Parallel workflows for computational science and engineering: FEniCS

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FEniCS-HPC

DOLFIN

- Hybrid parallelization
- MPI+OpenMP
- MPI+PGAS
- Parallel I/O (MPI I/O)

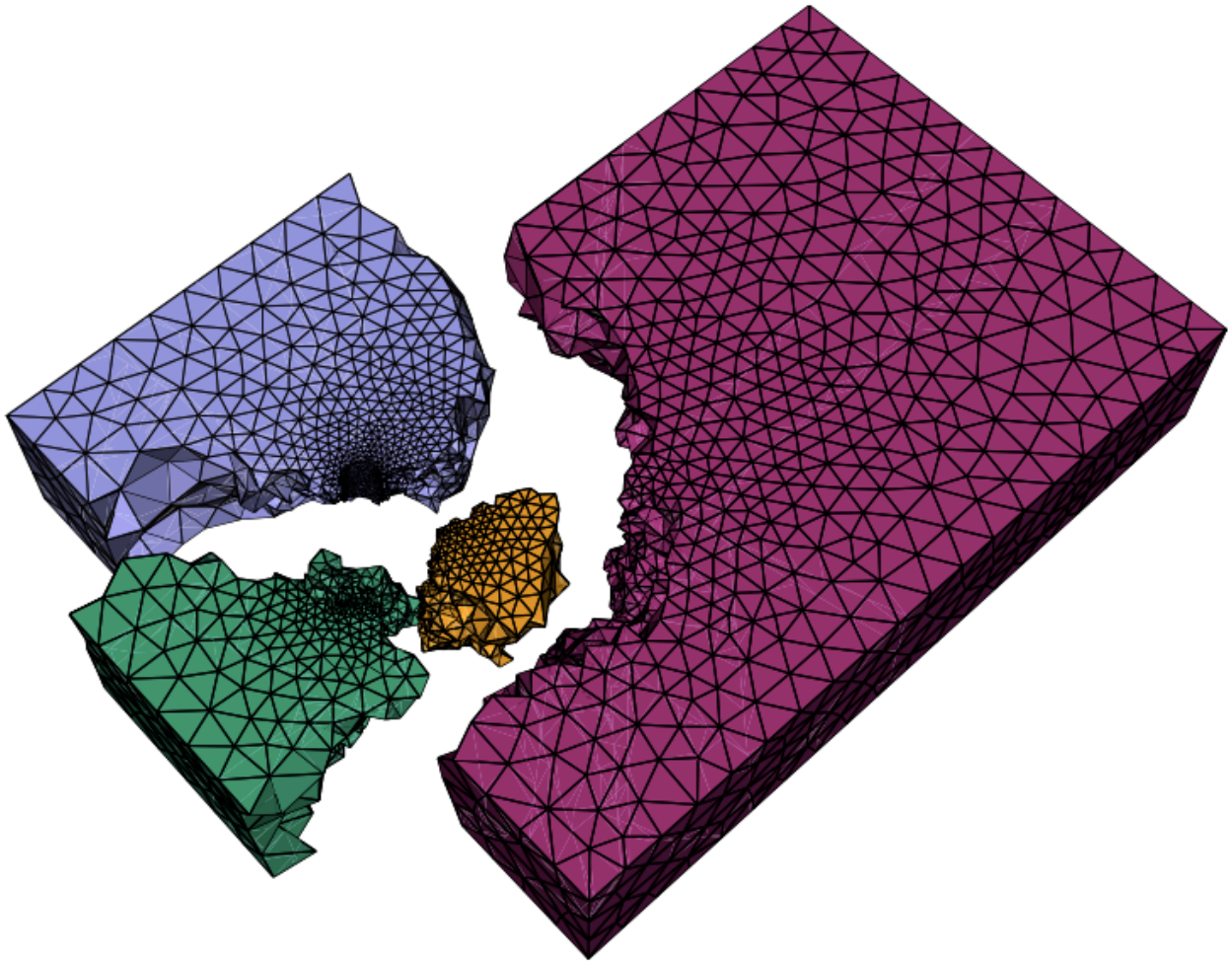
Unicorn

- Adaptive continuum mechanics solver
- Deforming/moving mesh algorithms

Dependencies

- autotools
- DOLFIN
  - PETSc
  - ParMETIS
  - UFC
  - MPI
  - FFC
- Unicorn
  - BLAS
  - Cray’s libsci (FORTRAN blas)

Distributed mesh



Distributed mesh

- Each core has a separate mesh
- Glued together using `MeshDistributedData`
- Shared entities are `shared` or `ghost`
- Mapping from local to global indices
- Mapping from global to local indices
- Iterators for shared and ghosted entities

Mesh algorithms

- Recursive longest edge bisection
  - Local serial refinement on each PE (concurrently)
  - Global propagation
  - Fully distributed termination criterion
- Dynamic load balancing
  - Scratch and remap (based on PLUM)
  - A priori work load estimation (serial LEPP)
- Mesh smoothing
  - Linear elastic analogy (PDE solve)

Functions and linear algebra

Functions

- Defined by a mesh and a vector of dofs
- `dofmap` tabulated for each cell

Linear algebra

- Row-wise data distributions
- Non-local data accessed through ghost points
- PETSc, Janpack

Binary file format

Mesh

```
Mesh mesh("mesh.bin");
File m_out("mesh_out.bin");
m_out << mesh;
```

Functions

```
Function u;
File file("primal.bin");
file << u;
```

The flat binary files can be converted to Paraview or Visit

High Re turbulent flow

- High Reynolds number turbulent flow, shocks, boundary layers, complex geometry, fluid-structure interaction
- Full computational resolution in DNS impossible
- State of the art: RANS, or LES for moderate Re
- Ad hoc mesh design: non-optimal and expensive

G2 Adaptive FEM Implicit LES

- Approximate turbulence as weak solutions by FEM with residual based stabilization (General Galerkin (G2)/Adaptive DNS/LES)
  - No RANS/LES averaging/filtering
  - No explicit turbulence/subgrid model (parameter free model)
  - Turbulent dissipation only from numerical stabilization (cf. Implicit LES, MILES [Fureby/Grinstein AIAA 99], VMM-LES [Bazilevs et.al. CMAME 07, Guasch/Codina 07])
- Error control with respect to output functionals of weak solutions (e.g. forces, mean values, etc.): $|M(u)-M(U)|$
- Automatic mesh design: by (parallel) adaptive algorithms based on a posteriori error control of $|M(u)-M(U)|$
- Modeling the effect of turbulent boundary layers by a cheap wall shear stress model (cf. [Schumann JCP 75])

[Hoffman SISC 05, JFM 06, CM 06, IJNMF 08, Hoffman/Johnson CMAME 06, Springer 07]

G2 Adaptive FEM Implicit LES

- [G2/GLS] For (v,q) in W_h : find (U,P) in V_h such that

$$(U_t + U\cdot\nabla U,v) + (\nu\nabla U,\nabla v) - (P,\nabla\cdot v) + (q,\nabla\cdot U)$$
$$+ (\delta R(U,P),R(v,q)) = (f,v)$$

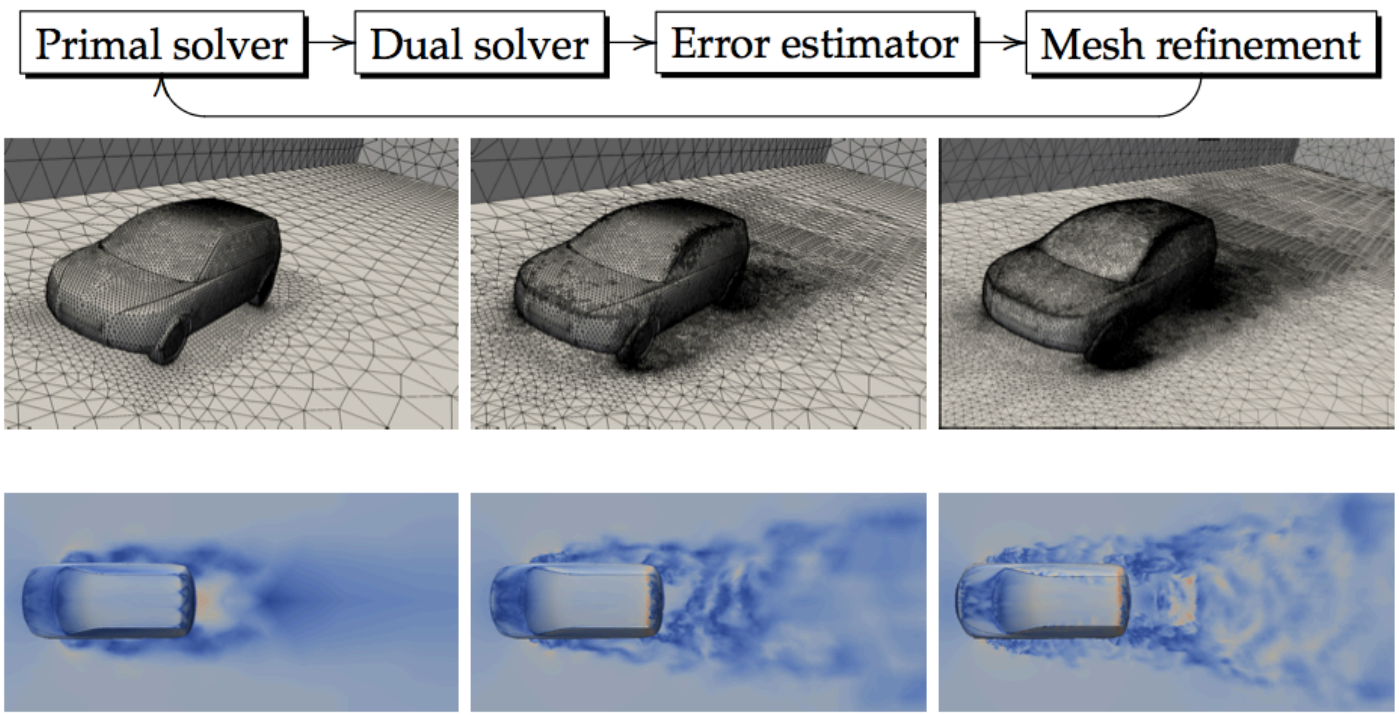
- Slip (no penetration) velocity: $u\cdot n = 0$ (strong BC)
- Wall shear stress: $\tau = n^T\sigma t = \beta(u\cdot t)$ (weak BC: β friction coeff.)

- Least squares stabilization of a residual: R(U,P), with $\delta \sim h$
- No explicit (physics based) subgrid model of unresolved scales
- Dissipation: $- dK/dt = ||\beta^{1/2}u\cdot t||^2 + ||\nu^{1/2}\nabla U||^2 + ||\delta^{1/2}R(U,P)||^2$

[Hoffman SISC 05, JFM 06, CM 06, IJNMF 08, Hoffman/Johnson CMAME 06, Springer 07]

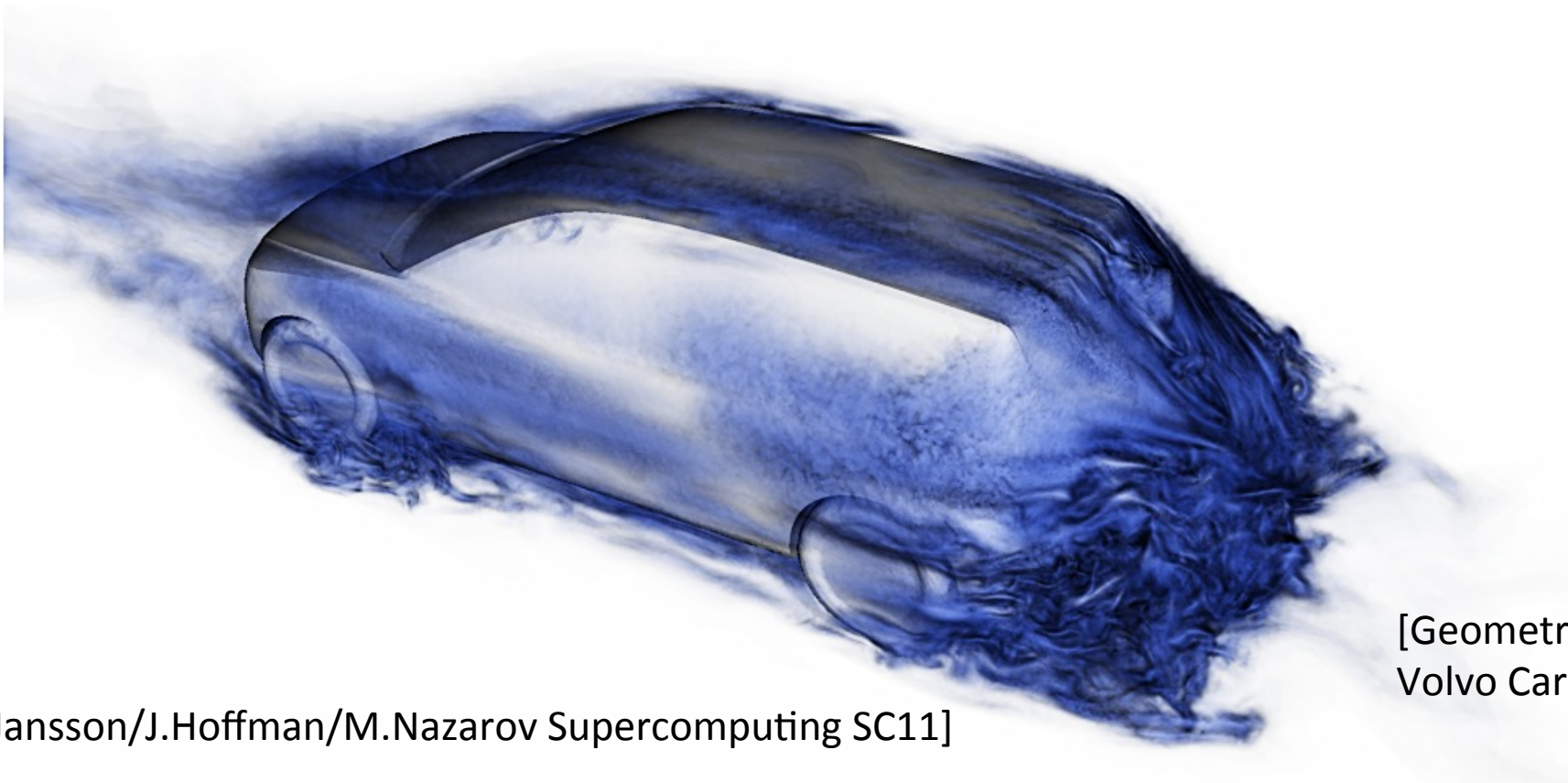
G2 Adaptive FEM Implicit LES

- A posteriori error estimate: $|M(u) - M(U)| \leq \sum_K E_K$ (cells K)
- Error indicator $E_K = S_K \times h_K|R_K|$ (S_K stability weight, R_K residual)
- Output sensitivity of $M(\cdot)$ by adjoint equation: stability weight S_K
- Adjoint equation: $-\partial\phi/\partial t - (u\cdot\nabla)\phi + \nabla U^T\phi + \nabla\theta = \psi, \quad \nabla\cdot\phi = 0$



G2 - Adaptive FEM for turbulence

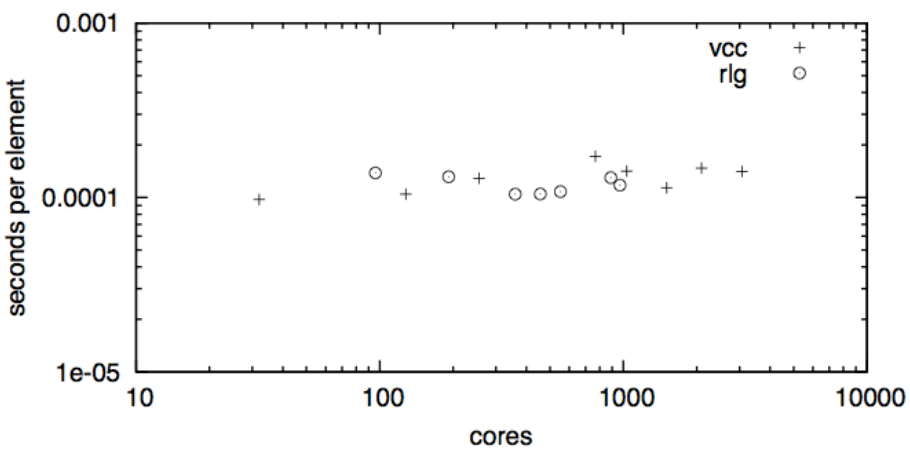
Adjoint solution show sensitivity with respect to drag

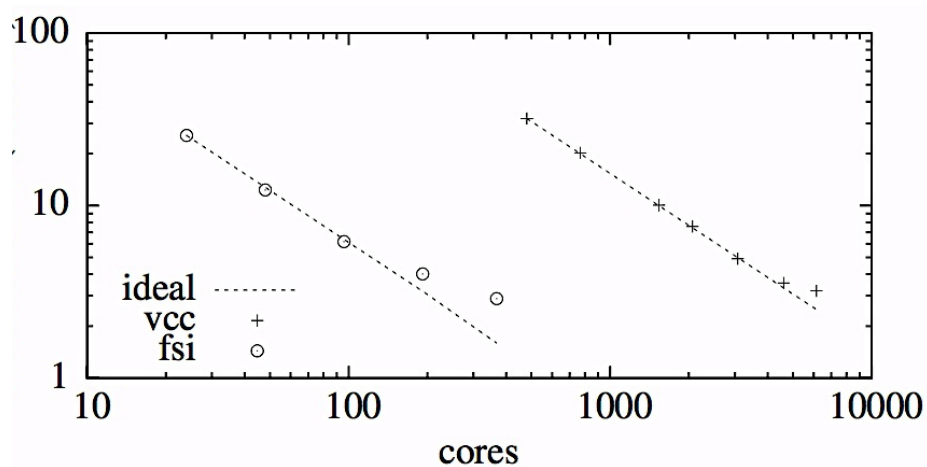


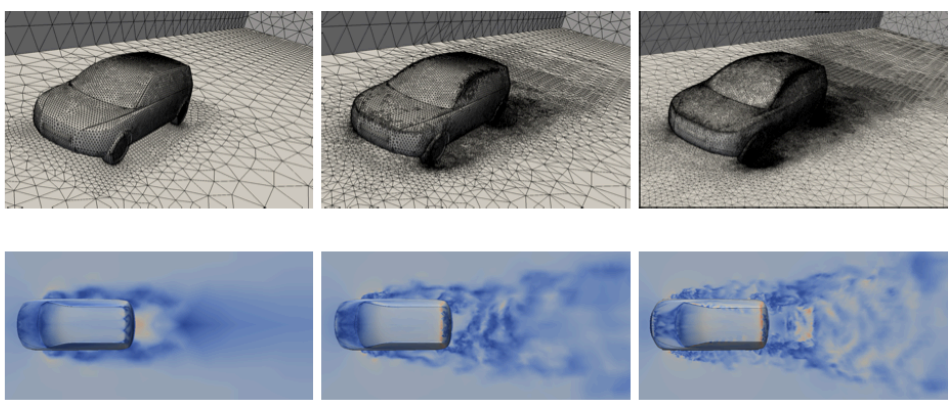
[Geometry by Volvo Cars]

