# FEniCS at KTH: projects, challenges and future plans

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# Overview

- FEniCS at KTH today
- A FEniCS prototype
- Ongoing projects
- Challenges
- Future plans

# FEniCS at KTH today

- JH + JJ + 1 PhD + 3 MSc
- Dag Lindbo/Gunilla Kreiss - 2-phase flow/level set
- 1 PhD/Anders Szepessy - Hamilton Jacobi eqns.
- 1 PhD/Dan Henningsson (JH) - transition
- 1 MSc/Luca Brandt (JH) - optimal disturbances
- Gustav Amberg group (Femlego) - testing
- MSc FEM course (JH) - Puffin ($\rightarrow$ Dolfin/FFC/FIAT)
- MSc CFD project course (JJ?) - Dolfin/FFC/FIAT
- Wide general interest in the project

# TACO - Techn. for Advanced Comp.

- Johan Hoffman
- Johan Jansson
- Murtazo Nazarov (PhD): compressible turbulence
- Oana Marin (MSc): free surface flow, level sets
- Alessio Quaglino (MSc): large def. solid mech., contact
- Michael Stöckli (MSc): fluid-structure, ALE

# TACO - Techn. for Advanced Comp.

TACO projects today:

- G2: turbulent flow in complex geometries
- G2: friction bc for turbulent flow
- G2: thermodynamics (turbulent compressible flow)
- Mesh refinement/coarsening/smoothing/flipping/...
- Free surface flow/level set
- ALE fluid structure interaction
- Large deformation structure mechanics/contact

# A FEniCS prototype

Vision of FEniCS: automation of

- ☐ discretization: done?
- ☐ discrete solver
- ☐ adaptivity/error control
- ☐ modeling
- ☐ optimization

# A FEniCS prototype

Vision: Automation of

- discretization:
  1. DE $\longrightarrow$ Form: not done?
  2. Form $\longrightarrow$ element matrix: FFC/FIAT
- discrete solver: not done?
- adaptivity/error control: not done?
- modeling: not done?
- optimization: not done?

# A FEniCS prototype

FEniCS prototype for turbulent flow: Dolfin NSE solver

- discretization:
  1. DE $\longrightarrow$ Form: General Galerkin G2
  2. Form $\longrightarrow$ element matrix: FFC/FIAT
- discrete solver: not done (PETSc + MG)
- adaptivity/error control: mesh refinement based on output error control by duality.
- turbulence modeling: G2
- optimization: not done

# Navier-Stokes Equations (NSE)

$$R(\hat{u}) = \begin{pmatrix} \dot{u} + u \cdot \nabla u - \nu \Delta u + \nabla p - f \\ \nabla \cdot u \end{pmatrix} = 0$$

$\hat{u} = (u, p)$: $u$ velocity, $p$ pressure, $\nu$ viscosity, $f = 0$

- Pointwise existence & uniqueness unknown: $R(\hat{u}) = 0$ (Clay Institute $1 million Prize Problem)
- Existence (but not uniq.) of weak solution (Leray 1934):

Find $\hat{u} \in \hat{V}$ : $\quad (R(\hat{u}), \hat{v}) = 0 \quad \forall \hat{v} = (v, q) \in \hat{V}$

$(R(\hat{u}), \hat{v}) \equiv (\dot{u}, v) + (u \cdot \nabla u, v) - (\nabla \cdot v, p) + (\nabla \cdot u, q) + (\nu \nabla u, \nabla v)$

$\hat{V} \subset H^1(Q)$, $Q = \Omega \times I$, $(v, w) = (v, w)_Q \equiv \int_Q v \cdot w \, dxdt$

# Turbulent incompressible flow

Typical scientific goals of today:

- Prove exist & uniq of pointwise NSE: $R(\hat{u}) = 0$
- Push limit of DNS (wrt $Re^3$ constraint, $Re = UL/\nu$)
- Turbulence modeling: find model for unresolved scales (filtering of NSE: Reynolds stresses, closure problem)

Alternative scientific goals:

- Approximate weak solution $\hat{U}$: weak uniqueness in (mean value) output $M(\hat{U})$: stability of $\hat{U}$ wrt $M(\cdot)$
- Adaptive algorithm: min #dof : $error(M(\hat{U})) < TOL$

# Existence of $\epsilon$-Weak Solutions

- $W_\epsilon = \{\hat{u} \in \hat{V} : |(R(\hat{u}), \hat{v})| \leq \epsilon \|\hat{v}\|_{\hat{V}} \quad \forall \hat{v} \in \hat{V} \subset H^1\}$

  (approximate weak solution: $\sim \|R(\hat{u})\|_{H^{-1}} \leq \epsilon$)

- Existence: Construction of $W_\epsilon$: General Galerkin G2

- Find $\hat{U} \in \hat{V}_h$: $\quad (R(\hat{U}), \hat{v}) + (hR(\hat{U}), R(\hat{v})) = 0 \quad \forall \hat{v} \in \hat{V}_h$

$$\frac{1}{2}\|U(t)\|^2 + ||\sqrt{\nu}\nabla U||_Q^2 + ||\sqrt{h}R(\hat{U})||_Q^2 = \frac{1}{2}\|U(0)\|^2$$

$$\begin{aligned}(R(\hat{U}), \hat{v}) &= (R(\hat{U}), \hat{v} - \pi_h \hat{v}) - (hR(\hat{U}), R(\pi_h \hat{v})) \\ &\leq (C + M_U)\, ||hR(\hat{U})||_Q\, \|\hat{v}\|_{\hat{V}} \leq C\sqrt{h}\, \|\hat{v}\|_{\hat{V}}\end{aligned}$$

- $\hat{U} \in$ G2 $\Rightarrow \hat{U} \in W_\epsilon \qquad \epsilon = (C + M_U)\, ||hR(\hat{U})||_Q$

# Weak Uniqueness: Duality

- Output (functional): $M(\hat{u}) \equiv (\hat{u}, \hat{\psi})$ (e.g. drag or lift)
- Adjoint Navier-Stokes equations (given by NSE):

Find $\hat{\varphi} = (\varphi, \theta)$ : $\quad a(\hat{u}, \hat{w}; \hat{v}, \hat{\varphi}) = M(\hat{v}) \quad \forall \hat{v} = (v, q) \in \hat{V}$

$$\begin{aligned} a(\hat{u}, \hat{w}; \hat{v}, \hat{\varphi}) \equiv & (\dot{v}, \varphi) + (u \cdot \nabla v, \varphi) + (v \cdot \nabla w, \varphi) \\ & - (\nabla \cdot \varphi, q) + (\nabla \cdot v, \theta) + (\nu \nabla v, \nabla \varphi) \end{aligned}$$

- Weak Uniqueness: $\hat{u}, \hat{w} \in W_\epsilon, \quad S_\epsilon(\hat{\psi}) \equiv \max_{\hat{u}, \hat{w} \in W_\epsilon} \|\hat{\varphi}\|_{\hat{V}}$

$$\begin{aligned} |M(\hat{u}) - M(\hat{w})| &= |a(\hat{u}, \hat{w}; \hat{u} - \hat{w}, \hat{\varphi})| \\ &= |(R(\hat{u}), \hat{\varphi}) - (R(\hat{w}), \hat{\varphi})| \leq 2\epsilon S_\epsilon(\hat{\psi}) \end{aligned}$$

- Exact solution ($\epsilon = 0$): stability information lost!

# Weak Uniqueness: Duality

- Weak Uniqueness: $\hat{u}, \hat{w} \in W_\epsilon$

$$|M(\hat{u}) - M(\hat{w})| \leq 2\epsilon S_\epsilon(\hat{\psi}) \quad \|R(\hat{u})\|_{H^{-1}}, \|R(\hat{w})\|_{H^{-1}} \leq \epsilon$$

- Computability: $\hat{u} \in W_\epsilon$ and $\hat{U} \in \ G2$

$$|M(\hat{u}) - M(\hat{U})| \ \leq \ (\epsilon + \epsilon_{G2})\ S_{\epsilon_{G2}}(\hat{\psi}) \quad \epsilon_{G2} = C\|hR(\hat{U})\|$$

- Residual only needs to be small in a weak norm!!! (for weak uniqueness)
- $\|R(\hat{u})\|_{H^{-1}}$ & $\|hR(\hat{U})\|_{L_2}$ vs $\|R(\hat{u})\|_{L_2}$
- Weak uniqueness characterized by stability factor $S_\epsilon(\hat{\psi})$

# Automation of turbulence simulation

NSE: $R(\hat{u}) = 0$

G2: $\hat{U} \in \hat{V}_h : (R(\hat{U}), \hat{v}) + SD_\delta(\hat{U}; \hat{v}) = 0 \quad \forall \hat{v} \in \hat{V}_h$

Functional output: $M(\hat{u}) = (\hat{u}, \hat{\psi})$ (drag, lift,...)

$$|M(\hat{u}) - M(\hat{U})| = |a(\hat{u}, \hat{U}; \hat{u} - \hat{U}, \hat{\varphi})| = |(R(\hat{u}), \hat{\varphi}) - (R(\hat{U}), \hat{\varphi})|$$

$$\leq \epsilon S_\epsilon + |(R(\hat{U}), \hat{\varphi})| = \epsilon S_\epsilon + |(R(\hat{U}), \hat{\varphi} - \hat{\Phi}) + SD_\delta(\hat{U}; \hat{\Phi})|$$

for all $\hat{\Phi} \in \hat{V}_h$, in particular for the interpolant of $\hat{\varphi}^h$ in $\hat{V}_h$

Use interpolation estimates: $\|h^{-1}(\hat{\varphi} - \hat{\varphi}^h)\| \leq C_i \|\hat{\varphi}\|_1$

Compute (using G2) approx. dual solution $\hat{\varphi}_h = (\varphi_h, \theta_h)$

# Automation of turbulence simulation

- G2 for NSE: No filtering. No Reynolds stresses. G2 automatic "turbulence model".
- Adaptive algorithm captures separation points, and "correct" (finite limit) dissipation in the turbulent wake.
- Mean value output (drag, lift, frequencies, separation points, pressure coeff,...) computable up to a tolerance corresponding to experimental accuracy ($\approx$ 1-5%).
- About 10-100 times less mesh points needed to compute drag than in non-adaptive LES.
- Simple/complex geometry: laptop/cluster.

