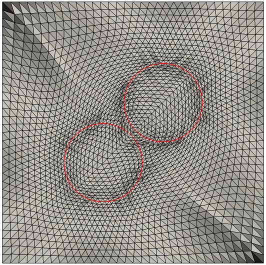
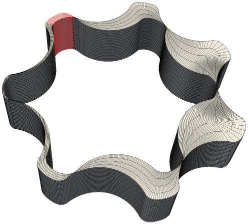
fakultät für mathematik

technische universität dortmund

Nonlinear Hyperelasticity-based Mesh Optimisation

Jordi Paul





Why we need “good” meshes

The task

On $\Omega \subset \mathbb{R}^d$ with a mesh $\mathcal{T}_h$, use the Finite Element Method to solve some kind of PDE, describing e.g.

1. transport phenomena,
2. deformations in solid mechanics,
3. incompressible flows.

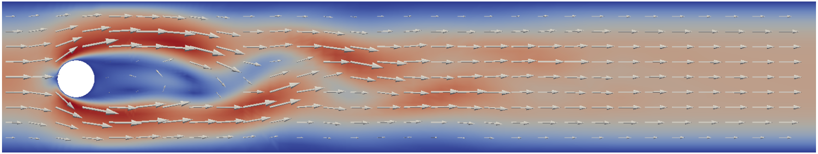


Figure: Navier-Stokes Bench 1: Velocity field

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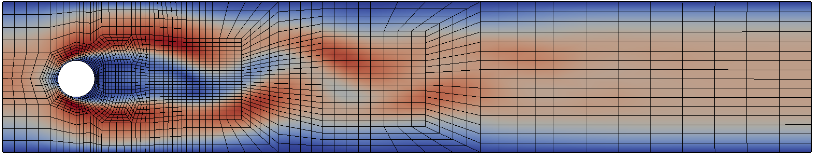
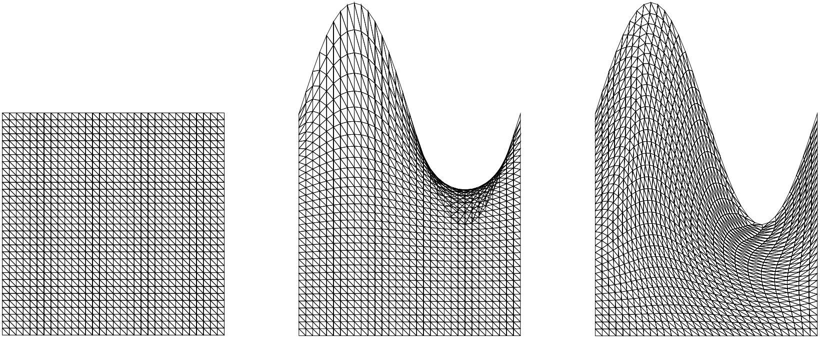


Figure: Navier-Stokes Bench 1: Underlying mesh

Requirements for $\mathcal{T}_h$

Requirement for the Finite Element Method

1. $\mathcal{T}_h$ must be free of intersecting cells

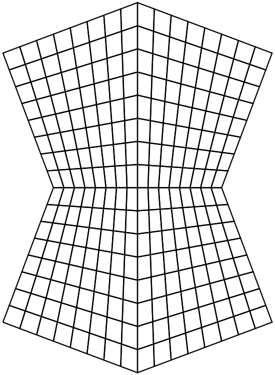


Initial mesh. Bad: Intersecting cells. Goal: No intersections.

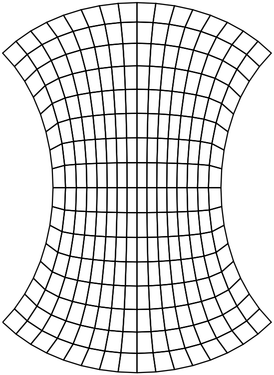
Requirements for $\mathcal{T}_h$

Reality is not polygonally bounded

2. $\mathcal{T}_h$ must capture the geometry of Ω.



Geometry insufficiently resolved.

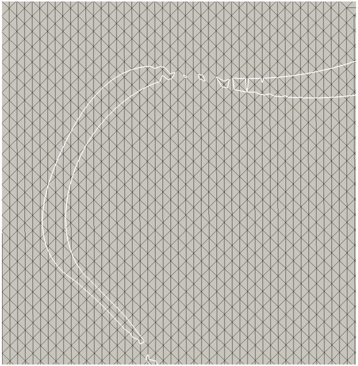


Good resolution of the boundary.

