Un método de elementos finitos adaptativo para problemas de optimización de forma

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En colaboración con

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Introduction: Shape Optimization Problem

Shape Calculus

AFEM for Shape Optimization

Numerical Results

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Shape optimization problems

- Cost functional $J = J(\Omega, u(\Omega))$
- $\blacktriangleright \ \Omega \subset \mathbb{R}^d$
- $u = u(\Omega)$ solution to a PDE $\mathcal{A}u(\Omega) = f$ in Ω
- Minimization problem:

$$\text{find } \Omega^* \in \mathcal{U}_{\mathrm{ad}}: \qquad J(\Omega^*, u(\Omega^*)) = \min_{\Omega \in \mathcal{U}_{\mathrm{ad}}} J(\Omega, u(\Omega))$$

 $\mathcal{U}_{\mathsf{ad}}:$ set of admissible domains

$$\begin{array}{lll} \mbox{Minimize} & J = J(\Omega, u(\Omega)) \\ \mbox{.t.} & \Omega \in \mathcal{U}_{\sf ad} & \mathcal{A}u(\Omega) = f \end{array}$$

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Example: Minimization of an obstacle drag

$$\begin{split} & -\nabla \cdot \boldsymbol{T}(\boldsymbol{u},p) = 0 & \text{in } \Omega \\ & \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \\ & \boldsymbol{u} = \boldsymbol{u}_d & \text{on } \Gamma_{\text{in}} \cup \Gamma_s \cup \Gamma_w \\ \boldsymbol{T}(\boldsymbol{u},p) \cdot \boldsymbol{n} = 0 & \text{on } \Gamma_{\text{out}} \\ \end{split}$$

$$\boldsymbol{T}(\boldsymbol{u},p) = 2\nu\varepsilon(\boldsymbol{u}) - p\boldsymbol{I}, \quad \varepsilon(\boldsymbol{u}) = \frac{\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T}{2}, \quad \boldsymbol{u}_d = \begin{cases} V_\infty \boldsymbol{i} & \text{on } \Gamma_{\text{in}} \\ \boldsymbol{0} & \text{on } \Gamma_w \cup \Gamma_s \\ \boldsymbol{0} & \text{on } \Gamma_w \cup \Gamma_s \end{cases} \\ \end{split}$$

$$\begin{aligned} & \text{Drag Functional:} \qquad J(\Omega, [\boldsymbol{u},p]) = -\int_{\Gamma_s} \left(\boldsymbol{T}(\boldsymbol{u},p)\,\boldsymbol{n}\right) \cdot \boldsymbol{i} \,\,d\Gamma \end{cases}$$

 $\mathcal{U}_{\mathsf{ad}} = \{ \Omega : |\Omega| = V, \text{ with } \Gamma_{\mathsf{in}}, \Gamma_{\mathsf{out}}, \Gamma_w \text{ fixed} \}$

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Numerical Results

We can define the shape derivative of a cost functional $J(\Omega)$ at Ω , in the direction of a vector field \boldsymbol{v} : $dJ(\Omega; \boldsymbol{v})$.

The velocity method: Let v be a smooth vector field. Define

$$\frac{d}{dt}X(t;x) = v(X(t;x)) \quad t > 0$$

$$X(0,x) = x$$

Let Ω_t be the image under $X(t; \cdot)$ of Ω

$$\Omega_t := \left\{ X(t;x) : x \in \Omega \right\}$$

We then define the shape derivative of $J(\Omega)$ in the direction \boldsymbol{v} as

$$dJ(\Omega; \boldsymbol{v}) = \lim_{t \to 0} \frac{J(\Omega_t) - J(\Omega)}{t}.$$

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Hadamard-Zolesio Theorem: There exists a function $g(\Omega)$ defined on $\partial\Omega$

$$dJ(\Omega;oldsymbol{v}) = \int_{\partial\Omega} g(\Omega)(oldsymbol{v}\cdotoldsymbol{n}) \, d\Gamma$$

The shape derivative depends only on the normal component of m v on $\partial\Omega.$

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Volume $J(\Omega) = \int_{\Omega} dx$ $dJ(\Omega; \boldsymbol{v}) = \int_{\Omega} \nabla \cdot \boldsymbol{v} \, dx = \int_{\Gamma} \mathbf{1}(\boldsymbol{v} \cdot \boldsymbol{n}) \, d\Gamma$ ・ロン ・四 ・ ・ ヨ ・ ・ ヨ ・ ・