# Automation of turbulence simulation

$$|M(\hat{u}) - M(\hat{U})| \leq \sum_{K \in \mathcal{T}} \mathcal{E}_K = \sum_{K \in \mathcal{T}} \|hR(\hat{U})\| \|\hat{\varphi}_h\|_1 + |SD_\delta(\hat{U}; \hat{\varphi}_h)|$$

Galerkin discretization error + stabilization modeling error

Adaptive algorithm: From coarse mesh $\mathcal{T}^0$ do

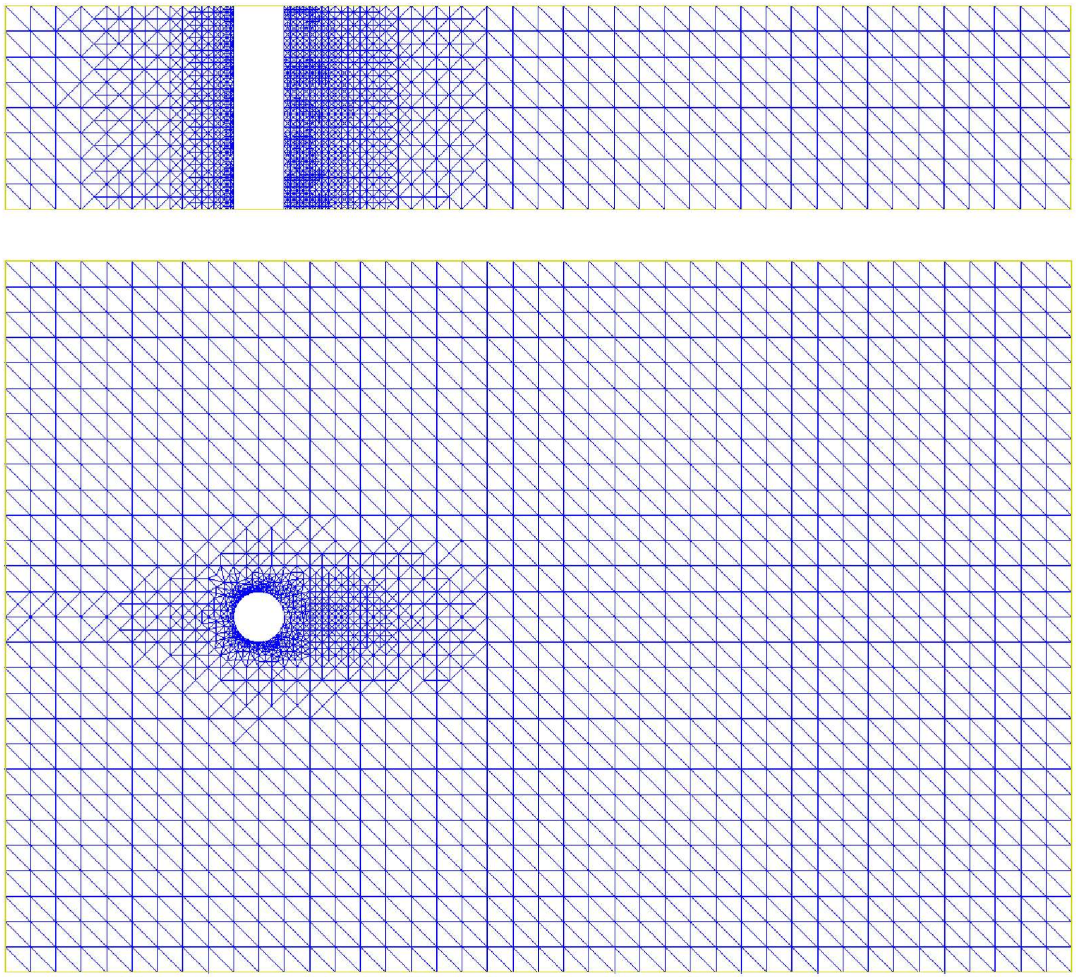
(1) compute primal and dual problem on $\mathcal{T}^k$

(2) if $\sum_{K \in \mathcal{T}^k} \mathcal{E}_K^k < \text{TOL}$ then STOP, else

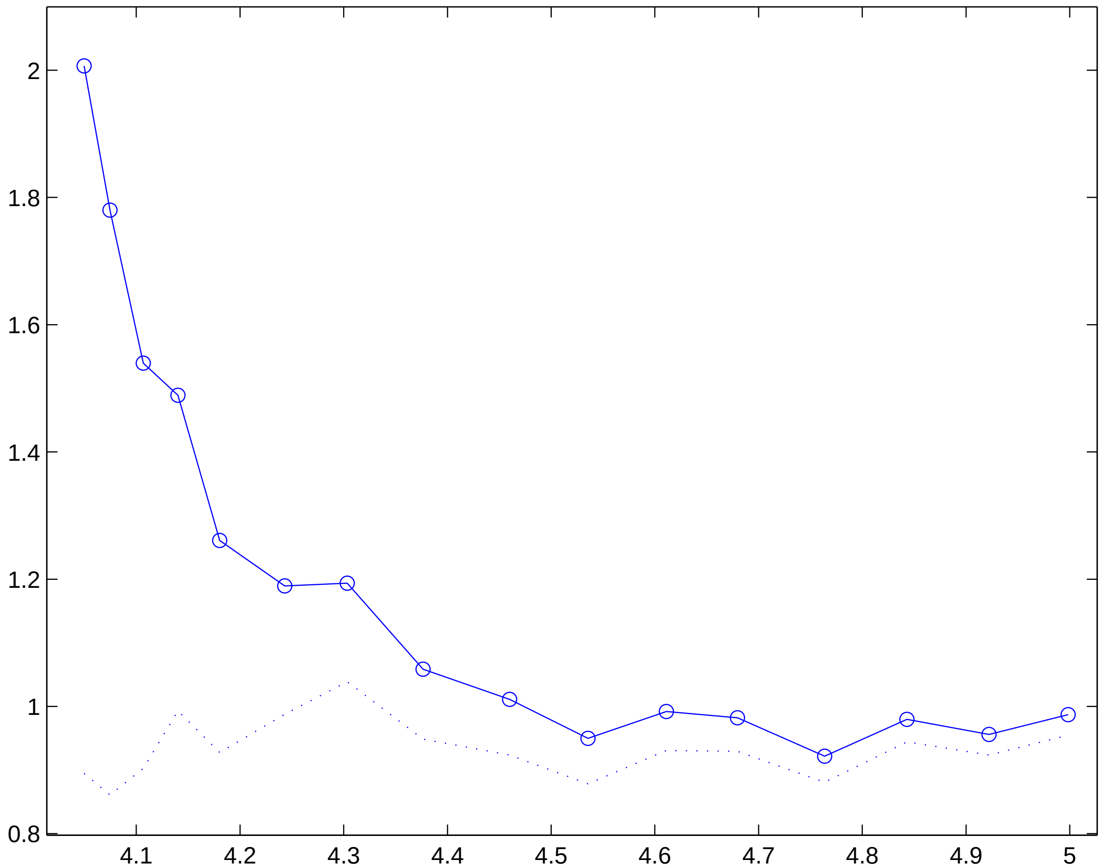
(3) refine elements $K \in \mathcal{T}^k$ with largest $\mathcal{E}_K^k \quad \rightarrow \quad \mathcal{T}^{k+1}$

(4) set $k = k + 1$, then goto (1)