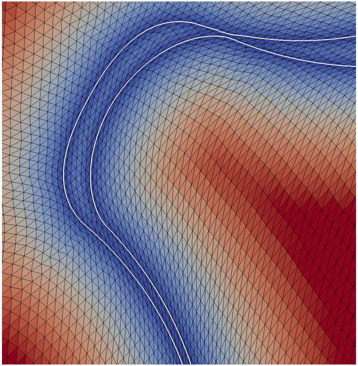
Requirements for $\mathcal{T}_h$

What is "fine enough"?

3. $\mathcal{T}_h$ must sufficiently resolve the solution u_h.



Insufficient resolution of the 0-levelset.



Good resolution of the 0-levelset by r-adaptivity.

Generic mesh optimisation problem

For a *mesh quality functional* $\mathcal{F}$ find an optimal deformation

$$\Phi^* = \operatorname{argmin}_{\Phi \in \mathcal{D}} \mathcal{F}(\Phi), \mathcal{D} \subset \left\{ \Phi : \Omega \to \mathbb{R}^d : \forall x \in \Omega : \det(\nabla \Phi(x)) > 0 \right\}$$

The orientation preserving property

$\det(\nabla \Phi(x)) > 0$ is crucial for applying the Finite Element Method.

(a) Initial configuration. (b) After applying the mapping Φ.

Figure: Overlap of cells resulting from one cell changing orientation.

My goals

Find a class of mesh quality functionals $\mathcal{F}$ such that

1. $\det(\nabla\Phi) > 0$ is enforced (robustness),
2. it is applicable in $2d$ and $3d$ for both simplex and hypercube meshes,
3. optimal cell sizes can be defined directly (r-adaptivity),
4. flexible boundary conditions are possible.

Such a method is available - in “theory“[1]

[1] M. Rumpf. “A variational approach to optimal meshes”. In: *Numerische Mathematik* (1996).

My goals

Find a class of mesh quality functionals $\mathcal{F}$ such that

1. $\det(\nabla\Phi) > 0$ is enforced (robustness),
2. it is applicable in 2*d* and 3*d* for both simplex and hypercube meshes,
3. optimal cell sizes can be defined directly (*r*-adaptivity),
4. flexible boundary conditions are possible.

Such a method is available - in “theory“[1]

- Not for hypercube meshes.
- *r*-adaptivity only mentioned.
- Additional theory required.
- Efficient nonlinear solvers not readily available.
- HPC-level implementation (MPI parallel, numerically efficient) using FEAT3.
- Application to complex geometries and ”large“ problems.

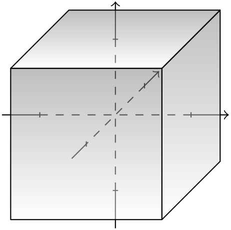
[1] M. Rumpf. “A variational approach to optimal meshes”. In: *Numerische Mathematik* (1996).

Reference cells, isotropic case

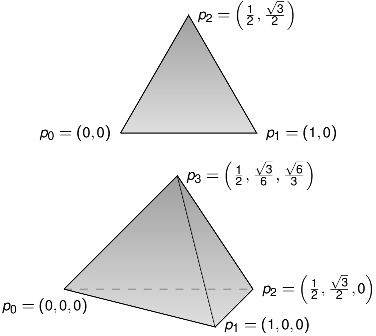
Assumptions

1. $\forall K \in \mathcal{T}_h$ there exists an optimal reference cell $\hat{K}$.

Hypercubes: $\hat{K}_n = [-1, 1]^d$



Simplices:



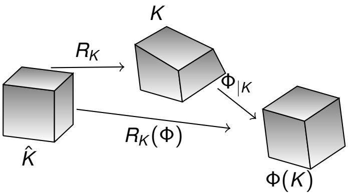
Optimal shape $\hat{K}_n$ and optimal scale $h(K)$

Can be individually chosen: $\hat{K} = h(K)\hat{K}_n$.