[N.Jansson/J.Hoffman/M.Nazarov Supercomputing SC11]

Optimal scaling – adaptive CFD/FSI



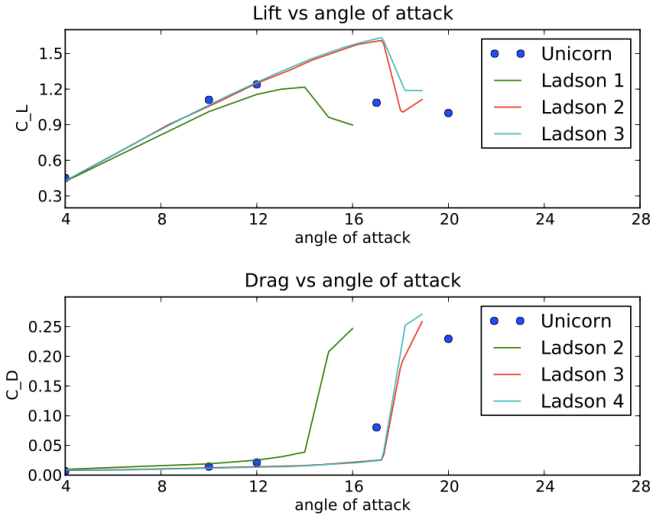


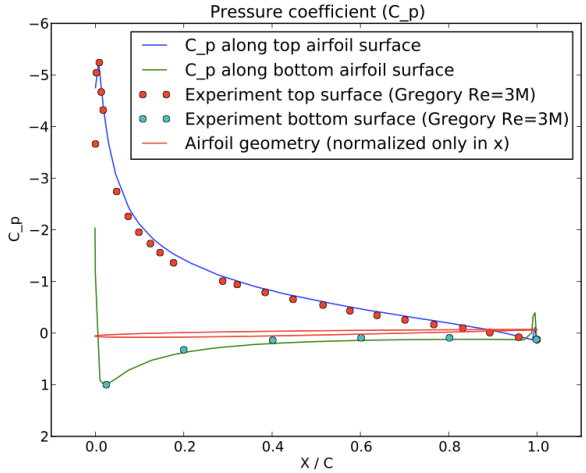


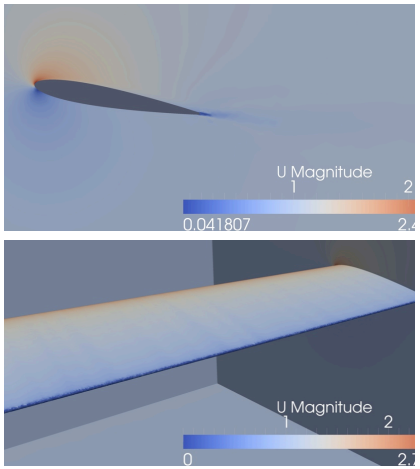
Full adaptive cycle:
primal problem, dual,
error estimation and
mesh refinement
[Cray XE6 Lindgren at PDC/KTH]

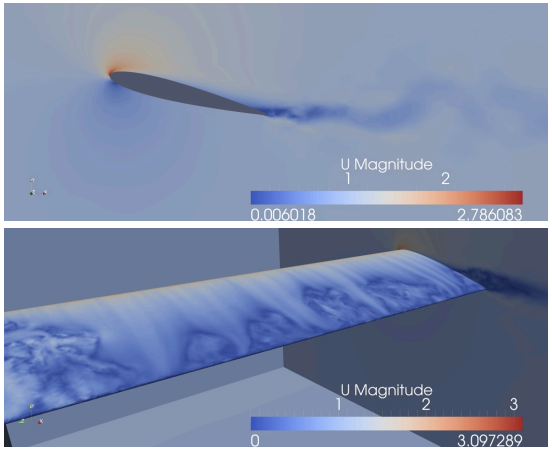
[N.Jansson/J.Hoffman/M.Nazarov Supercomputing SC11]

G2 validation: basic benchmarks









- NACA 0012 Re = 10^6 [Jansson/Jansson/JH, 2012]
- Cube Re = "∞" [JH/Jansson/Vilela, CMAME 2011]
- Circular cylinder Re = 3900 [JH, IJNMF 2009]
- Sphere Re = 10000 [JH, JFM 2006]
- Square cylinder Re=22000 [JH, SISC 2005]
- Surface mounted cube Re = 40000 [JH, SISC 2005]

Workshop on Benchmark problems for Airframe Noise Computations (BANC-I)

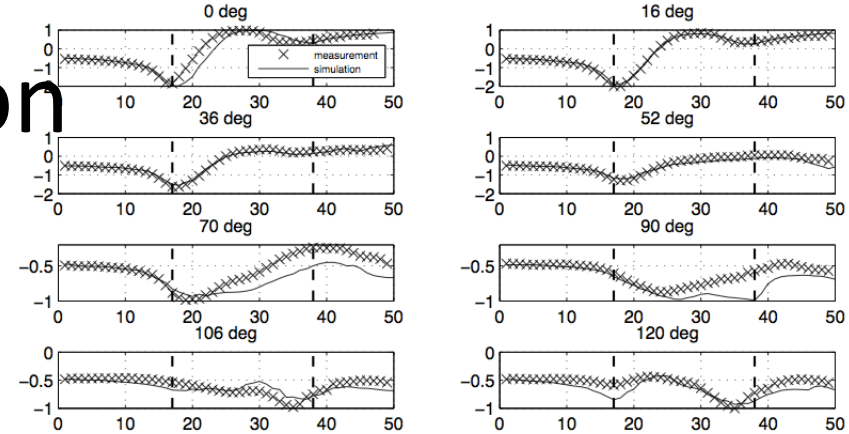
Landing gear test case
Re = 10^6, boundary layers tripped

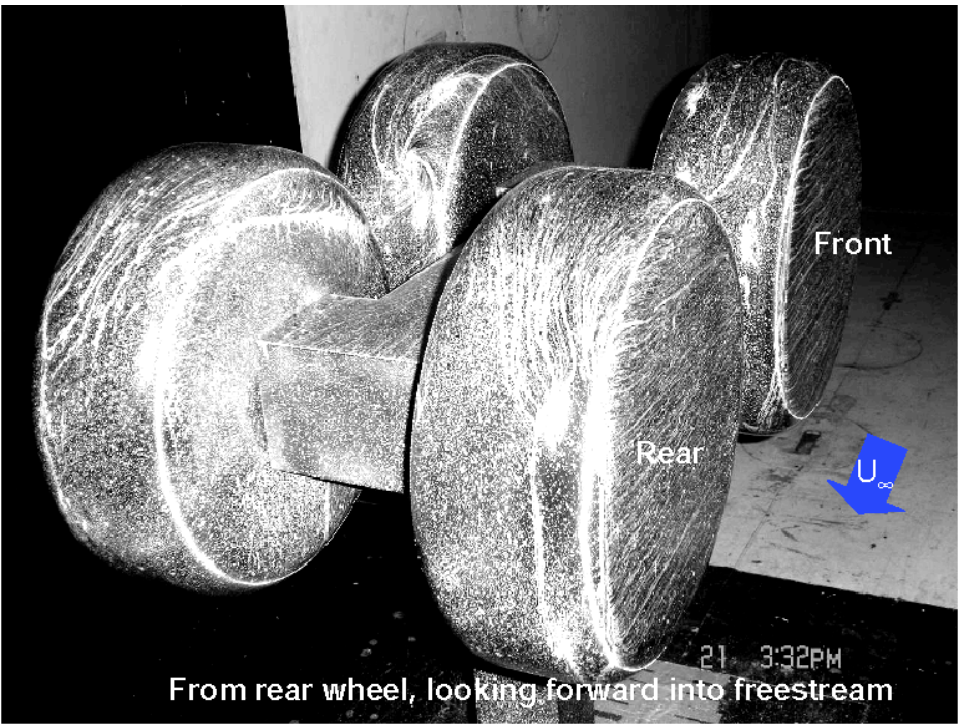
Experimental results [Boeing/Nasa]
Cx = 1.60
SPLmax = 149 dB

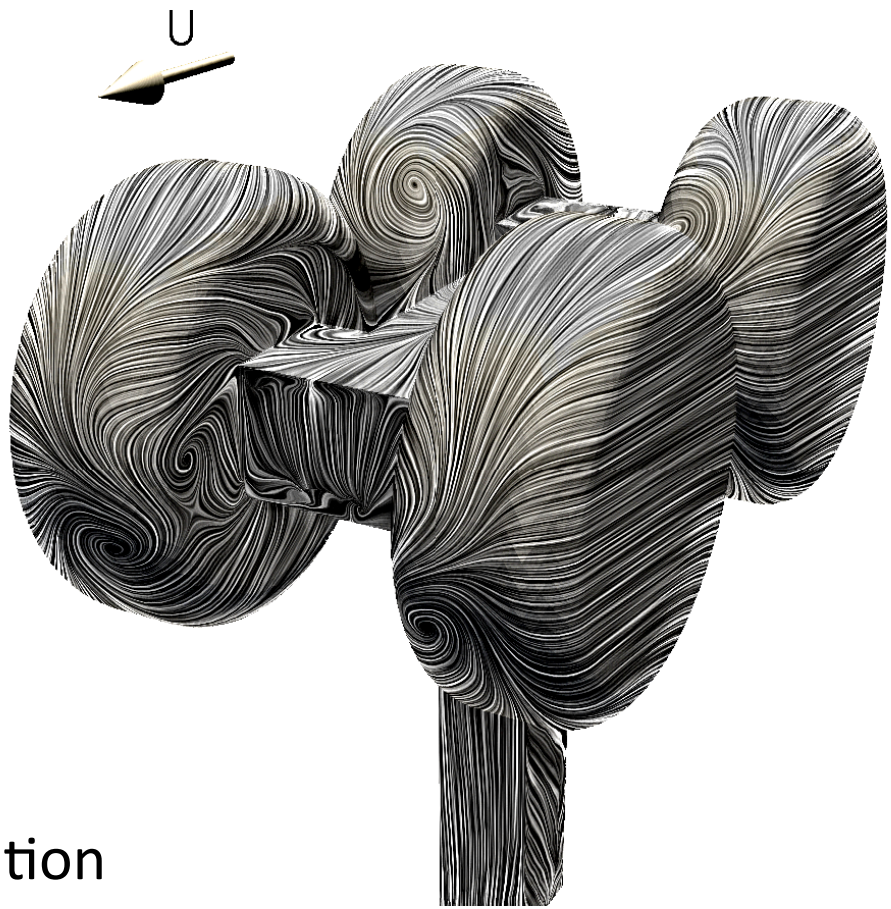
Computation: G2/free slip bc (β=0)
Turbulent BL left unresolved!
Cx = 1.62
SPLmax = 152 dB

[Vilela De Abreu/Jansson/Hoffman BANC-I 2010, AIAA 2011]

Experiment/Simulation
- surface pressures
- oil film visualization



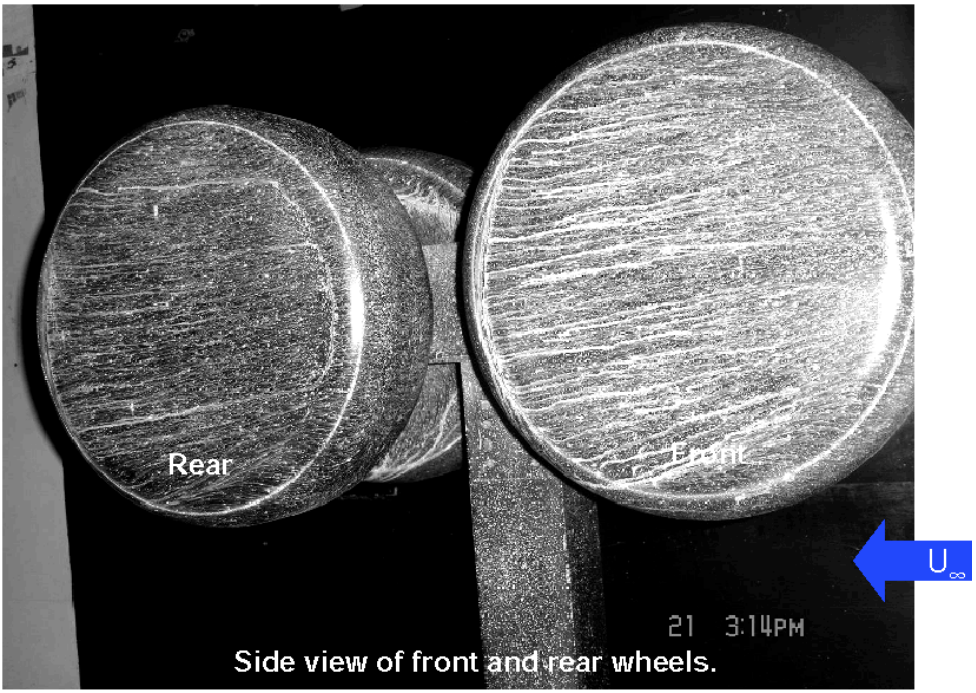


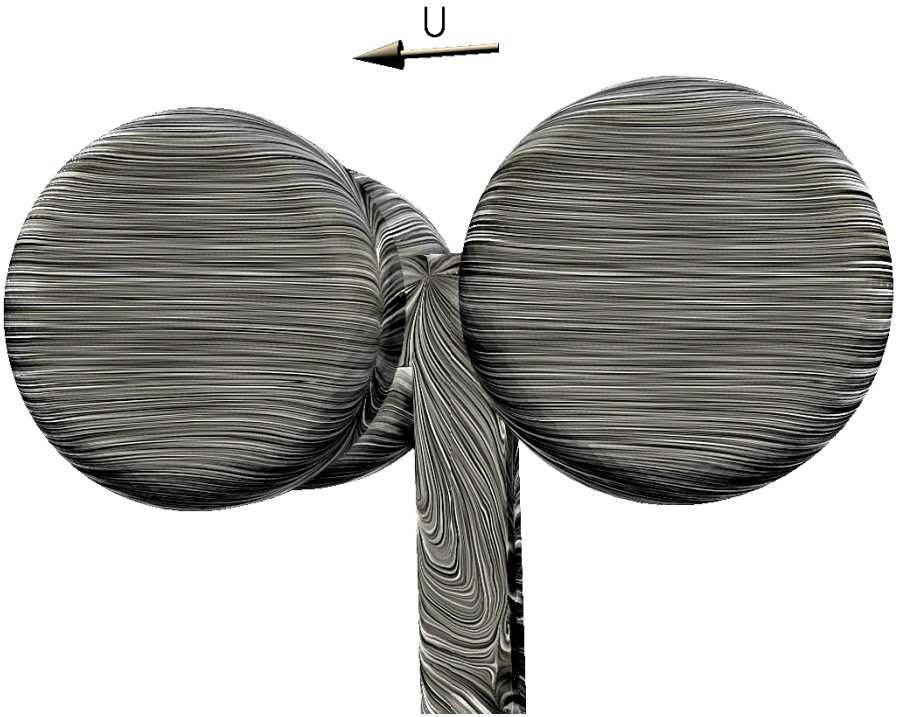


Surface flow separation patterns

No boundary layer - inviscid separation

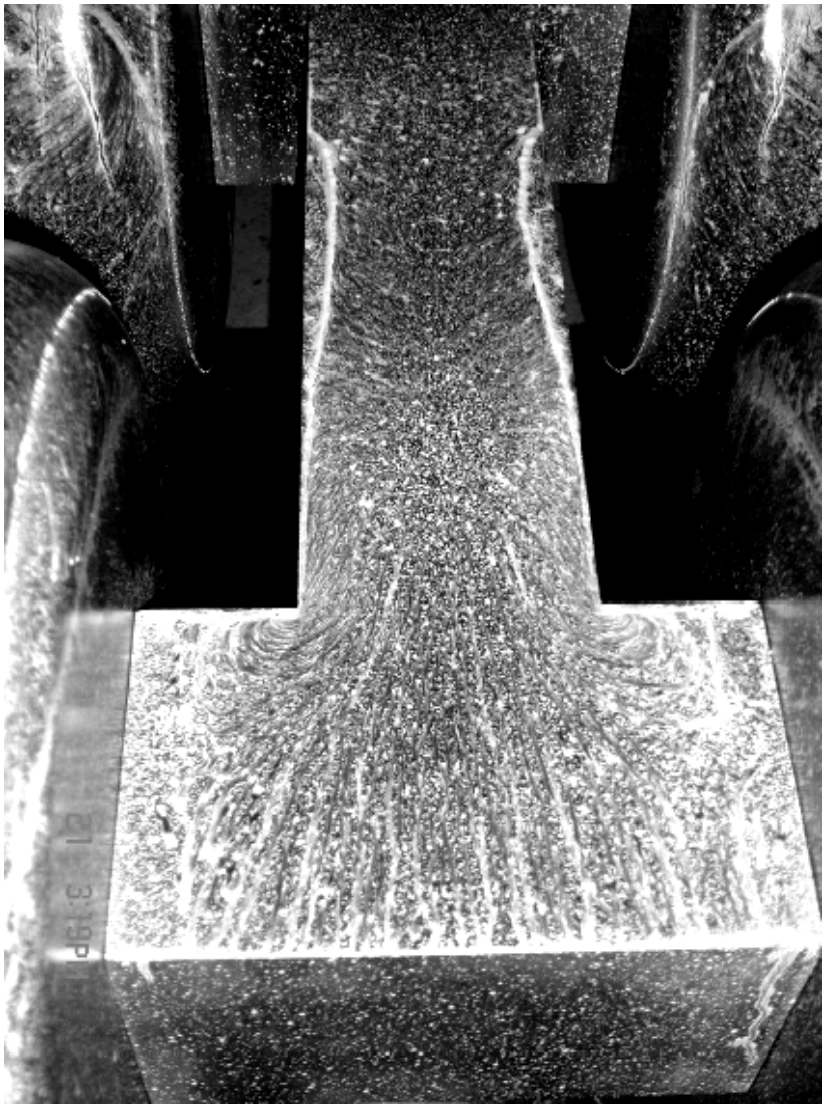
Experiment vs Simulation oil film visualization





