Homogenization with Non Separated Scales

Houman Owhadi
L. Berlyand, M. Desbrun, R. Donaldson, M. Federov
L. Kharevych, P. Mullen, L. Berlyand, L. Zhang

Thin space

$$\text{(2)} \quad \begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

$$g \in H^{-1}(\Omega) \Rightarrow u \in H_0^1(\Omega)$$

$$g \in L^2(\Omega) \Rightarrow u \in V \subset H_0^1(\Omega)$$

V is a "thin" subspace of $H_0^1(\Omega)$ (isomorphic to H^2)

The flux norm

For $k \in (L^2(\Omega))^d$, denote by k_{pot} the potential portion of the Weyl-Helmholtz decomposition of k (the orthogonal projection of k onto the closure of the space $\{\nabla f \,:\, f \in C_0^\infty(\Omega)\}$ in $(L^2(\Omega))^d$). For $\psi \in H_0^1(\Omega)$, define

$$\|\psi\|_{a-flux} := \|(a\nabla\psi)_{pot}\|_{(L^2(\Omega))^d}.$$

Theorem

$\|.\|_{a-flux}$ is a norm on $H_0^1(\Omega)$.
Furthermore, for all $\psi \in H_0^1(\Omega)$

$$\boxed{\lambda_{\min}(a)\|\nabla\psi\|_{(L^2(\Omega))^d} \leq \|\psi\|_{a-flux} \leq \lambda_{\max}(a)\|\nabla\psi\|_{(L^2(\Omega))^d}}$$

Motivations for the flux norm

- *Energy norm blows up for high contrast*: e.g., $a =$ const. (piecewise const)

$$\int_\Omega (\nabla u)^T a \nabla u = \frac{1}{a} \|\nabla \Delta^{-1} f\|^2_{(L^2(\Omega))^d}, \quad u = a^{-1} \triangle^{-1} f, a \ll 1.$$

  On contrary, *flux norm of solution of* (6) *is independent on a*: rewrite (6) as $div(a\nabla u + \nabla\Delta^{-1} f) = 0 \Rightarrow a\nabla u + \nabla\Delta^{-1} f$ is a divergence free vector field, it: potential part is 0. Thus $(a\nabla u)_{pot} + \nabla\Delta^{-1} f = 0 \Rightarrow \|u\|_{a\text{-flux}} = \|\nabla\Delta^{-1} f\|_{L^2}$.
- Why $(\cdot)_{\text{pot}}$? *Fluxes ξ (heat, stress) are of interest*

$$\int_{\partial\Omega} \xi \cdot n ds = \int_\Omega \text{div}(\xi) dx = \int_\Omega \text{div}(\xi_{\text{pot}}) dx.$$

- In classical homogenization convergence of energies (Γ-convergence) or convergence of fluxes (G-, H-convergence) $a^\epsilon \nabla u^\epsilon \rightharpoonup a^0 \nabla u^0$. Fluxes converge weakly, no flux norm was needed.

Notations

For a finite-dimensional linear subspace $V \subset H_0^1(\Omega)$, define $(\operatorname{div} a\nabla V)$, a finite-dim. subspace of $H^{-1}(\Omega)$, by

$$(\operatorname{div} a\nabla V) := \{\operatorname{div}(a\nabla v) \,:\, v \in V\}.$$

THM (Transfer property of the flux norm) *Let V and V' be finite-dimensional (approximation) subspaces of $H_0^1(\Omega)$. For $f \in L^2(\Omega)$*

- *let u solve* $\operatorname{div}(a\nabla u) = f$ *with conductivity $a(x)$,*
- *let u' sove* $\operatorname{div}(a'\nabla u') = f$ *with conductivity $a'(x)$.*

If $(diva\nabla V) = (diva'\nabla V')$, then approximation errors are equal:

$$\sup_{f\in L^2(\Omega)} \inf_{v\in V} \frac{\|u - v\|_{a\text{-flux}}}{\|f\|_{L^2(\Omega)}} = \sup_{f\in L^2(\Omega)} \inf_{v\in V'} \frac{\|u' - v\|_{a'\text{-flux}}}{\|f\|_{L^2(\Omega)}}.$$

Why is this useful? E.g., need $\mathcal{O}(h)$ error in H^1 norm.

Consider $a' = I$ so that $\operatorname{div} a'\nabla = \Delta$. Then $u' \in H^2$ and V' can be chosen as, e.g., the standard piecewise linear FEM space $\mathcal{L}_0^h$ with basis $\{\varphi_i\}$. The space V is then defined by its basis $\{\psi_i\}$, determined by $\operatorname{div}(a\nabla\psi_i) = \Delta\varphi_i$ with zero Dirichlet BCs.
Eq-n (12) shows that the error estimate for a problem with arbitrarily rough coefficients is equal to the error estimate for Laplace's equation.

Key: *choose appropriate a' and V'.*

Challenge: Localize the basis (work in progress) Zhang-Berlyand-Owhadi

φ_k localized piecewise linear nodal basis elements of $\mathcal{L}_0^h$. Introduce

$$\begin{cases} -\operatorname{div}\left(a(x)\nabla\Phi_k(x)\right) = \Delta\varphi_k & \text{in } \Omega \\ \Phi_k = 0 & \text{on } \partial\Omega \end{cases} .$$

$$V_h := \operatorname{span}\{\Phi_k\},$$

THM *For any $f \in L^2(\Omega)$, let u be the solution of* $-\operatorname{div}(a(x)\nabla u) = f(x)$. *Then,*

$$\sup_{f\in L^2(\Omega)} \inf_{v\in V_h} \frac{\|u-v\|_{a\text{-flux}}}{\|f\|_{L^2(\Omega)}} \le Ch$$

where C depends only on Ω and the aspect ratios of the simplices of Ω_h.

Implies error bound in H^1 norm with $\lambda_{min}(a)$ in error constant

Basis for approximation with optimal error constant

$$\begin{cases} \operatorname{div}\left(a(x)\nabla\theta_k(x)\right) = \Delta\Psi_k & \text{in } \Omega \\ \theta_k = 0 & \text{on } \partial\Omega \end{cases}$$

$$\begin{cases} -\Delta\Psi_k = \lambda_k\Psi_k \quad x \in \Omega \\ \Psi_k = 0 \quad \text{on} \quad \partial\Omega. \end{cases}$$

$$\Theta_h := \operatorname{span}\{\theta_1, \ldots, \theta_{N(h)}\},$$

$N(h)$: the integer part of $|\Omega|/h^d$.

Transfer property of the flux-norm

Theorem

Let u solve $\operatorname{div}(a\nabla u) = f \in L^2(\Omega)$. $u = 0$ on $\partial\Omega$. Then, **(3)**

$$\lim_{h\to 0} \sup_{f\in L^2(\Omega)} \inf_{v\in\Theta_h} \frac{\|u-v\|_{a-flux}}{h\|f\|_{L^2(\Omega)}} = \frac{1}{2\sqrt{\pi}}\left(\frac{1}{\Gamma(1+\frac{d}{2})}\right)^{\frac{1}{d}}.$$

Furthermore the space Θ_h leads (asymptotically as $h \to 0$) to the smallest possible constant in the right hand side of **(3)** among all subspaces of $H_0^1(\Omega)$ with $N(h)$, the integer part of $|\Omega|/h^d$, elements.

$|\Omega|/h^d$: number of dof of piecewise linear functions on a regular triangulation of Ω of resolution h.

Optimality of the error constant

The constant in the right hand side of **(3)** is the classical Kolmogorov n-width $d_n(A, X)$, understood in the asymptotic sense as $h \to 0$ (because the Weyl formula is asymptotic).
n-width measures how accurately a given set of functions $A \subset X$ can be approximated by linear subspaces of dimension n

$$d_n(A, X) = \inf_{E_n} \sup_{w \in A} \inf_{g \in E_n} \|w - g\|_X$$

for a normed linear space X.
In our case X is $H^1_0(\Omega)$ with $\|\cdot\|_{a-\text{flux}}$-norm, A – set of all solutions of (2) as f spans L^2 ($\|\cdot\|_{a-\text{flux}}$ depends on $a(x)$ as opposed to the $H^1_0(\Omega)$-norm, $a(x)$ is fixed).
A surprising result of the theory of n-widths: the space realizing the optimal approximation is not unique, therefore there may be subspaces, other than Θ_h, providing the same asymptotic constant.
Melenk, approximation by piecewise polynomials, degree p. Error in terms of p rather than h: $\exists C, \sigma : Ce^{-\sigma p}$

Fundamental inequality

The following inequality will allow one to reduce the number of precomputed problems to d in the scalar case and d^2 in the vectorial case.

Conjecture: Let $b \in (L^\infty(\Omega))^{d\times d}$ be uniformly elliptic and divergence free matrix (e.g., columns divergence free). Then for $d \geq 3$ there exists $\gamma_a > 0$ such that for all $z \in H_0^1(\Omega) \cap H^2(\Omega)$,

$$\|\Delta z\|_{L^2(\Omega)} \leq \gamma_b(\Omega)\|div(\ b\nabla z)\|_{L^2(\Omega)} \qquad \textbf{(4)}$$

proved $d = 2$. Under Cordes cond. $d \geq 3$.
Why div-free conditions? Elliptic operators with div-free coefficients are in both divergence and non-divergence form. For example, in 2D non-divergence form PDE has H^2 solutions, inequality **(4)** holds for $d = 2$ (div-free in 2D – scalar potential).

Sufficient to establish improved regularity property: If u solves

$$b_{ij}\partial_i\partial_j u = f \in L^2(\Omega), \qquad u = 0 \ \text{ on } \partial\Omega$$

then $u \in H^2(\Omega)$, (b as in the conjecture).
Fundamental open question ($d \geq 3$). If b is not div free, counter example

Discrete geometric structures in Homogenization
Desbrun-Donaldson-Owhadi

$$\begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

F: Harmonic coordinates

$F := (F_1, F_2)$

$$\begin{cases} -\operatorname{div}(a\nabla F_i) = 0 & \Omega \\ F_i(x) = x_i & \partial\Omega \end{cases}$$

[Desbrun-Donaldson-Owhadi-09]

First solve d time independent problems

F: Harmonic coordinates associated to (1)

$$F := (F_1, \ldots, F_d)$$

$$\begin{cases} -\operatorname{div}(a\nabla F_i) = 0 & \Omega \\ F_i(x) = x_i & \partial\Omega \end{cases}$$

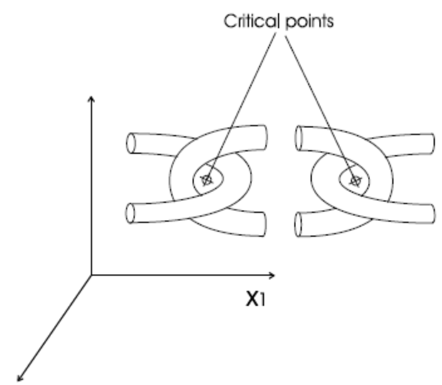
$$F : \Omega \to \Omega$$

$d = 2$, Ω convex $\Rightarrow$ F is an homeomorphism.

[Ancona-2002], [Alessandrini-Nesi-2003]

$d \geq 3$: F may be non-injective

[Ancona-2002], [Briane-Milton-Nesi-2004]

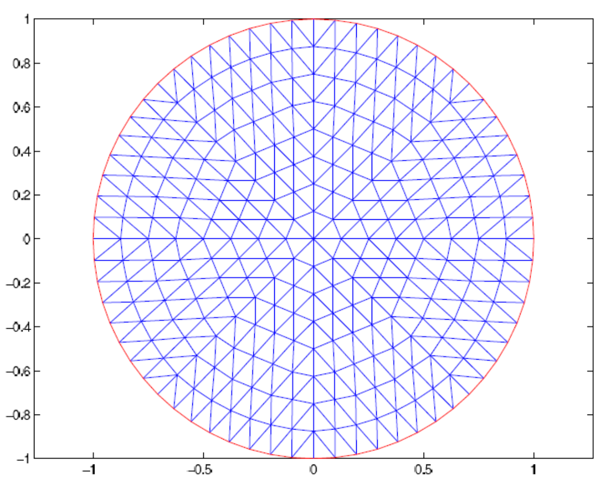


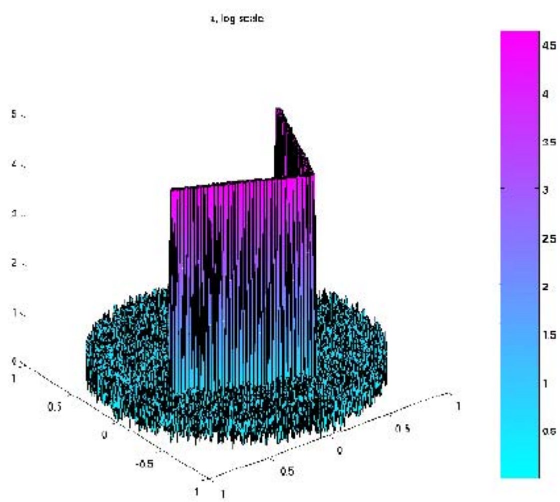
F: Harmonic coordinates associated to (1)