# Ref. Mesh wrt $c_D$: circular cylinder

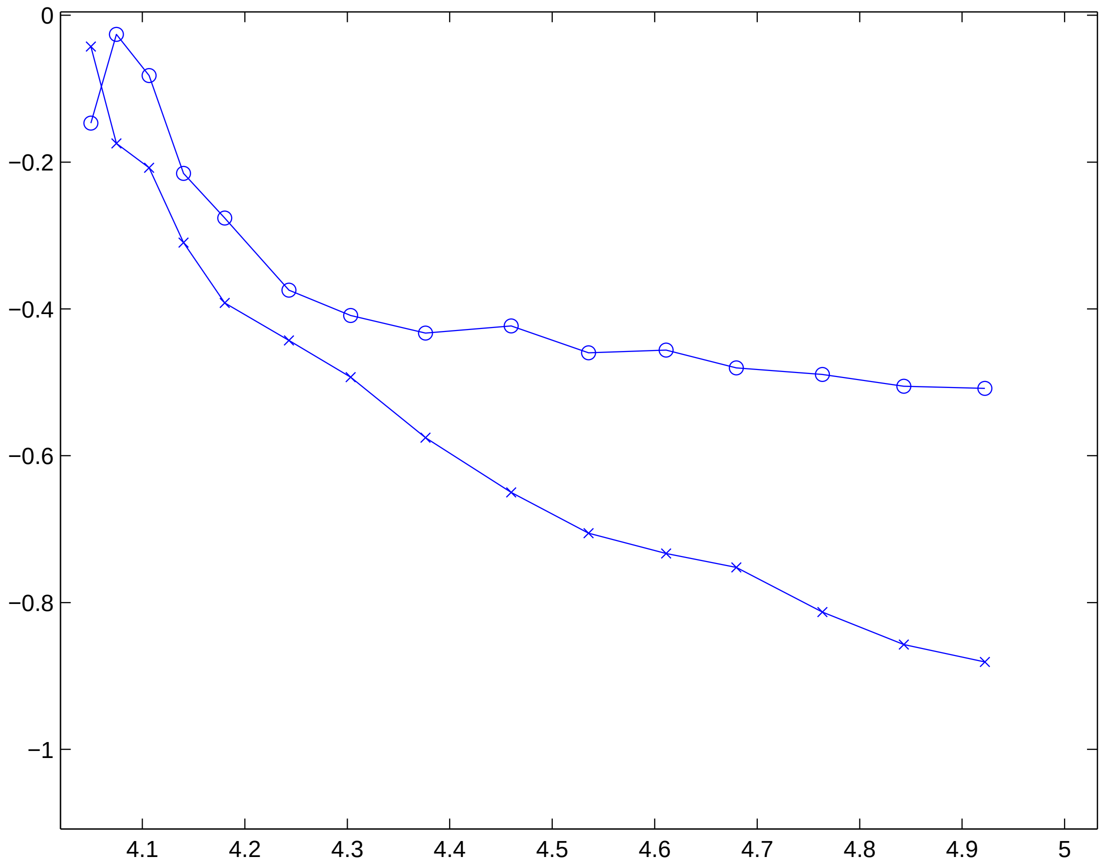


# Circular cylinder: $c_D \approx 1.0$

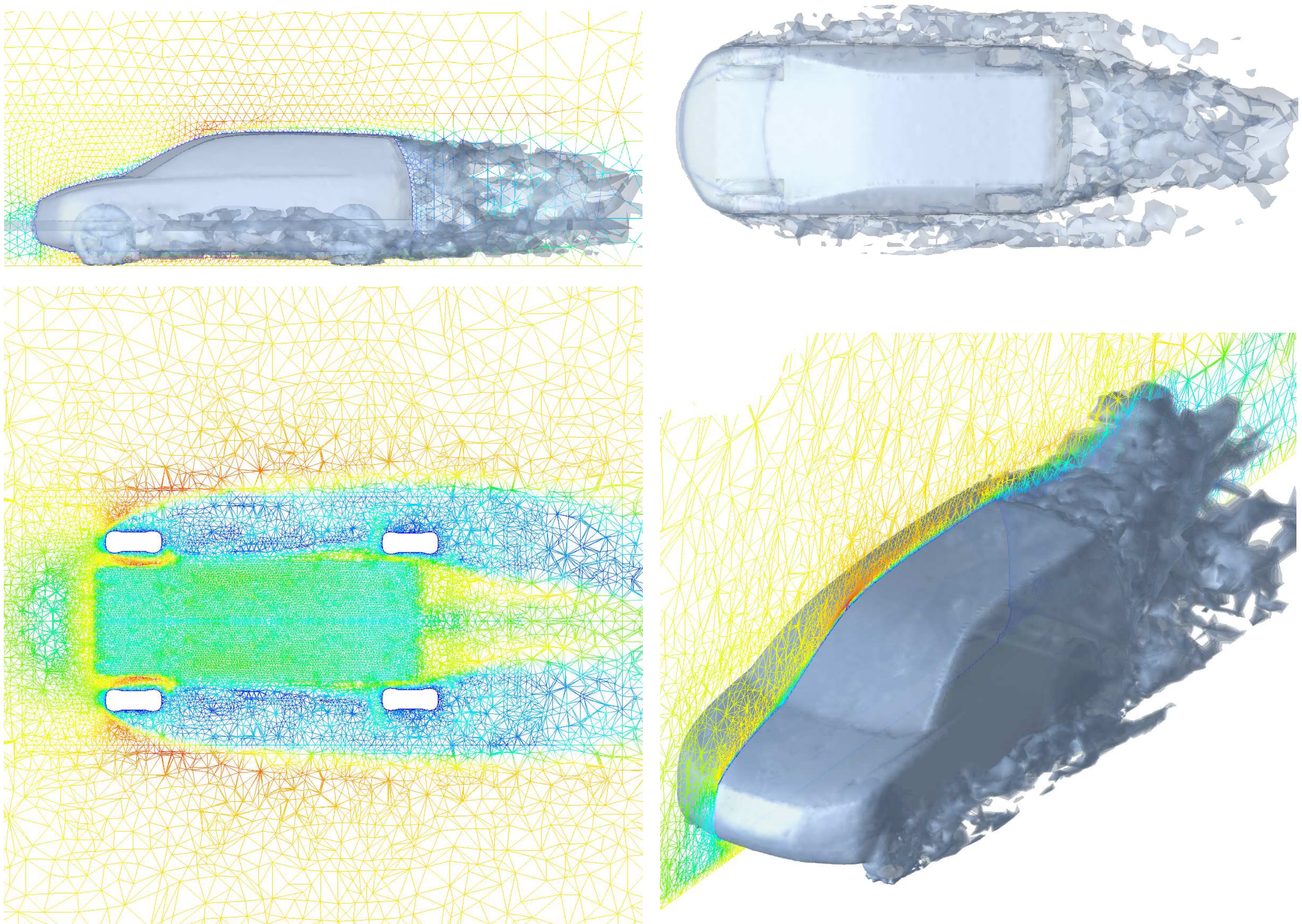



*circular cylinder* *dual solution*

# Circular cylinder: error estimates



# G2 for complex geometry (Volvo CC)

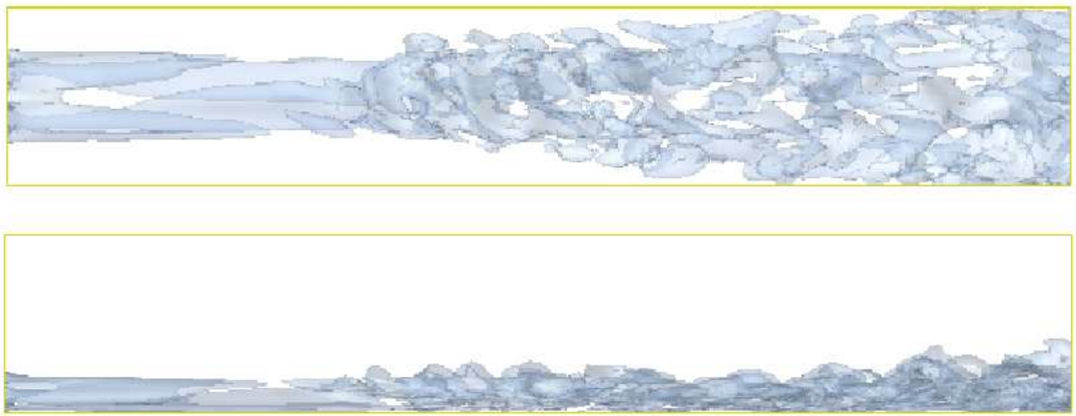


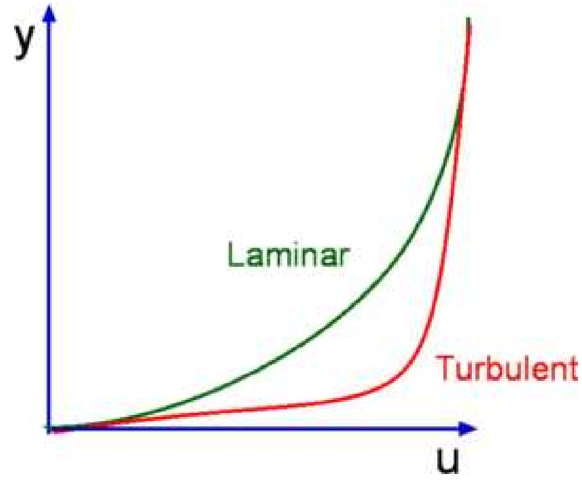
# Turbulent boundary layers

No slip boundary conditions ok for modeling laminar boundary layers.

For high $Re$ boundary layer undergoes transition.

Extremely expensive to resolve turbulent boundary layer: We need wall-model for correct separation and skin friction





# Turbulent boundary layers

Experiments: boundary skin friction $c_f \sim Re^{-0.2}$

That is: no Law of finite dissipation for $c_f$!

Skin friction $c_f$ depend on $Re$!

Cannot expect skin friction to be mesh independent:

We have to resolve/model the turbulent boundary layer!
(unless $c_f \approx 0$!!)

# Skin friction boundary condition

Slip with friction boundary condition [Maxwell, Navier,....]

Friction coefficient $\beta$; $\beta = 0$: slip b.c., $\beta = \infty$: no slip b.c.

[LES + Boundary Layer theory: Layton, John, Illiescu,....]

Simple wall model: $\beta \sim c_f$ (skin friction $c_f \sim Re^{-0.2}$)