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Area/Perimeter

$$J(\Omega) = \int_{\partial\Omega} d\Gamma$$

$$dJ(\Omega; \boldsymbol{v}) = \int_{\partial\Omega} \kappa(\boldsymbol{v} \cdot \boldsymbol{n}) d\Gamma$$

$$J(\Omega) = \int_{\partial\Omega} \phi \, d\Gamma \qquad (\phi : \mathbb{R}^d \to \mathbb{R})$$

$$dJ(\Omega; \boldsymbol{v}) = \int_{\partial\Omega} \left(\frac{\partial \phi}{\partial \boldsymbol{n}} + \phi \kappa \right) (\boldsymbol{v} \cdot \boldsymbol{n})$$

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The shape derivative depends only on the normal component of v on $\partial\Omega$. Obstacle Drag

$$dJ(\Omega; \boldsymbol{v}) = -2\nu \int_{\Gamma_s} [\varepsilon(\boldsymbol{u}) : \varepsilon(\boldsymbol{z})](\boldsymbol{v} \cdot \boldsymbol{n}) d\Gamma$$

With z solution to the adjoint problem

$$\begin{split} -\nabla \cdot \boldsymbol{T}(\boldsymbol{z},q) &= 0 & \text{ in } \Omega \\ \nabla \cdot \boldsymbol{z} &= 0 & \text{ in } \Omega \\ \boldsymbol{z} &= -\boldsymbol{i} & \text{ on } \Gamma_s \\ \boldsymbol{z} &= 0 & \text{ on } \Gamma_w \cup \Gamma_{\text{in}} \\ \boldsymbol{T}(\boldsymbol{z},q) \cdot \boldsymbol{n} &= 0 & \text{ on } \Gamma_{\text{out}} \end{split}$$



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Shape Optimization through Adaptive SQP

Goal: Design an algorithm to adaptively build $\{\Omega_k\}_{k\geq 0}$ converging to a local minimizer Ω^* of $J(\Omega, u(\Omega))$. Use low resolution at initial stages and improve accuracy upon convergence.

First Step: Design ∞ -SQP. An *ideal* Sequential Quadratic Programming algorithm assuming the PDE's can be solved exactly.

Second Step: Design a discrete counterpart of ∞ -SQP, using adaptivity to improve approximation upon convergence

→ Adaptive Sequential Quadratic Programming (ASQP)

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- $\mathbb{V}(\Gamma_k)$: Hilbert space defined on $\Gamma_k = \partial \Omega_k$ ($L^2(\Gamma_k)$, $H^1(\Gamma_k)$, etc)
- ▶ $b_k(\cdot, \cdot) : \mathbb{V}(\Gamma_k) \times \mathbb{V}(\Gamma_k) \to \mathbb{R}$ continuous and coercive bilinear form.
- ▶ Quadratic model of J at $\Omega_k \quad \rightsquigarrow \quad Q_k : \mathbb{V}(\Gamma_k) \to \mathbb{R}$

$$Q_k(w) = J(\Omega_k) + dJ(\Omega_k, w) + \frac{1}{2}b_k(w, w)$$

Search direction $v_k :=$ minimizer of $Q_k(w)$. Hence

$$v_k \in \mathbb{V}(\Gamma_k) : b_k(v_k, w) = -\langle g_k, w \rangle_k, \quad \forall w \in \mathbb{V}(\Gamma_k)$$

• v_k is a descent direction

$$0 \le b_k(v_k, v_k) = -\langle g_k, v_k \rangle_k = -dJ(\Omega_k, v_k)$$

The choice of b_k may have a *regularizing effect*

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∞ -SQP Algorithm

Given an initial domain Ω_0 , set k=0 and iterate:

(a) Compute $u_k = u(\Omega_k)$ by solving $\mathcal{A} u_k = f$

(b) Compute the Riesz representation $g_k = g(\Omega_k)$ of the shape derivative $dJ(\Omega_k, \cdot)$ (solve dual problem)

(c) Compute the search direction v_k by solving

$$v_k \in \mathbb{V}_k$$
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(d) Determine an admissible stepsize μ_k satisfying

 $J(\Omega_k + \mu_k \boldsymbol{v}_k) << J(\Omega_k)$ (line search)

(e) Update $\Omega_{k+1} \leftarrow \Omega_k + \mu_k \boldsymbol{v}_k$ $(\boldsymbol{v}_k = v_k \boldsymbol{n})$; $k \leftarrow k+1$.

NOT REALISTIC ∞ -dimensional problems

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Towards a realistic adaptive algorithm

Replace non-computable operations by adaptive finite approximations.

