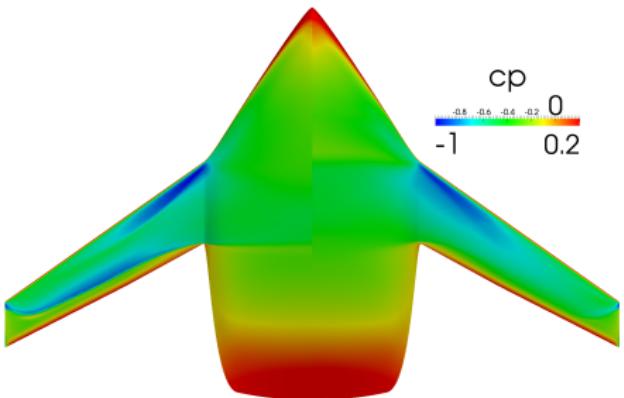


# Boundary and Volume Shape Newton Schemes

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Design study for blended wing-body configurations

- Transonic Inviscid Incompressible CFD
- > 460,000 surface node positions to be optimized
- Planform constant

# Acoustic Horn Design (joint with M. Berggren, E. Wadbro)



- General problem formulation allows treatment of general problems
- Design of acoustic (linear wave) horn antenna,  $3.5 \cdot 10^9$  unknowns!

# Generalized Problem

$$\min_{(\varphi, \Gamma_{\text{inc}})} J(\varphi, \Omega) := \frac{1}{2} \int_0^T \int_{\Gamma_{\text{i/o}}} \|B(n)(\varphi - \varphi_{\text{meas}})\|_2^2 \, dt \, ds + \delta \int_{\Gamma_{\text{inc}}} 1 \, ds$$

subject to

$$\dot{\varphi} + \operatorname{div} F(\varphi) = 0 \quad \text{in } \Omega$$

$$\text{BCs} = g \quad \text{on } \Gamma$$

Acoustics:

$$\begin{aligned}\frac{\partial u}{\partial t} + \nabla p &= 0 \text{ in } \Omega, \\ \frac{\partial p}{\partial t} + c^2 \operatorname{div} u &= 0 \text{ in } \Omega, \\ \frac{1}{2}(p - c\langle u, n \rangle) &= g \text{ on } \Gamma_{\text{i/o}}\end{aligned}$$

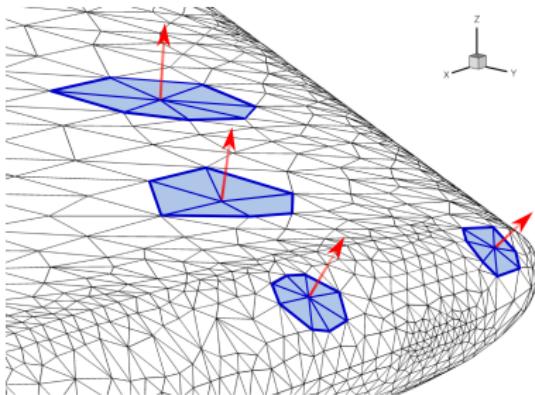
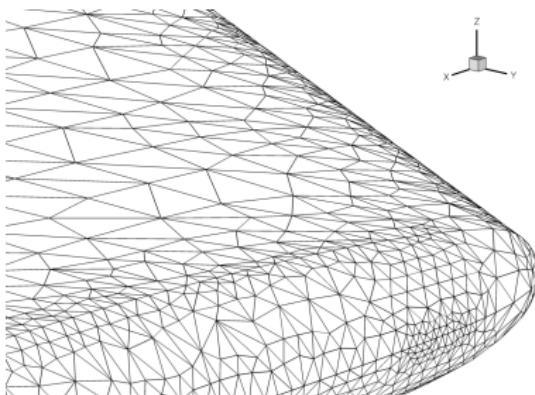
Electromagnetism:

$$\begin{aligned}\mu \frac{\partial H}{\partial t} &= -\nabla \times E \text{ in } \Omega, \\ \varepsilon \frac{\partial E}{\partial t} &= \nabla \times H - \sigma E \text{ in } \Omega, \\ \text{BCs} &= g \text{ on } \Gamma_{\text{i/o}}\end{aligned}$$

# Parameterization: From Numbers to Shapes

Use positions of surface nodes:

- Design  $\mathbf{q} = (\dots, x_i, y_i, z_i, \dots)^T$  coordinates of all surface nodes
- Very large scale,  $O(10^5)$
- Gradient based methods, higher order, smoothing
- Design unknowns coupled to CFD mesh
- Non-smooth parameterization



# Newton's Method

- Necessary optimality condition:  $\nabla J(q^*) = 0 \in \mathbb{R}^n$
- Newton's method can be used to find the roots of functions!