Reference mapping and local functionals

Assumptions

2. $\mathcal{F}(\Phi) = \sum_{K\in\mathcal{T}_h} \mu_K \int_K \tilde{\mathcal{L}}_K(\Phi)$ (Locality).
3. $\forall c \in \mathbb{R}^d : \tilde{\mathcal{L}}_K(\Phi + c) = \tilde{\mathcal{L}}_K(\Phi)$ (Translation invariance).
   $\Rightarrow\ \exists\mathcal{L} : \tilde{\mathcal{L}}_K(\Phi) = \mathcal{L}_K(\nabla\Phi)$



4. $\lim_{\det(\nabla\Phi)\to 0} \mathcal{L}_K(x, \nabla\Phi) = \infty$ (Regularity property).

- This enforces the orientation preserving property
- $\mathcal{L}_k$ cannot be convex in $\nabla\Phi$ but must be at least polyconvex

Observation

$\mathcal{L}$ is a *stored energy function* of a *hyperelastic material*.

[2] P. G. Ciarlet. *Mathematical elasticity Vol. I: Three-dimensional elasticity*. Studies in Mathematics and its Applications. Amsterdam: North-Holland Publishing Co., 1988

Stored energy functionals

Observation

$\mathcal{L}$ is a *stored energy function* of a *hyperelastic material*.

Existence theorem [2]:

Let $\Omega \subset \mathbb{R}^3$, $\partial\Omega = \Gamma_0 \cup \Gamma_1$, Γ_i $d\sigma$-measurable and $\mathrm{vol}_2(\Gamma_0) > 0$, $\mathcal{L} : \Omega \times \mathrm{SL}_3$ with the properties of

1. **Polyconvexity:** $\forall x \in \Omega$ *a.e.* $: \exists \tilde{L}(x,\cdot,\cdot,\cdot) : \mathrm{SL}_3 \times \mathrm{SL}_3 \times (0,\infty) \to \mathbb{R} :$ $\tilde{L}$ is convex and

$$\forall F \in \mathrm{SL}_3 : \quad \mathcal{L}(x,F) = \tilde{L}(x,F,\mathrm{Cof}(F),\det(F)),$$

2. **Stability**
3. **Coerciveness:** $\exists \alpha \in \mathbb{R}_+, \beta \in \mathbb{R}, 2 \le p \in \mathbb{N}, \frac{p}{p-1} \le q \in \mathbb{N}, 1 < r \in \mathbb{R} :$
   $\forall x \in \Omega$ *a.e.*$, \forall F \in \mathrm{SL}_3 :$

$$\mathcal{L}(x,F) \ge \alpha(\|F\|_F^p + \|\mathrm{Cof}(F)\|_F^q + \det(F)^r) + \beta$$

[2] P. G. Ciarlet. *Mathematical elasticity Vol. I: Three-dimensional elasticity*. Studies in Mathematics and its Applications. Amsterdam: North-Holland Publishing Co., 1988

Theory

Existence theorem [2]:

Let $\phi_0 \in L^1(\Gamma_0, \mathbb{R}^3)$ such that

$$\emptyset \neq \mathcal{D}_{\phi_0} := \{\Phi \in W^{1,p}(\Omega) : \mathrm{Cof}(\nabla\Phi) \in L^q(\Omega), \det(\nabla\Phi) \in L^r(\Omega),$$
$$\forall x \in \Omega \ a.e. : \det(\nabla\Phi)(x) > 0, \quad \forall x \in \Gamma_0 \ d\sigma \ a.e. : \Phi(x) = \phi_0(x)\}$$

Let $f \in L^p(\Omega)$ and $g \in L^s(\Gamma_1)$ such that the linear form

$$l : W^{1,p}(\Omega) \to \mathbb{R}, \quad l(\Phi) := \int_\Omega f \cdot \Phi dx + \int_{\Gamma_1} g \cdot \Phi d\sigma$$

is continuous and define

$$\mathcal{F}(\Phi) := \int_\Omega \mathcal{L}(x, \nabla\Phi(x)) dx - l(\Phi).$$

If $\exists \Phi \in \mathcal{D}_{\phi_0} : \mathcal{F}(\Phi) < +\infty$, there exists at least one

$$\Phi^* \in \mathcal{D}_{\phi_0} : \mathcal{F}(\Phi^*) = \inf_{\Phi \in \mathcal{D}_{\phi_0}} \mathcal{F}(\Phi).$$

Geometric interpretation and an example

h, $\hat{K}_n$ and R_K define a material behaviour

$$\mathcal{L}(\nabla\Phi)_{|K} = \mathcal{L}_K(\nabla R_K(\Phi))$$

1. $\|\nabla R_K(\Phi)\|_F^2$ measures length change of line segments.
2. $\|\mathrm{Cof}(\nabla R_K(\Phi))\|_F^2$ measures the facet deformation.
3. $\det(\nabla R_K(\Phi))$ measures the volume change.

