine, Barba et. al. "Reproducibility and Replicability in Science", Ionnidis "Why most published research findings are false"]

$\Rightarrow$

Can lead to reduced trust in the scientific community, key decisions based on non-scientific arguments.

Digital Math framework

We present the Digital Math framework as the foundation for modern science based on constructive digital mathematical computation. The computed result (coefficient vector, FEM function, plot, etc.) is a mathematical theorem, and the mathematical Open Source code, here in the FEniCS framework, and computation is the mathematical proof. We can also derive additional constructive proofs from the FEniCS and FEM formulation, such as stability.

Unlocks predictive aerodynamics and turbulence with DFS/Unicorn/FEniCS, reproducible science, motivation for Digital Math learning.

We build on the work by Turing, Gödel for mechanization/digitalization of math.

Satisfies reproducibility and replicability required by modern science [Barba et. al.]

FEniCS provides high abstraction level for FEM and PDE - understandable Digital Math.

Automated Digital Math - FEniCS

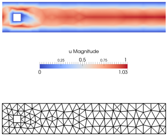
FEniCS(-HPC) open source FEM framework for automated solution of general PDE and Direct FEM Simulation (DFS). We started FEniCS 2003, today de-facto world-standard for mathematical FEM with 100s co-authors at highest level in academia:

Automated discretization (generate code for linear system from PDE):

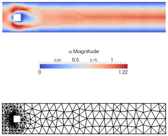
```
r = (inner(grad(u), grad(v)) - inner(f, v))*dx
```

$\Rightarrow$ `Poisson.cpp`

Automated error control (incl. parallel adaptive mesh refinement):



$+ \ |M(e)| \leq TOL \ \Rightarrow$



with $M(e)$ a goal functional of the computational error $e = u - U$.

Automated modeling of unresolved subscales (i.e. turbulence):

$(R(U), v) + h(R(U), R(v)) = 0, \forall v \in V_h$ (residual-based stabilization/dissipation)

Goal: Autom. generate the solution, mesh and program from PDE (residual) and goal functional $M(e)$ (e.g. drag).

Unified Continuum modeling - Unified Uman - FSI

Unified Continuum (UC) formulation for FSI

Conservation equations (momentum, mass) in Euler (laboratory) coordinates, stress σ as data, track discontinuous phase function θ with moving mesh/basis functions:

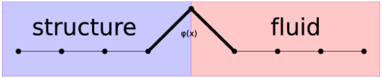
$$\begin{aligned}
\rho(\partial_t u + (u \cdot \nabla)u) - \nabla \cdot \sigma &= 0 && \text{in } Q,\\
\nabla \cdot u &= 0 && \text{in } Q,\\
\partial_t \rho + (u \cdot \nabla)\rho &= 0 && \text{in } Q,\\
\partial_t \theta + (u \cdot \nabla)\theta &= 0 && \text{in } Q,\\
u(\cdot, 0) &= u^0 && \text{in } \Omega,
\end{aligned}$$

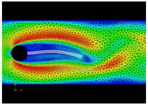
Different constitutive equations for phases:

$$\sigma = \bar{\sigma} - pI \quad \bar{\sigma} = \theta\bar{\sigma}_f + (1-\theta)\bar{\sigma}_s$$

$$D_t\bar{\sigma}_s = 2\mu_s\epsilon + \nabla u\bar{\sigma}_s + \bar{\sigma}_s\nabla u^\top \qquad \bar{\sigma}_f = 2\mu_f\epsilon$$

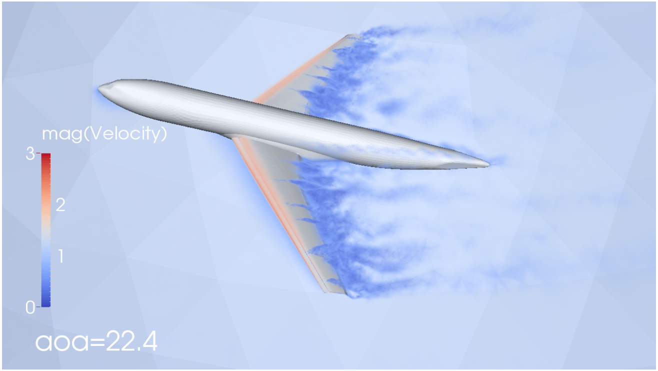
Discretize as one domain (exploited in error estimation, robustness):





FSI for human voice apparatus in EUNISON project

Unified continuum simulation with realistic geometry of the human voice apparatus in the EUNISON project with turbulent fluid-structure interaction with aeroacoustics and parallel contact based on solving an Eikonal equation, generating self-oscillation of the vocal folds and the expected glottal wave pattern. Adaptive method validated for 3D FSI benchmark.



Problem 3

Almost all students lose motivation for math/programming by high school [Swedish National Agency for Education].

$\Rightarrow$

Society today digital and automated - almost all activities soon based on computational math. Can lead to enormous divide, majority of population cannot contribute to societal development.