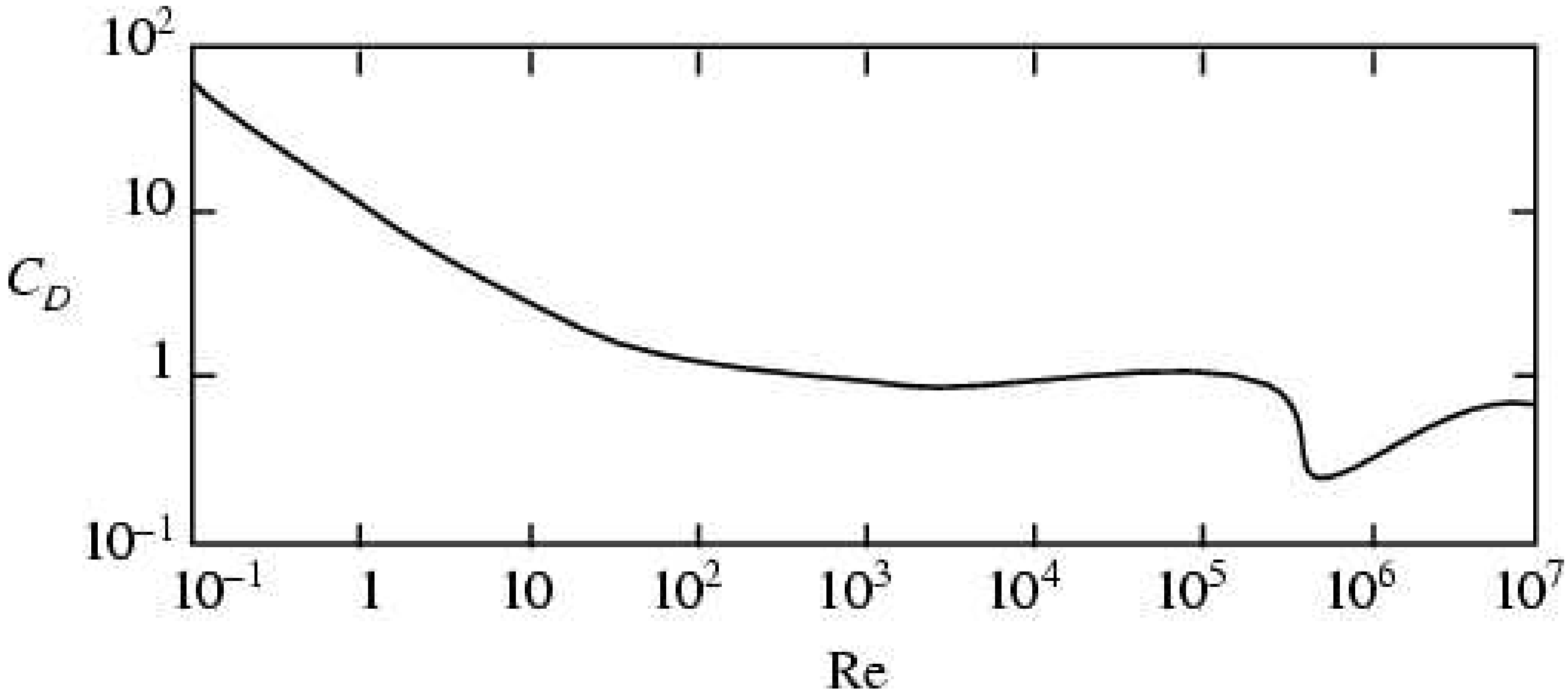
$\beta = \beta(Re, h)$; $\lim_{h \to 0} \beta = \infty$, $\lim_{Re \to \infty} \beta = 0$

$$\frac{1}{2}\|U(t)\|^2 + \sum_{i=1}^{2} ||\sqrt{\beta} u \cdot \tau_i||^2_{\Gamma \times I} + ||\sqrt{h} R(\hat{U})||^2_Q = \frac{1}{2}\|U(0)\|^2$$

(with $\nu$ small)

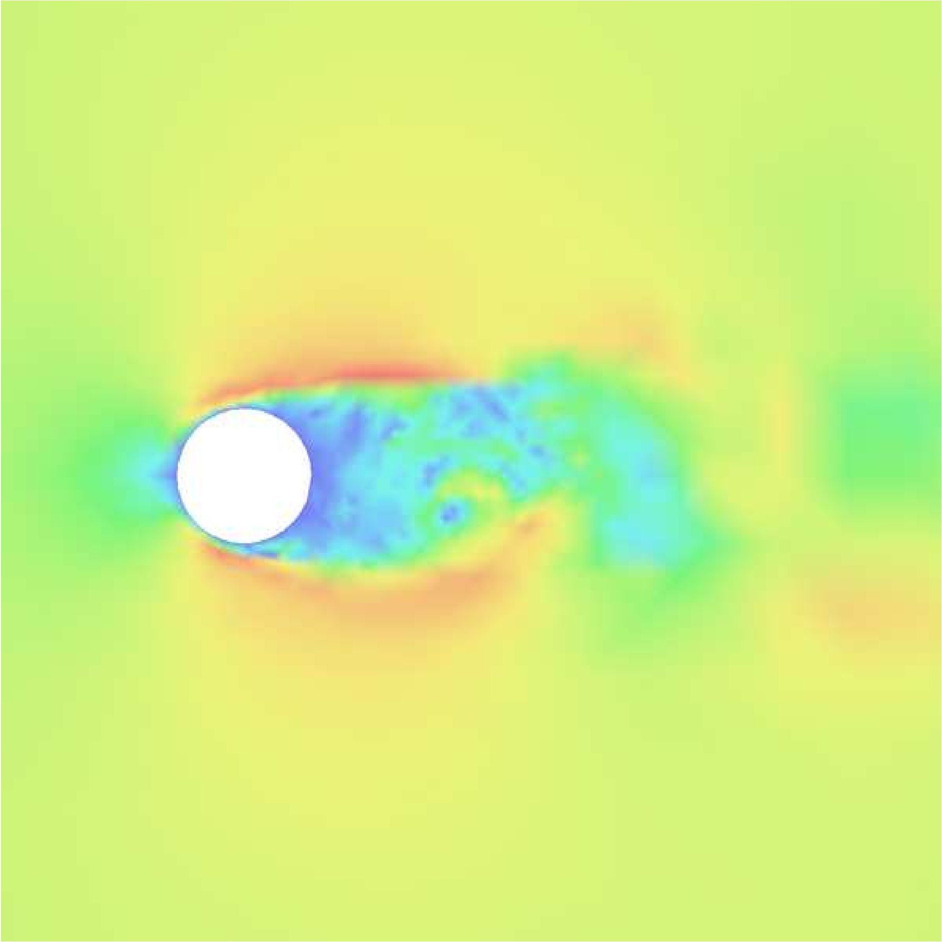
# Drag crisis for a cylinder

Turb. boundary layer $\Rightarrow$ high momentum near boundary $\Rightarrow$ delayed separation $\Rightarrow$ small wake $\Rightarrow$ drag crisis