Example for a local functional:

$$\begin{aligned}\mathcal{L}_K(\nabla R_K(\Phi)) = c_f(\|\nabla R_K(\Phi)\|_F^2 - d)^2 + \det(\nabla R_K(\Phi))^{p_d} \\ + \frac{c_d}{\left(\det(\nabla R_K(\Phi)) + \sqrt{\delta_r^2 + (\det(\nabla R_K(\Phi)))^2}\right)^{p_d}}\end{aligned}$$

Other methods not enforcing $\det(\nabla\Phi) > 0$

1. Harmonic energy: $\mathcal{F}(\Phi) = \|f - \Delta\Phi\|_{L^2(\mathcal{T}_h)}$
2. Biharmonic energy: $\mathcal{F}(\Phi) = \|f - \Delta^2\Phi\|_{L^2(\mathcal{T}_h)}$
3. Linearised elasticity:

$$\mathcal{F}(\Phi) = \|f - \nabla \cdot (\lambda \nabla \cdot \Phi + \frac{\mu}{2}(\nabla\Phi + (\nabla\Phi)^T)\|_{L^2(\mathcal{T}_h)}$$

Properties

+ Numerically “cheap”
+ Well-known problems
- Orientation preserving property coincidental
- Not robust enough for surface alignment
- Efficient solvers not readily available for all cases

Computational aspects

The hyperelasticity-based functional is hard to treat numerically:

1. Highly nonlinear.
2. Nonconvex with many local minimisers due to the polyconvexity.
3. Many local singularities.

How to find a minimiser?

Solve the Euler-Lagrange equations:

$$-\nabla \cdot \frac{\partial \mathcal{L}}{\partial F}(x, \nabla\Phi(x)) = f(x, \Phi(x))$$

But: Strong assumptions needed for the minimiser to be a solution.

Nonlinear solver

- Newton's method not applicable because $\mathcal{F}''$ is not positive definite
- Use line search based methods instead

Fréchet derivatives

Let $M : \mathbb{R} \to \mathbb{R}^{n\times n}$.

$$\frac{d}{dt}\det M(t) = \det M(t)\,\mathrm{tr}\left(M(t)^{-1}\frac{d}{dt}M(t)\right).$$

Using $M(t) := \nabla\phi + t\nabla\eta$:

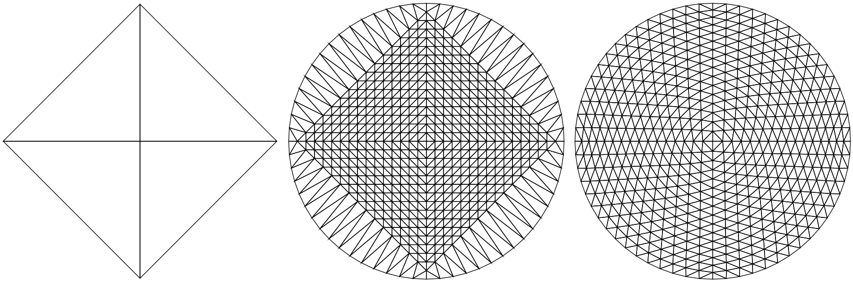
$$G_1(\Phi) := (\|\nabla\Phi\|_F^2 - d)^2, \quad G_1'(\Phi)\eta = 4\left(\|\nabla\Phi\|_F^2 - d\right)\nabla\Phi : \nabla\eta,$$

$$G_2(\Phi) := \left(\|\operatorname{Cof}(\nabla\Phi)\|_F^2 - d\right)^2$$

$$\begin{aligned} G_2(\Phi)'\eta =& 4(\|\operatorname{Cof}(\nabla\Phi)\|_F^2 - d)\ \operatorname{Cof}(\nabla\Phi) : \\ & \left[\left(\left([(\nabla\Phi)^{-1} : \nabla\eta]\ I_d - (\nabla\Phi)^{-1}\nabla\eta\right)\right)\operatorname{Cof}(\nabla\Phi)\right] \end{aligned}$$

$$G_3(\Phi) := \det(\nabla\Phi)^{p_d}, \quad G_3'(\Phi)\eta = p_d\det(\nabla\Phi)^{p_d}(\nabla\Phi)^{-T} : \nabla\eta$$

Degenerating family of meshes



(a) $\mathcal{T}_{h,0}$. (b) $\mathcal{T}_{h,4}$. (c) $\Phi^*(\mathcal{T}_{h,4})$.