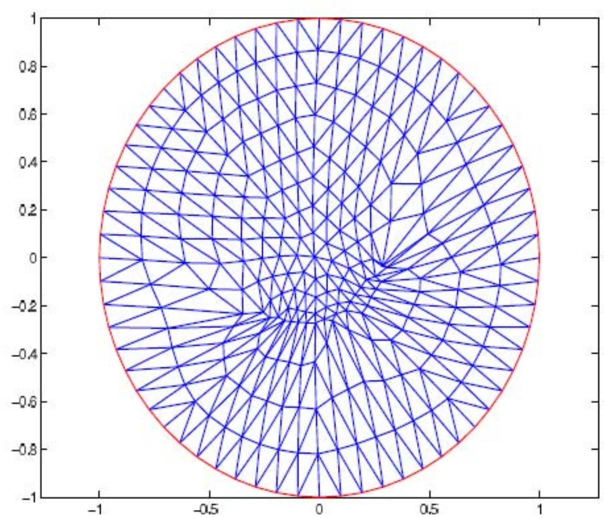
$F := (F_1, \ldots, F_d)$

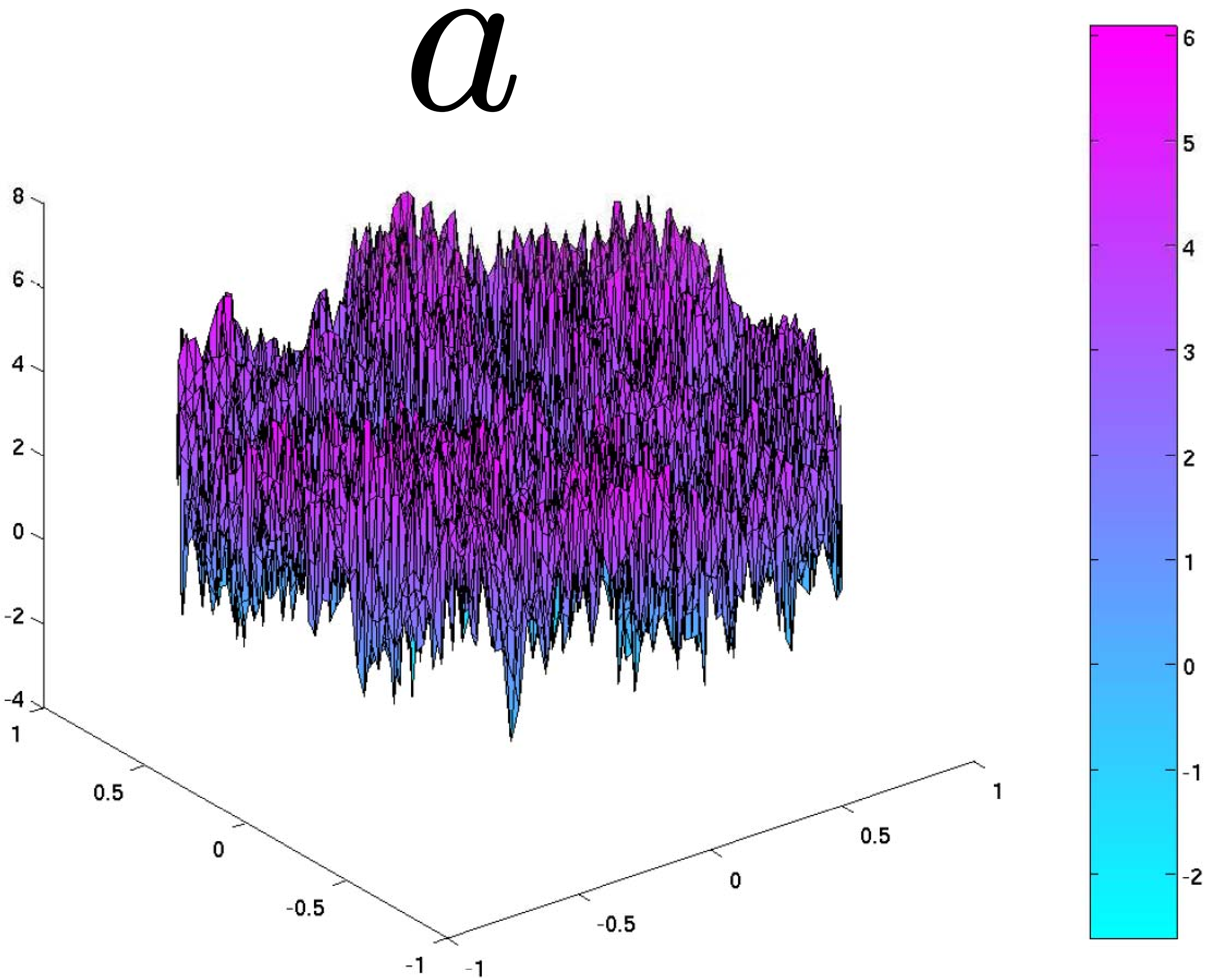
$$\begin{cases} -\operatorname{div}(a \nabla F_i) = 0 & \Omega \\ F_i(x) = x_i & \partial\Omega \end{cases}$$