MOOC - KTH/edX online course on adaptive FEM and FEniCS

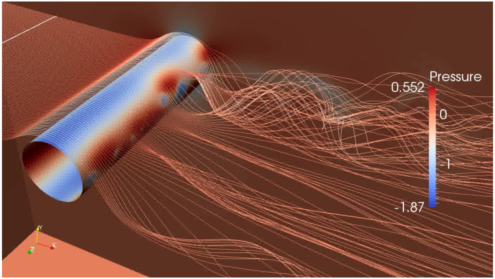
High Performance Finite Element Modeling MOOC supported by KTH.

Opened on October 17, 2017, already 10000+ students, join the fun!

Advanced part 2 on DFS, turbulence and HPC opened mid-April 2018. Participants can reproduce DFS flight results.

DigiMat

Vinnova DigiMat project for Digital Math education from pre-school to professionals.



Easy “elastic supercomputing” interface with Amazon AWS

We have verified large scale industrial cases both on traditional supercomputers, and now also on Amazon AWS, where we show better performance than the Cray supercomputer at KTH, and which represents a paradigm shift, allowing easy ”elastic supercomputing” in a web browser.

Possibility to run, reproduce, modify our simulations in an easy “one-click” AWS supercomputer web interface. Please let me know if you’re interested!

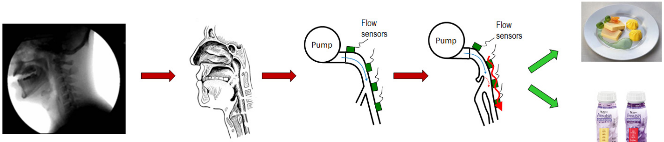
Current and recent research projects 2015-2022

Severo Ochoa Center of Excellence (BCAM), 4M EUR.
H2020 Marie Curie solid mechanics project (ENABLE), 3M EUR
H2020 Marie Curie Aerosimulat, 200kEUR
H2020 Cloud-HPC project (MSO4SC), 3M EUR
Formas Swallow, 300kEUR
VINNOVA Swedish Innovation Agency project DigiMat education, 200kEUR
VINNOVA Swedish Innovation Agency project ELISE electric aircraft, 50kEUR + 2MEUR
FP7 EUNISON project for voice modeling, 3M EUR
Basque ELKARTEK projects with Tecnalia for floating wind turbines (Best poster award at Bilbao Marine Energy Week) and with CTA/ITP/Rolls Royce for jet engine modeling. ca. 100kEUR
MINECO MTM mathematics ("Spanish VR") two projects, ca. 40kEUR.
VINNOVA Swedish Innovation Agency project for commercialization
Spanish CIEN project for 3D printing, ca. 70kEUR.
Bilbao Water Consortium project, ca. 20kEUR.

New project: Swallow

Simulate swallowing with FEniCS - non-Newtonian FSI.

Validate against Gothenburg throat experiments.



Videoflouroscopy
X-ray + contrast medium

Swallowing tract
geometry, disorders

Model 1
solid pipes, sensors

Model 2
Elastic, 3D, sensors

Food and nutrition for swallowing disorders

Focus on 3 grand challenges in science, industry and education

1. Predictive aerodynamics - stall of a full aircraft
2. Reproducibility and replicability in science
3. Math and computer programming education

The Digital Math program is a unified solution to all 3 challenges, with realization for FEM and PDE in Open Source FEniCS.

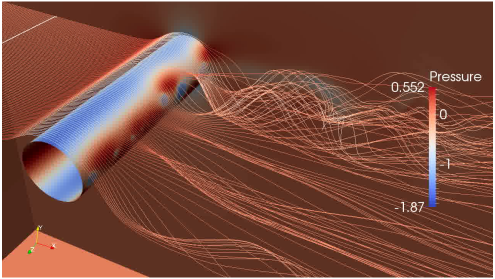
`http://digimat.tech`

Open Source commercialization/industrialization:
Icarus Digital Math - `http://icarusmath.com`

Appendix

Slip separation

The methodology is based on our new resolution of d'Alembert's paradox showing that slightly viscous bluff body flow can be viewed as zero-drag/lift potential flow modified by 3d rotational slip separation arising from a specific separation instability of potential flow, into turbulent flow with nonzero drag/lift. Detailed Direct FEM Simulation (DFS) of incompressible Euler with slip BC validating the theory for full aircraft, NACA0012 airfoil and cylinder model problem with adaptive error control.