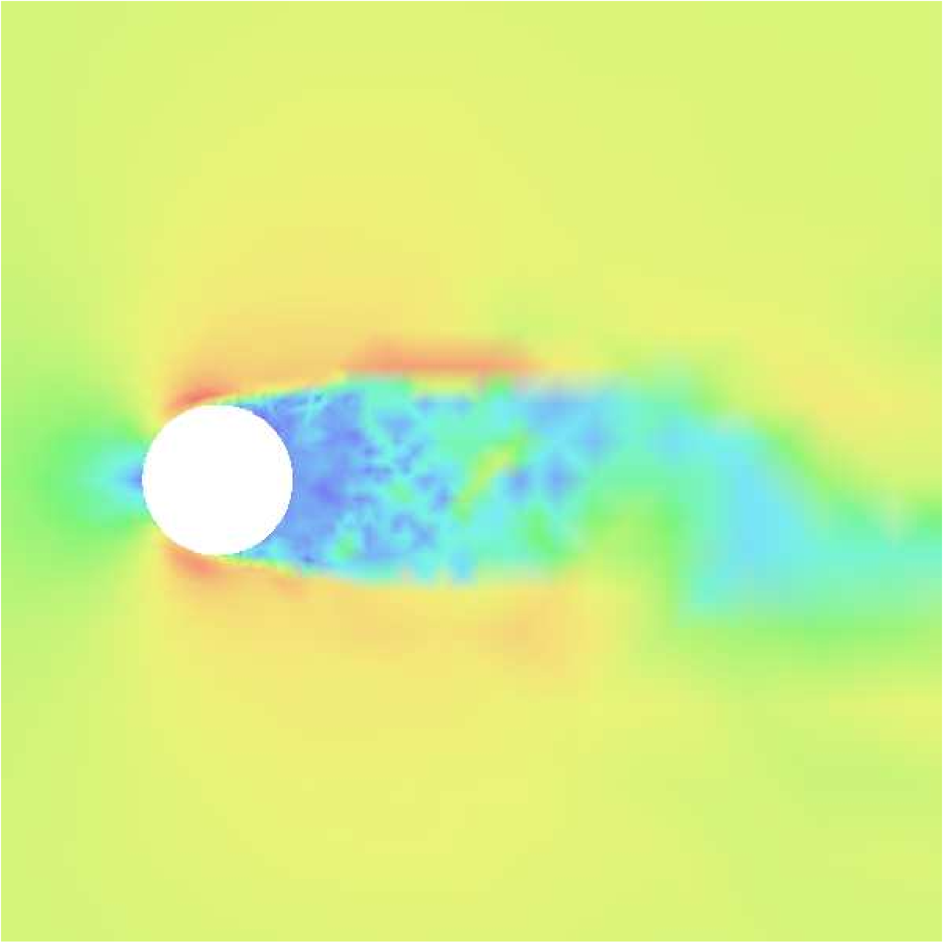



Drag crisis for a circular cylinder at $Re \sim 10^5 - 10^6$

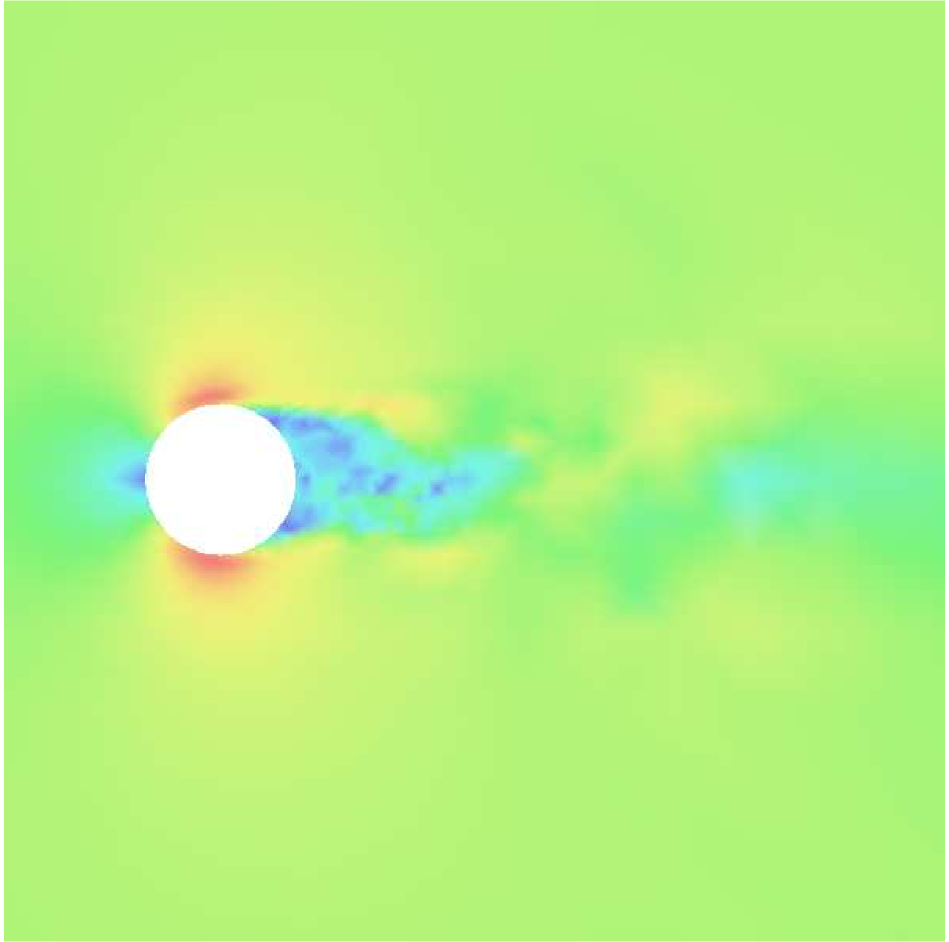
# drag crisis; $\beta = 1$: $c_D \approx 1.0$



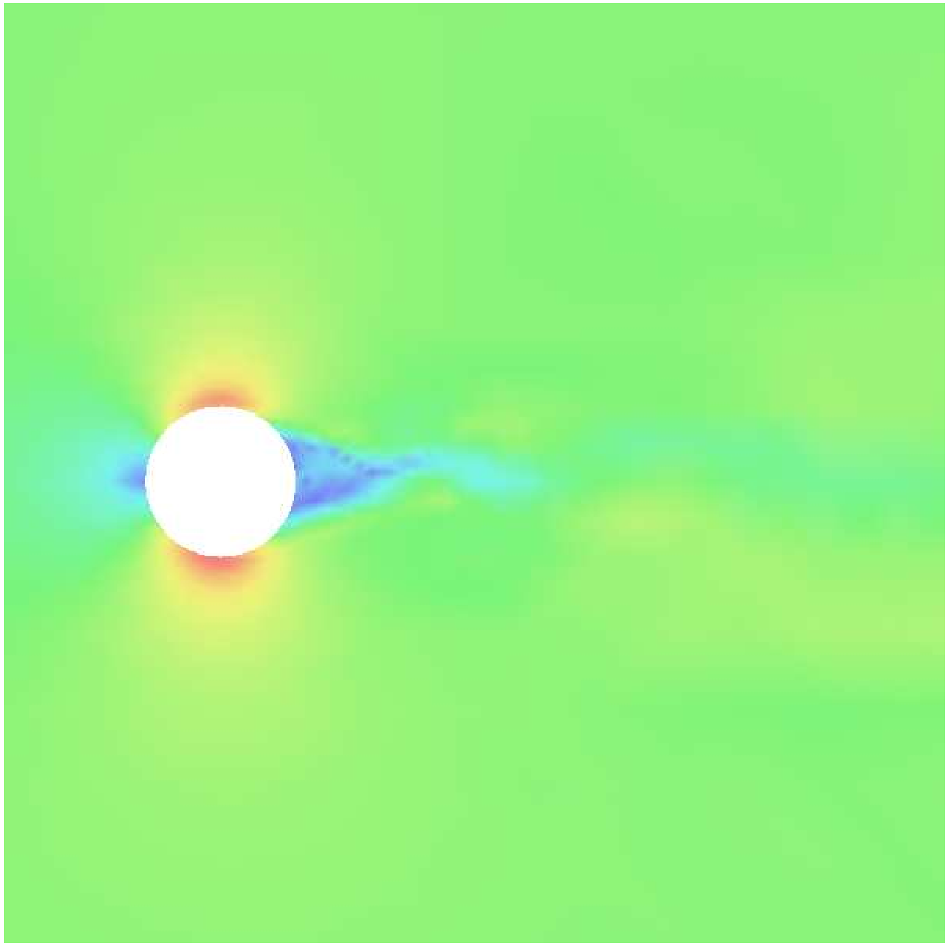
# drag crisis; $\beta = 2 \times 10^{-2}$: $c_D \approx 0.7$



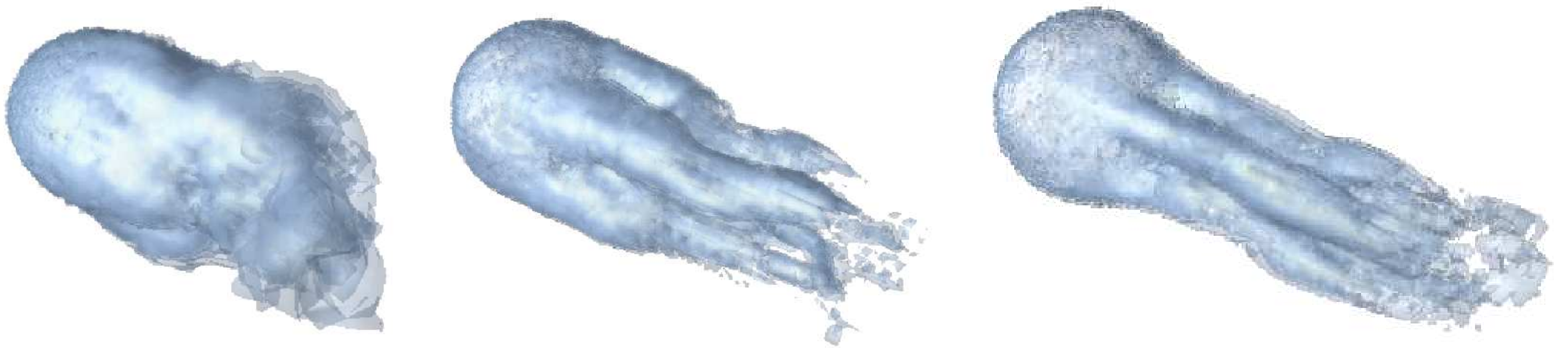
# drag crisis: $\beta = 1 \times 10^{-2}$; $c_D \approx 0.5$