$F : \Omega \to \Omega$



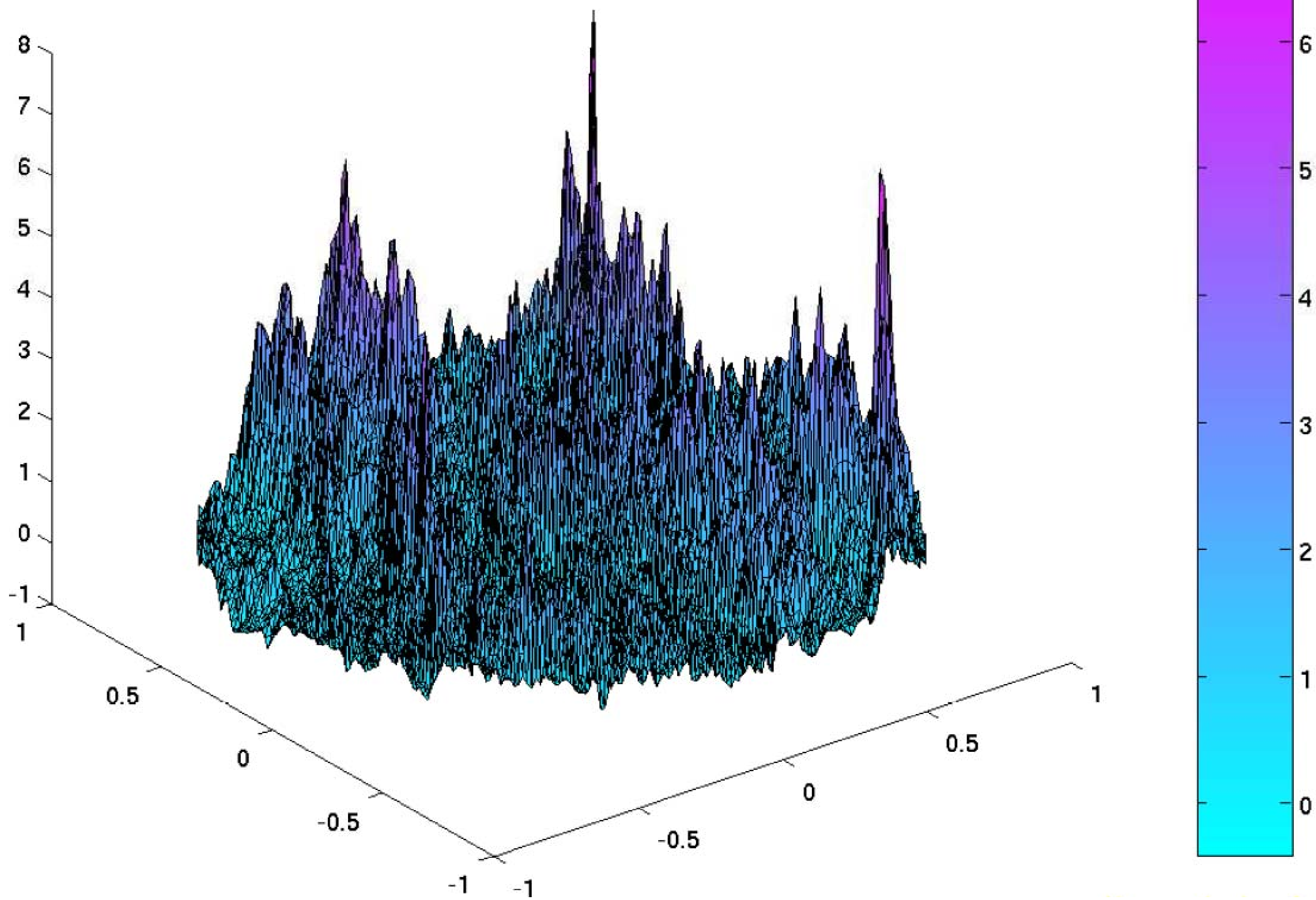


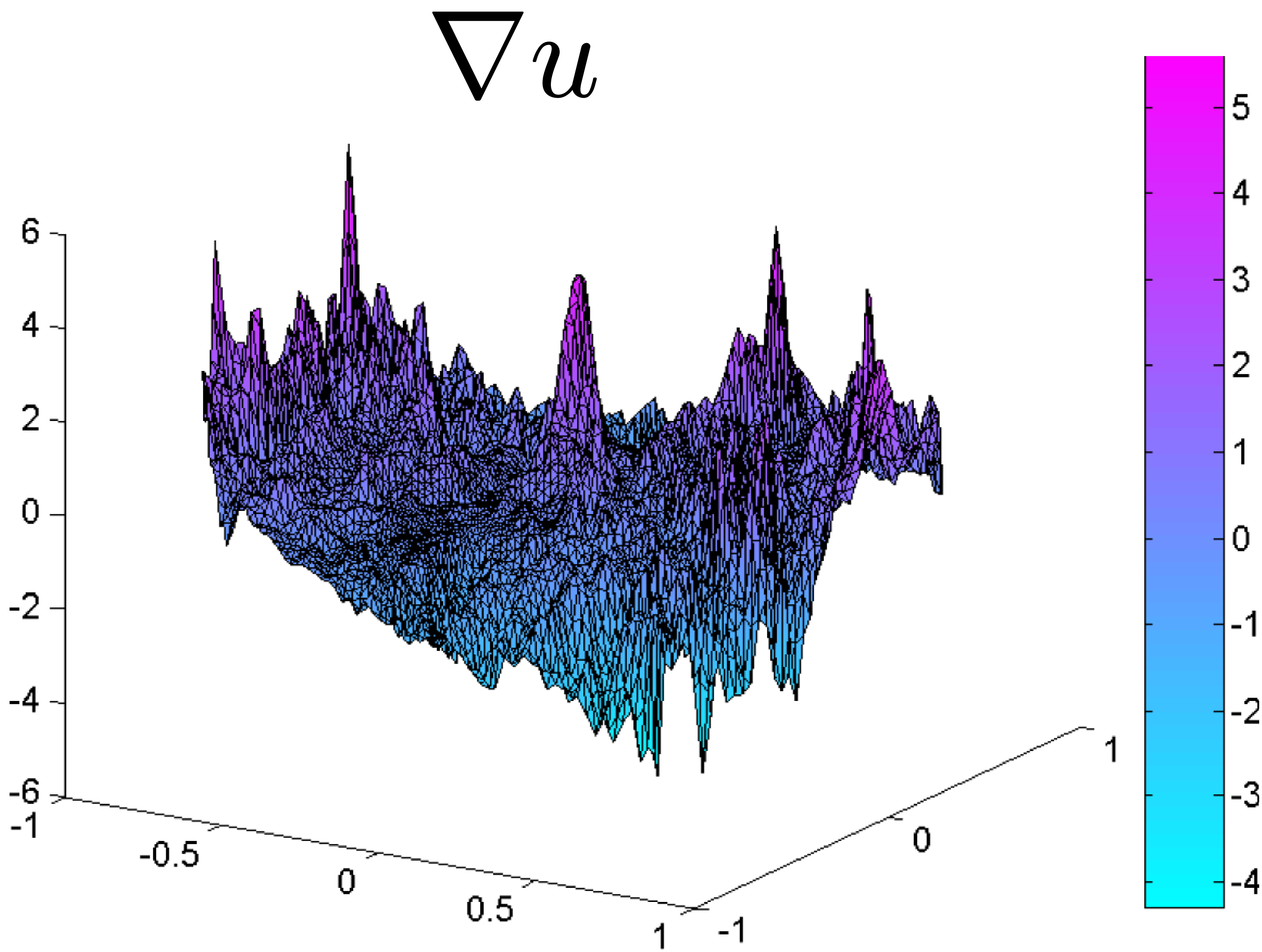


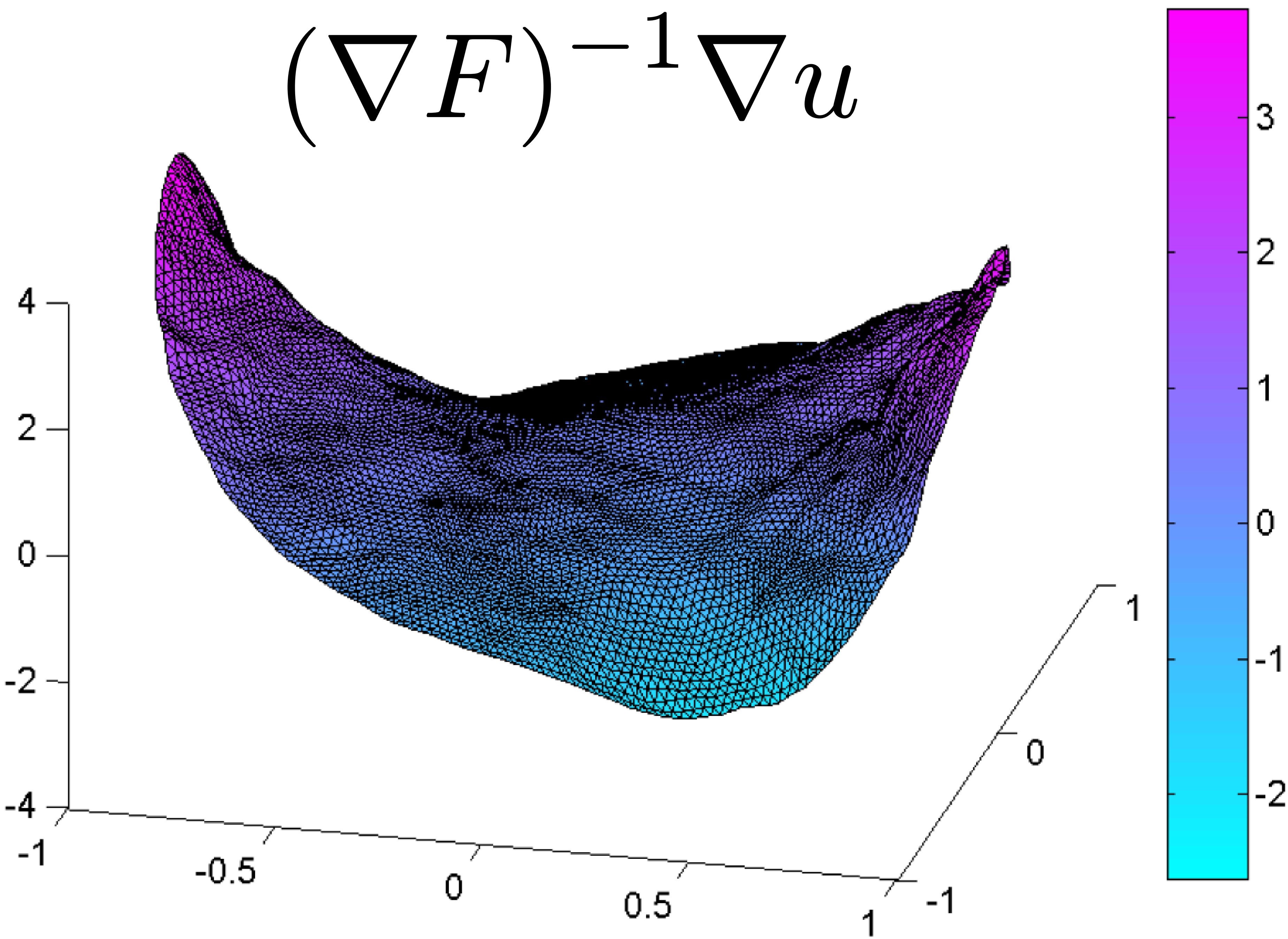


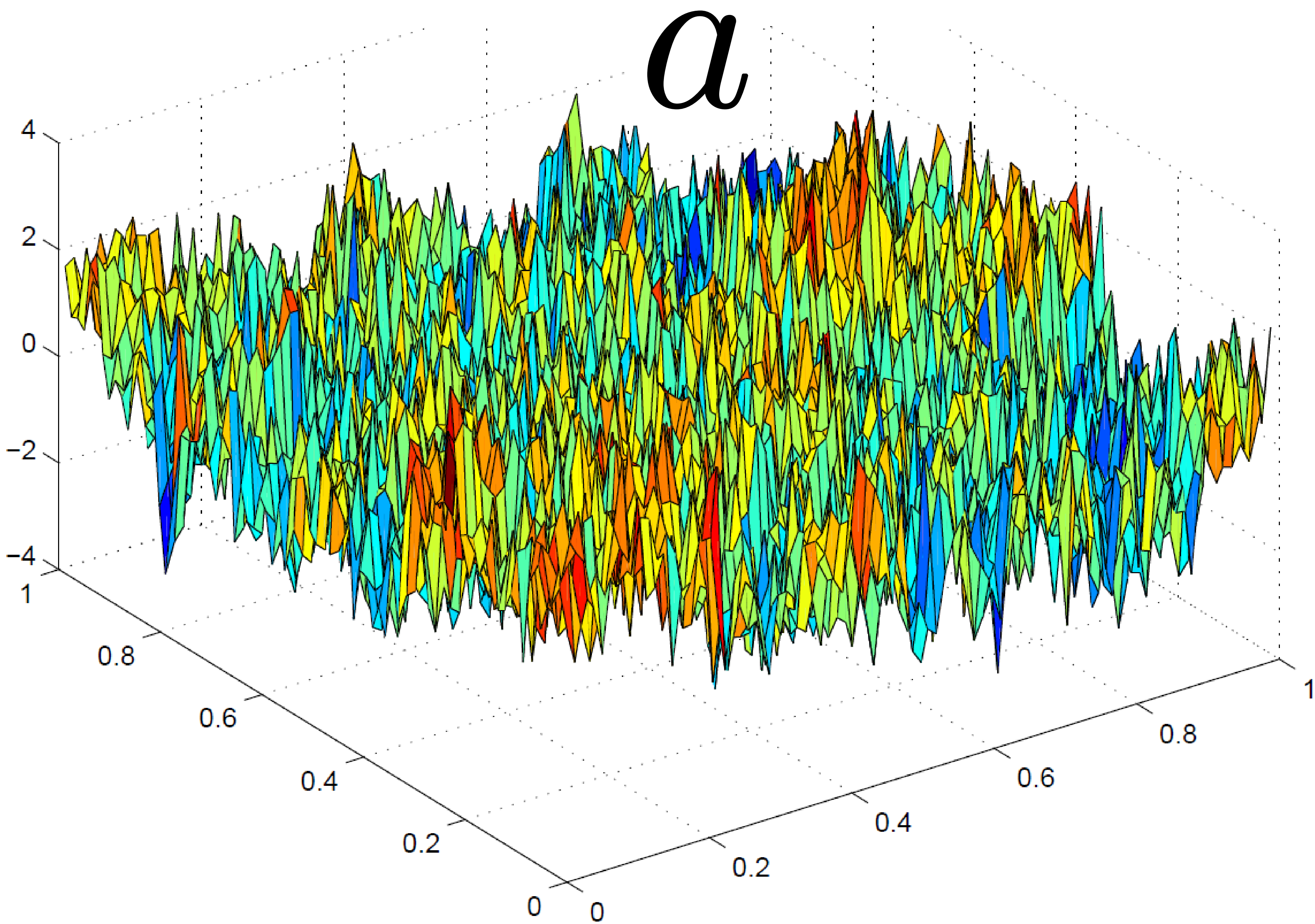
a
8
6
4
2
0
-2
-4
1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1
6
5
4
3
2
1
0
-1
-2

∇F

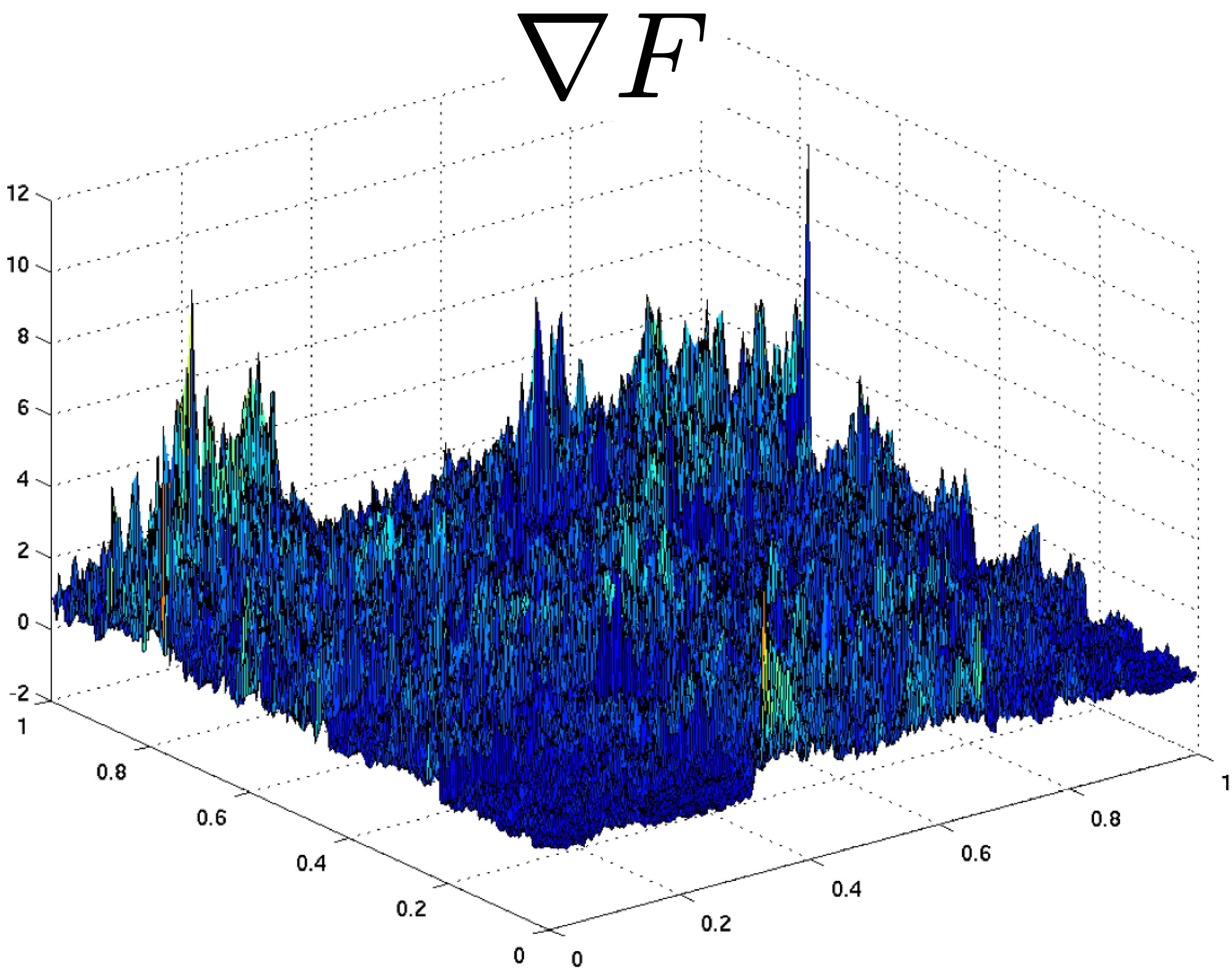



∇u
6
4
2
0
-2
-4
-6
-1
-0.5
0
0.5
1
-1
0
1
5
4
3
2
1
0
-1
-2
-3
-4

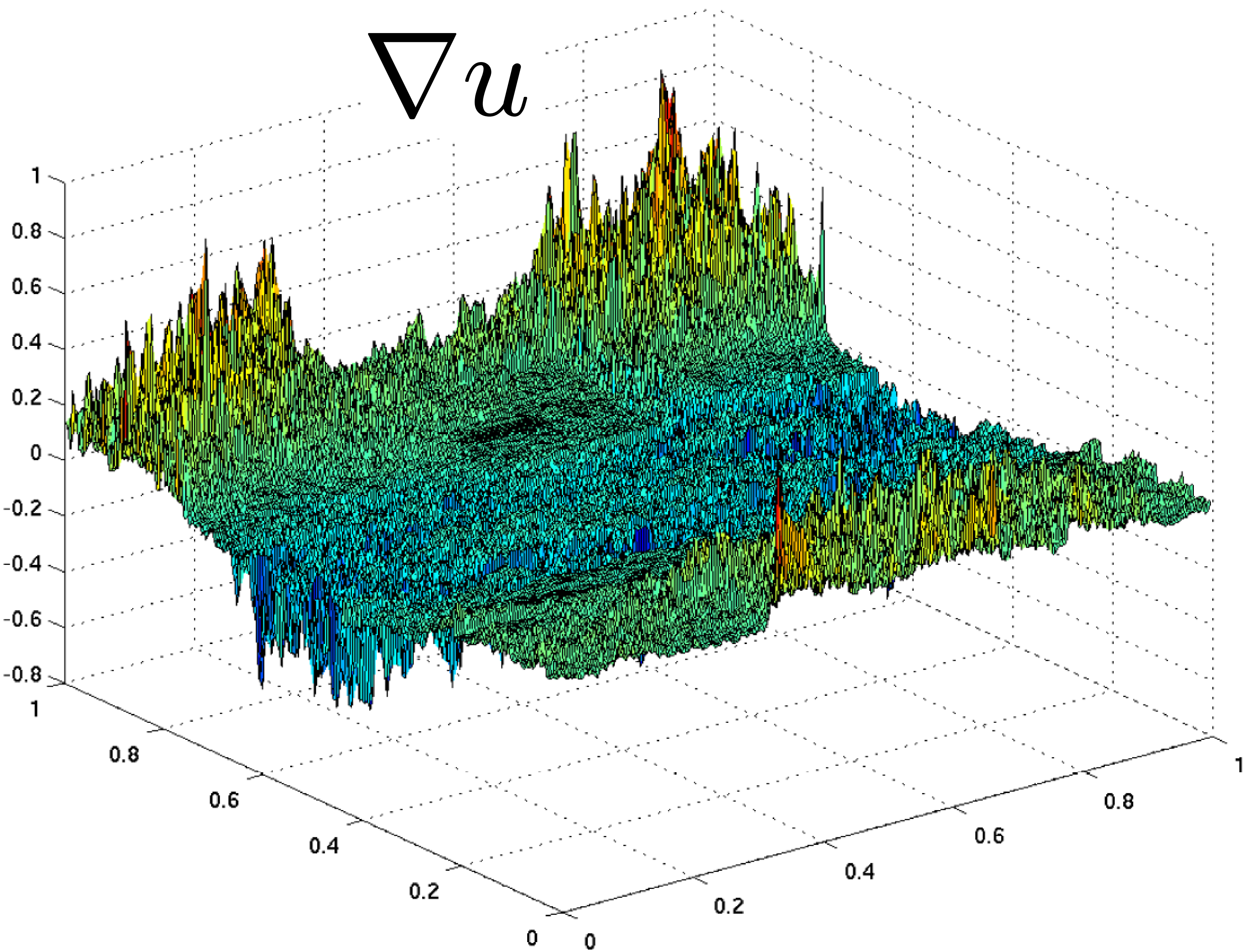

$(\nabla F)^{-1}\nabla u$
4
2
0
-2
-4
-1
-0.5
0
0.5
1
-1
0
1
3
2
1
0
-1
-2



a
4
2
0
−2
−4
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1

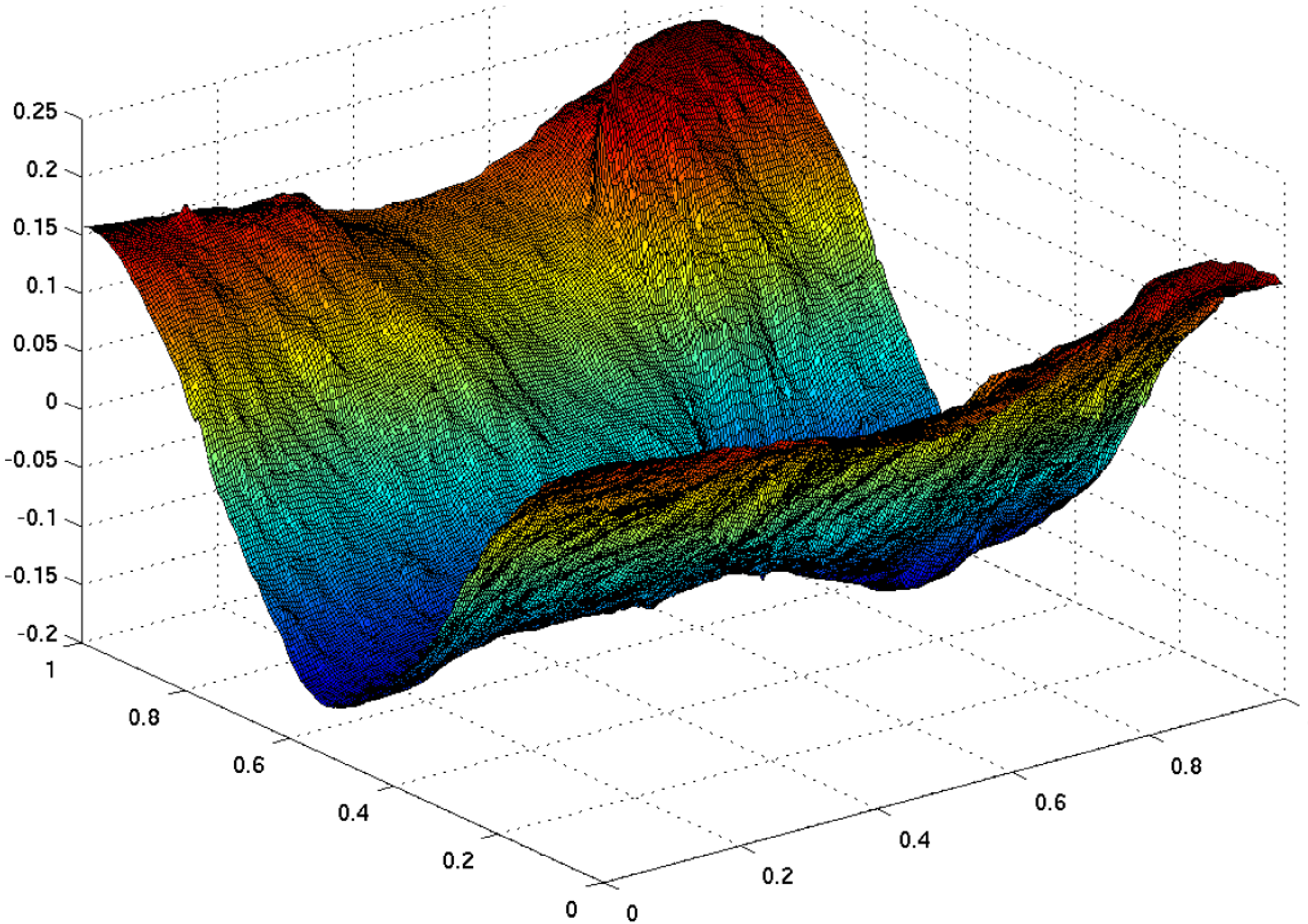


∇F
12
10
8
6
4
2
0
-2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1



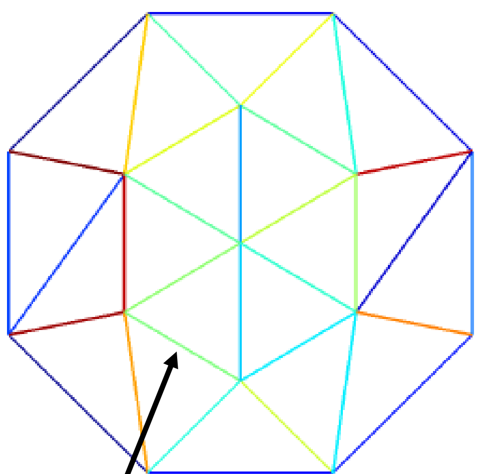
∇u
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1