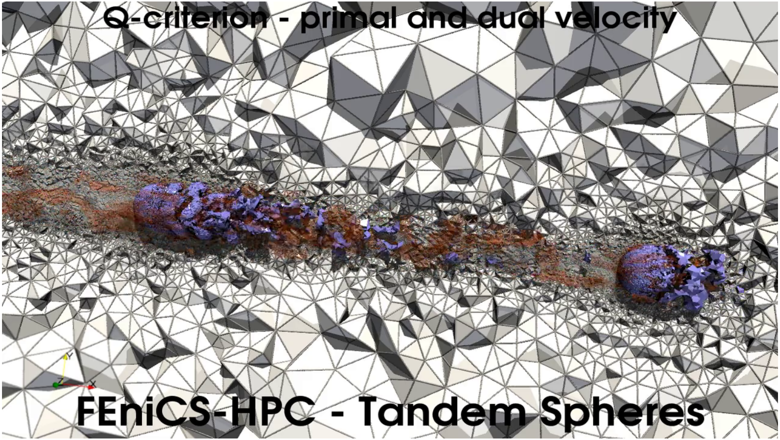
3D slip separation.

What about high order?

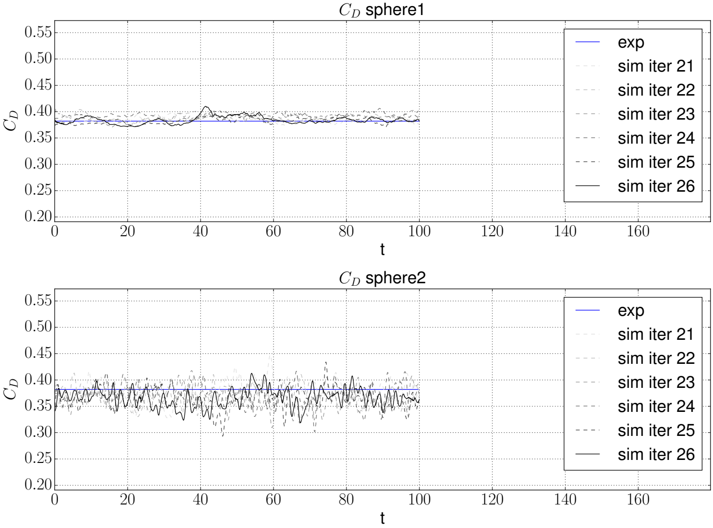
CS1: Viz of adaptive results

AIAA 5th International Workshop on High-order CFD methods

Goal quantity: drag $M(\hat{u})$
Recall err. rep.: $M(\hat{e}) = (-R(\hat{U}), \hat{\phi})$
Adjoint $\hat{\phi}$ weights error indicators upstream, zero weight downstream of downstream sphere, residual $R(\hat{U})$ weights turbulent wakes.



Time-evolution of C_D



Time evolution of the drag coefficient for various iterations of our adaptive procedure.

Convergence order

We hope to contribute an interesting perspective on convergence order in the setting of adaptive methods.

What is the order of convergence of an adaptive h-refinement method?

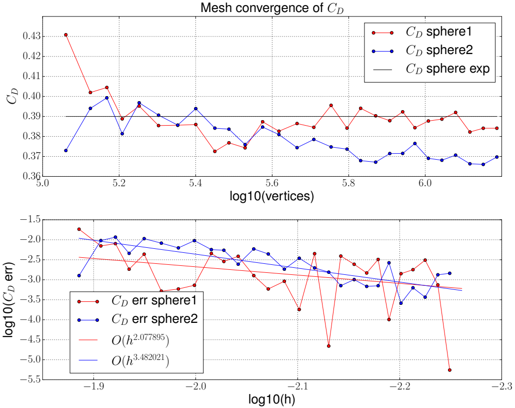
- Generalized length scale $h = N_{DOF}^{\frac{1}{d}}$
- Order of convergence $e(h) = Ch^p$ or $log(e(h)) = p\, log(Ch)$
- Compute convergence sequence (e_i, h_i)
- Least-squares fit for p gives "effective order of convergence".

Adaptive DNS/LES $\Rightarrow$ asymptotic regime is DNS

We are interested in efficient computation $\Rightarrow$ as coarse meshes as possible typically in ILES regime which is non-smooth (refinement uncovers finer scales).

Uniform refinement quasi-optimal for smooth solutions.

Adaptive mesh convergence

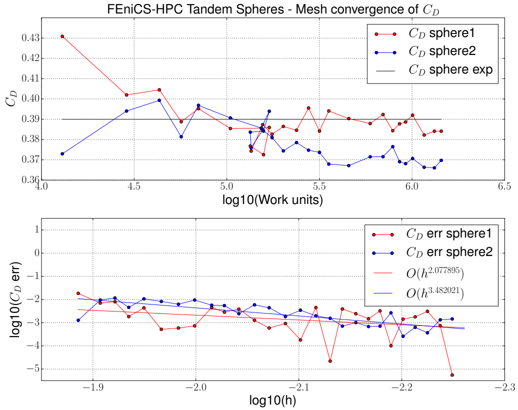


Mesh convergence of the drag coefficients of the two spheres. Effective order of convergence > 3. However, not interesting with asymptotic behavior. Allowing coarsening could give different behavior, (Couchman/Galbraith).

We see a clear drag reduction for the downstream sphere, consistent with a "slipstream" phenomenon.

2% away from experimental reference for upstream sphere.

Adaptive mesh convergence



Mesh convergence of the drag coefficients of the two spheres.