# drag crisis; $\beta = 5 \times 10^{-3}$: $c_D \approx 0.45$



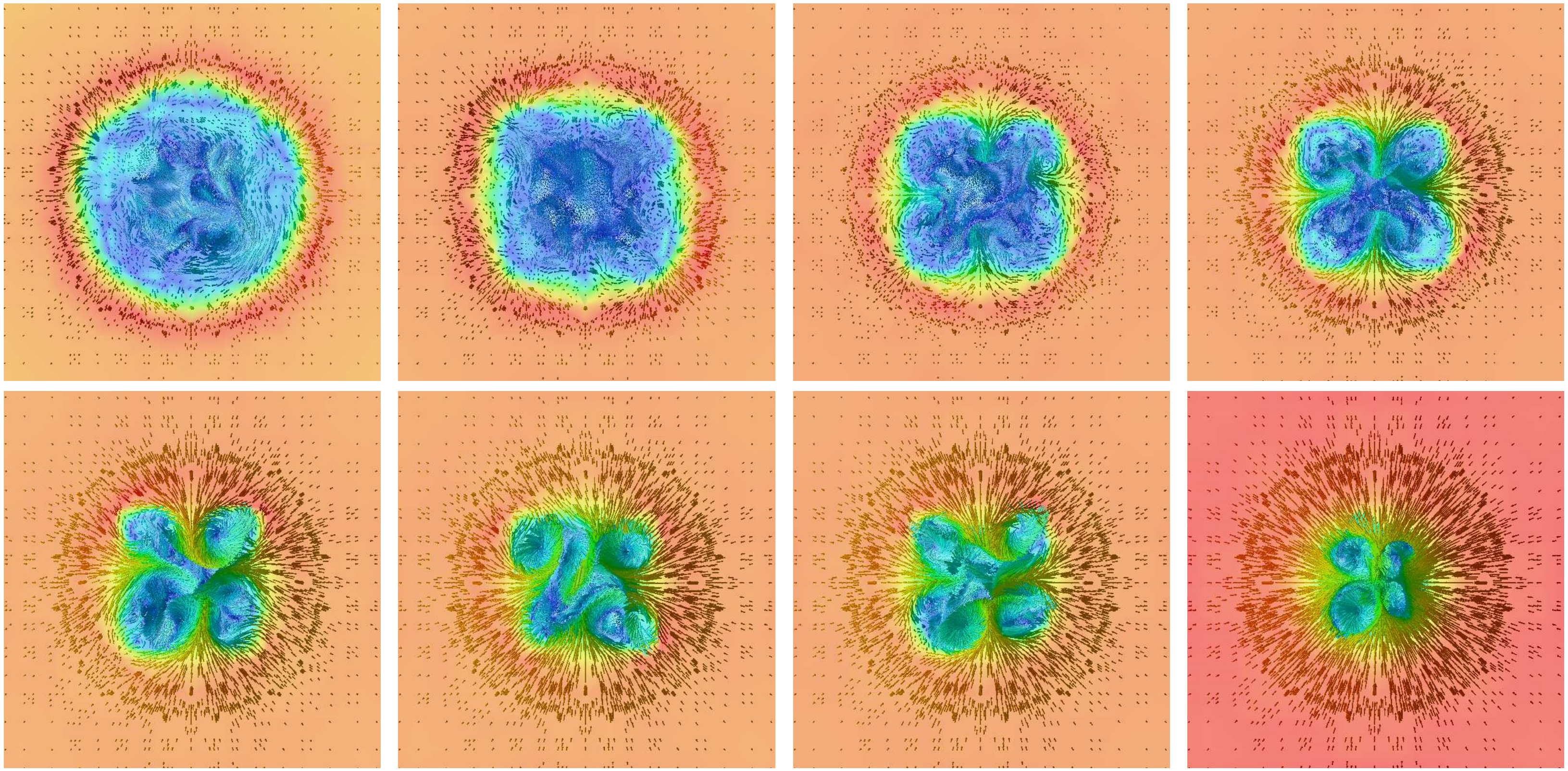
# Drag crisis for a sphere



Modeling of drag crisis for a sphere by skin friction model

Friction coeff. $\beta = 0.1 \rightarrow 0.01$ : $c_D = 0.4 \rightarrow 0.2$

# Drag crisis for a sphere

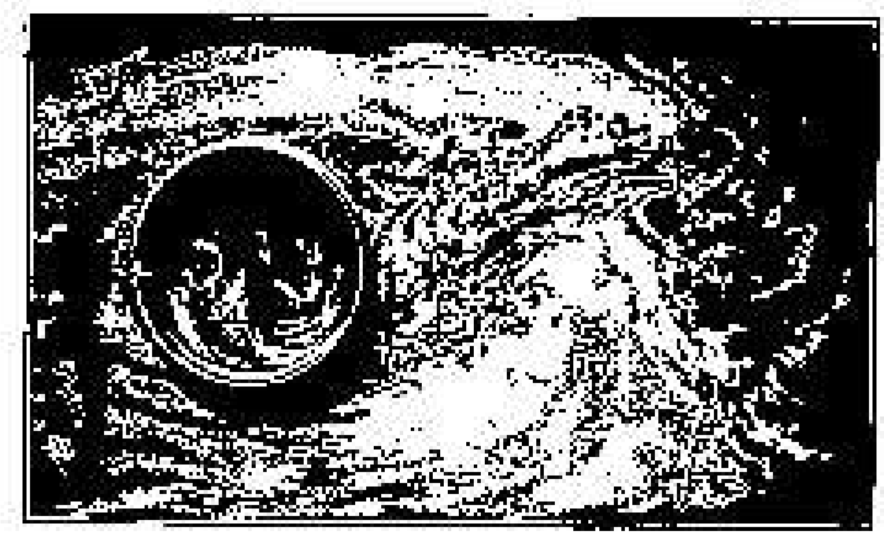


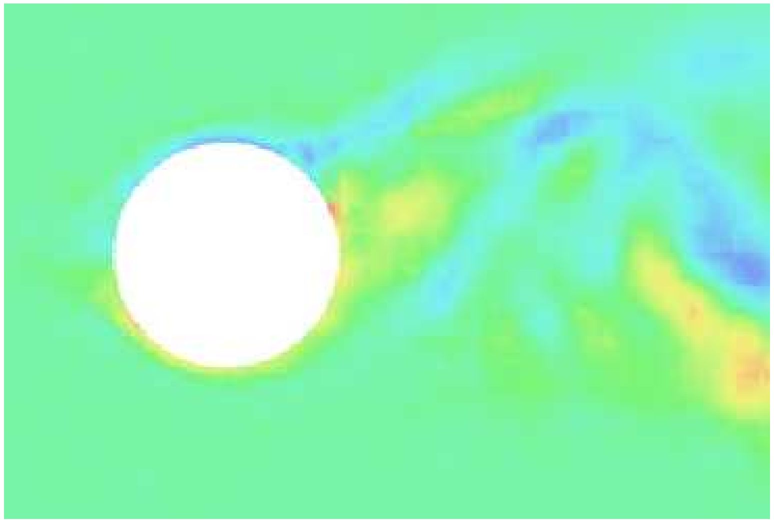
# EG2 and Turbulent Euler solutions

$\beta \rightarrow 0$; $Re \rightarrow \infty$ ($\nu \rightarrow 0$) $\Rightarrow$ Euler/G2 + slip b.c. (EG2)

EG2: no empirical parameters; only $h$ (very general...)

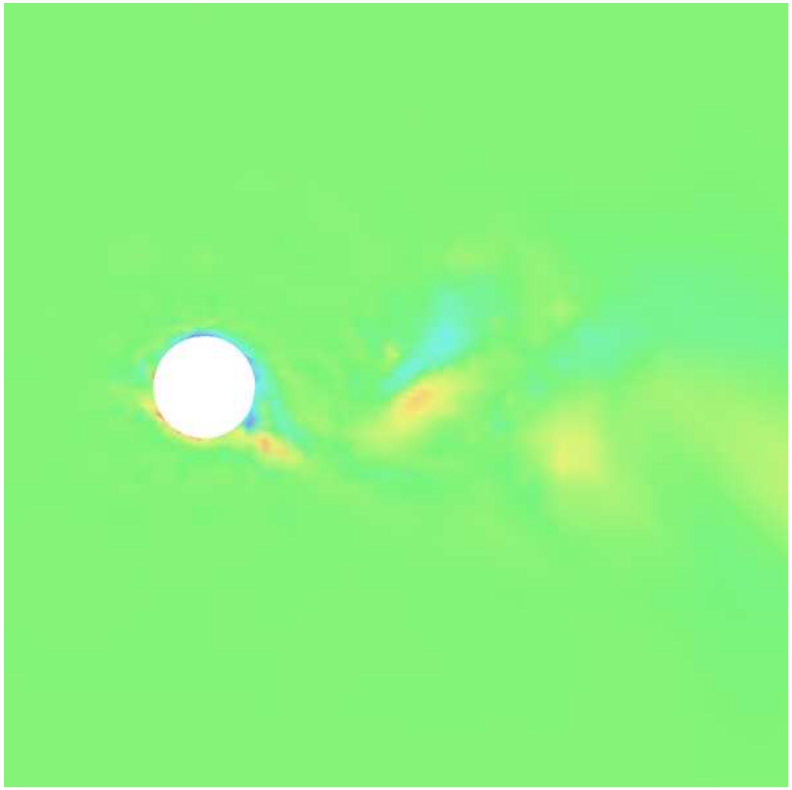
No experimental results for cylinder at $Re > 10^7$





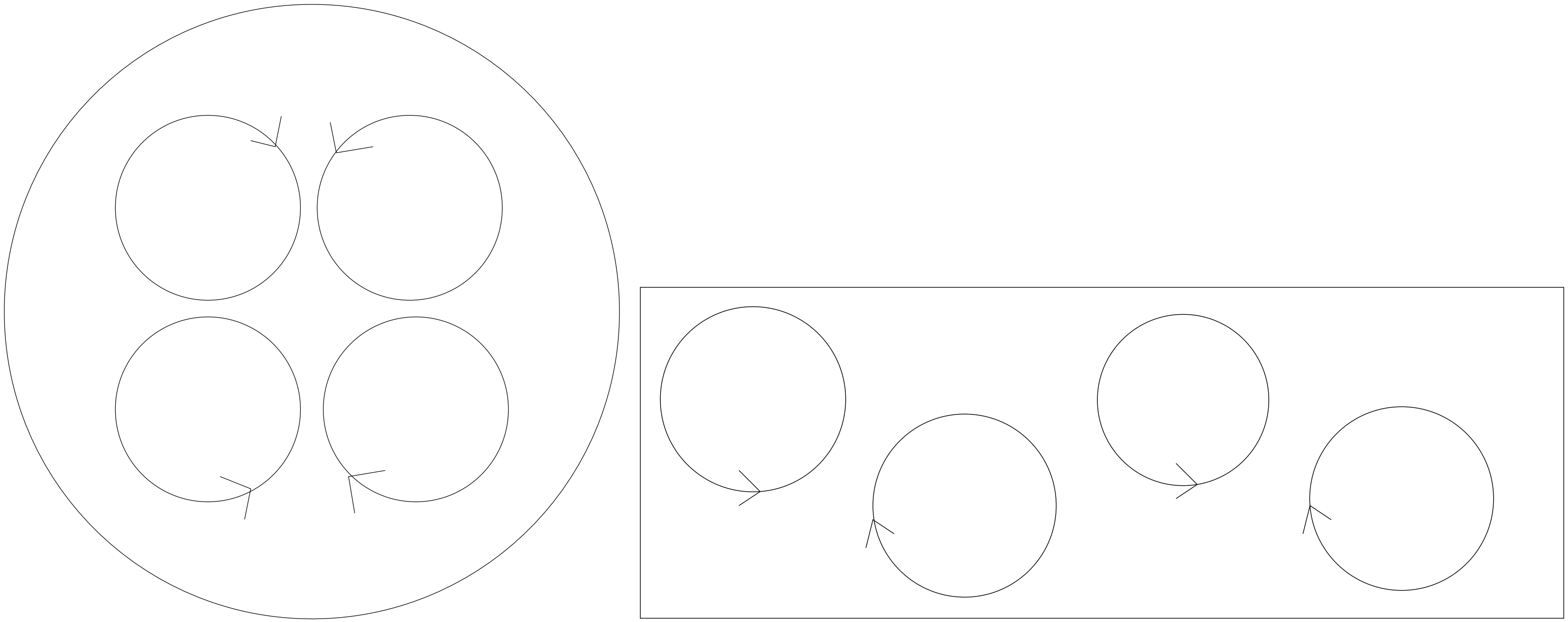
$u$ $p$ $\omega_1$, $xy$ $\omega_1$, $xz$ $\omega_1$, $yz$