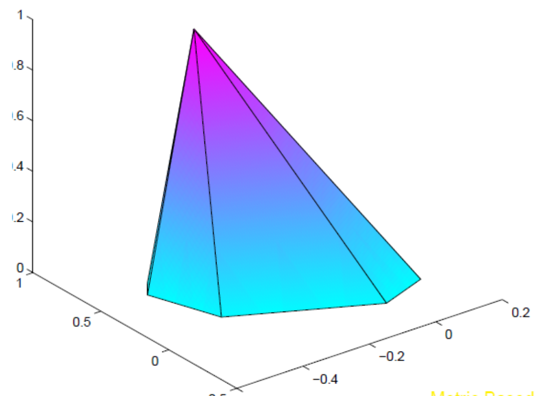
$$(\nabla F)^{-1}\nabla u$$

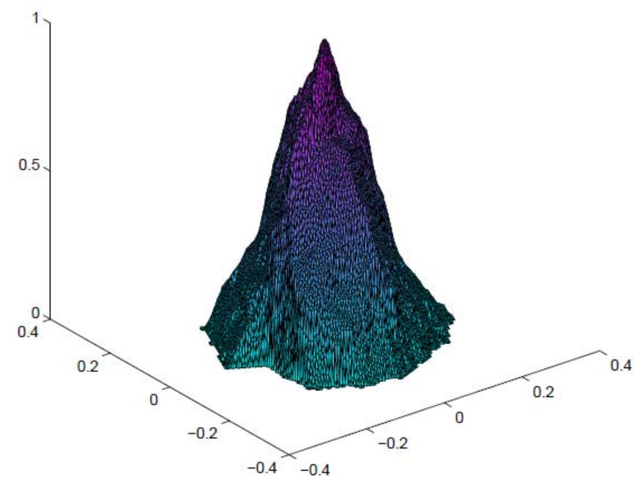


Edges effective conductivities

Ω_h $\qquad$ φ_i $\qquad$ $\varphi_i \circ F$







$$q_{ij}^h := -\int_\Omega (\nabla(\varphi_i \circ F))^T a(x) \nabla(\varphi_j \circ F)\, dx$$

Homogenization without scale separation

$$(1) \quad \begin{cases} \partial_t u - \operatorname{div}(a\nabla u) = g & \Omega \times [0,T] \\ u = 0 & \partial\Omega \times [0,T] \cup \Omega \times \{t=0\} \end{cases}$$

- $\Omega \subset \mathbb{R}^d$, bounded, convex, C^2
- a: $d \times d$, symmetric, uniformly elliptic, $a_{i,j} \in L^\infty(\Omega)$
- $g \in L^2(\Omega \times (0,T))$

How to homogenize eq-(1)?

[Owhadi-Zhang-2007]

Laminar (1d) elliptic case: method I (SFEM) of [Babuška-Caloz-Osborn-1994]

First solve d time independent problems

F: Harmonic coordinates associated to (1)

$$F := (F_1, \ldots, F_d)$$

$$\begin{cases} -\operatorname{div}(a\nabla F_i) = 0 & \Omega \\ F_i(x) = x_i & \partial\Omega \end{cases}$$

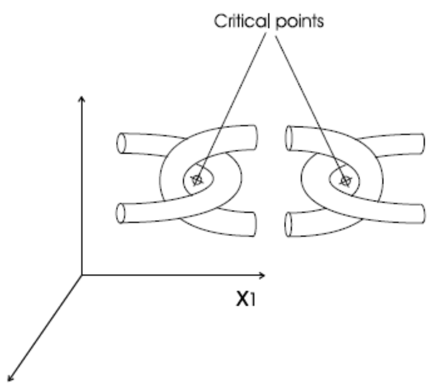
$$F : \Omega \to \Omega$$

$d = 2$, Ω convex $\Rightarrow$ F is an homeomorphism.

[Ancona-2002], [Alessandrini-Nesi-2003]

$d \geq 3$: F may be non-injective

[Ancona-2002], [Briane-Milton-Nesi-2004]

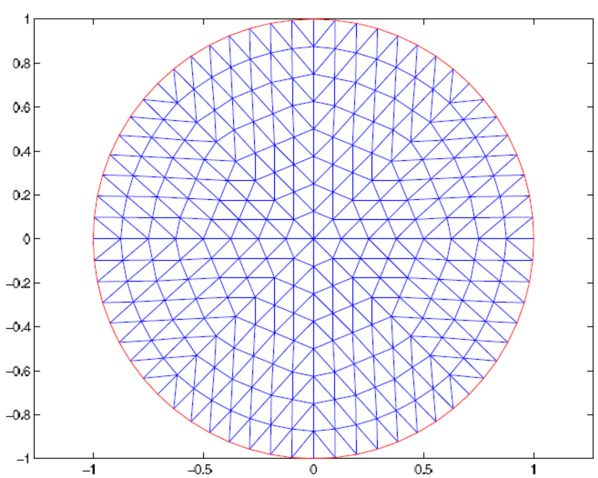


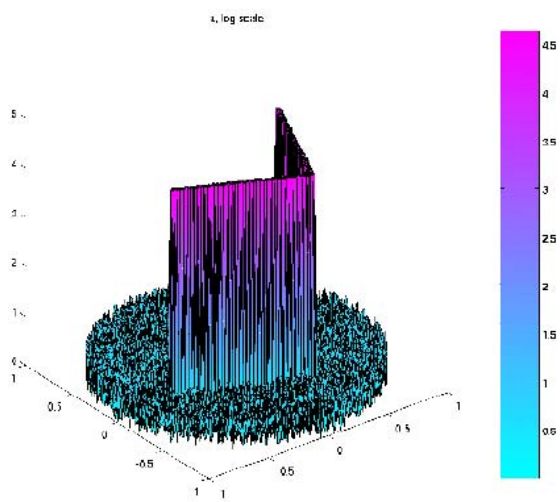
F: Harmonic coordinates associated to (1)

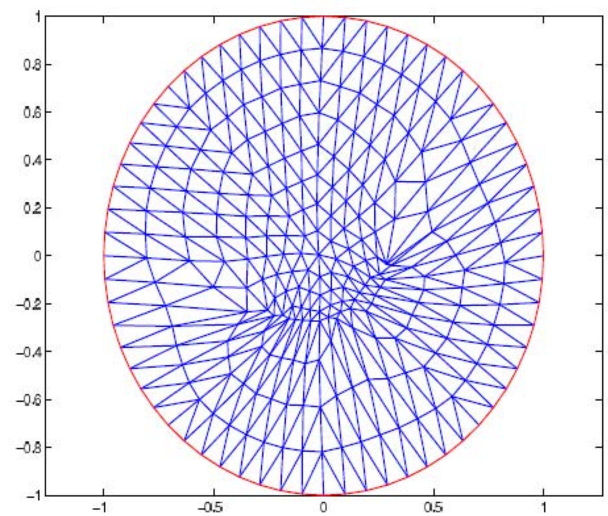
$$F := (F_1, \ldots, F_d)$$

$$\begin{cases} -\operatorname{div}(a \nabla F_i) = 0 & \Omega \\ F_i(x) = x_i & \partial\Omega \end{cases}$$

$$F : \Omega \to \Omega$$







$$u \in L^2(0,T,H_0^1(\Omega))$$

Theorem [Owhadi-Zhang-2007]

If M satisfies (CTC) then

$$u \circ F^{-1} \in L^2(0,T,W^{2,2}(\Omega)) \text{ and}$$

$$\left\| u \circ F^{-1} \right\|_{L^2(0,T,W^{2,2}(\Omega))} \leq C \, \|g\|_{L^2(\Omega_T)}$$

$$\|v\|^2_{L^2(0,T,W^{2,2}(\Omega))} := \int_0^T \int_\Omega \sum_{i,j} (\partial_i \partial_j v)^2$$

(CTC) on

$$M := (\nabla F)^T a \nabla F$$

$$\beta_M := \operatorname{ess\,sup}_\Omega \, d - \frac{\Big(\mathrm{Trace}[M]\Big)^2}{\mathrm{Trace}[M^T M]} < 1$$

Remark: **d=2**

$$\beta_\sigma < 1 \Leftrightarrow \operatorname{ess\,sup}_\Omega \frac{\lambda_{\max}[M(x)]}{\lambda_{\min}[M(x)]} < \infty$$

Homogenization of (1)

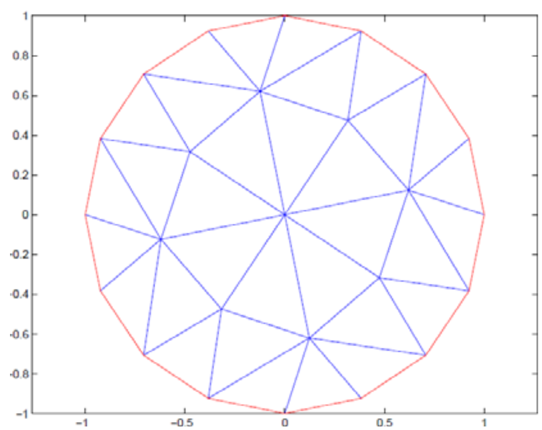
[Owhadi-Zhang-2007]
Generalization of the space introduced in method I (SFEM) of [Babuška-Caloz-Osborn-1994]

X_h: Finite dimensional linear sub-space of $H^1_0(\Omega)$

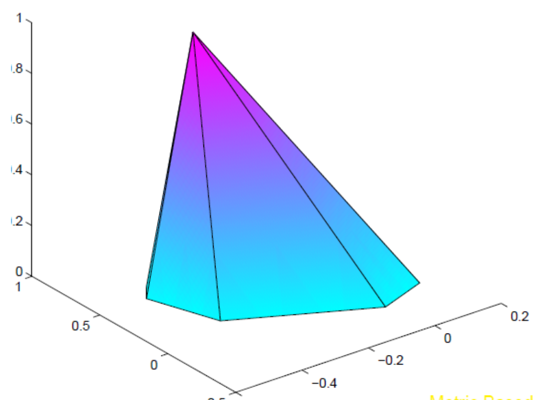
Property $\exists C_X > 0 \; : \; \forall f \in C^\infty_0(\Omega)$

$$\inf_{v\in X_h} \|f-v\|_{H^1_0(\Omega)} \leq C_X h \|f\|_{W^{2,2}(\Omega)}$$

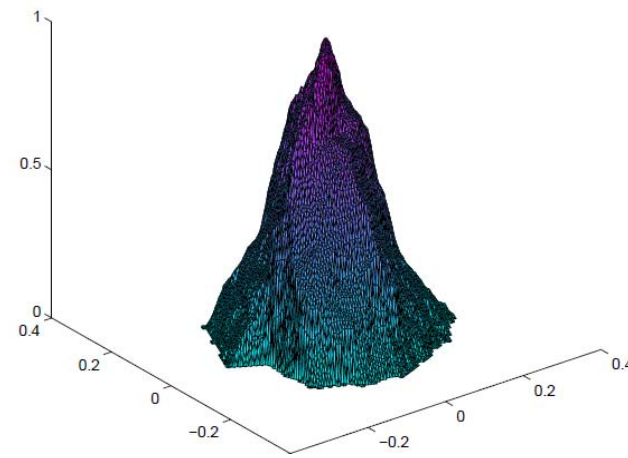
$$V_h := \{\varphi \circ F \; : \; \varphi \in X_h\}$$



Ω_h



φ_i



$\varphi_i \circ F$

$u \in L^2(0, T, H_0^1(\Omega))$

u_h F.E. solution of (1) in $L^2(0, T, V_h)$

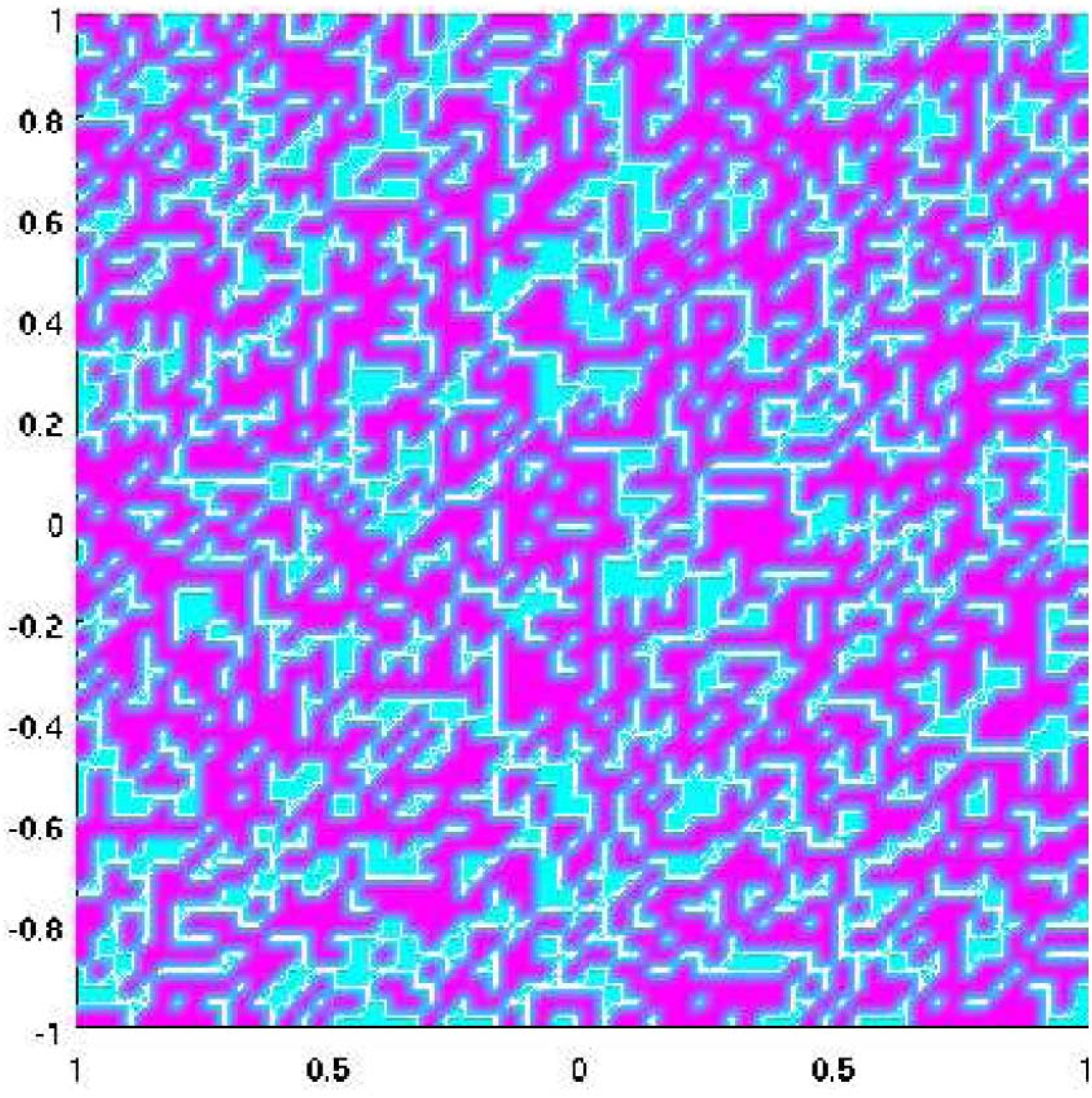
$$u_h = \sum_i c_i(t)\, \varphi_i \circ F(x)$$