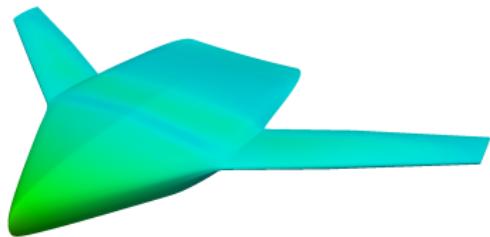
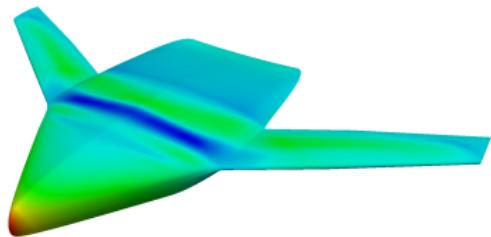
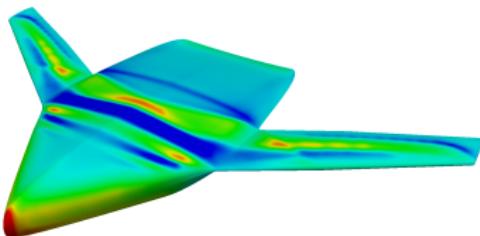
## Newton's Method

Update  $q_{k+1} = q_k + \Delta q$ , where  $\Delta q$  solves

$$\text{Hess } J(q_k) \Delta q = -\nabla J(q_k)$$

⇒ Second derivative Hess  $J$  is needed!

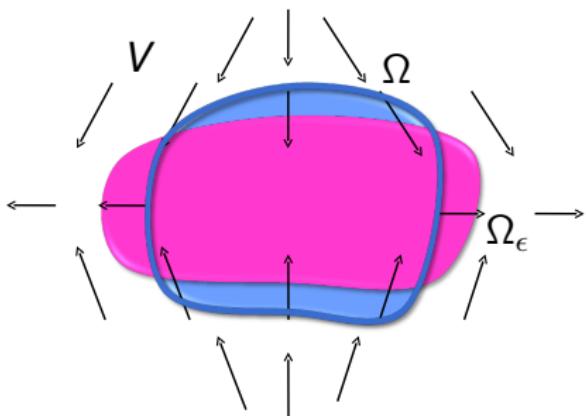
# Hessian Approximation by Gradient Smoothing



Sobolev Method:

Use tangential Laplace operator  $\Delta_\Gamma$  for Hess results in gradient smoothing. When and why is this a good idea?

# Introduction to Shape Optimization



- Shape is modeled by set  $\Omega$
- $\Omega_\epsilon := \{x + \epsilon V(x) : x \in \Omega\}$
- $J : \mathcal{P}(\Omega) \supseteq \mathcal{D} \rightarrow \mathbb{R}$ : target function
- (Directional) derivative of  $J$  with respect to  $\Omega$ ?

- Directional Derivative

$$dJ(\Omega)[V] := \lim_{\epsilon \rightarrow 0^+} \frac{J(\Omega_\epsilon) - J(\Omega)}{\epsilon}$$

# The Shape Derivative

- Objective function:

$$J_1(\epsilon, \Omega) := \int_{\Omega(\epsilon)} f(\epsilon, x_\epsilon) \, d x_\epsilon \text{ or } J_2(\epsilon, \Omega) := \int_{\Gamma(\epsilon)} g(\epsilon, s_\epsilon) \, d s_\epsilon$$

- Take Limit:

$$dJ_1(\Omega)[V] = \frac{d}{d\epsilon} \Big|_{\epsilon=0} \int_{\Omega(\epsilon)} f(\epsilon, x_\epsilon) \, d x_\epsilon \text{ or } dJ_2(\Omega)[V] = \frac{d}{d\epsilon} \Big|_{\epsilon=0} \int_{\Gamma(\epsilon)} g(\epsilon, s_\epsilon) \, d s_\epsilon$$