# EG2 and Turbulent Euler solutions



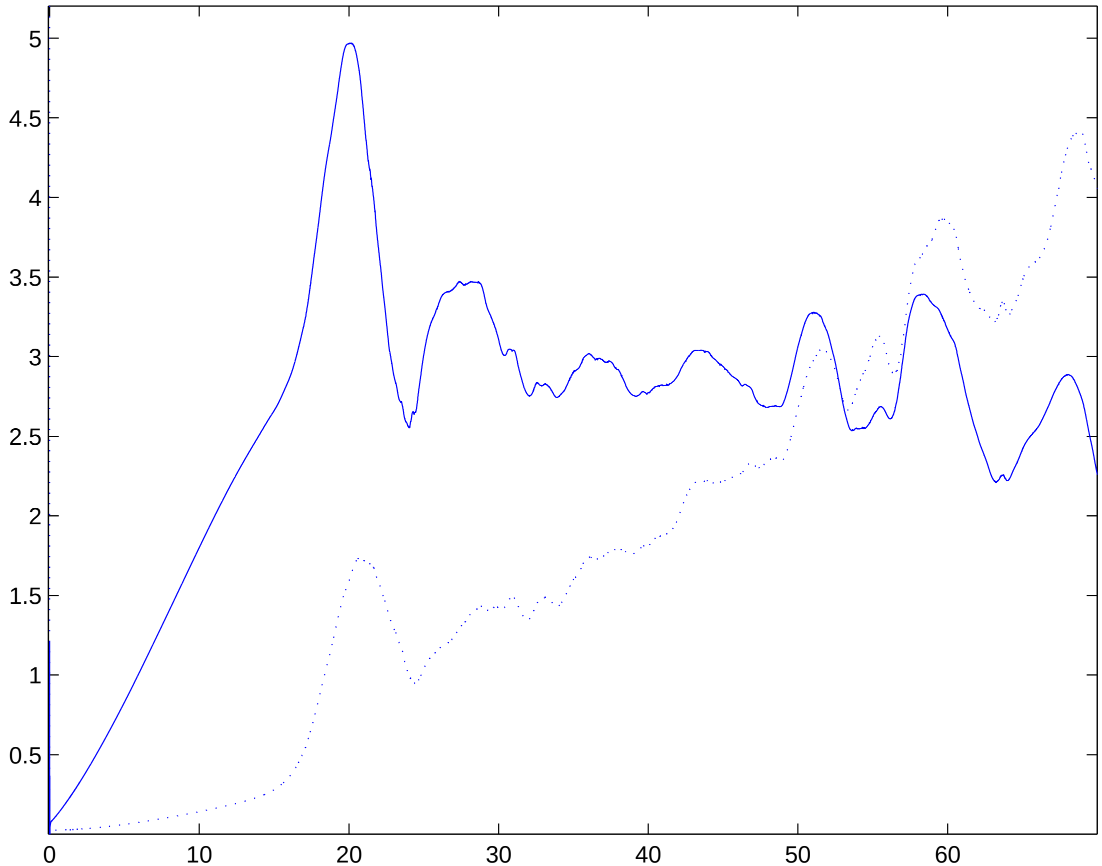
Euler relevant for very large $Re$: geophysical flow!

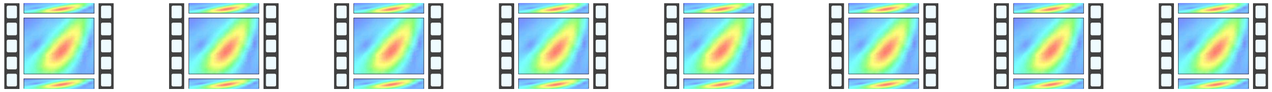
# EG2 solutions: sphere and cylinder



EG2 solutions of physical relevance for (very) high $Re$?

# Simulation of take-off: lift vs drag



# Turbulent Compressible Flow

EG2 for the compressible Euler equations:

- ☐ Conservation of total mass, momentum, and energy
- ☐ Automatic satisfaction of 2nd Law.

$$\dot{\rho} + \nabla \cdot (u\rho) = 0$$

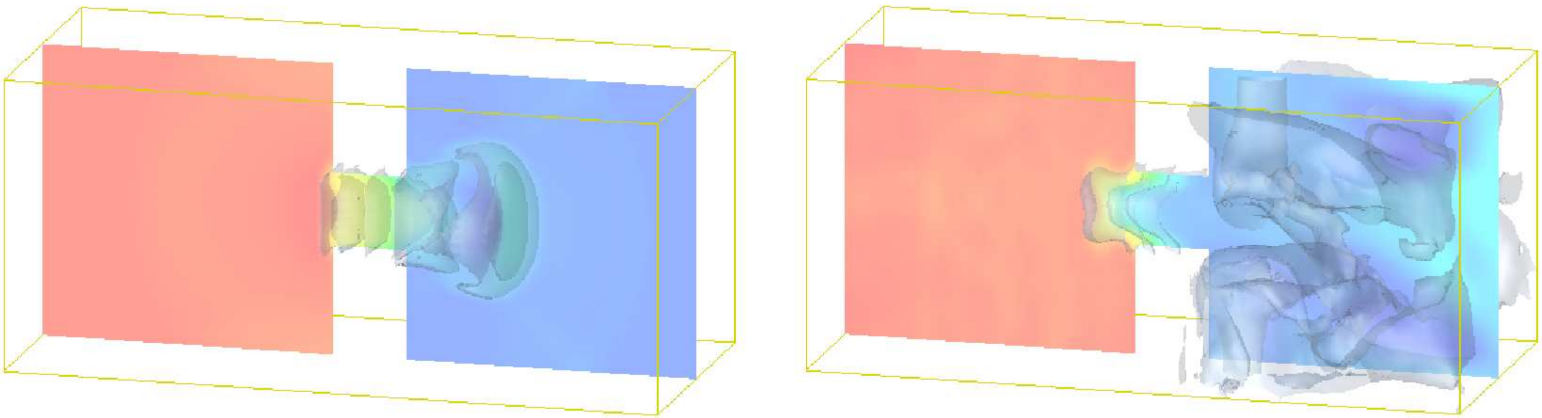
$$\dot{m} + \nabla \cdot (um) + \nabla p = 0$$

$$\dot{e} + \nabla \cdot (ue) + \nabla \cdot (up) = 0$$

# Turbulent Compressible Flow

EG2 for the compressible Euler equations:

- Conservation of total mass, momentum, and energy
- Automatic satisfaction of 2nd Law.

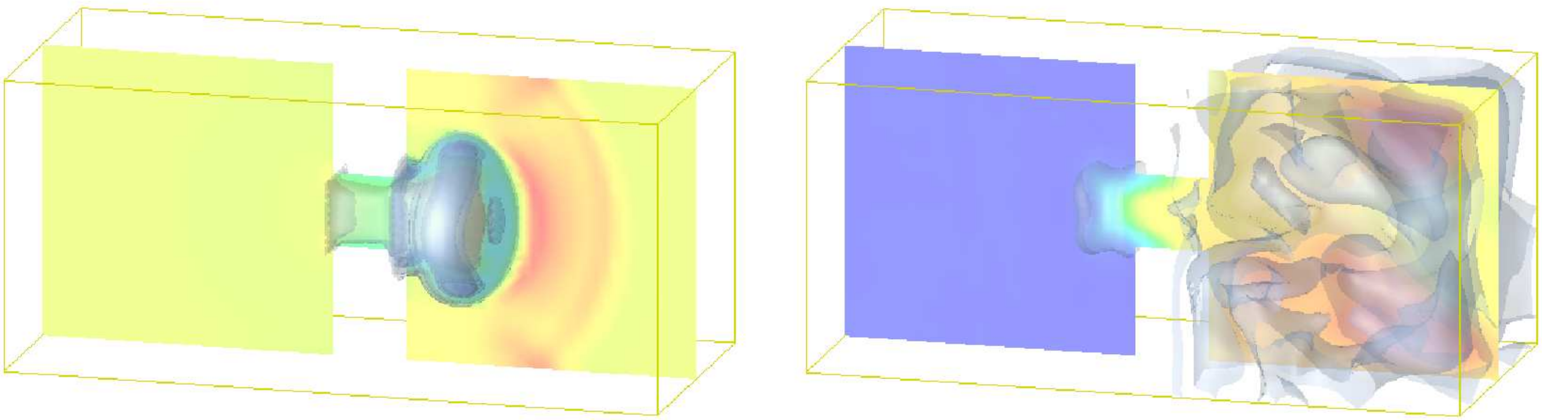


Density

# Turbulent Compressible Flow

EG2 for the compressible Euler equations:

- Conservation of total mass, momentum, and energy
- Automatic satisfaction of 2nd Law.

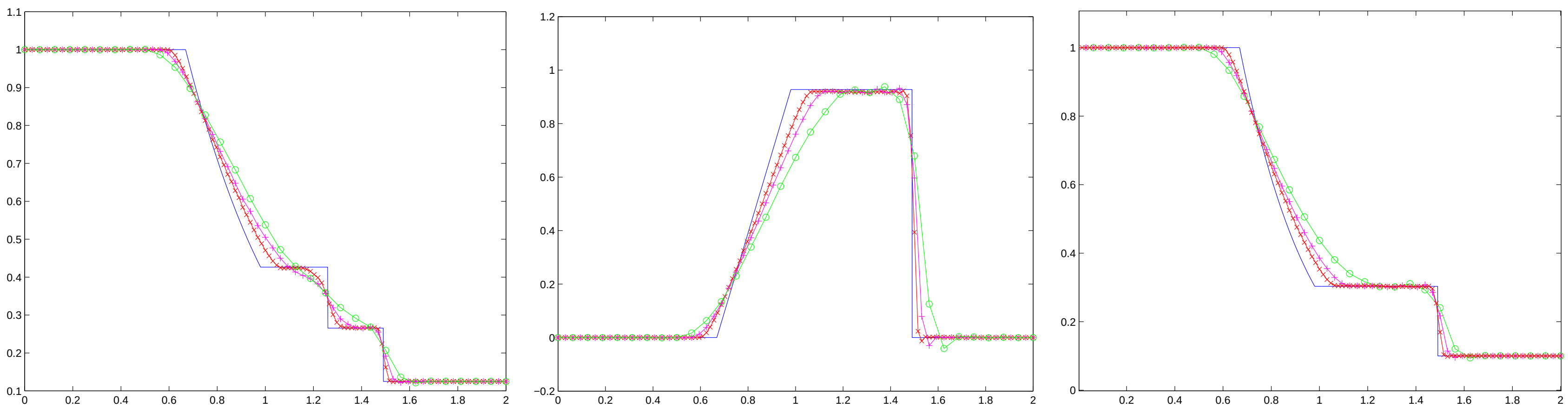


Temperature

# Turbulent Compressible Flow

EG2 for the compressible Euler equations:

- ☐ Conservation of total mass, momentum, and energy
- ☐ Automatic satisfaction of 2nd Law.