- → two main sources of error:
 - Adaptive approximation of PDE (PDE Error) $\rightsquigarrow u_k, J, dJ (g_k)$ Adaptive approximation of domain (Geometric Error) $\rightsquigarrow v_k$

Goals:

- distribute the computational effort between the two sources of error and adjust the accuracies along the iteration
 it is wasteful to impose PDE Error finer than Geometric Error
- sort out whether geometric singularities are genuine to the problem or due to lack of resolution
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ASQP algorithm

- \mathcal{T}_k : triangulation of Ω_k
- $\mathbb{S}_k = \mathbb{S}_k(\Omega_k)$: finite element space defined on Ω_k
- $\mathbb{V}_k = \mathbb{V}_k(\Gamma_k)$: finite element space defined on Γ_k
- $\blacktriangleright \ \mathcal{E}_k = (\Omega_k, \mathbb{S}_k, \mathbb{V}_k)$

The ASQP algorithm is an iteration of the form:

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Adaptivity is carried out in APPROXJ and DIRECTION

- ▶ APPROXJ acts on PDE Error
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APPROXJ enriches/coarsens PDE space \mathbb{S}_k to control the error in the approximate functional value $J_k(\Omega_k + \mu_k V_k)$ to the prescribed tolerance ε (Goal oriented adaptivity / DWR method)

We choose $\varepsilon := \gamma \mu_k \|V_k\|_{\Gamma_k}^2$, $\gamma > 0$

 $\begin{array}{ll} \text{APPROXJ} & \Rightarrow & \left| J(\Omega_k + \mu_k \boldsymbol{V}_k) - J_k(\Omega_k + \mu_k \boldsymbol{V}_k)) \right| \leq \gamma \mu_k \|V_k\|_{\Gamma_k}^2 \end{array}$

- ► The value of ε is not very demanding ~→ coarse meshes at the beginning and a combination of refinement and coarsening later on.
- ▶ DWR detects geometric singularities, such as corners, and refines/coarsen what is necessary for computing *J* accurately

Dual Weighted Residual method (DWR) [Becker, Rannacher '96 & '01]

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ASQP (Module DIRECTION)