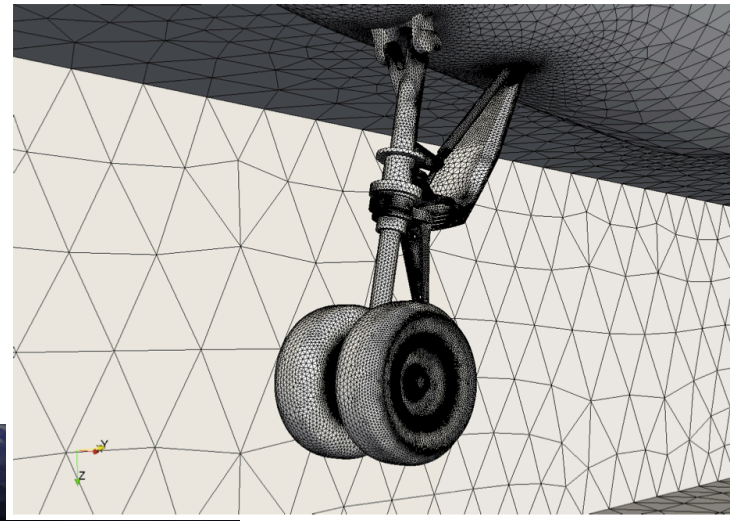
[Vilela De Abreu/Jansson/Hoffman BANC-I 2010, AIAA 2011]

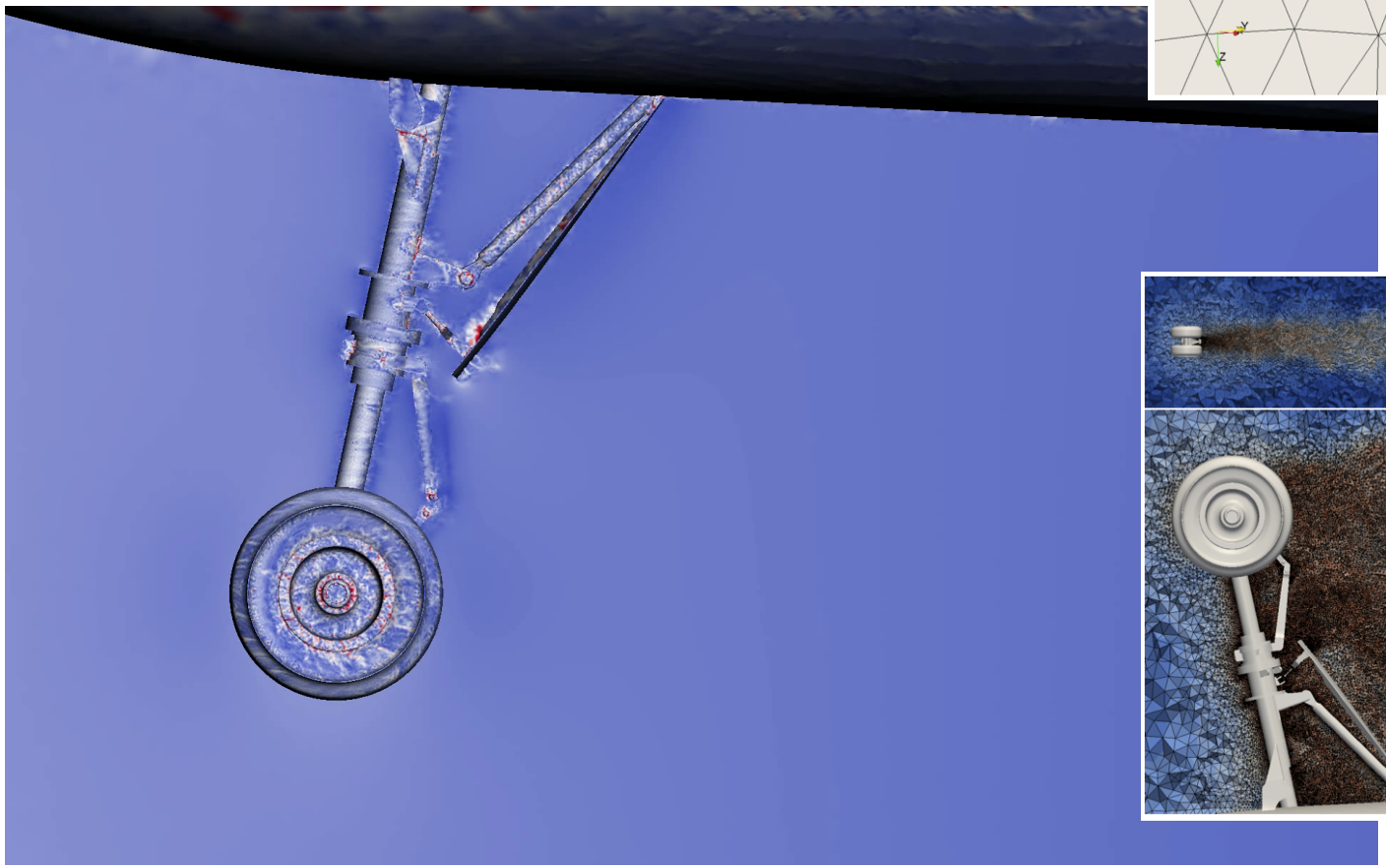
Experiment vs Simulation
oil film visualization

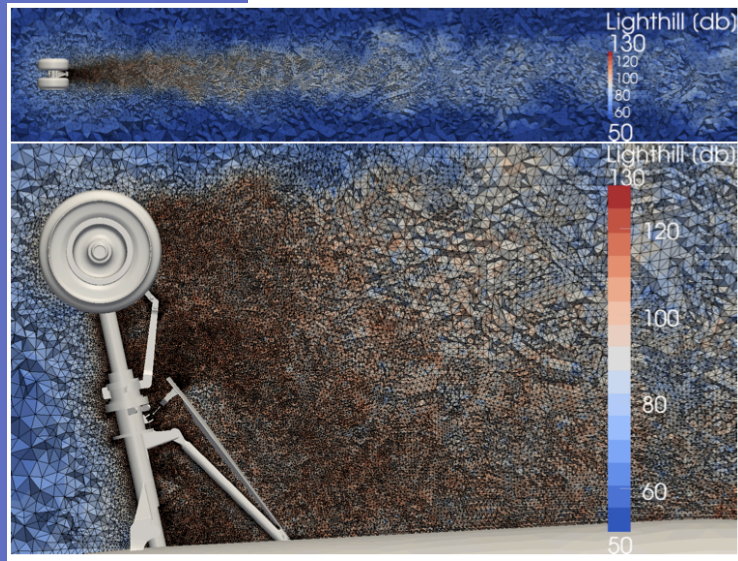


BANC-II 2012
AFEM for aeroacoustics

[Initial mesh by ANSA, postprocessing by SAAZ]

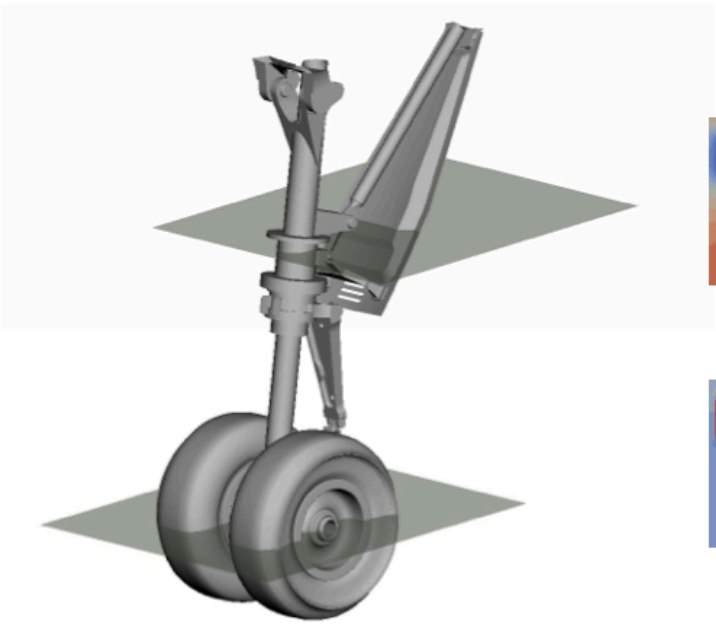


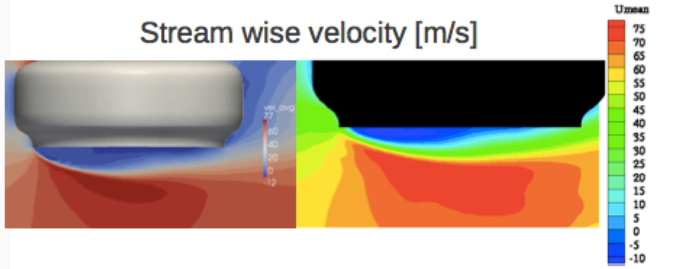


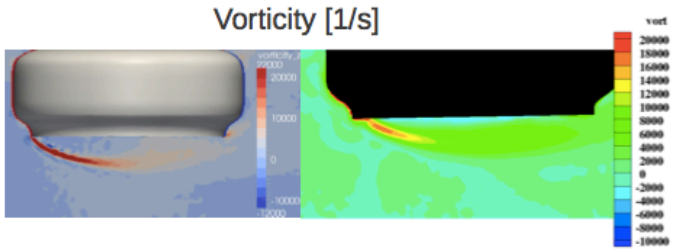


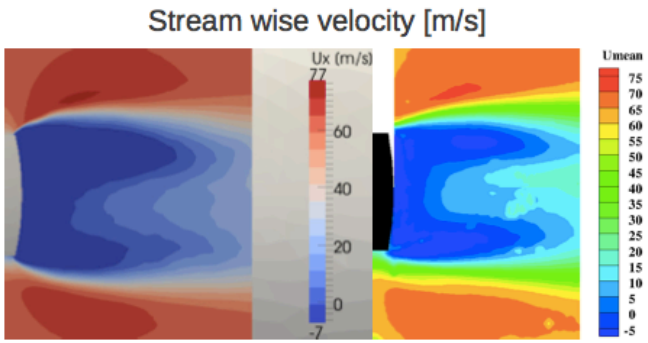
[Vilela De Abreu/Jansson/Hoffman BANC-II 2012, AIAA conference 2012]

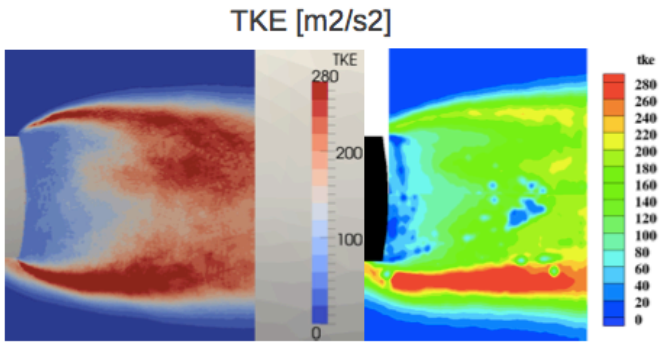
Validation against experiments





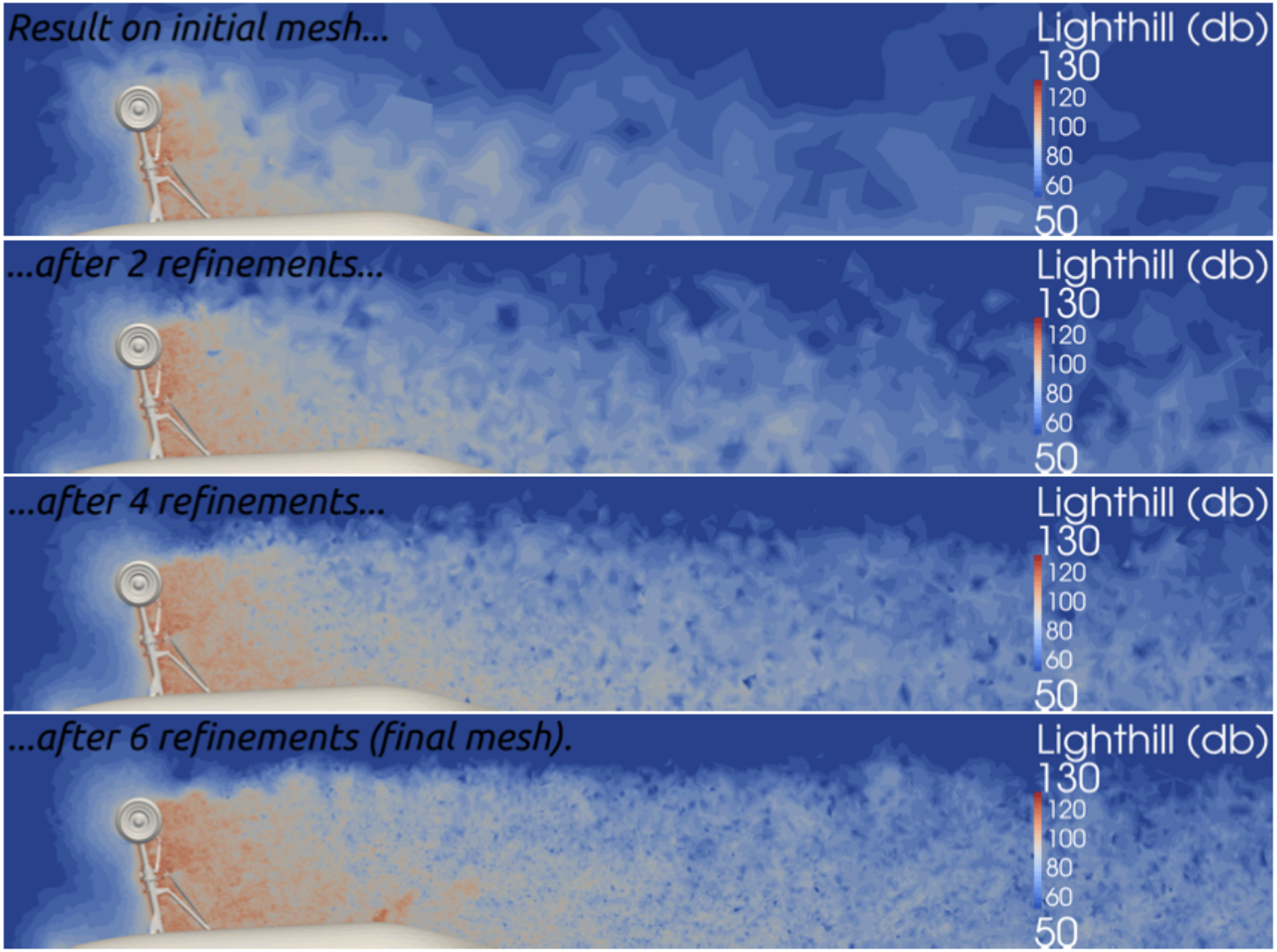




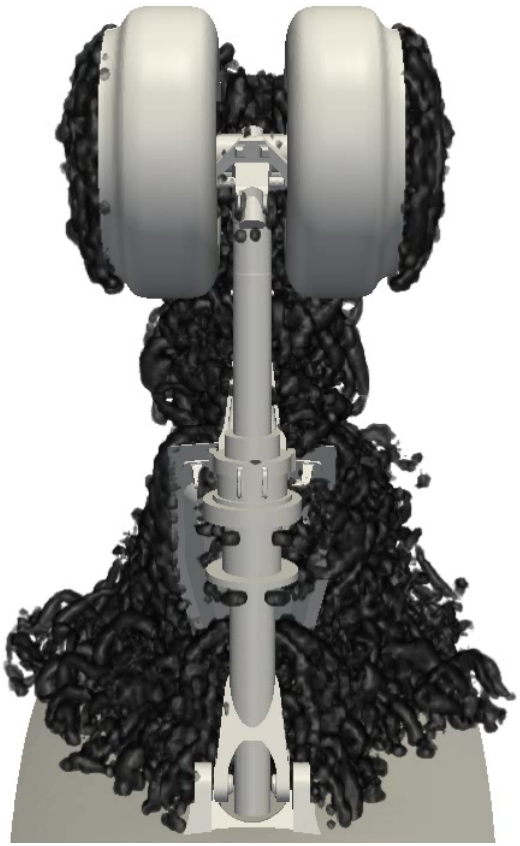


[Vilela De Abreu/Jansson/Hoffman BANC-II 2012, AIAA conference 2012]