Theorem [Owhadi-Zhang-2007]

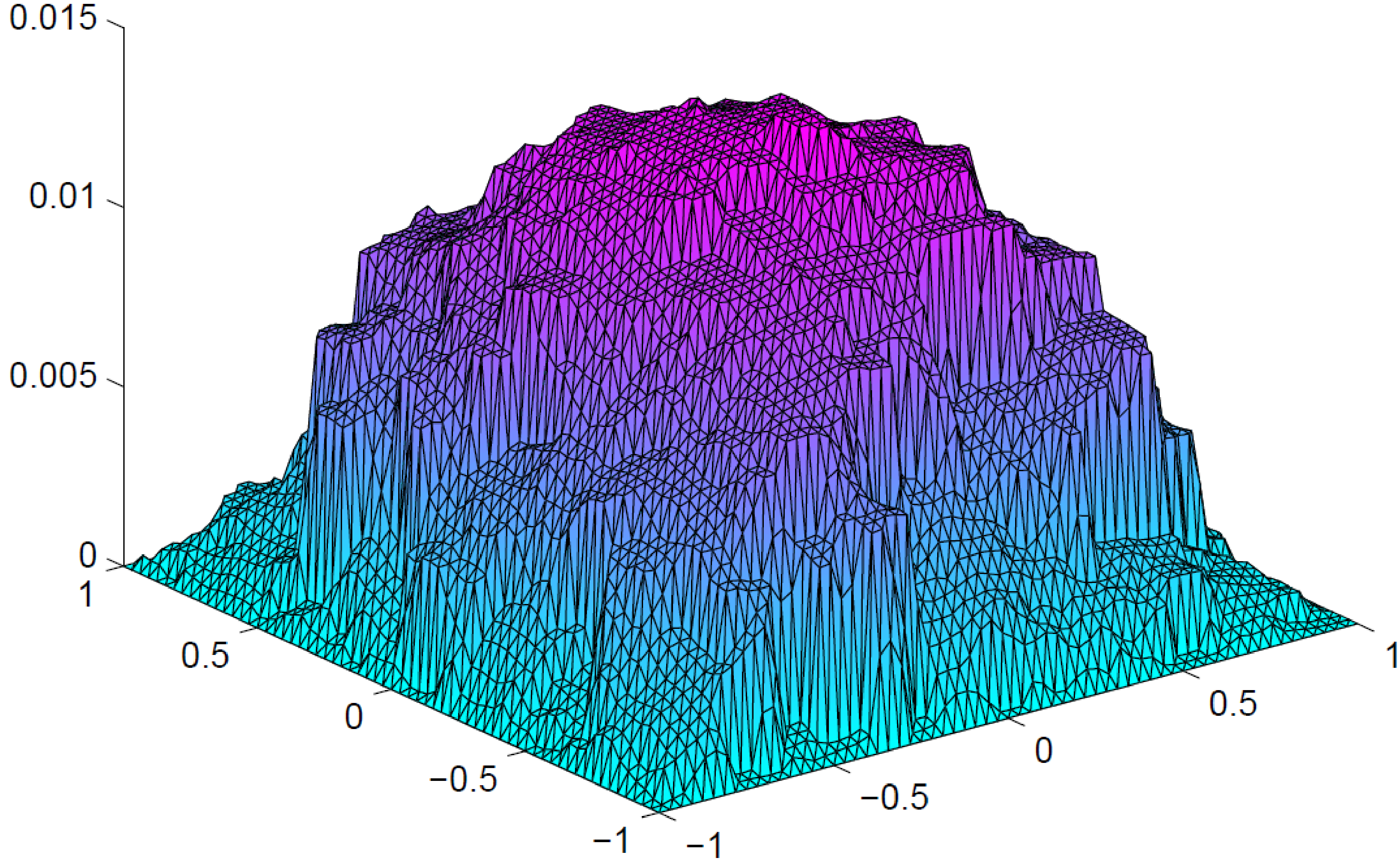
If M satisfies (CTC) then

$$\big\|(u - u_h)(.,T)\big\|_{L^2(\Omega)} + \|u - u_h\|_{L^2(0,T,H_0^1(\Omega))} \leq C\, h\, \|g\|_{L^2(\Omega_T)}$$

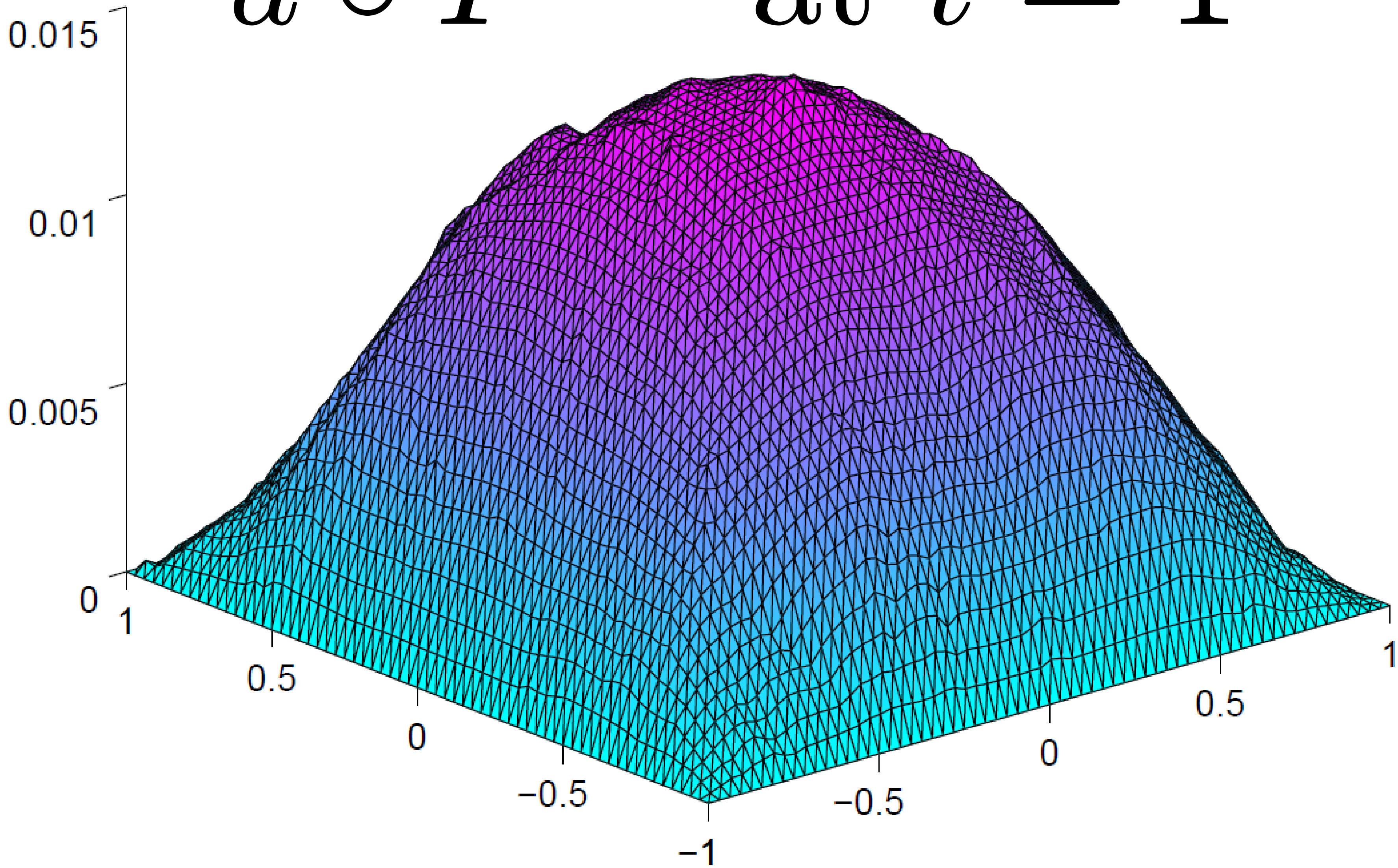
a

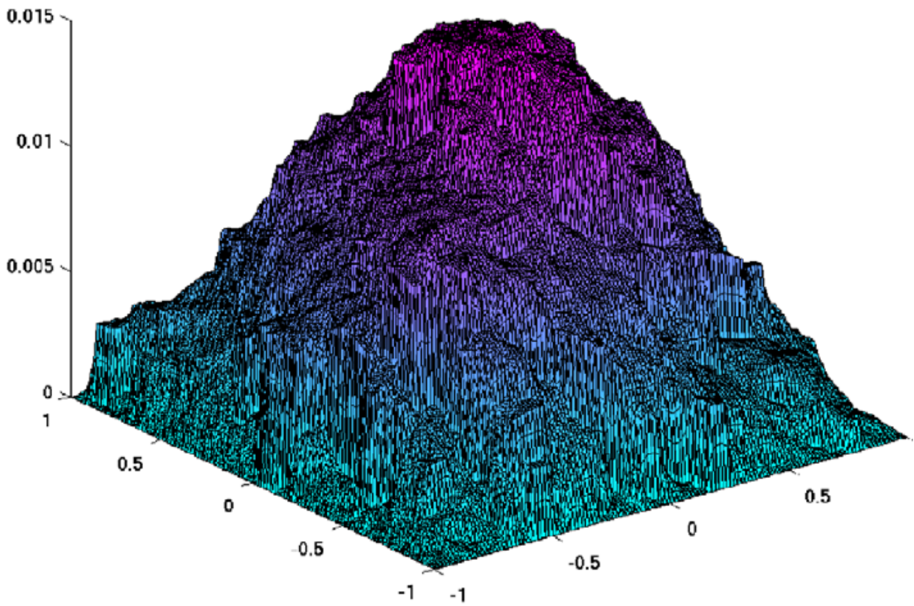


u at $t = 1$

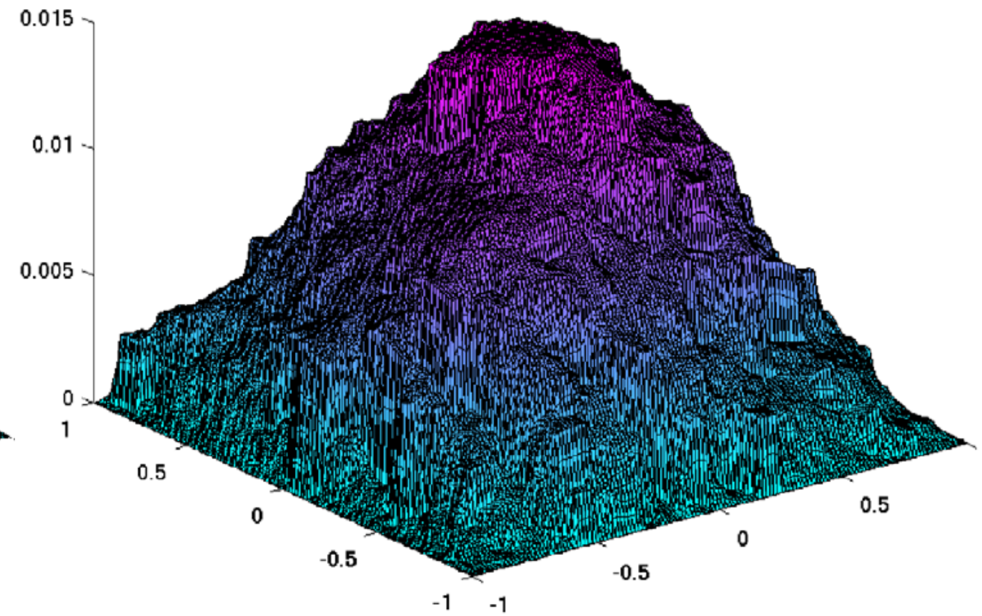


$u \circ F^{-1}$ at $t = 1$





u computed on 16641 degrees of freedom (interior nodes)



$u_{h,\Delta t}$ computed on 9 d.o.f
L^1-relative error: 0.0196
H^1-relative error: 0.0312

Extension to wave equations

$$\begin{cases} K^{-1}(x)\partial_t^2 u = \mathrm{div}(\rho^{-1}(x)\nabla u(x,t)) + g \quad \text{in} \quad \Omega \times (0,T). \\ u(x,t) = 0 \quad \text{for} \quad (x,t) \in \partial\Omega \times (0,T). \\ u(x,t) = u(x,0) \quad \text{for} \quad (x,t) \in \Omega \times \{t=0\}. \\ \partial_t u(x,t) = u_t(x,0) \quad \text{for} \quad (x,t) \in \Omega \times \{t=0\}. \end{cases}$$

K: bulk modulus ρ: Density $a := \rho^{-1}$

Theorem

Assume that M satisfies condition **CTC**, $\partial_t g \in L^2(\Omega_T)$, $g \in L^\infty(0,T,L^2(\Omega))$, $\mathrm{div}\, a\nabla u(x,0) \in L^2(\Omega)$ and $\partial_t u(x,0) \in H^1(\Omega)$ then $u \circ F^{-1} \in L^2(0,T,H^2(\Omega))$ and

$$\begin{aligned} \|u \circ F^{-1}\|_{L^\infty(0,T,H^2(\Omega))} \leq C \quad & \big(\|g\|_{L^\infty(0,T,L^2(\Omega))} + \|\,\mathrm{div}\, a\nabla u(x,0)\|_{L^2(\Omega)} \\ & + \|\partial_t u(x,0)\|_{H^1(\Omega)} + \|\partial_t g\|_{L^2(\Omega_T)}\big). \end{aligned}$$