- G_k approximation to shape derivative $g(\Omega_k)$
- $v_k \in \mathbb{V}(\Gamma_k)$ exact solution of $\mathcal{B}_k v_k = -G_k$
- $V_k \in \mathbb{V}(\Gamma_k)$ finite element approximation to v_k .

```
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```

 $\|V_k - v_k\|_{\Gamma_k} \le \theta \|V_k\|_{\Gamma_k} \qquad (\theta \le 1/2)$

 $\begin{array}{l} \mbox{Example: } \mathcal{B}_k = -\Delta_{\Gamma_k} \Rightarrow \mbox{Adaptivity for Laplace-Beltrami} \\ \mbox{[Demlow, Dziuk '07], [Mekchay, M., Nochetto '09]} \end{array}$

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$$\begin{aligned} \left| J(\Omega_k + \mu_k \boldsymbol{V}_k) - J(\Omega_k + \mu_k \boldsymbol{v}_k) \right| &\simeq \mu_k \left| dJ(\Omega_k; \boldsymbol{V}_k - \boldsymbol{v}_k) \right| \\ &= \mu_k \left| b_k(v_k, V_k - v_k) \right| \\ &\leq \delta \mu_k \|V_k\|_{\Gamma_k}^2 \qquad (\delta = M \, \theta \, (1 + \theta)) \end{aligned}$$

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ASQP

- $\blacktriangleright \text{ APPROXJ } \Rightarrow \left|J(\Omega_k + \mu_k \boldsymbol{V}_k) J_k(\Omega_k + \mu_k \boldsymbol{V}_k))\right| \leq \gamma \mu_k \|V_k\|_{\Gamma_k}^2$
- ► DIRECTION ⇒ $\left|J(\Omega_k + \mu_k \boldsymbol{V}_k) J(\Omega_k + \mu_k \boldsymbol{v}_k)\right| \le \delta \mu_k \|V_k\|_{\Gamma_k}^2$
- APPROXJ + DIRECTION \Rightarrow bound on local error at iteration k

$\left|J_k(\Omega_k + \mu_k \boldsymbol{V}_k) - J(\Omega_k + \mu_k \boldsymbol{v}_k)\right| \le (\gamma + \delta) \mu_k \|V_k\|_{\Gamma_k}^2$

(choose $\gamma \simeq \delta \
ightarrow$ balance computational loads)

Consistency check of ASQP

If ASQP converges to a stationary point $(\mu_k || V_k ||_{\Gamma_k}^2 \to 0)$

- ▶ DIRECTION and APPROXJ approximate the descent direction v_k and functional $J(\Omega_k)$ increasingly better
- \blacktriangleright PDE and Geometric Error progressively decrease as $k \rightarrow \infty$

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Layout

Introduction: Shape Optimization Problem

Shape Calculus

AFEM for Shape Optimization

Numerical Results

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Minimization of an obstacle drag

Initial and Final Shape (DRAG minimization)



Numerical simulations 🛶 toolbox ALBERTA www.alberta-fem.de 🗄 🛛 🗄 🔊 🌣

Further Ingredients

- Mesh quality: is maintained through an optimization routine that works locally. We try to avoid *remeshing*, but sometimes it is necessary.
- Timestep: is controlled to ensure proper reduction and to avoid node crossing. Remeshing helps to allow bigger timesteps.
- Volume or perimeter constraints: are handled with Lagrange multipliers and maintained up to machine precision.
- Refinement on the moving boundary: is done in a geometrically consistent way, to avoid overrefinement around fake corners and bad approximation of curvature.

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Conclusions

- ► We developed an adaptive finite element method for shape optimization, based on an adaptive finite dimensional version of an ∞-dimensional SQP algorithm ~> ASQP
- ► The adaptive refinement acts on two different sources of error:
 - PDE error due to discretization
 - Geometric Error due to boundary approximation
- A dynamically varying accuracy balances the computational effort between the two sources of error
- The algorithm is able to sort out whether geometric singularities are genuine to the problem or due to lack of numerical resolution, and to correct the effects of early (and no longer necessary) mesh refinements

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The Module APPROXJ

$$\begin{split} [\mathcal{T}_*, U_*, Z_*, J_*, G_*] &= \texttt{APPROXJ}(\Omega, \mathcal{T}, \varepsilon) \\ \Omega_* &= \Omega \\ \texttt{do} \\ & [U_*, Z_*] &= \texttt{SOLVE}(\Omega, \mathcal{T}_*) \\ & \{\eta_*(T)\}_{T \in \mathcal{T}_*} &= \texttt{ESTIMATE}(U_*, Z_*, \mathbb{S}_* \\ & [\mathcal{R}_*, \mathcal{C}_*] &= \texttt{MARK}(\mathcal{T}_*, \{\eta_*(T)\}_{T \in \mathcal{T}_*}) \\ & \texttt{if} \ (\eta_*(\mathcal{T}_*) > \varepsilon) \\ & & [\mathcal{T}_*, \mathcal{C}_*] &= \texttt{REFINE}(\mathcal{T}_*, \mathcal{R}_*) \\ & \texttt{elseif} \ (\eta_*(\mathcal{C}_*) < \delta \varepsilon) \\ & \mathcal{T}_* &= \texttt{COARSEN}(\mathcal{T}_*, \mathcal{C}_*) \\ & \texttt{endif} \\ & \texttt{while} \ (\eta_*(\mathcal{T}_*) > \varepsilon) \\ & J_* &= \texttt{EVALJ}(\Omega, \mathcal{T}_*, U_*) \\ & G_* &= \texttt{RIESZ}(\Omega, \mathcal{T}_*, U_*, Z_*) \end{split}$$

SOLVE: solve the discrete system for the primal and dual variables U_* , Z_* .

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ESTIMATE: use DWR method to compute a posteriori error estimators taylored to approximate the functional J.

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MARK: use maximum strategy. Given $0 < \delta^- \ll \delta^+ < 1$, let $\eta_* = \max_{T \in \mathcal{T}_*} \eta_*(T)$ and

$$\eta_*(T) > \delta^+ \eta_* \quad \Rightarrow \quad T \in \mathcal{R}_*, \qquad \qquad \eta_*(T) < \delta^- \eta_* \quad \Rightarrow \quad T \in \mathcal{C}_*.$$