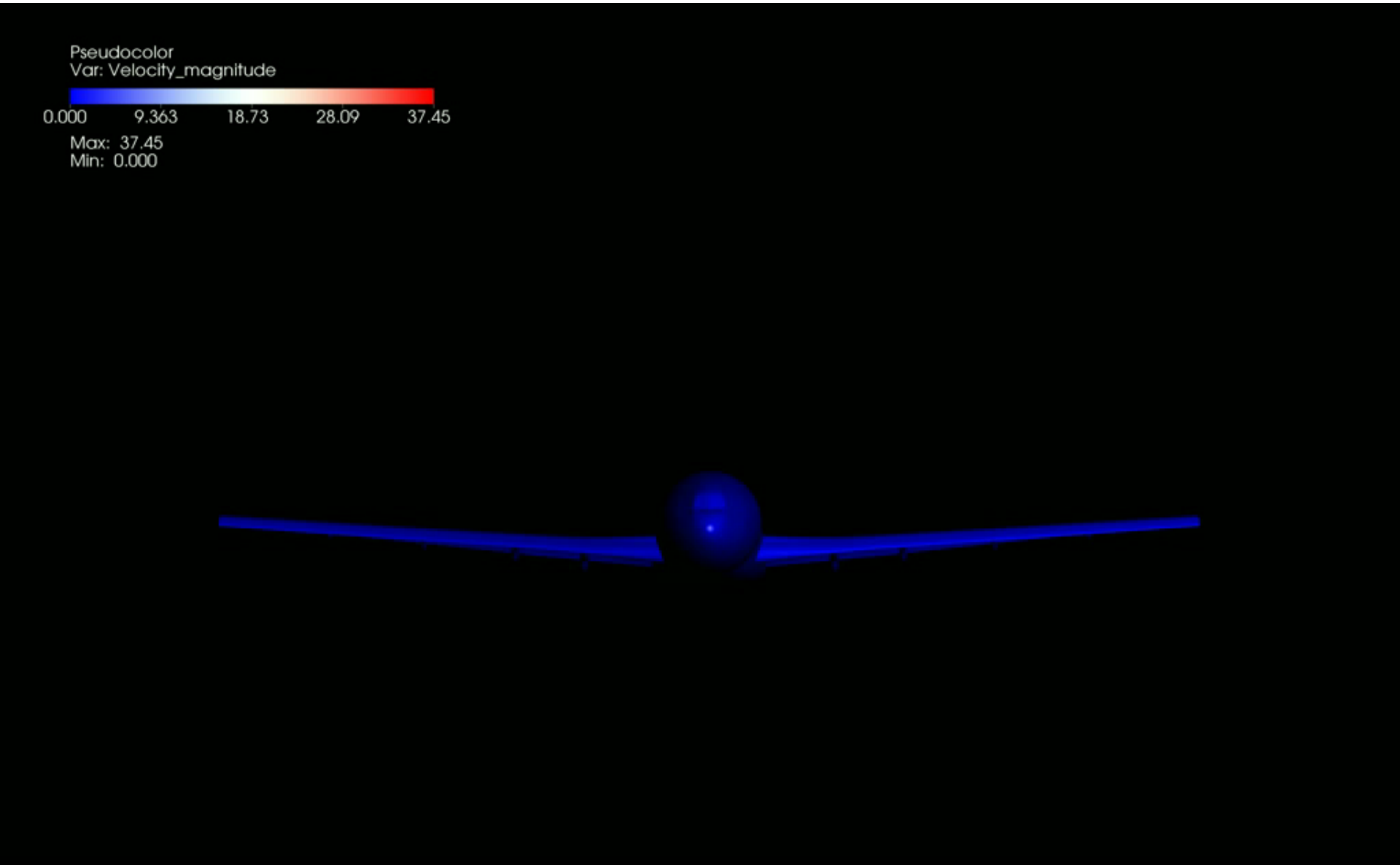
Lighthill source - mesh convergence



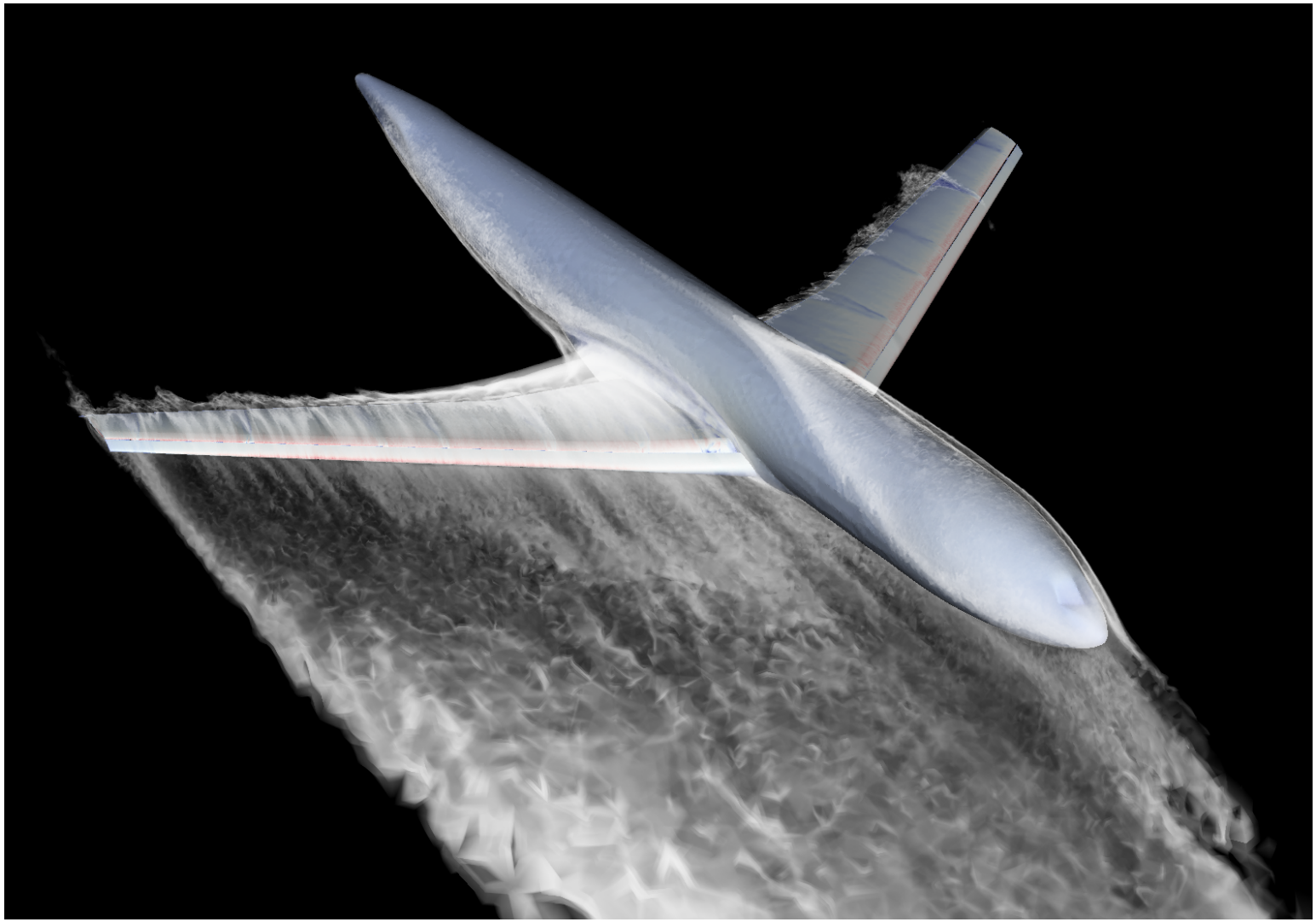
Lambda 2



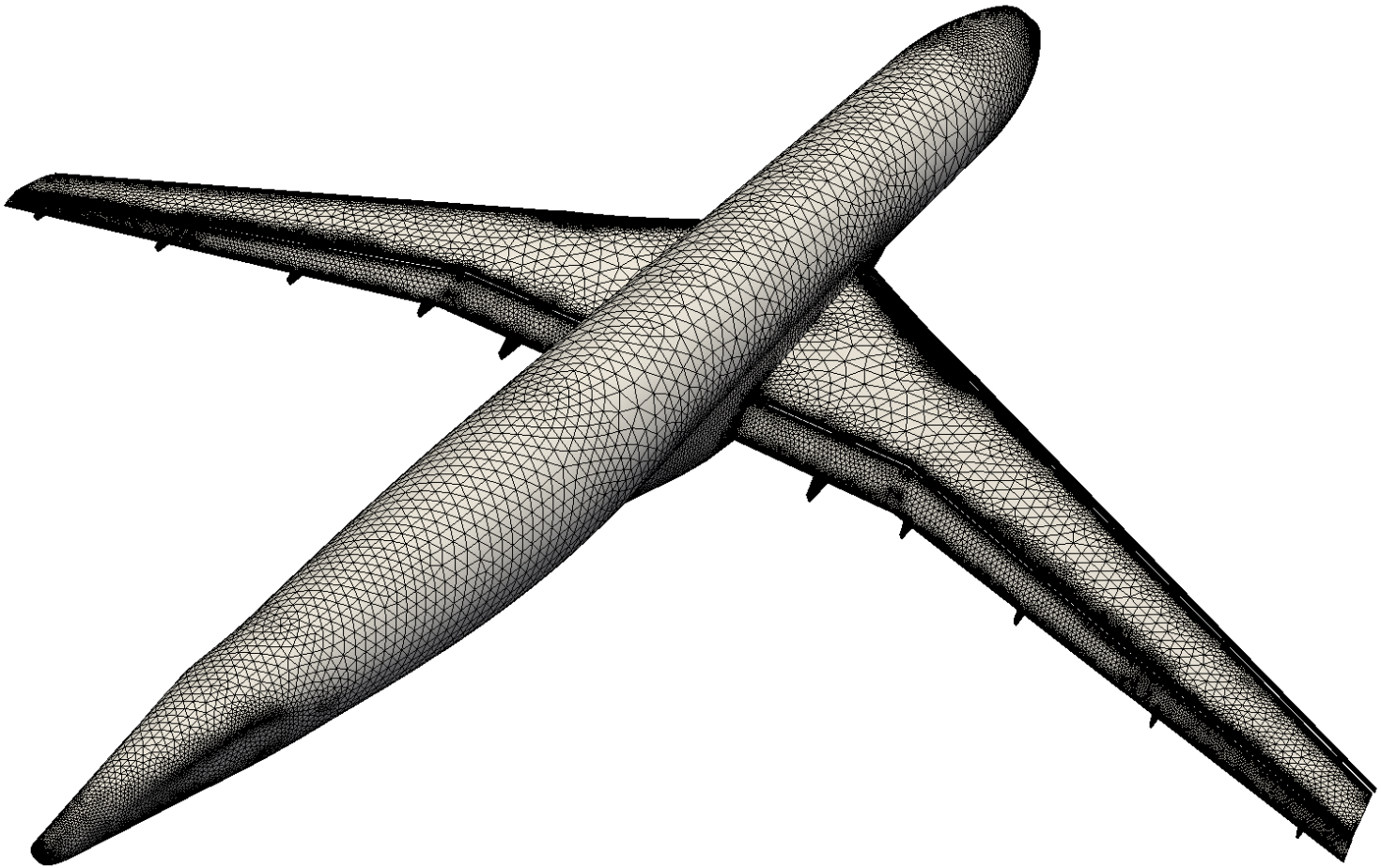
HiLiftPW-2 full aircraft aoa = 21°



Adjoint - drag of right halfplane

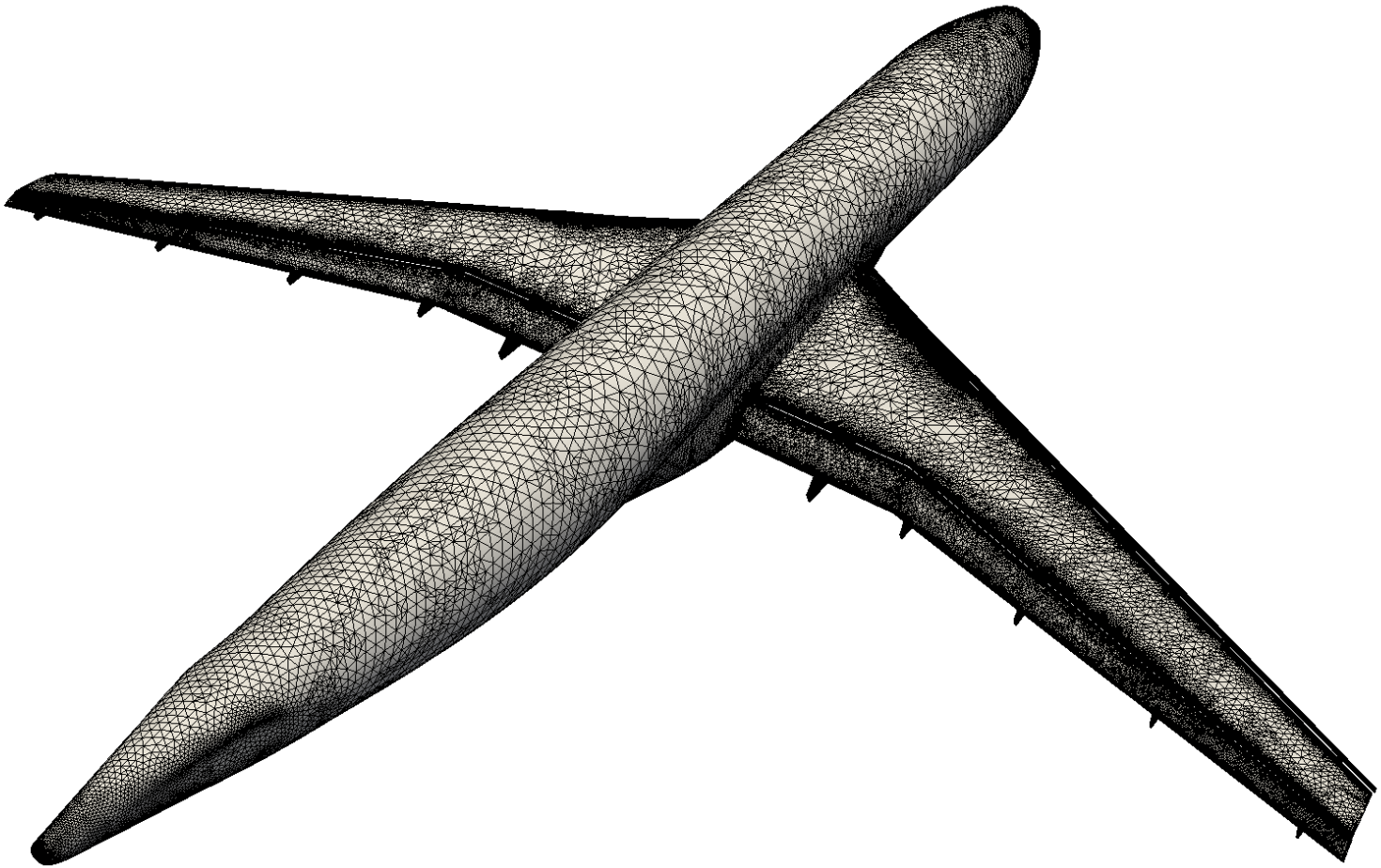


Mesh 700 k vertices



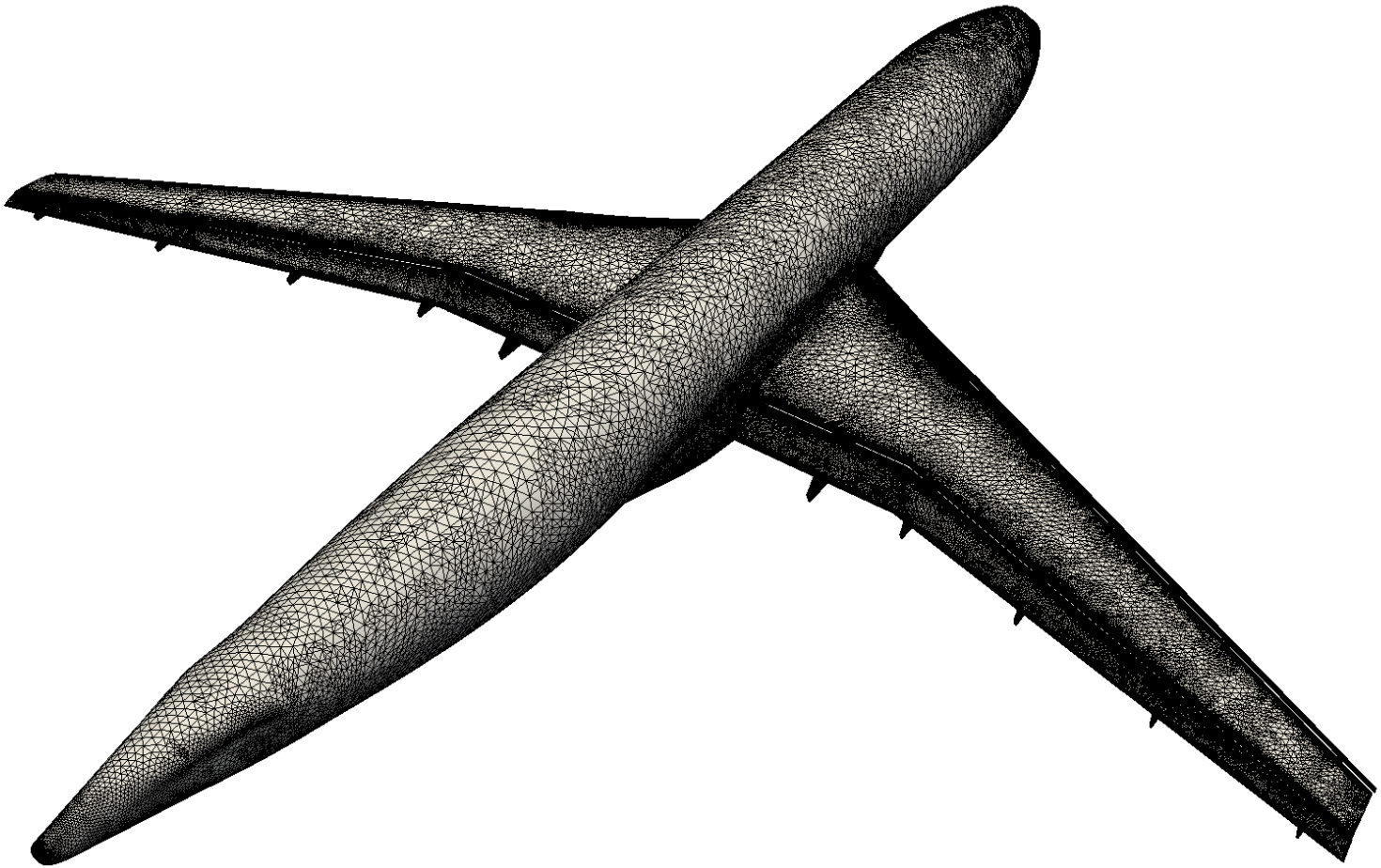
[Initial mesh by ANSA, postprocessing by SAAZ]