Extension to wave equations

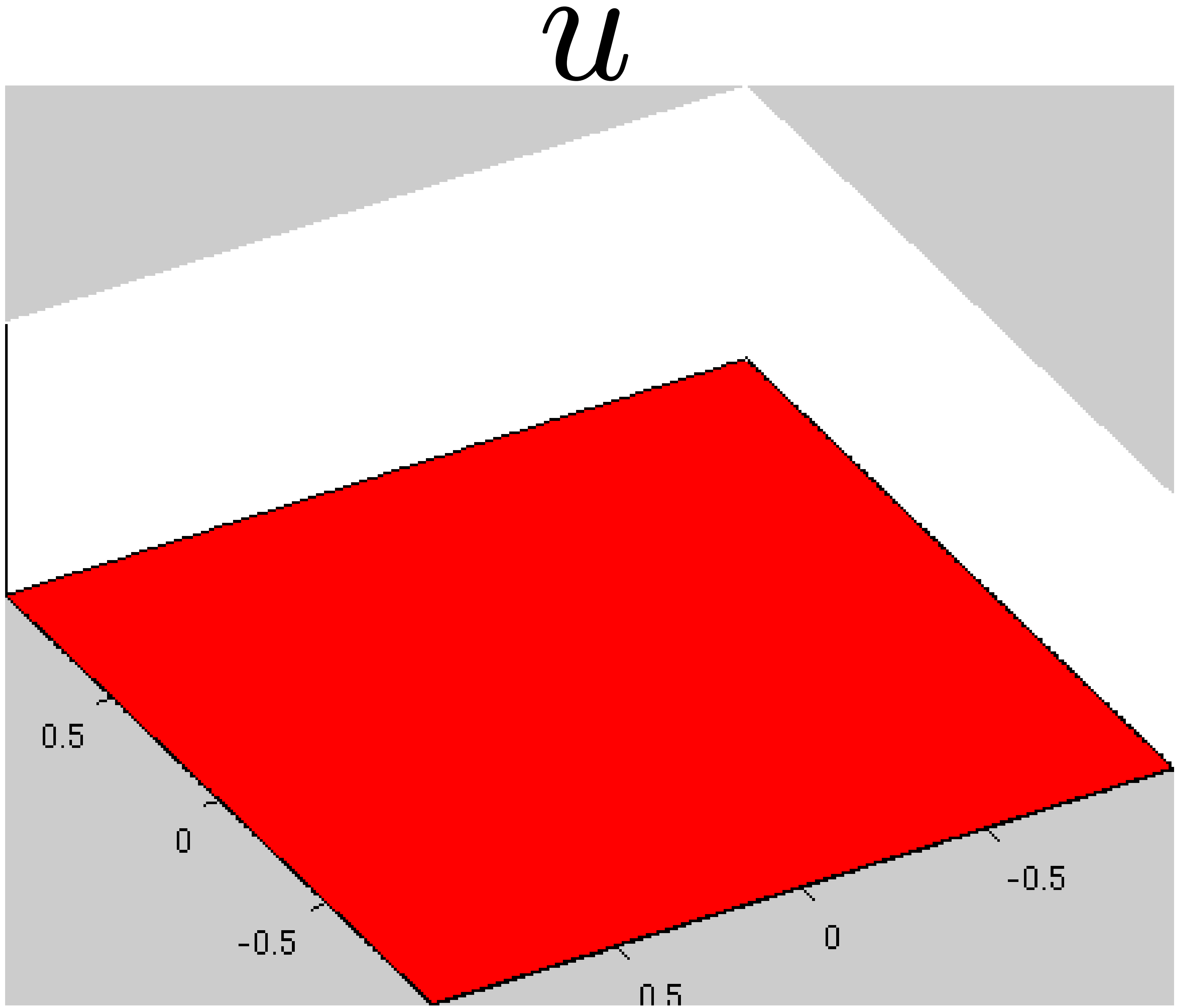
$$\begin{cases} K^{-1}(x)\partial_t^2 u = \mathrm{div}(\rho^{-1}(x)\nabla u(x,t)) + g \quad \text{in} \quad \Omega \times (0,T). \\ u(x,t) = 0 \quad \text{for} \quad (x,t) \in \partial\Omega \times (0,T). \\ u(x,t) = u(x,0) \quad \text{for} \quad (x,t) \in \Omega \times \{t=0\}. \\ \partial_t u(x,t) = u_t(x,0) \quad \text{for} \quad (x,t) \in \Omega \times \{t=0\}. \end{cases}$$

K: bulk modulus ρ: Density $a := \rho^{-1}$

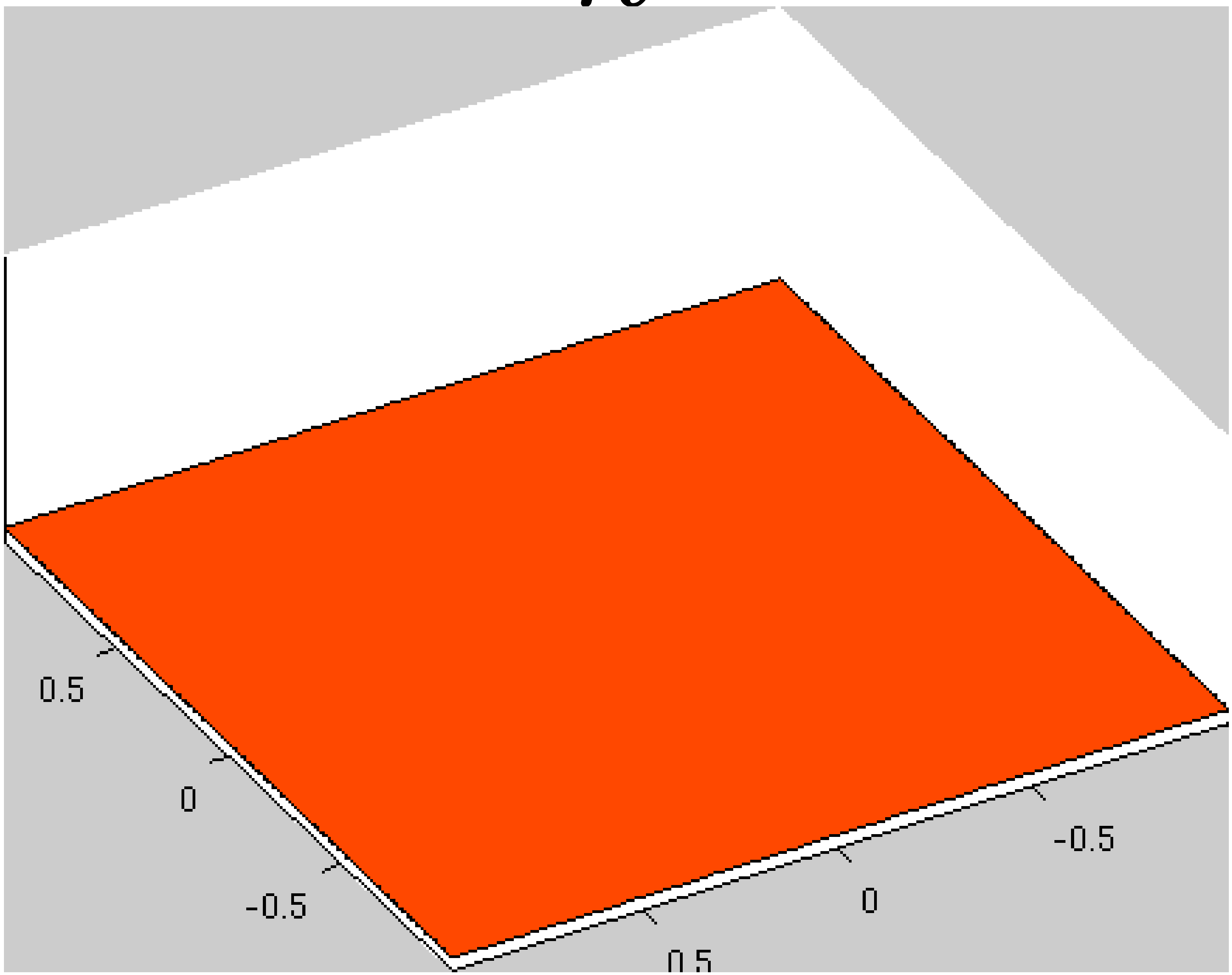
Theorem

Assume that M satisfies condition **CTC**, $g(x,0) \in L^2(\Omega)$, $\partial_t^2 g \in L^2(\Omega_T)$ and $\partial_t g \in L^\infty(0,T,L^2(\Omega))$ then

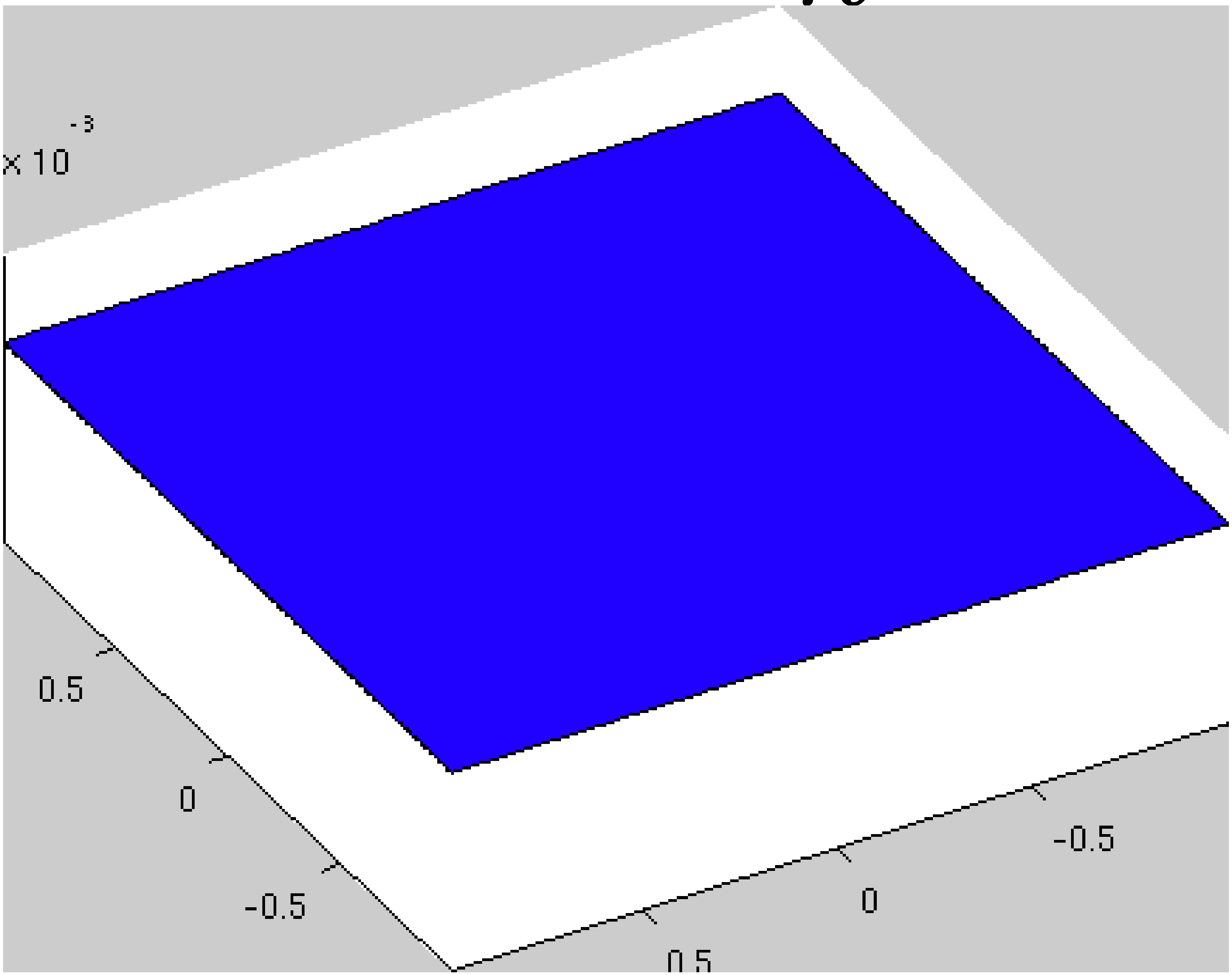
$$\big\|\partial_t(u-u_h)(.,T)\big\|_{L^2(\Omega)} + \big\|(u-u_h)(.,T)\big\|_{H_0^1(\Omega)} \le Ch\Big(\|\partial_t g\|_{L^\infty(0,T,L^2(\Omega))} + \|\partial_t^2 g\|_{L^2(\Omega_T)} + \|\,\mathrm{div}(a\nabla u(x,0))\|_{H^1(\Omega)} + \|\,\mathrm{div}(a\nabla\partial_t u(x,0))\|_{L^2(\Omega)}\Big).$$


u
0.5
0
-0.5
-0.5
0
0.5

u_h



$$u - u_h$$



Rough coefficients in space and time

$$(2) \quad \begin{cases} \partial_t u - \operatorname{div}(a\nabla u) = g & \Omega \times [0,T] \\ u = 0 & \partial\Omega \times [0,T] \cup \Omega \times \{t=0\} \end{cases}$$

$$g \in L^2(\Omega_T) \qquad \Omega_T := \Omega \times [0,T]$$

$$a = a(x,t), \text{ symmetric, uniformly elliptic}$$

$$a_{i,j} \in L^\infty(\Omega \times [0,T])$$

Caloric coordinates

$$F := (F_1, \ldots, F_d)$$

$$\begin{cases} \partial_t F_i - \operatorname{div}\big(a(x,t)\nabla F_i\big) = 0 & \Omega_T \\ F_i(x,t) = x_i & \partial\Omega \times [0,T] \\ -\operatorname{div}\big(a(x,0)\nabla F_i(x,0)\big) = 0 & \Omega \end{cases}$$

u_h F.E. solution of (3) in $Y_{h,\Delta t}$

$$u_h = \sum_i c_i(t)\, \varphi_i \circ F(x,t)$$

$c_i(t)$: piecewise constant on intervals $(t_i, t_{i+1}]$ of size Δt

Theorem [Owhadi-Zhang-2007]