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 $\begin{array}{l} \textbf{REFINE/COARSEN:} \ \text{Refine the marked elements (in \mathcal{R}_*) using a Geometrically Consistent} \\ \textbf{Refinement algorithm on the boundary; coarsen the elements in \mathcal{C}_*.} \end{array}$

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DWR for Drag functional

The following DWR error estimate holds

$$|J(\boldsymbol{u}, p) - J(\boldsymbol{U}, P)| \leq \sum_{T} \left\{ \|r(\boldsymbol{U}, P)\|_{T} \|\boldsymbol{z} - \boldsymbol{Z}\|_{T} + \|j(\boldsymbol{U}, P)\|_{\partial T} \|\boldsymbol{z} - \boldsymbol{Z}\|_{\partial T} \right\}$$
$$+ \sum_{T} \|\mathcal{R}(\boldsymbol{U})\|_{T} \|q - Q\|_{T},$$

with

$$r(\boldsymbol{U})|_T := -\nabla \cdot (2\nu\varepsilon(\boldsymbol{U}) - P\mathbf{I}) \qquad \mathcal{R}|_T := \nabla \cdot \boldsymbol{U},$$

$$j(\boldsymbol{U})|_{e} = \begin{cases} \frac{1}{2} [2\nu\varepsilon(\boldsymbol{U}) \cdot \boldsymbol{n} - P\boldsymbol{n}] & e \cap \partial\Omega = \emptyset\\ 2\nu\varepsilon(\boldsymbol{U}) \cdot \boldsymbol{n} - P\boldsymbol{n} & e \subset \Gamma_{out}\\ 0 & \text{otherwise,} \end{cases}$$

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SQP with constraint

- ▶ Quadratic model $Q(w) := J(\Omega) + \langle g, w \rangle + \frac{1}{2}b_{\Gamma}(w, w)$
- ► Volume $C(\Omega) = \int_{\Omega} dx \quad \rightsquigarrow \quad dC(\Omega; w) = \langle 1, w \rangle$

Lagrangian

$$\mathcal{L}(w,\lambda) = Q(w) + \lambda(C(\Omega+w) - VOL) \simeq Q(w) + \lambda(dC(\Omega,w))$$

▶ Find (v, λ) such that

$$\nabla_w Q(v) + \lambda = 0$$

$$C(\Omega + v\mathbf{n}) - VOL = 0$$

- $v = v_0 + \lambda v_1$, with $\mathcal{B}v_0 = -g$ and $\mathcal{B}v_1 = -1$
- Apply Newton's method to $c(\lambda) := \int_{\Omega + \mu(v_0 \boldsymbol{n} + \lambda v_1)} dx VOL = 0$

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The Module LINESEARCH

$$\begin{split} [\Omega_*,\mathcal{T}_*,\mu] &= \texttt{LINESEARCH}(\Omega,\mathcal{T},\boldsymbol{V},J,G,m) \\ \mu &= 2m\,,~\varphi = J\,,~\psi = \langle G,V\rangle_{\Gamma} \\ \texttt{do} \end{split}$$

$$\begin{split} \mu &\leftarrow \mu/2; \\ [\Omega_*,\mathcal{T}_*] = \texttt{UPDATE}(\Omega,\mathcal{T},\mathbf{V},\mu) \\ [U_*,Z_*] = \texttt{SOLVE}(\Omega_*,\mathcal{T}_*) \\ \varphi_* &= \texttt{EVALJ}(\Omega_*,\mathcal{T}_*,U_*) \\ \end{split}$$
 while ($\varphi_* > \varphi + \alpha \mu \psi$)

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Evolution of meshes (DRAG minimization)

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Initial Mesh



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Evolution of meshes (DRAG minimization)

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Mesh after 1 iteration



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Evolution of meshes (DRAG minimization)

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Mesh after 2 iterations



Evolution of meshes (DRAG minimization)

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Mesh after 3 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 4 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 5 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 6 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 9 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 10 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 15 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 16 iterations


Evolution of meshes (DRAG minimization)

go back

Mesh after 17 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 20 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 22 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 25 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 27 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 28 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 30 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 32 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 34 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 40 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 42 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 45 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 47 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 49 iterations



Evolution of meshes (DRAG minimization)

go back

Mesh after 52 iterations



go back



go back



go back



go back



go back



go back



go back



go back

Initial Mesh



go back

Mesh after 1 iteration



go back

Mesh after 2 iterations



go back

Mesh after 3 iterations



go back

Mesh after 4 iterations



go back

Mesh after 5 iterations



go back

Mesh after 6 iterations



go back

Mesh after 7 iterations



go back

Mesh after 8 iterations



go back

Mesh after 9 iterations



go back

Mesh after 10 iterations



go back

Mesh after 11 iterations



go back

Mesh after 12 iterations



go back

Mesh after 13 iterations


go back

Mesh after 14 iterations



go back

Mesh after 15 iterations



go back

Mesh after 16 iterations



go back

Mesh after 17 iterations



go back

Mesh after 18 iterations



go back

Mesh after 19 iterations