1.1 M vertices



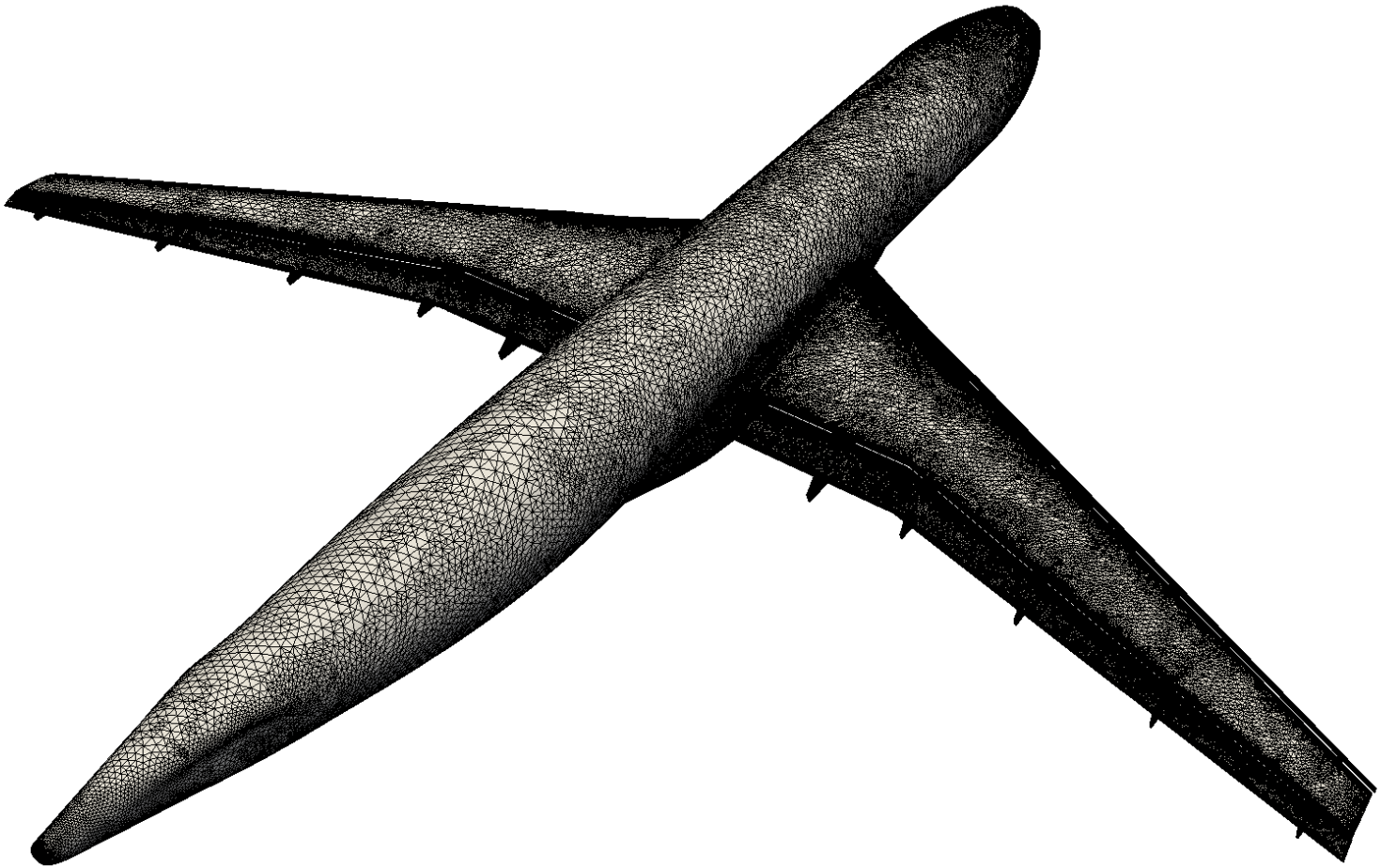
[Initial mesh by ANSA, postprocessing by SAAZ]

1.6 M vertices



[Initial mesh by ANSA, postprocessing by SAAZ]

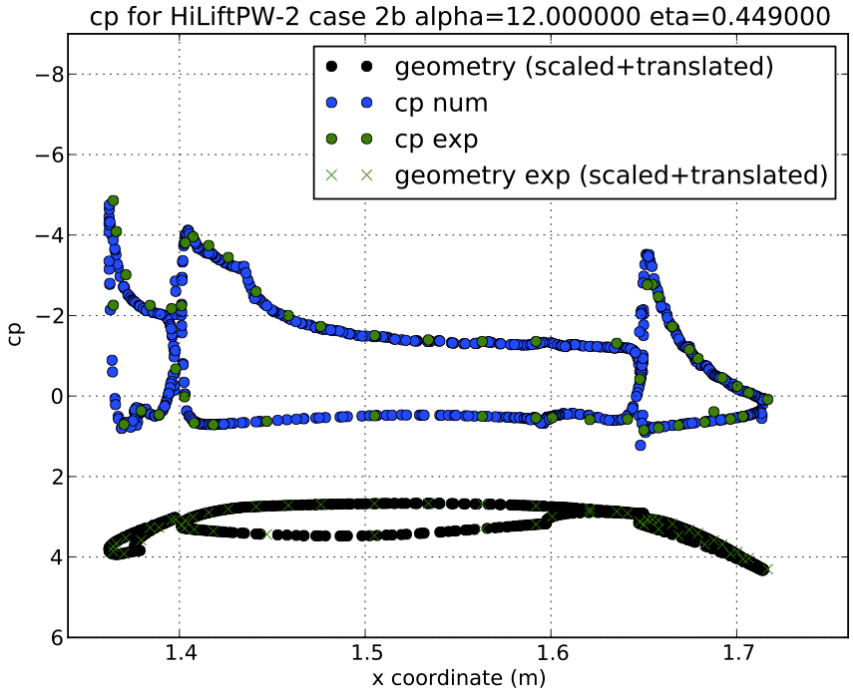
2.2 M vertices



[Initial mesh by ANSA, postprocessing by SAAZ]

3.1 M vertices

[Initial mesh by ANSA, postprocessing by SAAZ]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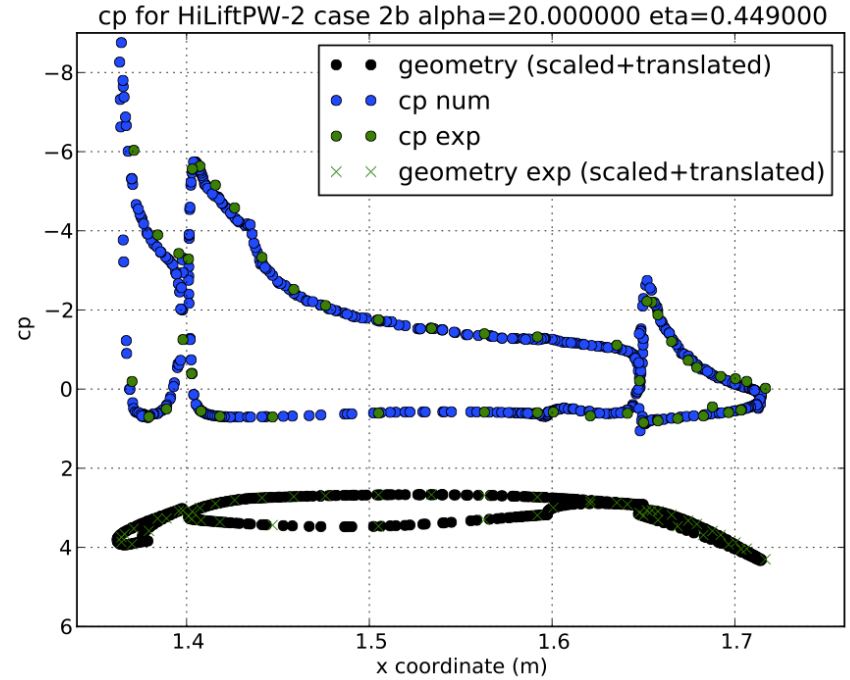
cp num
cp exp
geometry exp (scaled+translated)
cp
x coordinate (m)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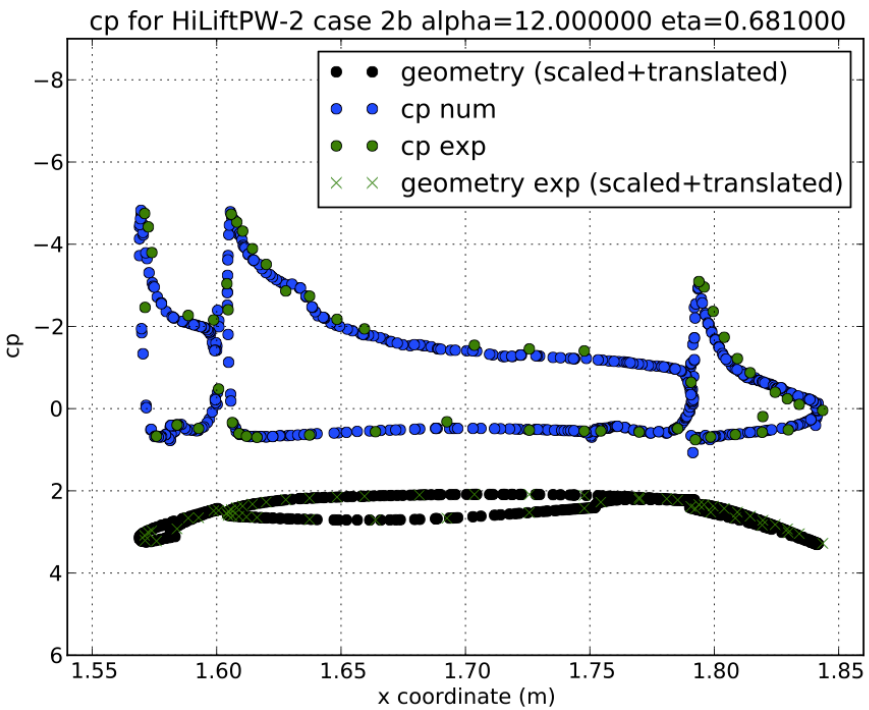
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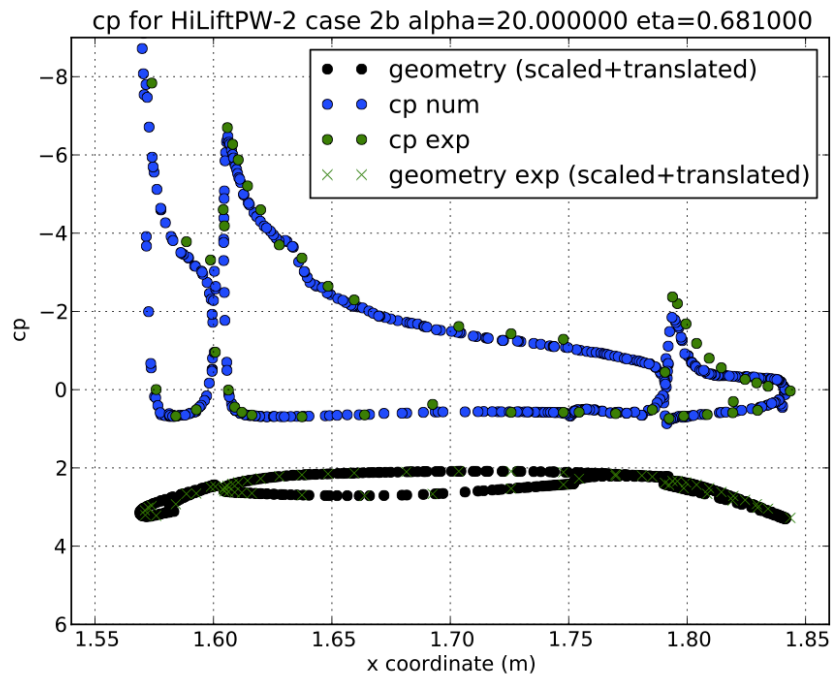
x coordinate (m)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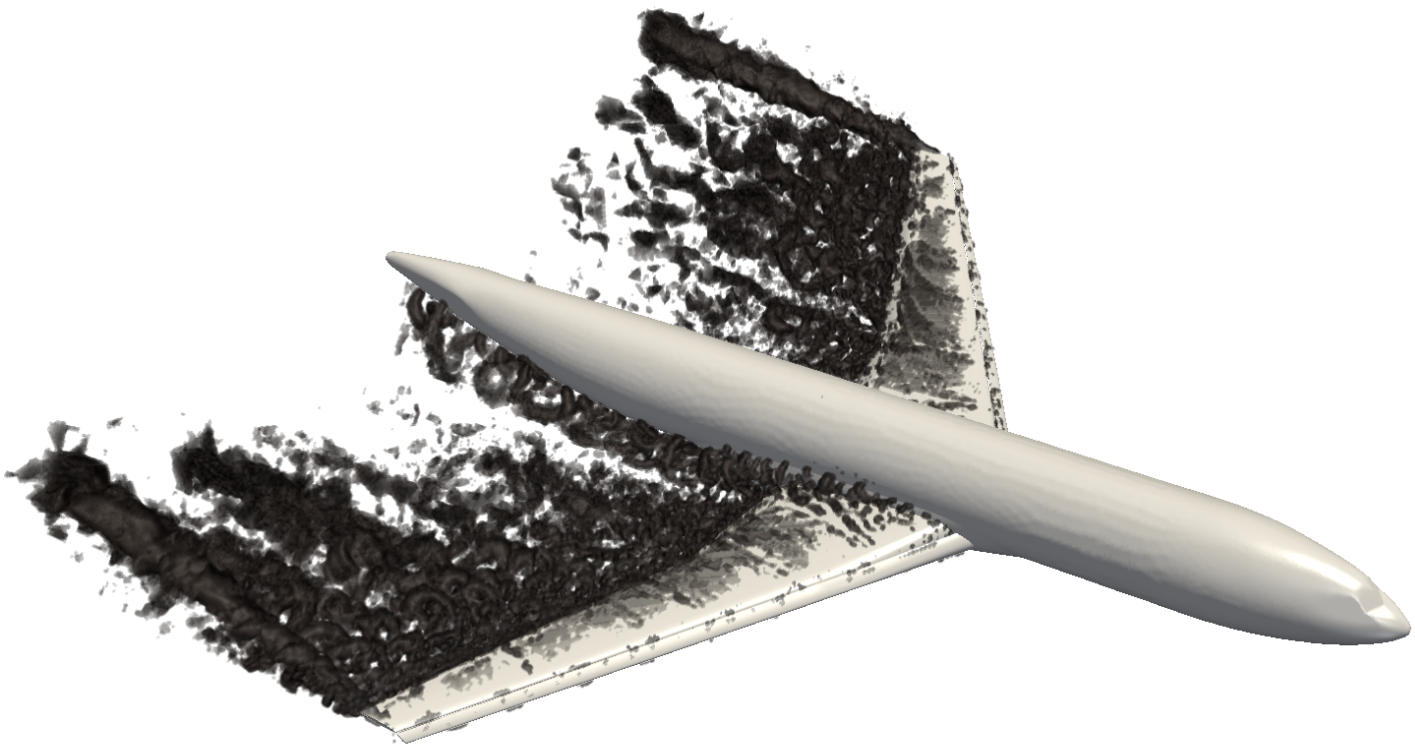
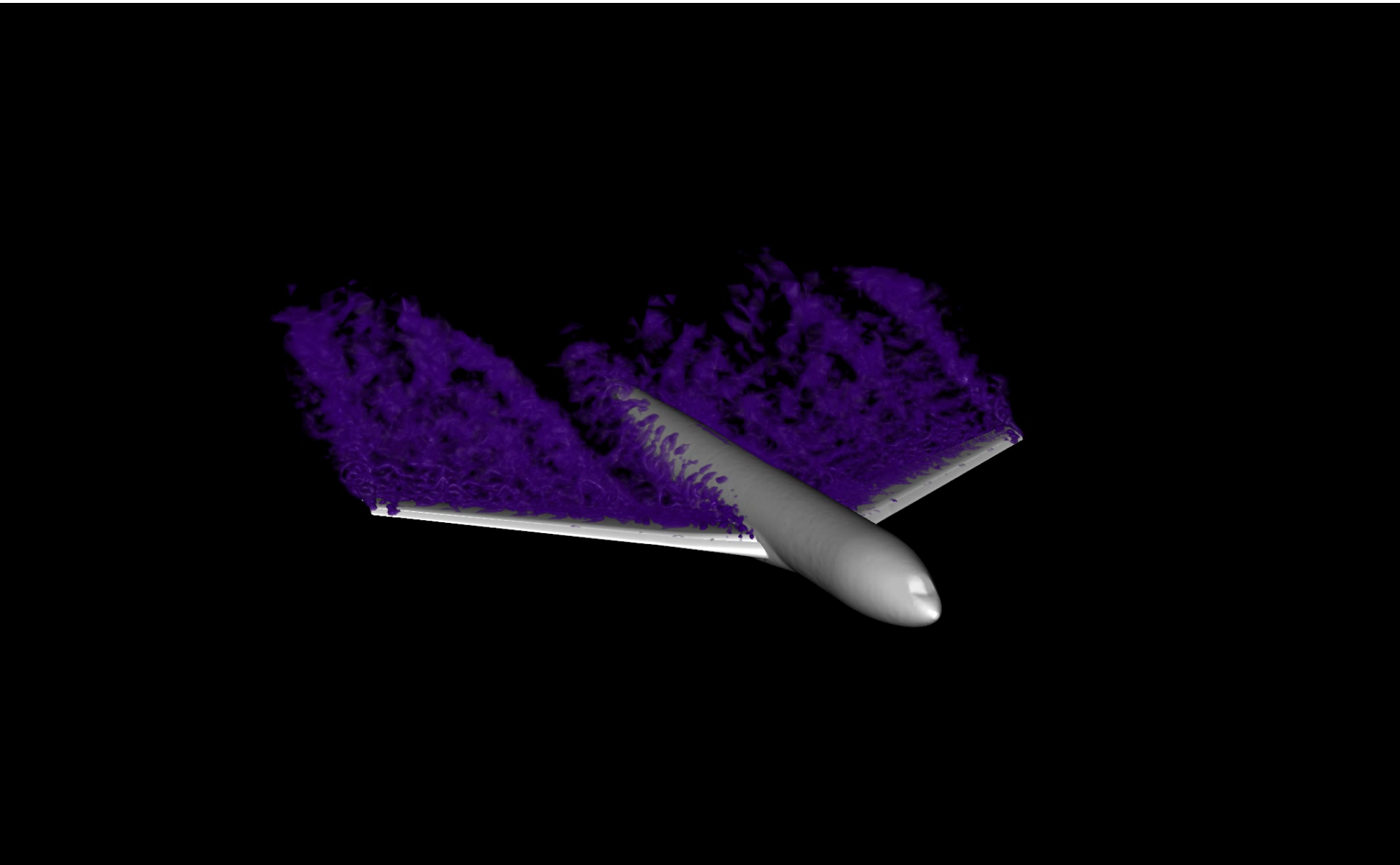
cp exp
geometry exp (scaled+translated)
cp
x coordinate (m)