- Change of Variables = Change in Domain

$$dJ_1(\Omega)[V] = \int_{\Omega} \frac{d}{d\epsilon} \Big|_{\epsilon=0} \left[ f(T_\epsilon(x)) \cdot |\det DT_\epsilon(x)| \right] + f'(x)[V] \, d x$$

$$dJ_2(\Omega)[V] = \int_{\Gamma} \frac{d}{d\epsilon} \Big|_{\epsilon=0} \left[ g(T_\epsilon(s)) \cdot |\det DT_\epsilon(s)| \| (DT_\epsilon(s))^{-T} n(s) \|_2 \right] + g'(s)[V] \, d s$$

- Local / Shape Derivative:  $f'(x)[V] := \frac{\partial}{\partial \epsilon} f(0, x)$

# The Shape Derivative (Weak vs Strong)

- Material Derivative:  $df[V] := \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} f(\epsilon, T_\epsilon(x)) = \langle \nabla f, V \rangle + f'[V]$
- Local / Shape Derivative:  $f'(x)[V] := \left. \frac{\partial}{\partial \epsilon} \right|_{\epsilon=0} f(0, x)$

$$\begin{aligned} dJ_1(\Omega)[V] &= \int_{\Omega} f(0, x) \operatorname{div}(V) + \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} f(\epsilon, T_\epsilon(x)) dx \\ &= \int_{\Omega} f \operatorname{div} V + df[V] dx \quad (\text{Weak/Volume/Distributed Formulation}) \\ &= \int_{\Omega} \operatorname{div}(fV) + f'[V] dx = \int_{\Gamma} \langle V, n \rangle f ds + \int_{\Omega} f'[V] dx \quad (\text{Surface Formulation}) \end{aligned}$$

$$\begin{aligned} dJ_2(\Omega)[V] &= \int_{\Gamma} g \operatorname{div}_{\Gamma} V + dg[V] ds \quad (\text{Weak/Volume/Distributed Formulation}) \\ &\stackrel{V \text{ normal}}{=} \int_{\Gamma} \operatorname{div}_{\Gamma}(gV) + \langle V, n \rangle \frac{\partial g}{\partial n} + g'[V] ds \\ &= \int_{\Gamma} \langle V, n \rangle \left[ \frac{\partial g}{\partial n} + \kappa g \right] + g'[V] ds \end{aligned}$$

# Regularization, Approximate Newton, $H^1$ -Descent

Assume:

$$R(\Gamma) = \int_{\Gamma} 1 \, ds$$

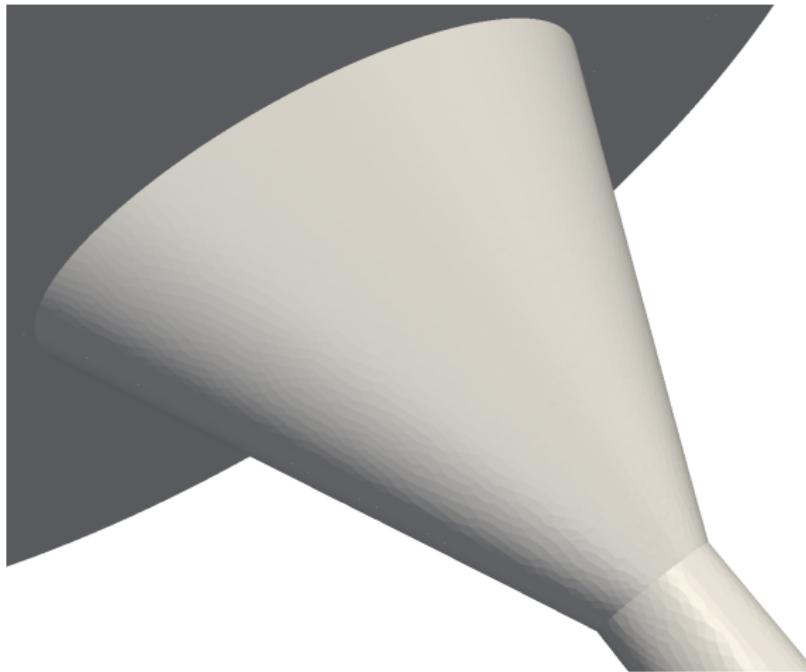
Then:

$$dR(\Gamma)[V] = \int_{\Gamma} \langle V, n \rangle \kappa \, ds$$

$$d^2 R(\Gamma)[V, W] = \int_{\Gamma} \langle \nabla_{\Gamma} \langle V, n \rangle, \nabla_{\Gamma} \langle W, n \rangle \rangle + \langle V, n \rangle \langle W, n \rangle \kappa^2 \, ds$$

Sobolev-Descent arises when surface area is penalized and the PDE is ignored in Newton's method.