Assume that σ satisfies (CDC') then

$$u \circ F^{-1} \in L^2(0,T,W^{2,2}(\Omega))$$

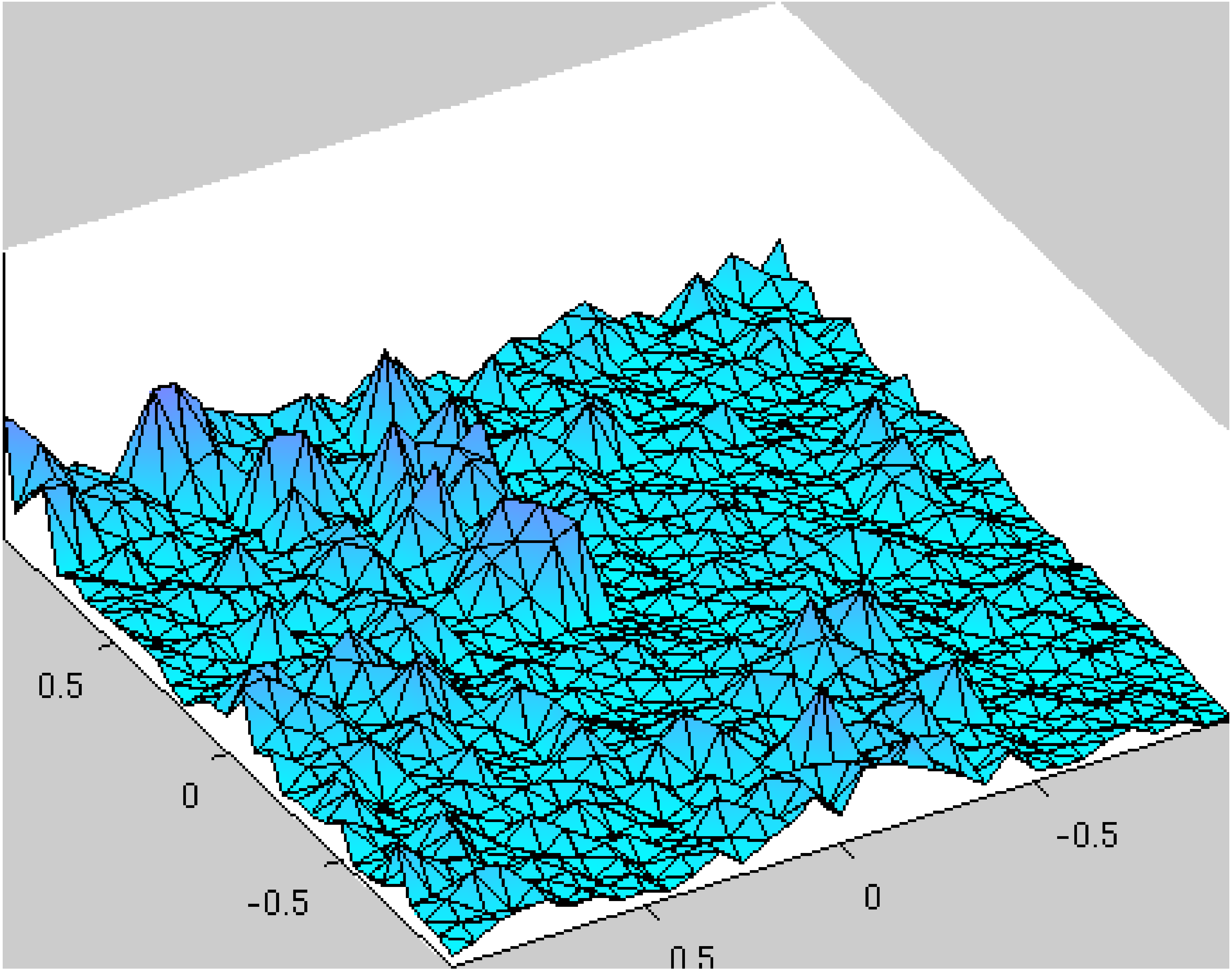
$$u \in L^2(0,T,H^1_0(\Omega))$$

$$\partial_t (u \circ F^{-1}) \in L^2(\Omega_T)$$

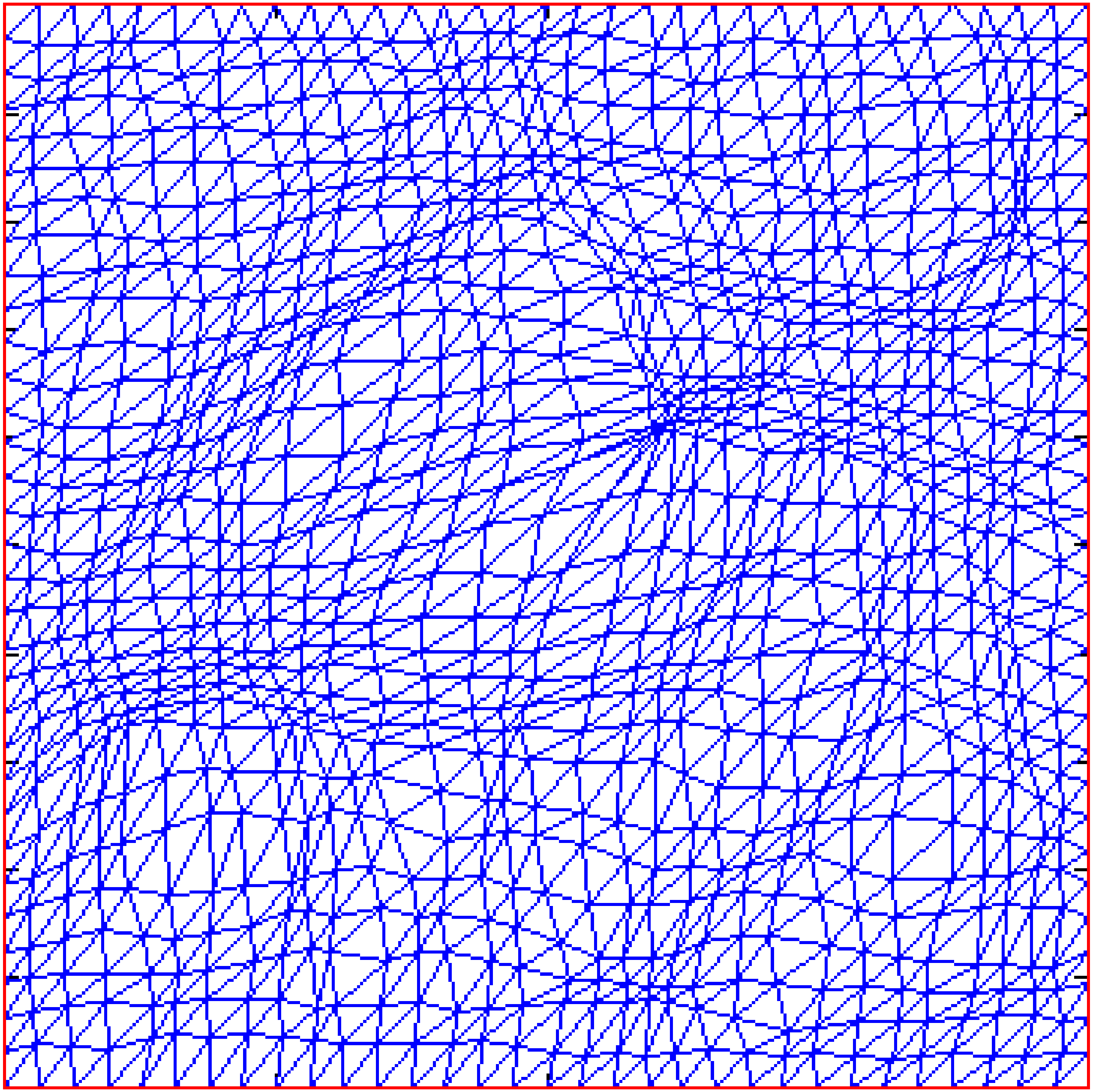
$$\partial_t u \in L^2(0,T,H^{-1}(\Omega))$$

$$\left\| u \circ F^{-1} \right\|_{L^2(0,T,W^{2,2}(\Omega))} + \left\| \partial_t (u \circ F^{-1}) \right\|_{L^2(\Omega_T)} \leq C \|g\|_{L^2(\Omega_T)}$$

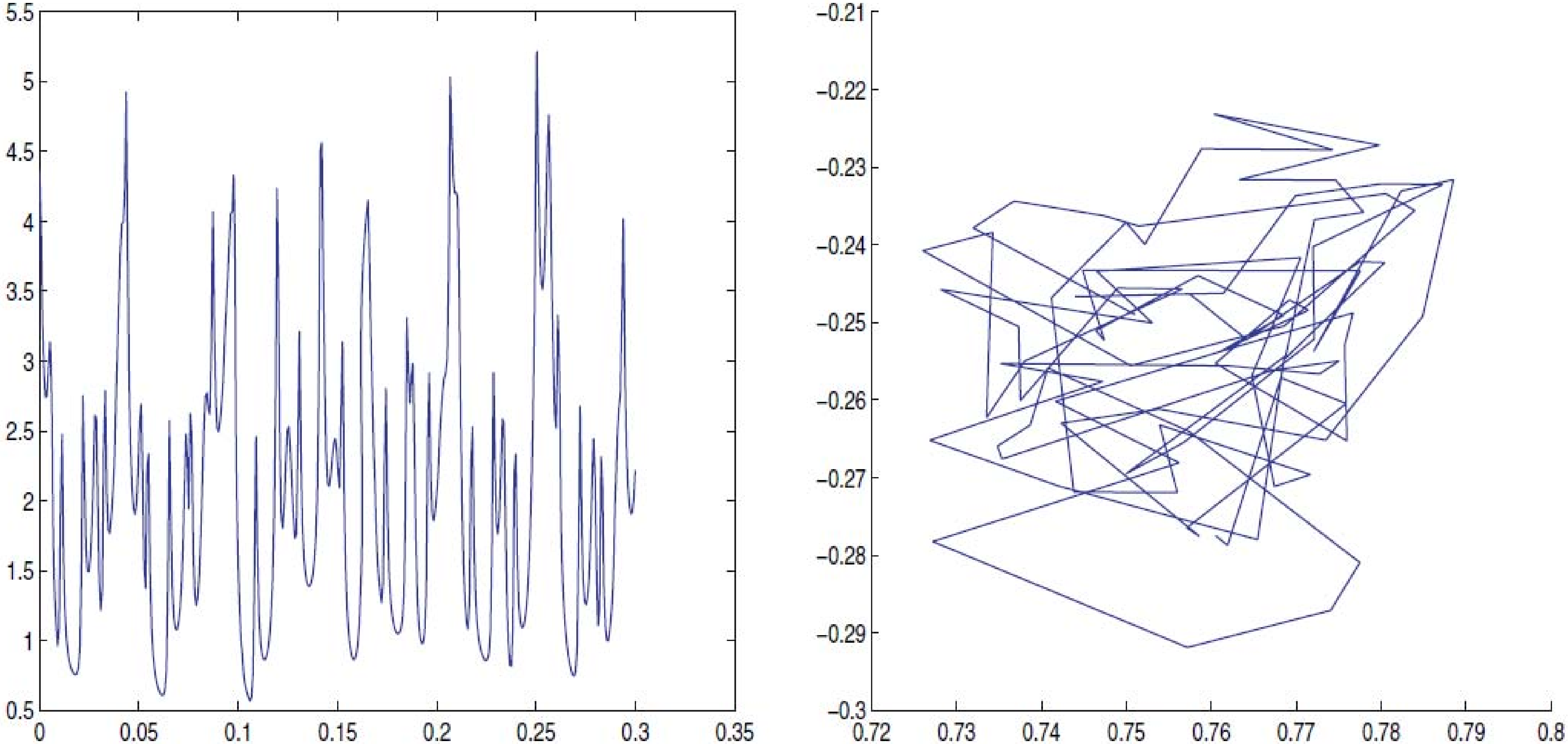
$$\left\| (u - u_h)(.,T) \right\|_{L^2(\Omega)} + \|u - u_h\|_{L^2(0,T,H^1_0(\Omega))} \leq C \left(h + \frac{\Delta t}{h}\right) \|g\|_{L^2(\Omega_T)}$$