HiLiftPW-2 aoa=12
(Lambda 2 visualization in an box)



HiLiftPW-2 aoa=12



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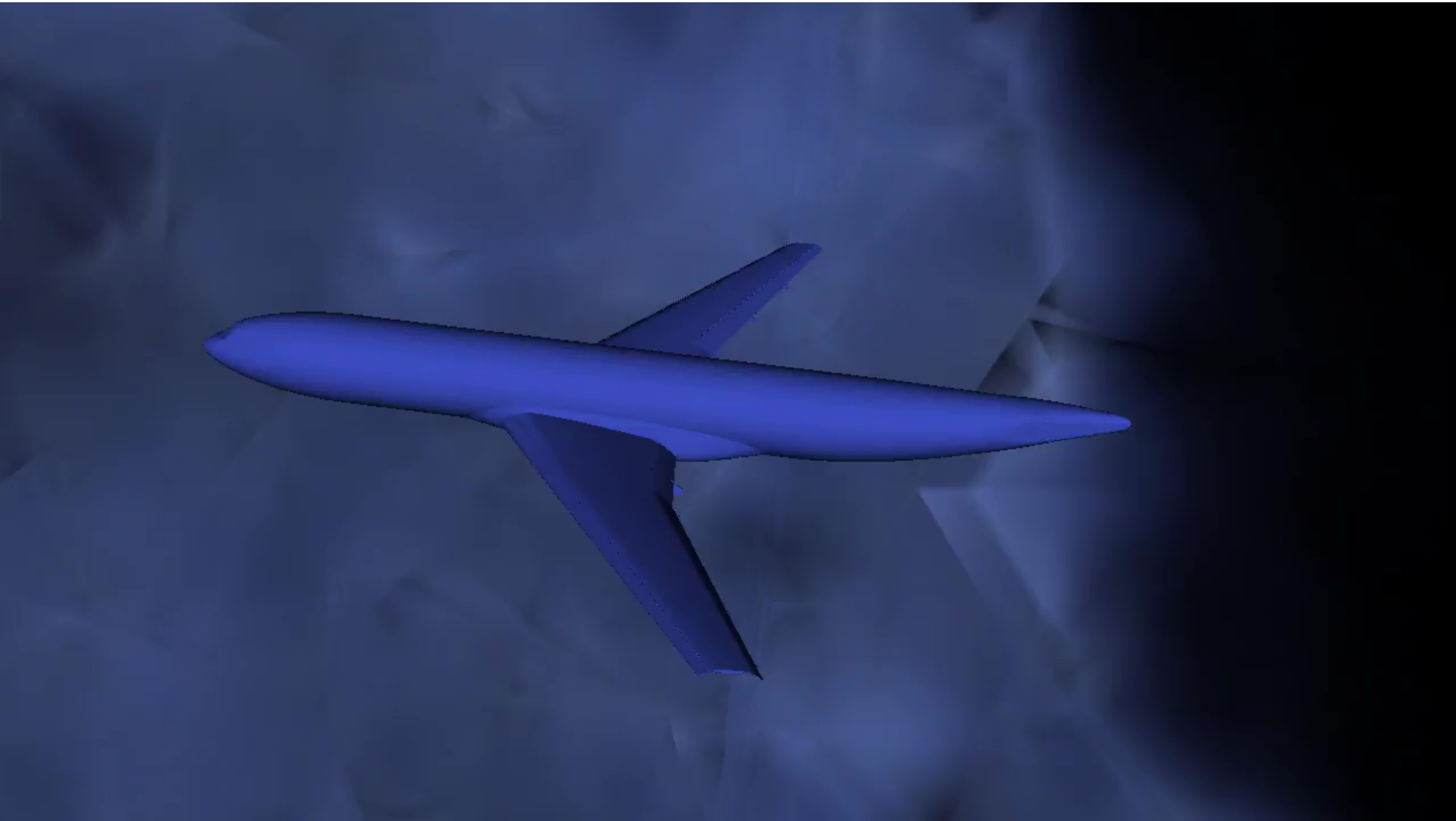

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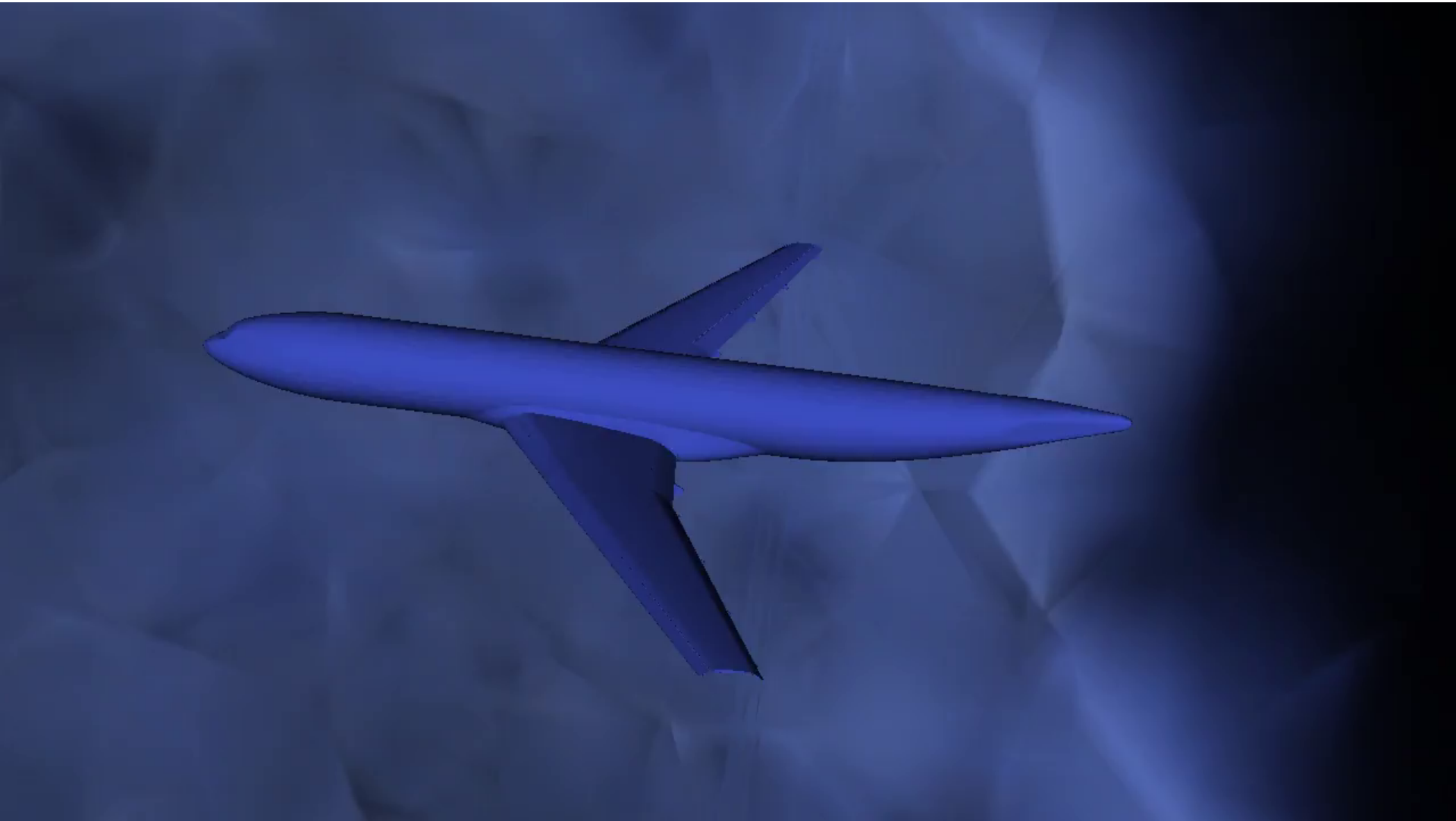
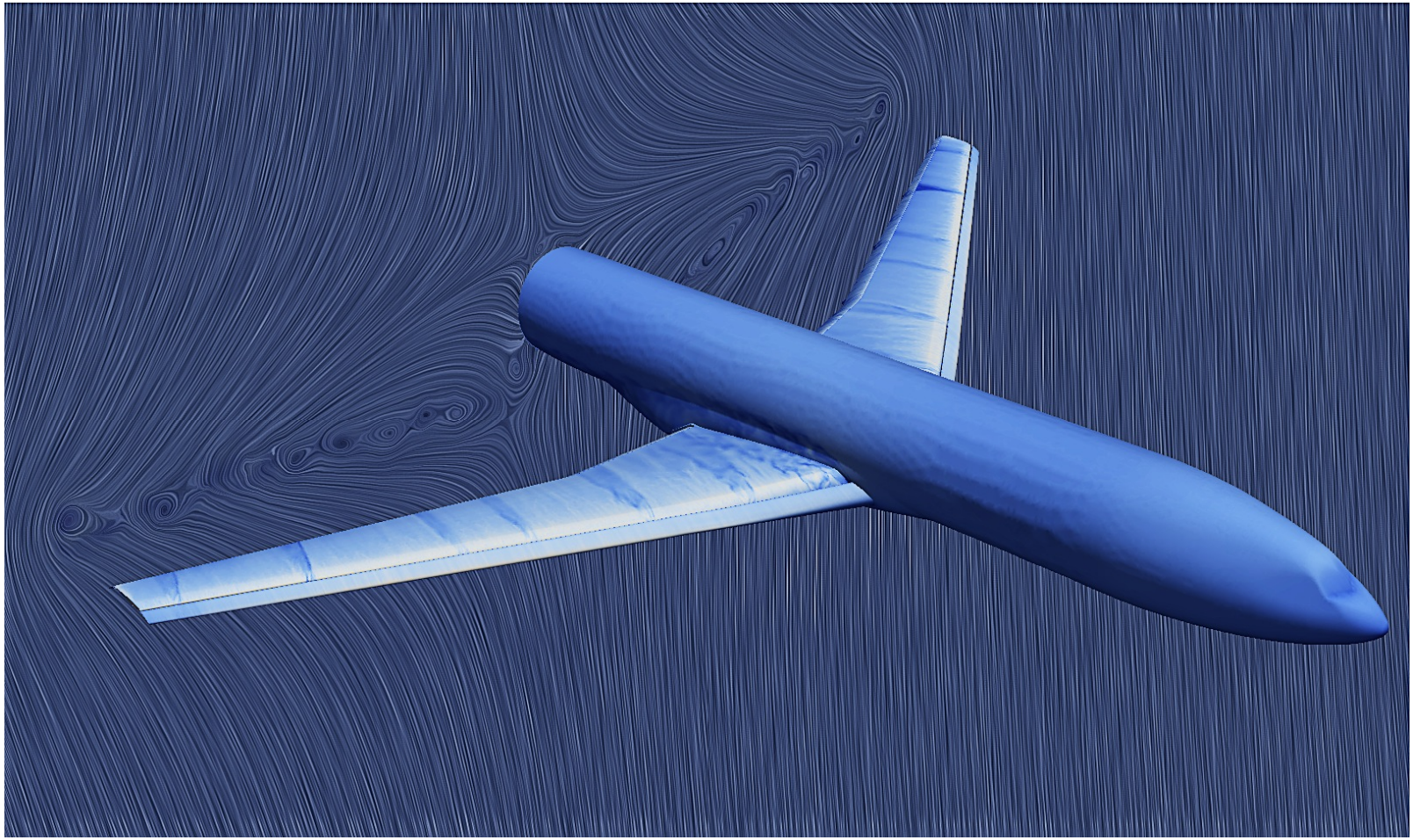
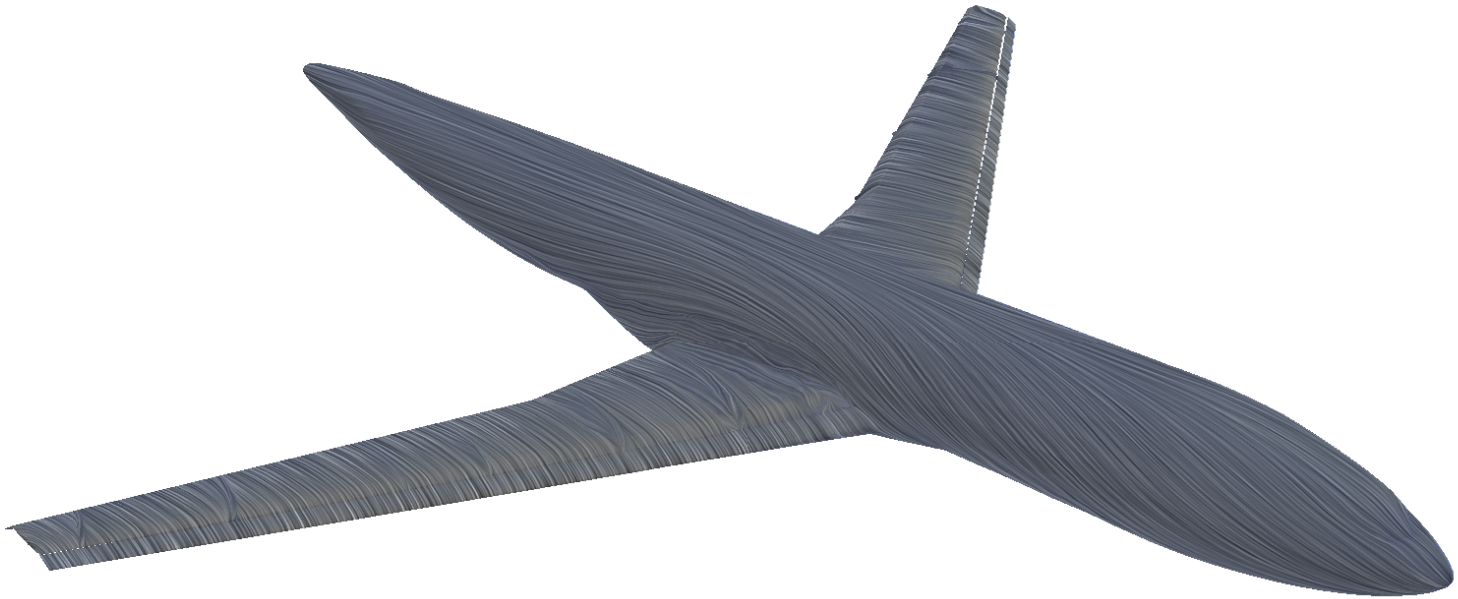


aoa = 12



Oilfilm visualization



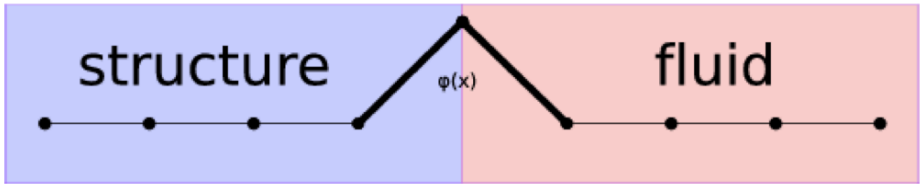
Unified Continuum FSI (UC-FSI)

[Hoffman/Jansson/Stöckli M3AS, 2011]

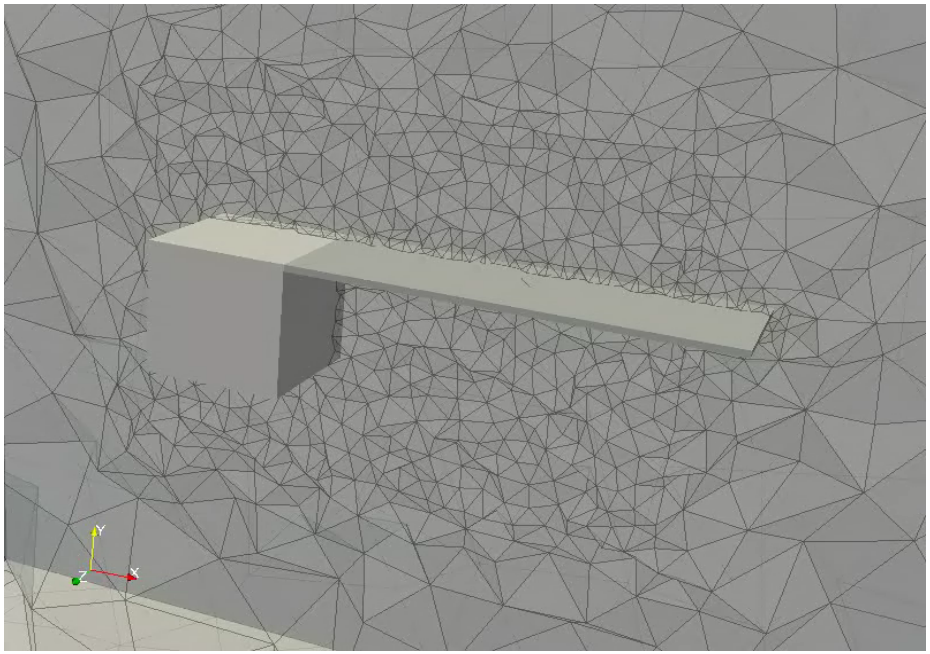
$$\rho\left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)=\frac{\partial}{\partial x_j}\sigma_{ij}+f_i,$$
$$\frac{\partial u_j}{\partial x_j}=0,$$
$$\frac{\partial \theta}{\partial t}+u_j\frac{\partial \theta}{\partial x_j}=0.$$

$$\sigma=\theta\sigma^f+(1-\theta)\sigma^s$$
$$\sigma_{ij}=\sigma^D_{ij}-p\delta_{ij}$$

$$\sigma^f_{ij}=2\mu_f\epsilon(u)_{ij}$$
$$\frac{\partial\sigma^s_{ij}}{\partial t}=2\mu_s\epsilon(u)_{ij}+\frac{\partial u_i}{\partial x_k}\sigma^s_{kj}+\sigma^s_{ik}\frac{\partial u_k}{\partial x_j}$$