1. Refinement lets $\alpha_{\text{min}} \to 0$
2. Simple problem to study mesh dependence

Degenerating family of meshes

l	DoF	NLCG # its	NLCG $t[s]$	NLSD-lBFGS # its	NLSD-lBFGS $t[s]$
3	290	44	$6.4e{-3}$	40	$6.2e{-3}$
4	1090	103	$4.3e{-2}$	94	$3.9e{-2}$
5	4226	208	$3e{-1}$	184	$3.1e{-1}$
6	16642	400	$2.1e{+0}$	377	$3.4e{+0}$
7	66050	1081	$2.9e{+1}$	791	$3e{+1}$
8	263170	3908	$6.8e{+2}$	1915	$3.7e{+2}$
9	1050626	1156	$1.4e{+3}$	389	$5.8e{+2}$
10	4198402	388	$1.1e{+3}$	507	$4.1e{+3}$
11	16785410	359	$4e{+3}$	759	$7.4e{+3}$

Table: Solver stagnated or stopped early.

Increasing iteration numbers and runtimes

Find PDE-based preconditioner instead.

Nonlinear Conjugate Gradient Method

Algorithm 1 Preconditioned nonlinear Conjugate Gradient (NLCG).

For a given Φ_0, preconditioner $B : \mathbb{R}^d \to \mathbb{R}^d$ and initial search direction $d^{(0)}$ do $k = 0, \ldots, N$:

1. Use a *line search* to compute $\alpha^{(k)}$: $\mathcal{F}(\Phi^{(k)} + \alpha d^{(k)}) < \mathcal{F}(\Phi)$.
2. Set $\Phi^{k+1} = \Phi^{(k)} + \alpha d^{(k)}$.
3. Compute a new descent direction

$$d^{(k+1)} = -B^{-1}\, \mathcal{F}'(\Phi^{(k)}) + \beta^{(k)} d^{(k)}$$

- Efficient line searches are non-trivial
- Implementation uses FEAT3's MPI parallel structures
- Preconditioner should use the most powerful tools available (parallel geometric multigrid)

Preconditioning with a second order operator

Recall

$$\left(\|\nabla\Phi\|_F^2 - d)^2\right)'\eta = 4\left(\|\nabla\Phi\|_F^2 - d\right)\nabla\Phi : \nabla\eta$$

Linear operator for preconditioning

$$A : \mathcal{D}_{\phi_0} \to \mathcal{D}_0', (A\Phi,\eta) := (\mathbf{D}(\Phi),\mathbf{D}(\eta)), \quad \mathbf{D}(\Phi) = \frac{1}{2}(\nabla\Phi + (\nabla\Phi)^T)$$

1. Another positive definite approximation for the Hessian $\mathcal{F}''$.
2. Solver for A_h defines the choice of preconditioner $B = (\tilde{A}_h)^{-1}$.
3. Efficient parallel solvers (e.g. PCG-MG) available.

Degenerating family of meshes

l	DoF	NLCG # its	NLCG $t[s]$	NLSD-lBFGS # its	NLSD-lBFGS $t[s]$	NLCG-$\tilde{A}_h^{s,M}$ # its	NLCG-$\tilde{A}_h^{s,M}$ $t[s]$
3	290	44	$6.4e{-}3$	40	$6.2e{-}3$	24	$2.3e{-}2$
4	1090	103	$4.3e{-}2$	94	$3.9e{-}2$	30	$9.2e{-}2$
5	4226	208	$3e{-}1$	184	$3.1e{-}1$	32	$3.8e{-}1$
6	16642	400	$2.1e{+}0$	377	$3.4e{+}0$	36	$1.7e{+}0$
7	66050	1081	$2.9e{+}1$	791	$3e{+}1$	38	$8.2e{+}0$
8	263170	3908	$6.8e{+}2$	1915	$3.7e{+}2$	43	$5.6e{+}1$
9	1050626	1156	$1.4e{+}3$	389	$5.8e{+}2$	39	$1.7e{+}2$
10	4198402	388	$1.1e{+}3$	507	$4.1e{+}3$	76	$2.1e{+}3$
11	16785410	359	$4e{+}3$	759	$7.4e{+}3$	29	$3.7e{+}3$

Table: Solver stagnated or stopped early.