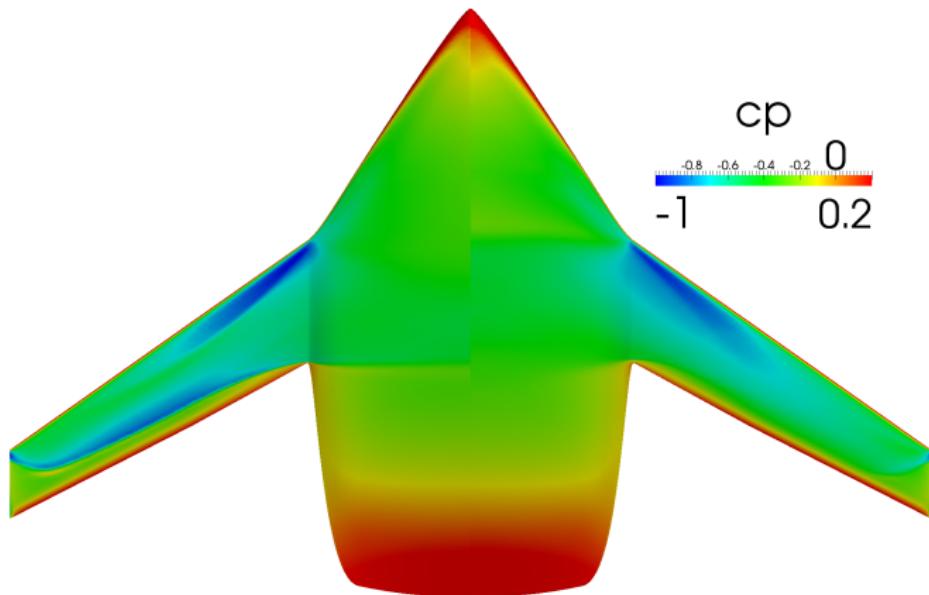
# Optimal Emitter for Acoustics



Boundary Data Compression:

$3.5 \cdot 10^9$  unknowns: 26 TB to 3.26 GB, 3 Months on 48 CPUs  
(S., Wadbro, Berggren, 2016)

# 3D Euler Flow: VELA



Shape	$C_D$	%	$C_L$	%
460,517	$3.342 \cdot 10^{-3}$	-30.06%	$1.775 \cdot 10^{-1}$	-0.67%

(S., Ilic, Schulz, Gauger 2013)

# The Regularization Term

(joint with R. Herzog, J. Vidal-Nuñez M. Herrmann, H. Kröner)

Better regularization than surface area?

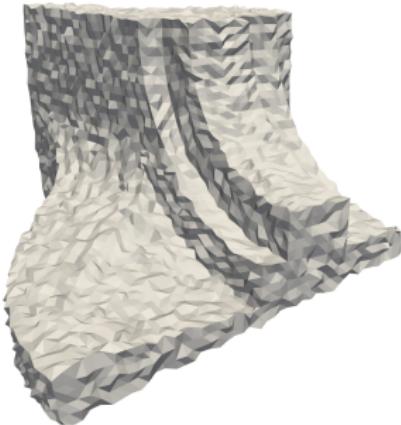
$$\min_{(\varphi, \Gamma_{\text{inc}})} \frac{1}{2} \int_0^T \int_{\Gamma_{\text{i/o}}} \|B(n)(\varphi - \varphi_{\text{meas}})\|_2^2 \, dt \, ds + \delta R(\Gamma_{\text{inc}})$$

subject to

$$\dot{\varphi} + \operatorname{div} F(\varphi) = 0 \quad \text{in } \Omega$$

$$\text{BCs} = g \quad \text{on } \Gamma$$

- Previously:  
*R* surface area:  
Laplace Smoothing/Curvature Flow
- Idea: Regularization to favor kinks
- Idea:  $R = TV(n) \doteq \sum_E \|[\![n]\!]\|_2$   
Total Variation of the normal