- Mesh smoothing/local remeshing
- Validated for 2D benchmark [Turek]

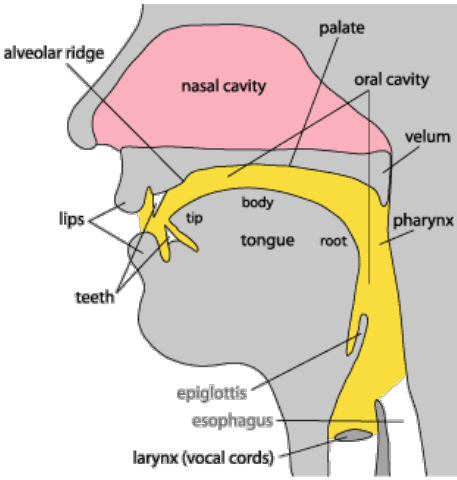


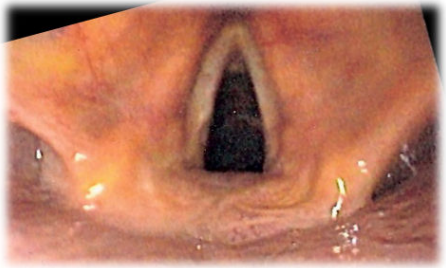
FP7 Eunison - the human voice

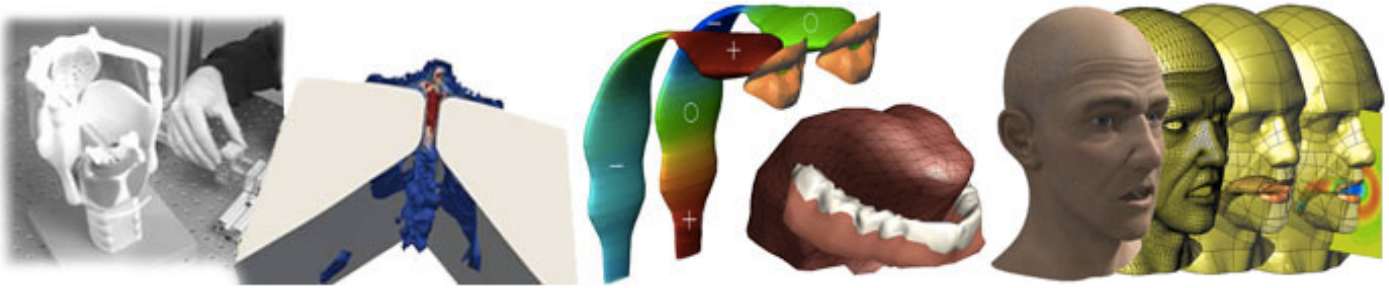
Goal: unified simulation of the human voice

- FSI of flow through vocal folds
- UC-FSI continuum contact model
- Acoustic propagation in vocal tract
- Implementation in FEniCS

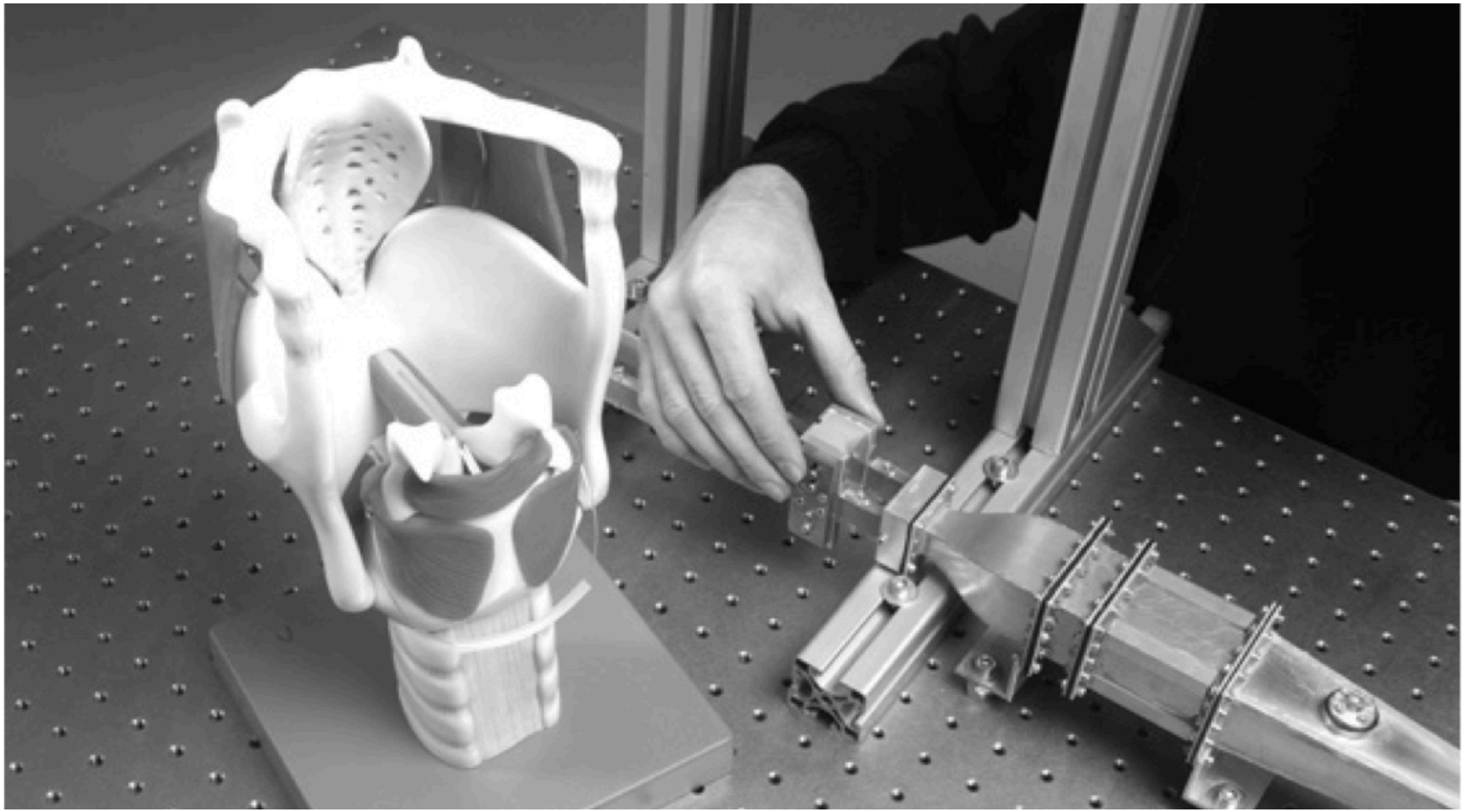
- Future and Emerging Technologies (FET)
- Partners: KTH, Erlangen (FAU), Grenoble (CNRS-GIPSA), Barcelona (CIMNE, La Salle)







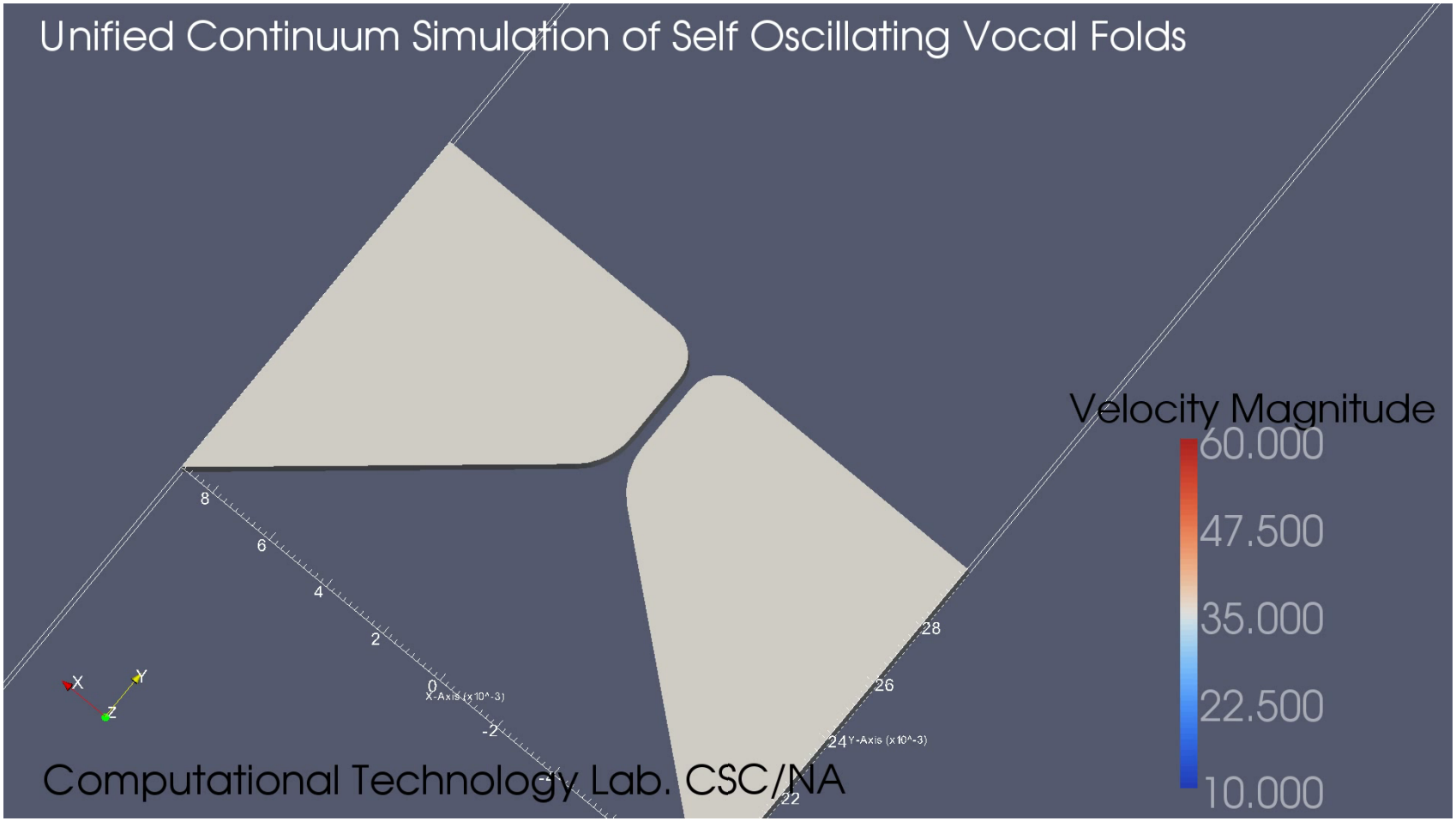
Vocal folds replica – FAU Erlangen



FSI: Self-oscillation with contact

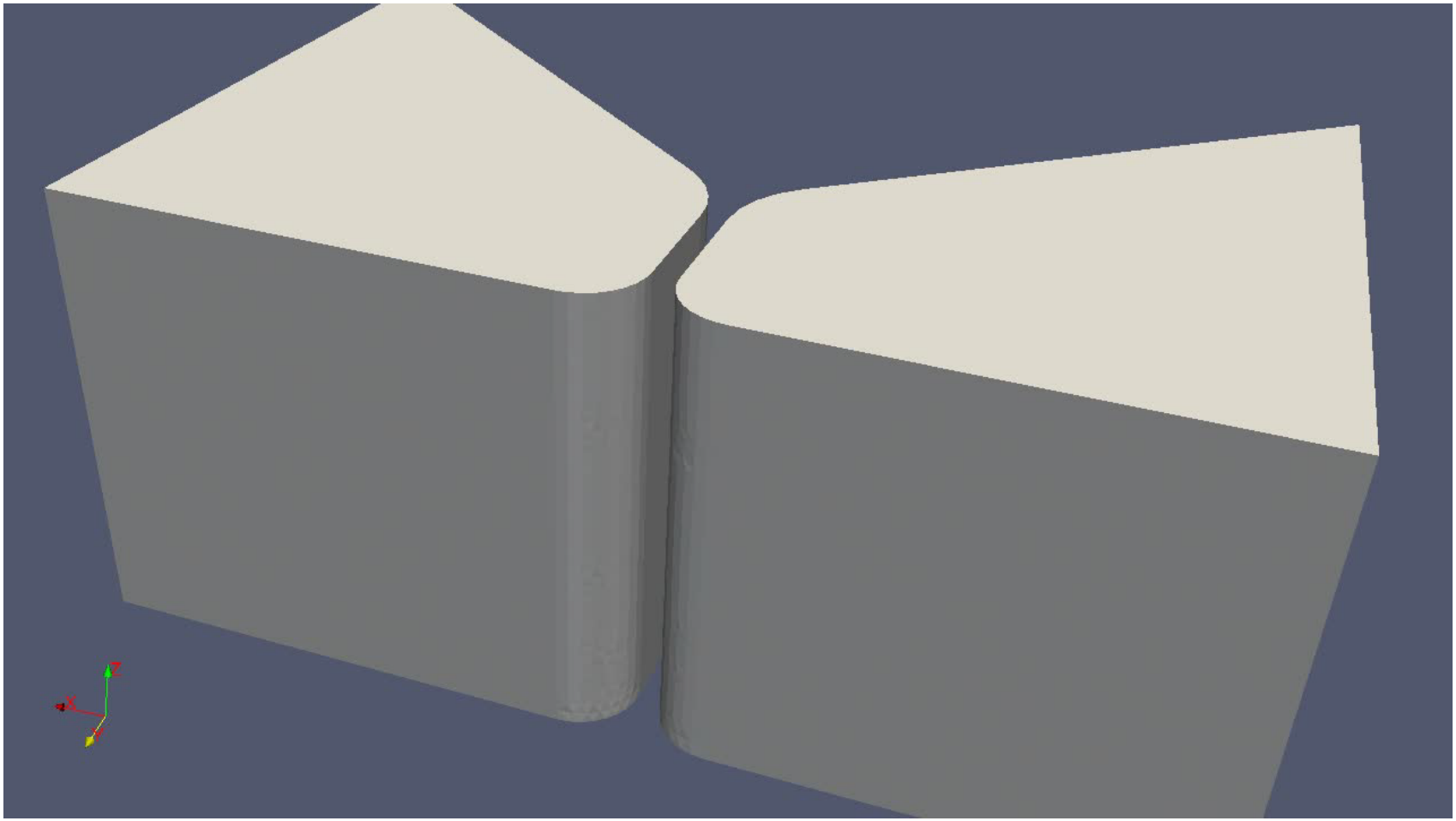
[C.Degirmenci/J.Jansson/JH, 2012]

FSI: Self-oscillation with contact



[C.Degirmenci/J.Jansson/JH]

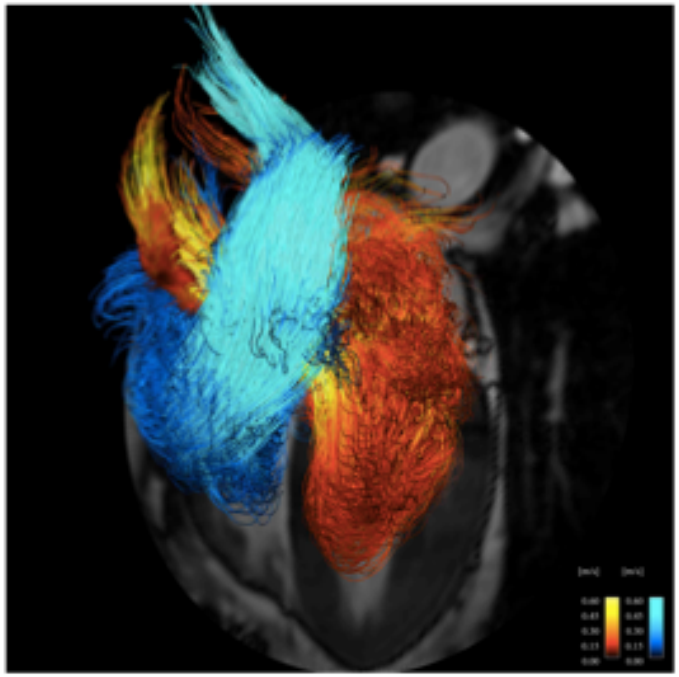
FSI: Self-oscillation with contact

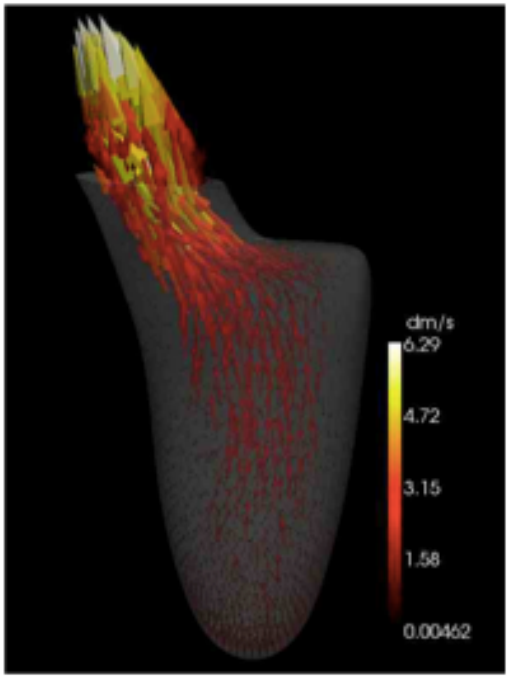


[C.Degirmenci/J.Jansson/JH]