Numerical effort still considerable

1. Optimise mesh on coarser level than the PDE
2. Post-optimisation adaption necessary
3. Extrude from $2d$ to $3d$ if possible

Software used

FEAT3

Common successor to FEAT2 and FEAST, developed since 2011

- MPI-parallel high-performance cross-platform general purpose FEM toolkit
- Full (unstructured) $2d/3d$ support: trias, quads, tetras and hexas
- C++11 standard conforming, well-documented, automated regression testing
- Very powerful (non-)linear solver framework including mixed-arch/-prec/MKL/GPU support
- Designed for academic research, student projects, HPC and industry applications
- In active development, but lacking real world applications

Robustness

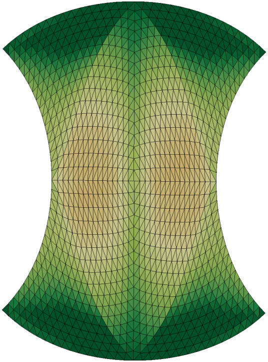


Figure: $t = 0$.

Moving boundary

- Stop when $\alpha_{\min} < 1^\circ$
- NLCG-$(\tilde{A}_h)^{-1}$
- Colouring from red (1°) to green (45°).

$$\varphi_b : [0, \bar{t}] \times \partial\Omega(0) \to \mathbb{R}^2, \varphi_b(t,x) = x + t \begin{pmatrix} (x_1 - \xi_1) + (x_2 - \xi_2)^3 \\ -(x_1 - \xi_1) + (x_2 - \xi_2)^3 + (x_2 - \xi_2)^3 \end{pmatrix}$$

r-adaptivity, surface alignment[3], topology changes

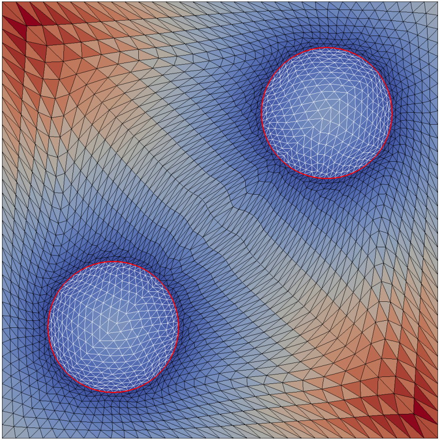


Figure: $t = 0$.

Moving implicit surfaces $\Gamma_{1,2}$

- Optimal scales according to distance to Γ_i
- Cell size varies by factor of 20
- Additional nonlinearity $\mathcal{L} = \mathcal{L}(\nabla R_{K,n}, h(K))$
- Efficient preconditioner not available
- Colouring according to cell size (blue: 5e-5, red: 1e-3)
- Mesh *aligned* with moving surfaces

[3] S. Basting and M. Weismann. "A hybrid level set front tracking finite element approach for fluid–structure interaction and two-phase flow applications". In: *Journal of Computational Physics* (2013).

Why surface alignment?

Elliptic interface problem with different coefficients $\beta_{1,2}$[4].

$$\begin{aligned} \nabla\cdot(\beta\nabla u) &= f \text{ in } \Omega, \\ u &= 0 \text{ on } \partial\Omega, \\ [u]_\Gamma &:= (u_{1|\Gamma} - u_{2|\Gamma}) = 0, \\ [\beta\partial_\nu u]_\Gamma &:= (\beta_1\partial_{\nu_1}u_1 + \beta_2\partial_{\nu_2}u_2) = 0 \end{aligned}$$

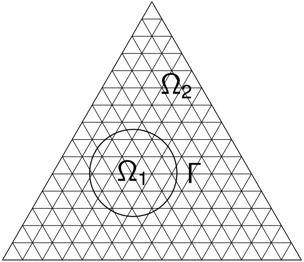


Figure: Domain of interest.

[4] J. Li et al. "Optimal a Priori Estimates for Higher Order Finite Elements for Elliptic Interface Problems". In: *Applied Numerical Mathematics* 1-2 (Jan. 2010).

Why surface alignment?