# Dealing with Non-Smoothness: ADMM

Introduce new variables until an “easy” problem arises [Goldstein, Osher 2009]

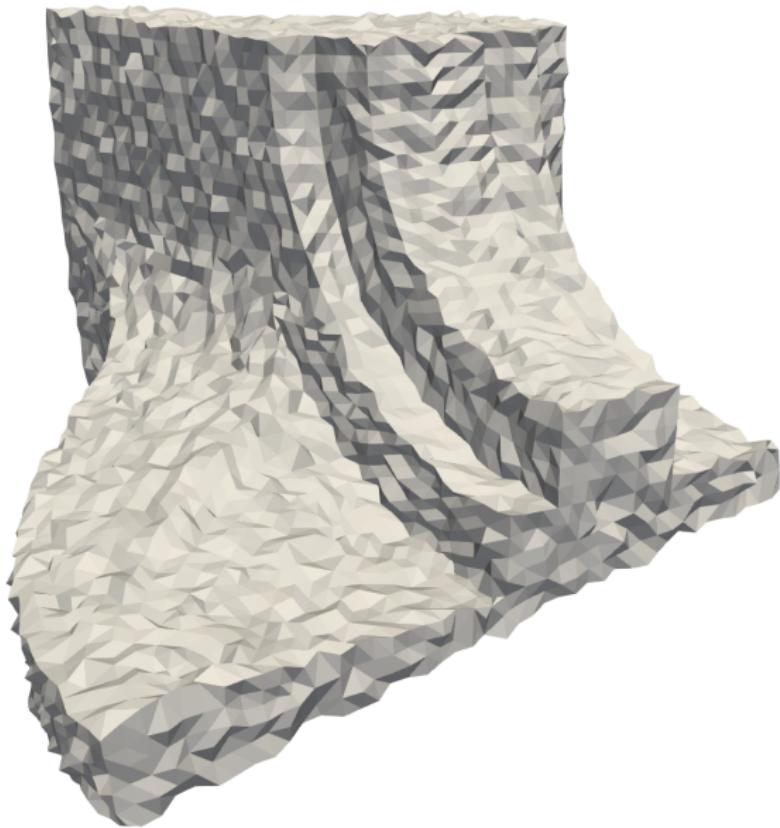
- New variable for gradient / edge jump:  $d_E := [\![n]\!]_E$
- Space:  $\mathcal{DG}_0$  on edges: “HDivTrace”
- New problem:  $\min \theta(\Gamma, d_E, b_e)$  with

$$\theta(\Gamma, d_E, b_e) = J(\Gamma) + \delta \sum_E |d_E| \ell_E + \frac{\lambda}{2} \sum_E |d_E - [\![n]\!]_E - b_E|^2 \ell_E$$

Algorithm:

- ①  $\Gamma^{k+1} := \arg \min_{\Gamma} \theta(\Gamma^k, d_E^k, b_E^k)$
- ②  $d_E^{k+1} := \arg \min_{d_E} \theta(\Gamma^{k+1}, d_E^k, b_E^k)$   
still non-smooth, but solvable via shrinkage!
- ③ Update  $b_E^{k+1} = b_E^k + (\Omega^{k+1} - d_E^{k+1})$

# Results



# CFD, Regularity and Higher Order Methods

## Model Problem: Incompressible Navier–Stokes

$$\min_{(u,p,\Omega)} E_{NS}(u, p, \Omega) := \frac{1}{2} \int_{\Omega} \mu \sum_{j,k=1}^3 \left( \frac{\partial u_k}{\partial x_j} \right)^2 dA$$

subject to

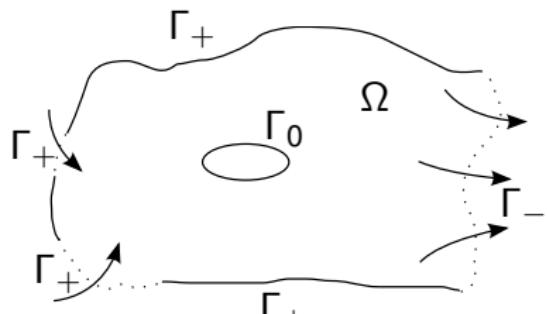
$$-\mu \Delta u + \rho u \nabla u + \nabla p = 0 \quad \text{in } \Omega$$

$$\operatorname{div} u = 0$$

$$u = u_+ \quad \text{on } \Gamma_+$$

$$u = 0 \quad \text{on } \Gamma_0$$

$$pn - \mu \frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_-$$



# Weak Shape Hessians

Strategy:

Use adjoint approach to eliminate material derivatives  $du$ , not  $u'$

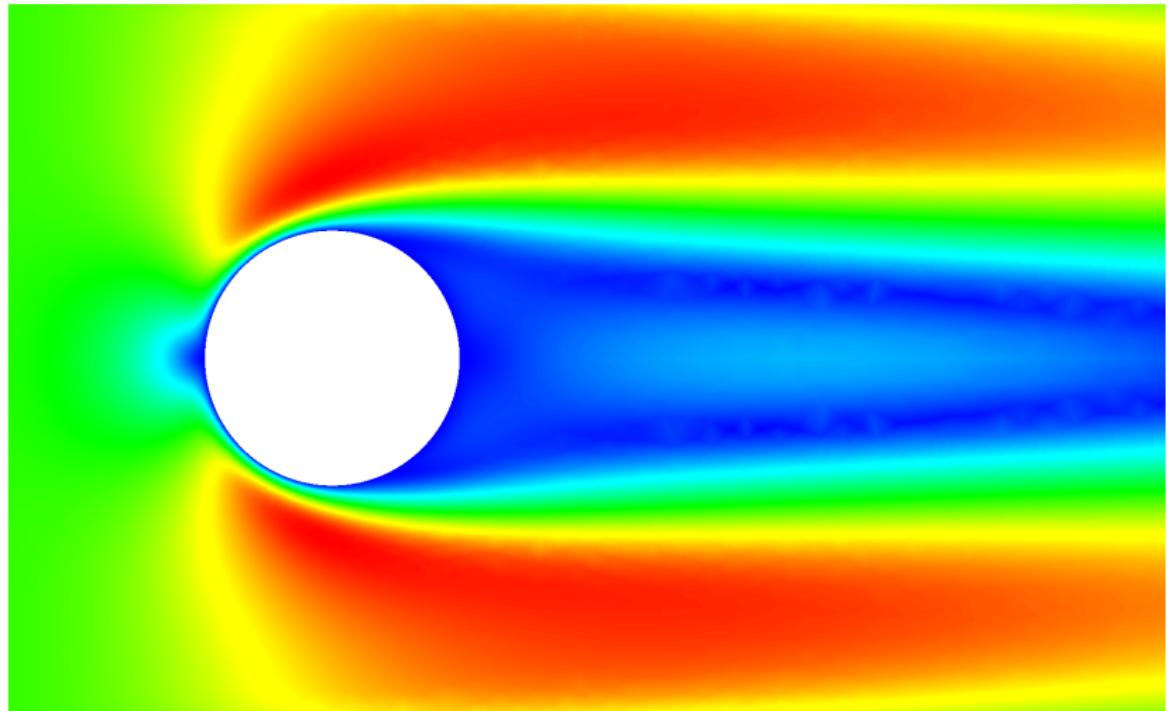
Result:

$$d^2 J_1[V, W] = \int_{\Omega} f \operatorname{div} V \operatorname{div} W + df[V] \operatorname{div} W + df[W] \operatorname{div} V - f \operatorname{tr}(D V D W) + d^2 f[V, W] \, dx$$

$$\begin{aligned} & d^2 J_2[V, W] \\ &= \int_{\Gamma} g \operatorname{div}_{\Gamma} V \operatorname{div}_{\Gamma} W + df[V] \operatorname{div}_{\Gamma} W + df[W] \operatorname{div}_{\Gamma} V - f \operatorname{tr}(D V D W) + d^2 g[V, W] \\ &+ g \left( \langle (DV)^T n, DW n \rangle + \langle DV n, (DW)^T n \rangle + \langle (DW)^T n, (DV)^T n \rangle - 2 \langle DV n, n \rangle \langle DW n, n \rangle \right) \end{aligned}$$

- ~ Excessively long expressions with normal, curvature or PDEs
- ~ Automatic symbolic generation!!

# Results



# Conclusions and Outlook

- Sobolev Smoothing is area penalization
- Total Variation Regularization vastly superior
- Shape SQP-Methods for incompressible Navier–Stokes
- How to do this in SU2?  
(PDEs on surfaces and on edges necessary)