Shocktube on coarse meshes: density, velocity, pressure

# Fluid-structure: ALE

- Ex: blood flow with elastic walls,...
- ALE: mesh moving/smoothing, object in a box,...
- Splitting of discrete system: NS + Ko
- Turbulence, transition, separation,...
- Adaptivity: moving domain, splitting, h-p-r,...

*no ale* *ale* *pinch* *pinch move*

*oib mesh* *oib vel* *oib rot mesh*

# Mesh algorithms

- Mesh refinement/coarsening
- Mesh smoothing (Laplacian, optimization,...)
- Edge flip/face swap
- Local remesh
- Projection between general meshes
- Hierarchy vs. one mesh
- GMG vs. AMG
- Optimal alg. vs. simple alg. + smooth/flip/swap

# Mesh refinement

Goals for (tetrahedral) mesh refinement:

1. cut edges (reduce $h$)
2. avoid adding edges to node (avoid small angles)
3. avoid hanging nodes (localization)

- ☐ Edge vertex insertion (1 0 1)
- ☐ Face vertex insertion (0 0 1)
- ☐ Cell vertex insertion (0 0 1)
- ☐ Uniform cell refinement (1 1 0)

# Mesh coarsening

Goals for (tetrahedral) mesh coarsening:

1. increase $h$
2. avoid adding edges to node (avoid small angles)
3. localization

- ☐ Edge collapse
- ☐ Face collapse
- ☐ Cell collapse

Alt. 1: coarsen by mesh hierarchy (use parent-child info).

Alt. 2: coarsen by “Matt-algorithm”.

# Free surface flow - level sets

Applications: dam break, flow past structures, ships,...

Challenges: topology changes, turbulence, wetting bc,...

Method: G2, variable density/viscosity, “level set”,...

# Large deformation - contact

Physics engine for animation using Ko/DOLFIN/FFC/FIAT

Industrial partner: plug-in for gaming, simulators,...

Real-time: efficiency, contact model,...

# FEniCS - Challenges

Challenges

- Dolfin module developers - need stable kernel
- New users - simple build (including dependencies)
- Industrial partners (including software companies)

Solutions

- dolfin-dev + dolfin-stable
- scons/cmake/?
- A license that does not exclude industrial partners

# Expected input to FEniCS

- ☐ Automation of modeling: turbulent flow (G2)
- ☐ Mesh algorithms: refine/coarse/smooth/flip/...
- ☐ General function projections
- ☐ Modules: turbulence, free surface, ale, solid, contact,...
- ☐ Advanced modules/top applications
  $\longrightarrow$ new abstractions, users/developers, visibility,...
- ☐ New developers $\longrightarrow$ testing, contribution,...
- ☐ Use in education $\longrightarrow$ visibility, testing,...
- ☐ Industrial partners $\longrightarrow$ visibility, testing, funded devel.,...

# Future plans

FEniCS prototype: automation of

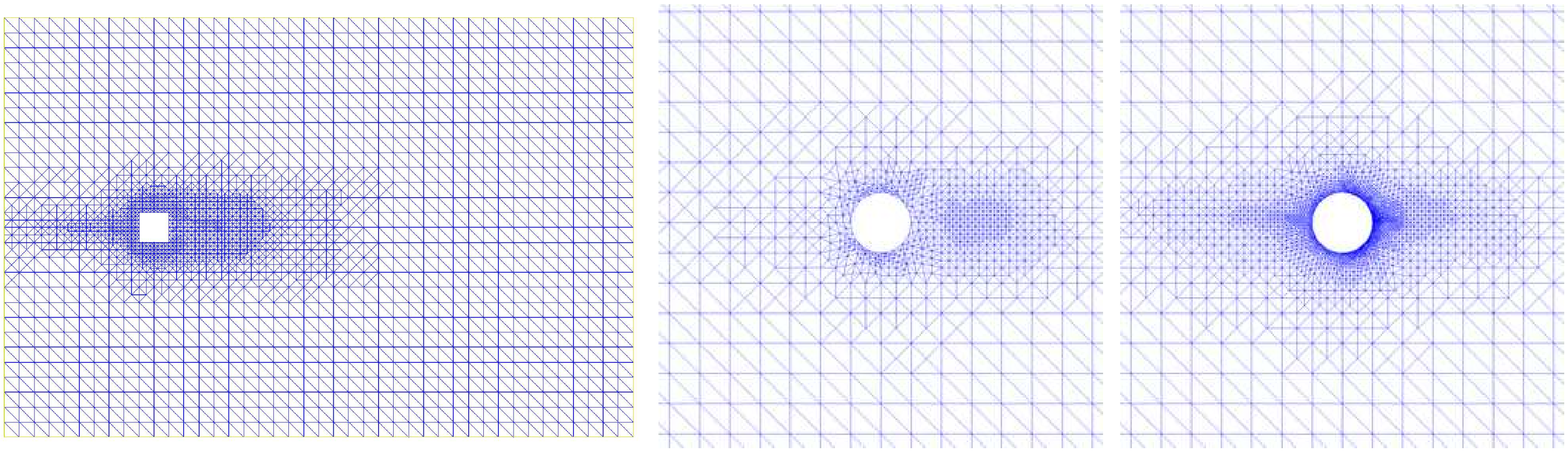
- turbulent incompressible/compressible flow,
- fluid-structure interaction,
- general free-surface problem,
- h-p-r adaptivity.

# G2 - automation of discretization

General Galerkin G2: Find $\hat{U} \in \hat{V}_h \subset \hat{V}$:

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

The G2 solution $\hat{U} \in \hat{V}_h$ is defined on a computational mesh, of size $h(x)$, which defines a smallest scale.



# G2 - automation of discretization

General Galerkin G2: Find $\hat{U} \in \hat{V}_h \subset \hat{V}$:

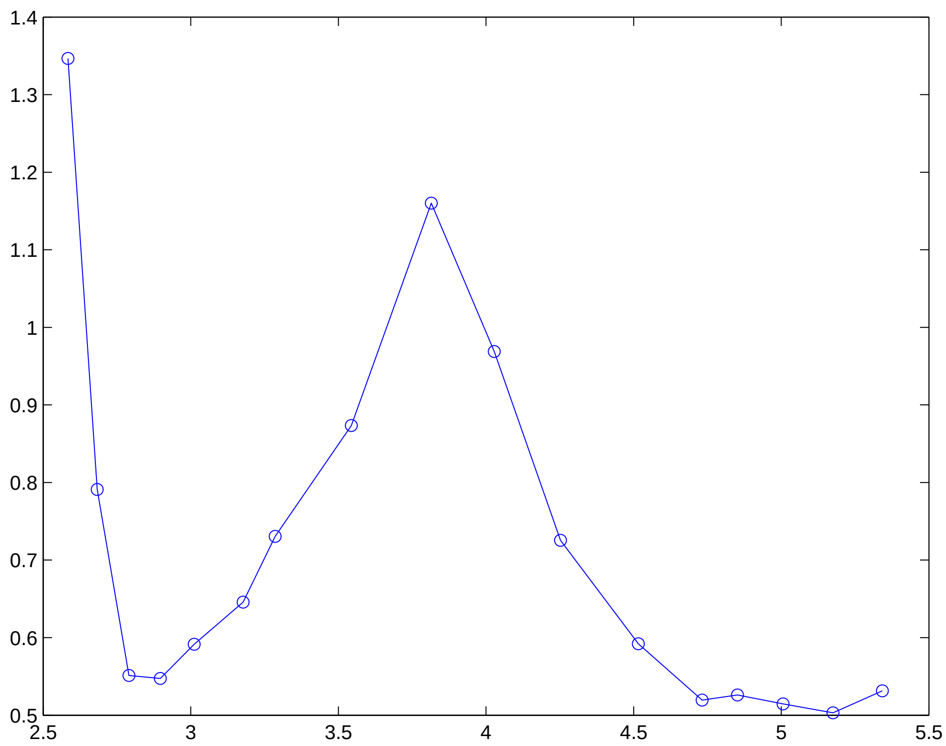
$$(R(\hat{U}), \hat{v}) + (hR(\hat{U}), R(\hat{v})) = 0 \quad \forall \hat{v} \in \hat{V}_h$$

Energy estimate for G2 (assuming $f = 0$): set $\hat{v} = \hat{U}$

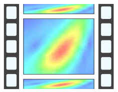
$$\frac{1}{2}\|U(t)\|^2 + ||\sqrt{\nu}\nabla U||_Q^2 + ||\sqrt{h}R(\hat{U})||_Q^2 = \frac{1}{2}\|U(0)\|^2$$

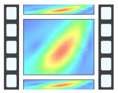
Total dissipation of energy: $||\sqrt{\nu}\nabla U||_Q^2 + ||\sqrt{h}R(\hat{U})||_Q^2$

# Law of Finite Energy Dissipation




Flow around cube:

 *Re=40 0000: xy*

 *Re=40 0000: xz*

The intensity of the stabilizing term $||\sqrt{h}R(\hat{U})||_Q^2$ in the wake is independent of $h$ after some mesh refinement.