If Γ is sufficiently smooth, $R_K \in \mathbb{P}_m(\hat{S})$, $u \in H^1(\Omega) \cap H^s(\Omega_1 \cup \Omega_2)$ for some $s \in [1, p+1]$

$$
\begin{aligned}
&\forall s \in \left[1, \frac{3}{2}\right) : \|u - u_h\|_{1,\Omega} \le C h^{s-1} \|u\|_{s,\Omega_1 \cup \Omega_2}, \\
&\forall s \in \left[\frac{3}{2}, p+1\right] \wedge \nabla u \in B^{\frac{1}{2}}_{2,1}(\Omega_1 \cup \Omega_2) \\
&\qquad \Rightarrow \|u - u_h\|_{1,\Omega} \le C h^{s-1} \|u\|_{s,\Omega_1 \cup \Omega_2} + \sqrt{\delta} \|\nabla u\|_{0,B^{\frac{1}{2}}_{2,1}(\Omega_1 \cup \Omega_2)}.
\end{aligned}
$$

Typical values for δ are

$$
\begin{aligned}
\delta &= O(h), \text{ (implicit representation of } \Gamma), \\
\delta &= O(h^{m+1}), \text{ (sharp interface representation with } R_K \in \mathbb{P}_m(\hat{S})).
\end{aligned}
$$

Industry-level application: Micro gear pump

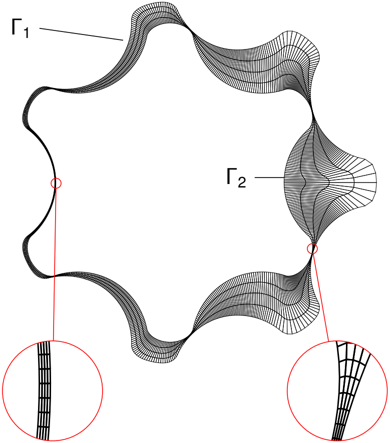


Figure: $t = 0$.

Micro gear pump

- Optimal scales according to gap width
- Boundaries rotate at different speeds
- Unilateral boundary conditions of place
- Extreme cell compression and expansion
- Mesh can be extruded to 3*d*

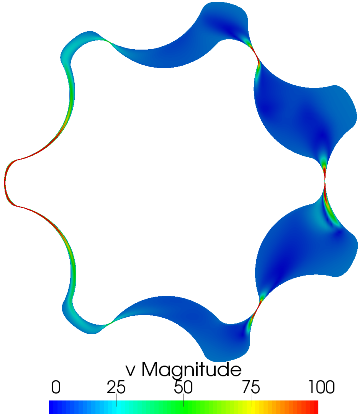
Unilateral boundary condition of place

For a given $\Gamma_2 \subset \mathbb{R}^d$ require that

$$\forall x \in \Gamma_2 \; d\sigma \; a.e. : \Phi(x) \in \Gamma_2$$

- Essential boundary condition
- Can be enforced by projection
- If Γ_2 is not planar, the projection operator is nonlinear
- Highly unstable if $\det(\nabla\Phi) > 0$ is not enforced directly

Industry-level application: Micro gear pump



Micro gear pump

- Mesh optimisation solved on coarser mesh than flow problem
- $Re \approx 6500$
- No inlet or outlet $\Rightarrow$ Flow field governed by incompressibility constraint

Summary

Theory

1. Extended class of mesh quality functionals to hypercubes
2. Direct control of $\det(\nabla\Phi)$ results in a robust method
3. Added r-adaptivity and nonlinear boundary conditions
4. Combined this with surface alignment

Implementation using FEAT3

1. Mesh deformation and optimisation framework
2. MPI parallel NLCG and efficient line search
3. PDE-based linear preconditioner for which efficient numerical methods are available (parallel geometric multigrid etc.)

Ready for non-academic problems.

Future Work

Theory

1. Extend preconditioner for r-adaptivity and surface alignment.
2. Variable metric preconditioners.
3. Surface alignment for hypercube meshes.
4. Anisotropic reference cells.
5. Derive mesh quality functionals from material laws.

Numerics

1. Hybrid linear/nonlinear methods.
2. GPU acceleration for nonlinear solvers.
3. Application to real world problems with complex geometries.

Literature

[1] S. Basting and M. Weismann. “A hybrid level set front tracking finite element approach for fluid–structure interaction and two-phase flow applications”. In: *Journal of Computational Physics* 255 (2013), pp. 228 –244.