Simulation in health care

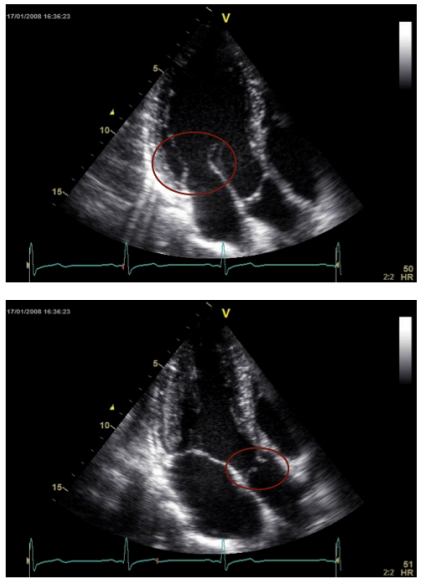
- Individualized diagnosis
- Treatment planning





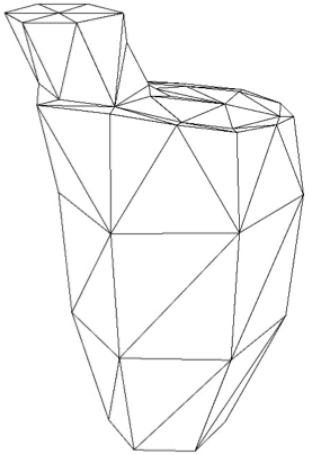
Patient specific LV heart model

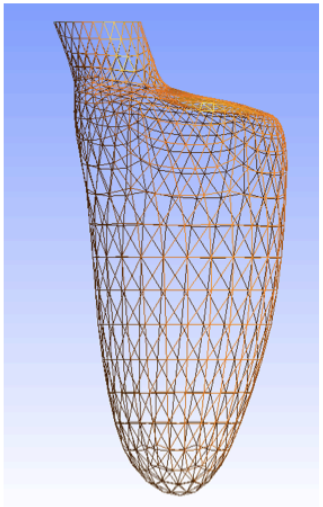
- Left ventricle (LV) geometry from ultrasound data
- Blood flow ALE simulation in deforming domain
- Validation: ultrasound, MRI, pressure measurements
- Basic research, decision support for diagnosis and treatment
- KTH-STH, Karolinska U Hospital, Umeå U, Linköping U

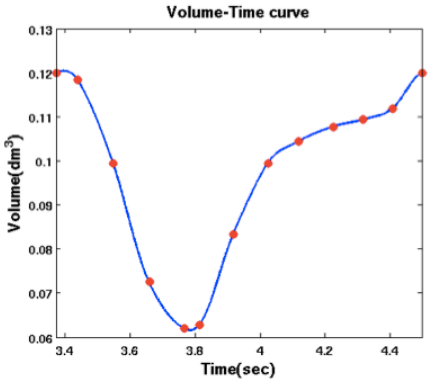


Diastole

Systole

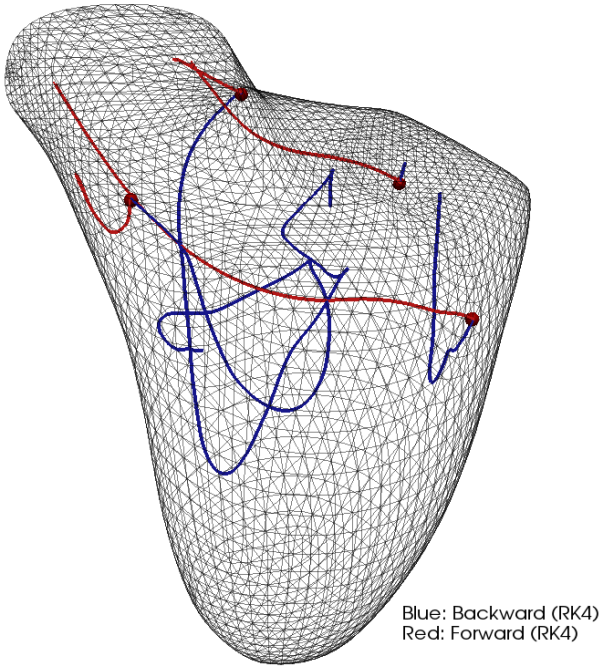


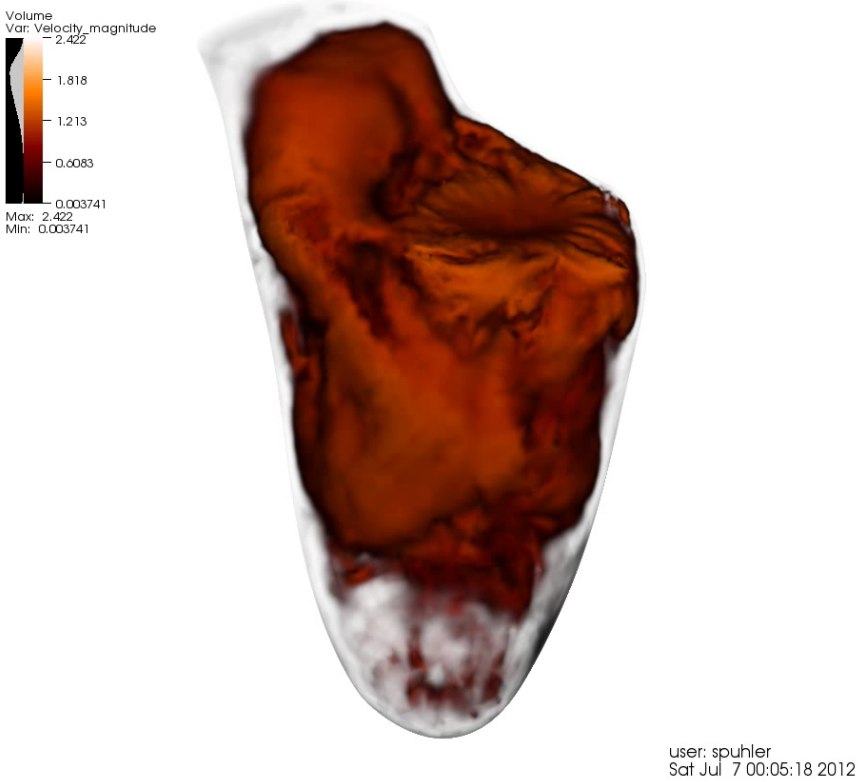


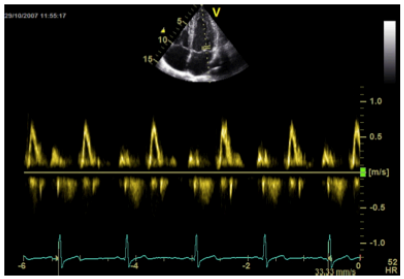


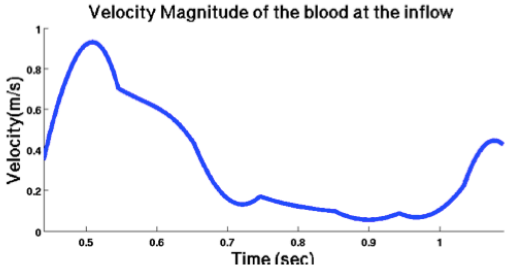
[P.Vesterlund/U.Gustafson/M.G.Larson (Umeå University)]

Blood flow in LV



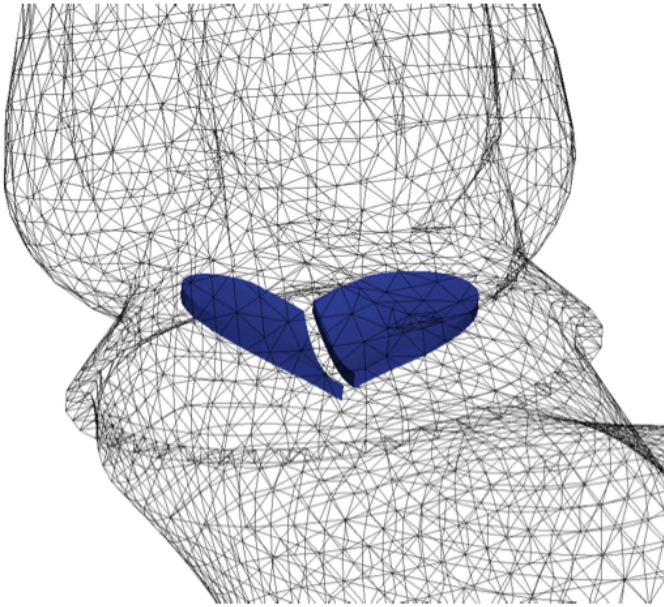




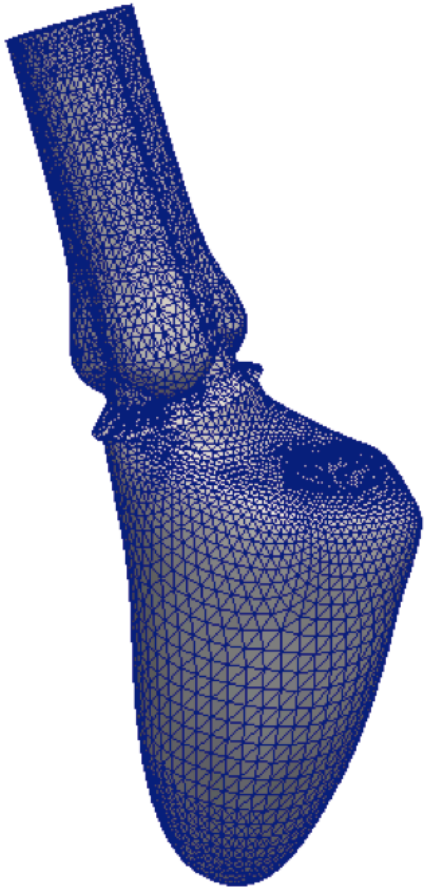


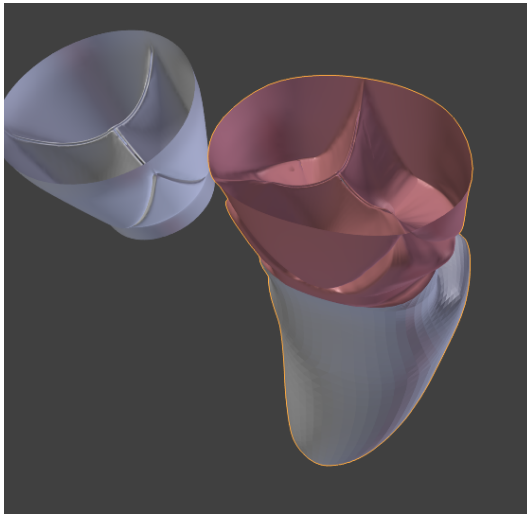
[J.Spühler/J.Jansson/N.Jansson/JH, 2012]

Embedding aortic heart valves



Mechanical bileaflet valves

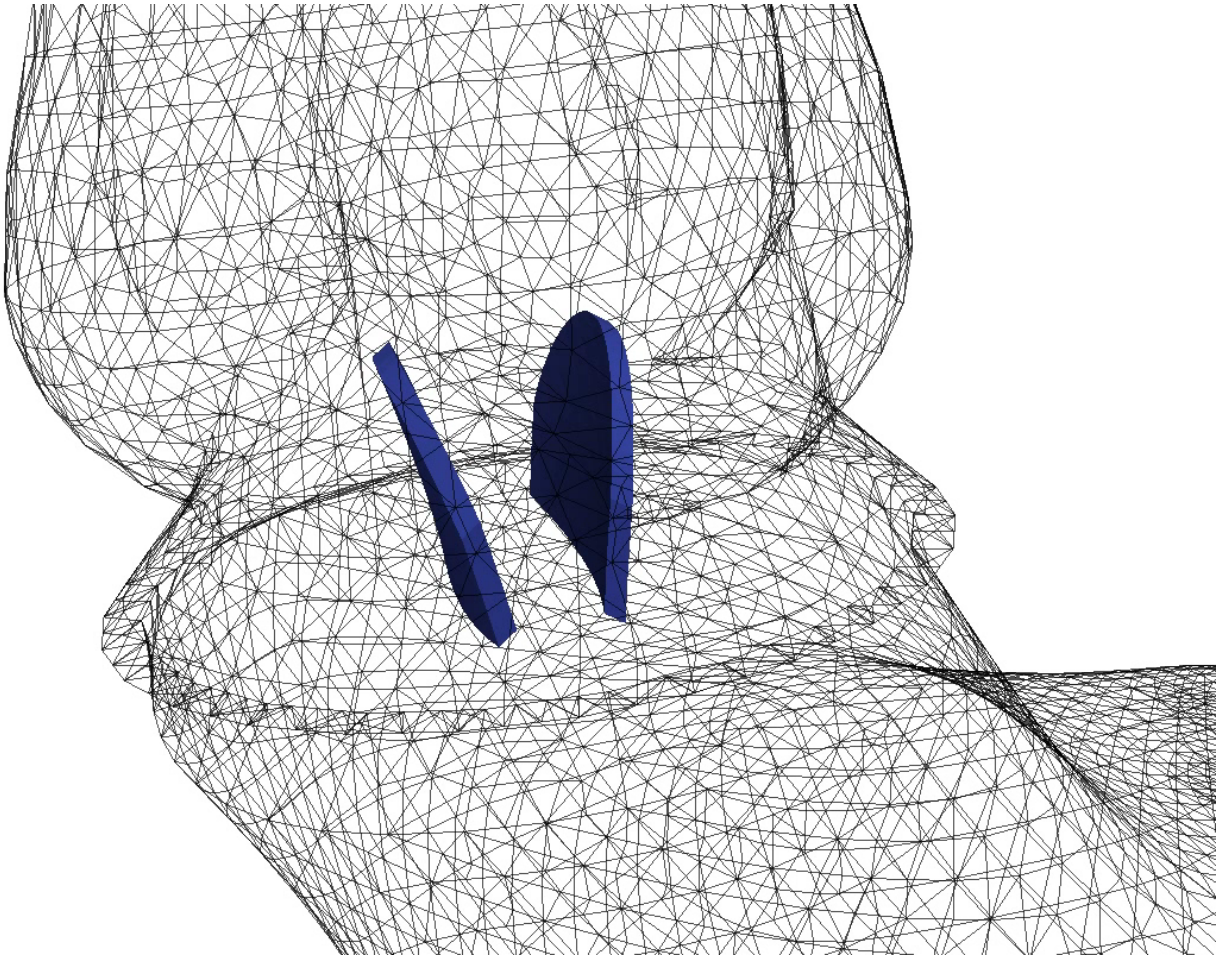




Biological aortic valves

[T.Nilsson/J.Spühler/J.Jansson/M.Broomé/P.Vesterlund/A.Waldenström/JH]

Work in progress



[T.Nilsson/J.Spühler/J.Jansson/M.Broomé/P.Vesterlund/A.Waldenström/JH]

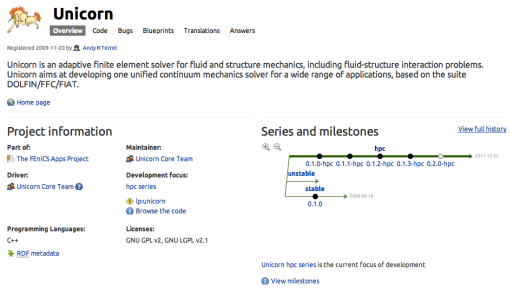
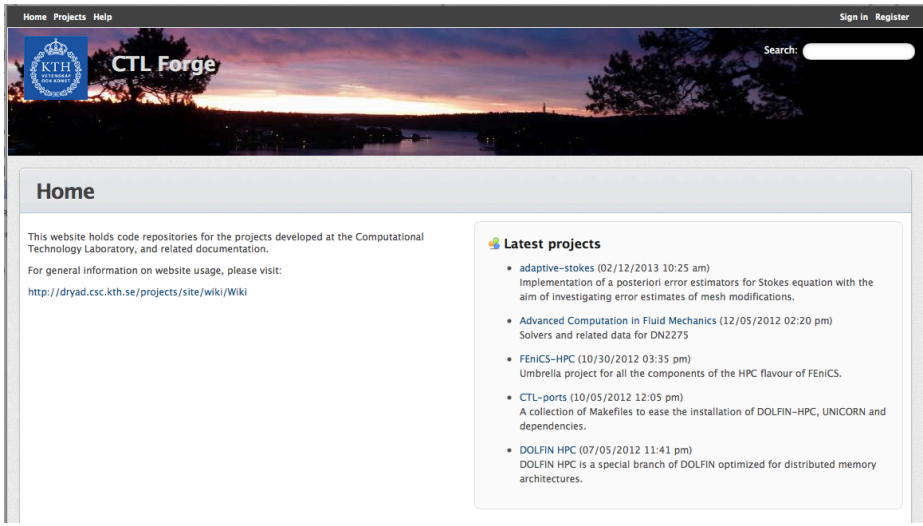
Interactive Visualization Demo

[F.Ioakeimidou, F.Ericson, J.Forsslund, A.Olwal, J.Spühler, J.Jansson, E.Sallnäs, JH]

FEniCS-HPC tool chain

- FEniCS-HPC tool chain: FIAT FFC **DOLFIN(-HPC) Unicorn**
- Fully distributed unstructured mesh, parallel I/O with MPI
- Hybrid parallel model MPI-OpenMP/MPI-PGAS
- LA back-end: PETSc, **Janpack** (MPI+PGAS)
- A posteriori error estimation based on adjoint problems
- Parallel adaptive mesh refinement, ALE moving mesh
- Turbulent flow, fluid-structure interaction, contact models
- Today installed at supercomputing centers in Sweden (under way: Finland, Spain,…)
- Central for a number of application projects: aerodynamics, aeroacoustics, geophysics and biomedcine

FEniCS-HPC tool chain



- Unicorn
- DOLFIN(-HPC)
- Janpack
- All projects available at fenicsproject.org/Launchpad (through Unicorn [https://launchpad.net/unicorn]) or at CTL Forge [http://dryad.csc.kth.se] (git/Redmine)