[2] P. G. Ciarlet. *Mathematical elasticity Vol. I: Three-dimensional elasticity*. Vol. 20. Studies in Mathematics and its Applications. Amsterdam: North-Holland Publishing Co., 1988.

[3] J. Li et al. “Optimal a Priori Estimates for Higher Order Finite Elements for Elliptic Interface Problems”. In: *Applied Numerical Mathematics* 60.1-2 (Jan. 2010), pp. 19–37.

[4] J. Paul. “Nonlinear Hyperelasticity-based Mesh Optimisation”. PhD thesis. TU Dortmund, 2016.

[5] M. Rumpf. “A variational approach to optimal meshes”. In: *Numerische Mathematik* 72 (1996), pp. 523–540.

Appendix: Optimal Variations

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ and $\partial\Omega = \biguplus_{m=0}^{d-1} \partial\Omega^m$, where $\partial\Omega^0$ is a set of singular points and $\partial\Omega^m$ are relatively open, smooth m-dimensional manifolds. Then Φ^* is an *optimal variation* of the partitioning $\mathcal{T}_h$ of Ω with respect to the functional $\mathcal{F}$ iff

$$\mathcal{F}(\Phi^*) = \min_{\Phi \in V} \mathcal{F}(\Phi) \text{ where}$$

$$V := \{\Phi : \mathcal{T}_h \to \mathbb{R}^d : \Phi \in \mathcal{C}^0(\mathcal{T}_h), \forall K \in \mathcal{T}_h : \nabla\Phi_{|K} \in SL_d,$$
$$\forall x \in \mathcal{E}^0(\mathcal{T}_h) : \forall m = 0, \dots, d-1 : x \in \partial\Omega^m \Rightarrow \Phi(x) \in \partial\Omega^m\}$$

Back to generic mesh optimisation problem

Appendix: ∇h

We need to express $\mathcal{L} = \mathcal{L}(\nabla R_{K,n}, h(K))$ to resolve the dependency on h.

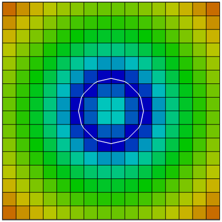
$$
\begin{aligned}
h(T) &= \sqrt[d]{\frac{c(T)}{\sum_{K\in\mathfrak{T}_h}} \sum_{K\in\mathfrak{T}_h} \det \nabla R_{K,n}(Id)} \\
\Rightarrow \frac{\partial h(T)}{\partial x_{ij}} &= \frac{1}{d}\left(\frac{c(T)}{\sum_{K\in\mathfrak{T}_h}} \sum_{K\in\mathfrak{T}_h} \det \nabla R_{K,n}(Id)\right)^{\frac{1}{d}-1} \left[\frac{c(T)}{\sum_{K\in\mathfrak{T}_h}} \frac{\partial}{\partial x_{ij}} \left(\sum_{K\in\mathfrak{T}_h} \det \nabla R_{K,n}(Id)\right)\right. \\
&\quad \left. + \left(\frac{\frac{\partial}{\partial x_{ij}}\left(\frac{c(T)}{\sum_{K\in\mathfrak{T}_h}}\right) + c(T)\sum_{K\in\mathfrak{T}_h c(K)} \frac{\partial c(K)}{\partial x_{ij}}}{\left(\sum_{K\in\mathfrak{T}_h} c(K)\right)^2}\right)\left(\sum_{K\in\mathfrak{T}_h} \nabla R_{K,n}(Id)\right)\right],
\end{aligned}
$$

where x_{ij} is the jth component of the local vertex i belonging to T.

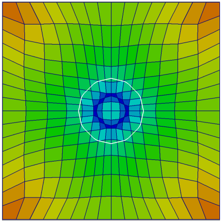
Appendix: Dependent Optimal Scales

Note the difference between

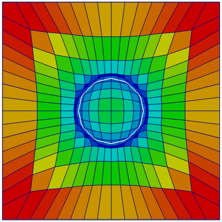
$$c_1(K) = f(\mathrm{dist}(s_{\Phi^*(K)}, \Gamma)) \text{ and } c_2(K) = f(\mathrm{dist}(s_K, \Gamma))$$



(a) $k = 0$.



(b) $k = 1$.



(c) $k = 50$.

Figure: Iterates $\Phi^{(k)}$ of a Picard iteration using c_2.