a

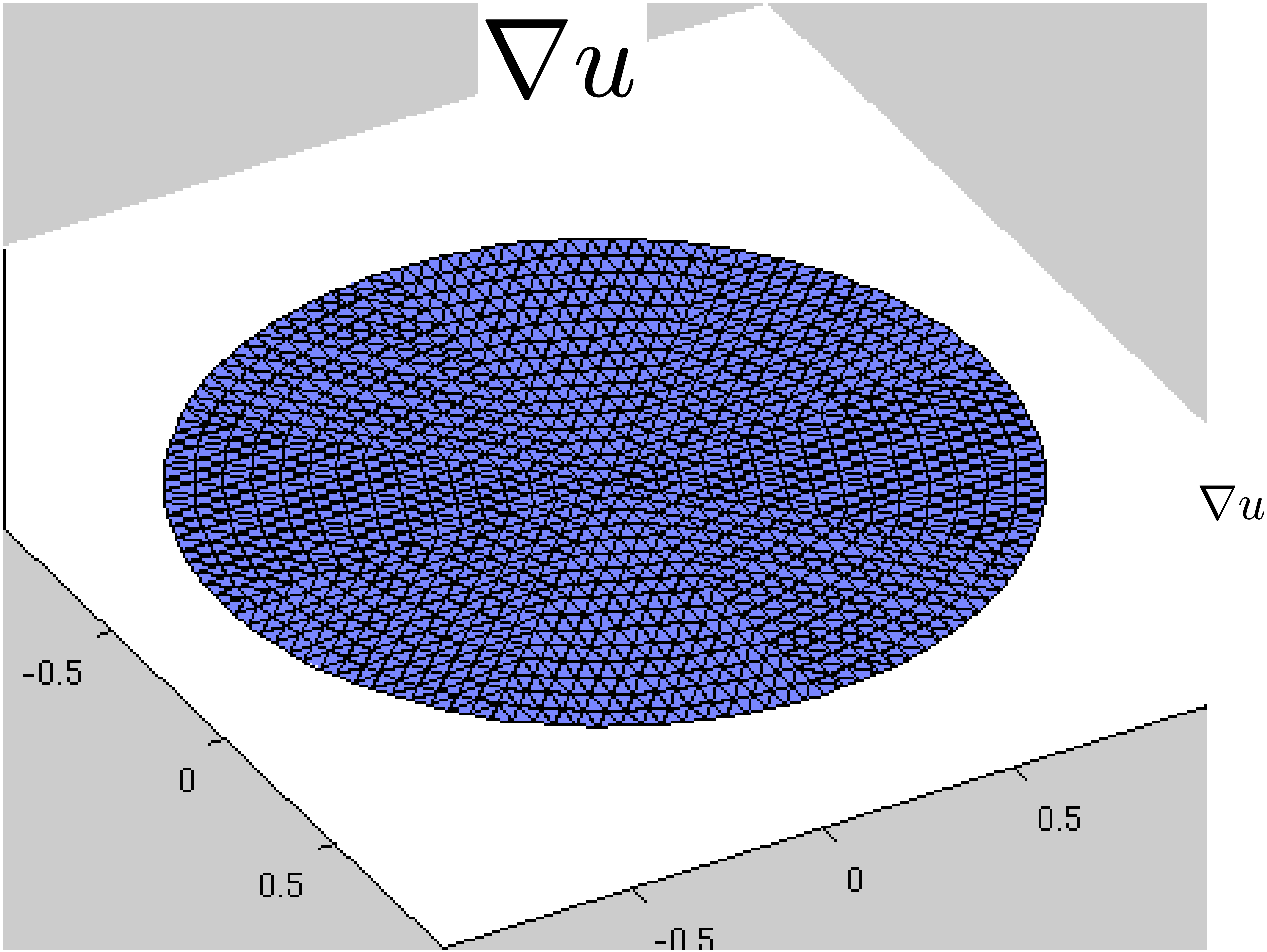


F

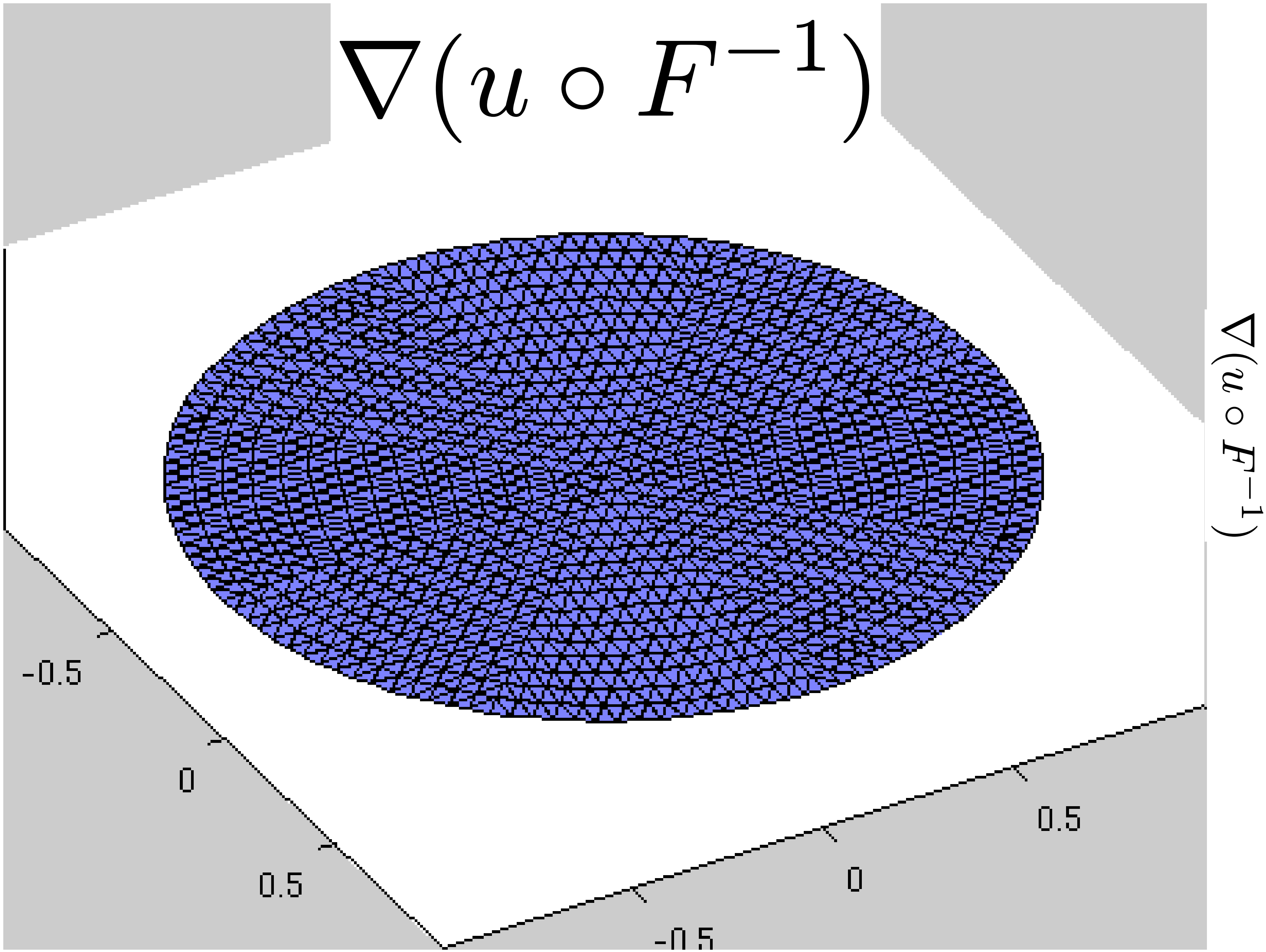


(a) $t \to a(x_0, t)$.

(b) Top view of $t \to F(x_0, t)$.



∇u
∇u
-0.5
0
0.5
0.5
0
-0.5



$\nabla(u \circ F^{-1})$
$\nabla(u \circ F^{-1})$
-0.5
0
0.5
0.5
0
-0.5

(CDC') on $\sigma := (\nabla F)^T a \nabla F$

$\exists \delta, \epsilon > 0$:

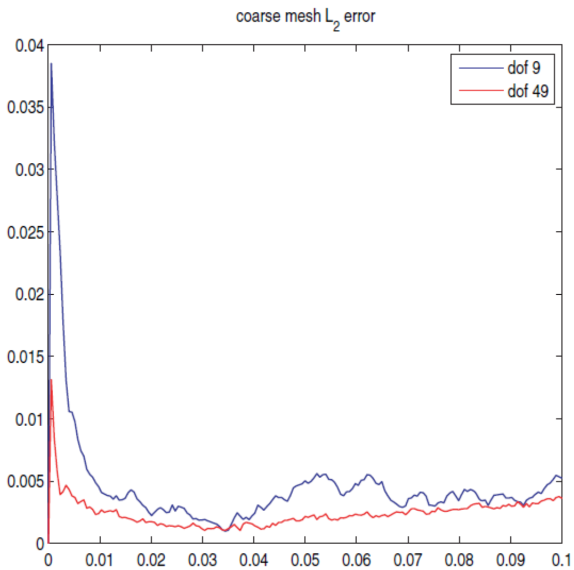
$$\operatorname{ess\,sup}_{\Omega_T} \frac{\delta^2 \operatorname{Trace}[\sigma^T \sigma]+1}{(\delta \operatorname{Trace}[\sigma]+1)^2} \leq \frac{1}{d+\epsilon}$$

Remark: If $y_\sigma := \| \operatorname{Trace}[\sigma]\|_{L^\infty(\Omega_T)} \left\|(\operatorname{Trace}[\sigma])^{-1}\right\|_{L^\infty(\Omega_T)} < \infty$

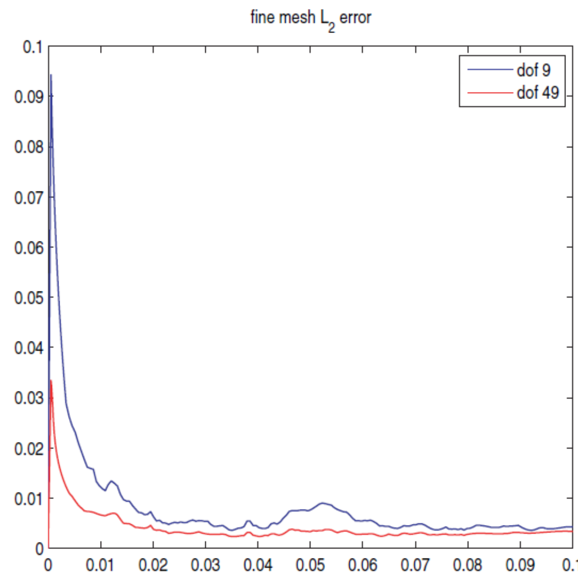
then (CDC') is satisfied with $\delta = d\left\|(\operatorname{Trace}[\sigma])^{-1}\right\|_{L^\infty(\Omega_T)}$ and $\epsilon = \frac{2y_\sigma - 1}{2y_\sigma^2}$

provided that $\operatorname{ess\,sup}_{\Omega_T} d\frac{\operatorname{Trace}[\sigma^T \sigma]}{(\operatorname{Trace}[\sigma])^2} \leq 1 + \frac{\epsilon}{d}$

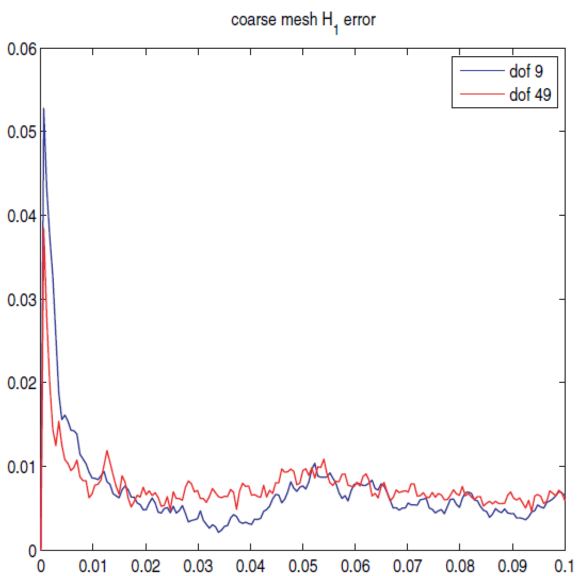
Experiment	dof	L^1	L^∞	L^2	H^1
Coarse mesh error. Time-independent percolation with $g = 1$.	9	0.0142	0.0389	0.0168	0.0366
	49	0.0077	0.0450	0.0101	0.0482
	225	0.0035	0.0228	0.0060	0.0293
Fine mesh error. Time-independent percolation with $g = 1$.	9	0.0196	0.0843	0.0251	0.1193
	49	0.0136	0.0698	0.0184	0.1028
	225	0.0040	0.0243	0.0070	0.0485
Coarse mesh error. Time-independent percolation with $g = \sin(2.4x - 1.8y + 2\pi t)$.	9	0.0236	0.0569	0.0262	0.0477
	49	0.0181	0.0571	0.0215	0.0558
	225	0.0119	0.0774	0.0167	0.0939
Fine mesh error. Time-independent percolation with $g = \sin(2.4x - 1.8y + 2\pi t)$.	9	0.0424	0.1099	0.0512	0.1712
	49	0.0277	0.0985	0.0348	0.1451
	225	0.0174	0.0886	0.0242	0.1192
Coarse mesh error. Multiscale trigonometric time-dependent. $g = 1$.	9	0.0018	0.0045	0.0019	0.0039
	49	0.0012	0.0054	0.0015	0.0060
Fine mesh error. Multiscale trigonometric time-dependent. $g = 1$.	9	0.0031	0.0096	0.0034	0.0242
	49	0.0014	0.0059	0.0016	0.0166
Coarse mesh error. Multiscale trigonometric time-dependent. $g = \sin(2.4x - 1.8y + 2\pi t)$.	9	0.0043	0.0087	0.0044	0.0085
	49	0.0033	0.0079	0.0035	0.0084
Fine mesh error. Multiscale trigonometric time-dependent medium. $g = \sin(2.4x - 1.8y + 2\pi t)$.	9	0.0082	0.0199	0.0087	0.0379
	49	0.0038	0.0104	0.0040	0.0244
Coarse mesh error. Time-dependent random fractal.	9	0.0046	0.0074	0.0052	0.0065
	49	0.0036	0.0046	0.0036	0.0059
Fine mesh error. Time-dependent random fractal.	9	0.0039	0.0082	0.0043	0.0222
	49	0.0033	0.0054	0.0034	0.0168



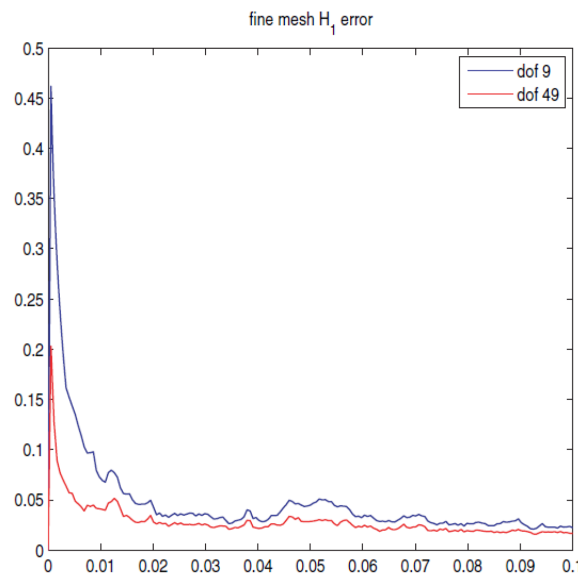
(a) coarse mesh L^2 error.



(b) Fine Mesh L^2 error.



(c) coarse Mesh H^1 error.



(d) fine Mesh H^1 error.

FIG. 3.4. *Time-dependent random fractal medium at* $t = 0.1$.

Discrete geometric structures in Homogenization
Desbrun-Donaldson-Owhadi

$$\begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

F: Harmonic coordinates

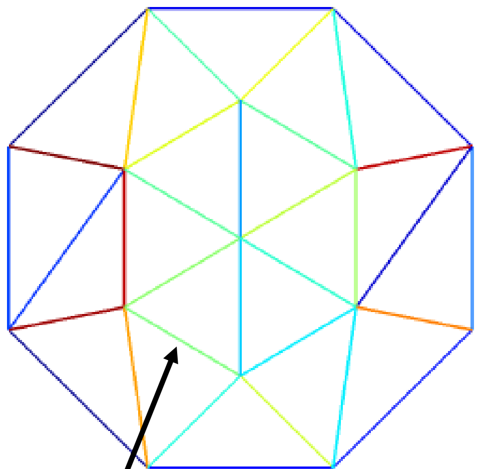
$$F := (F_1, F_2)$$

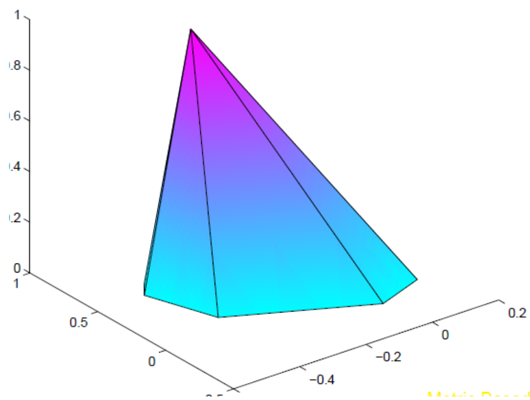
$$\begin{cases} -\operatorname{div}(a\nabla F_i) = 0 & \Omega \\ F_i(x) = x_i & \partial\Omega \end{cases}$$

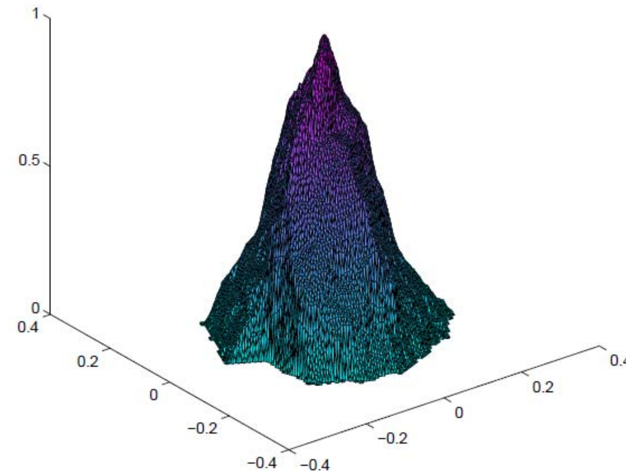
[Desbrun-Donaldson-Owhadi-09]

Edges effective conductivities

Ω_h φ_i $\varphi_i \circ F$







$$q_{ij}^h := -\int_\Omega (\nabla(\varphi_i \circ F))^T a(x) \nabla(\varphi_j \circ F)\, dx$$

Homogenization with edges effective conductivities

$$\sum_{j\sim i} q_{ij}^h (u_i^h - u_j^h) = \int_\Omega f(x)\varphi_i \circ F(x)\, dx$$

$$u_h := \sum_{i\in\mathcal{N}_h} u_i^h \varphi_i \circ F$$

Theorem **(Weak CDC** $\operatorname{ess\,sup}_\Omega \frac{\lambda_{\max}[(\nabla F)^T \nabla F(x)]}{\lambda_{\min}[(\nabla F)^T \nabla F(x)]} < \infty$ **d=2)**

$$\|u - u_h\|_{H_0^1(\Omega)} \leq Ch\|f\|_{L^2(\Omega)}$$

Physical conductivity space

$$a$$

Non linear and Non-injective

$$q_{ij}^h$$

Edges effective conductivities

$$q_{ij}^h := -\int_\Omega (\nabla(\varphi_i \circ F))^T a(x) \nabla(\varphi_j \circ F)\, dx$$

Divergence-free matrix Q

$$Q := \frac{(\nabla F)^T a \nabla F}{\det(\nabla F)} \circ F^{-1}$$

Theorem **Q is symmetric and positive**

$$\forall l \in \mathbb{R}^2 \;\; \operatorname{div}(Q \cdot l) = 0$$

$$q^h_{ij} := - \int_\Omega (\nabla \varphi_i)^T Q(x) \nabla \varphi_j \, dx$$

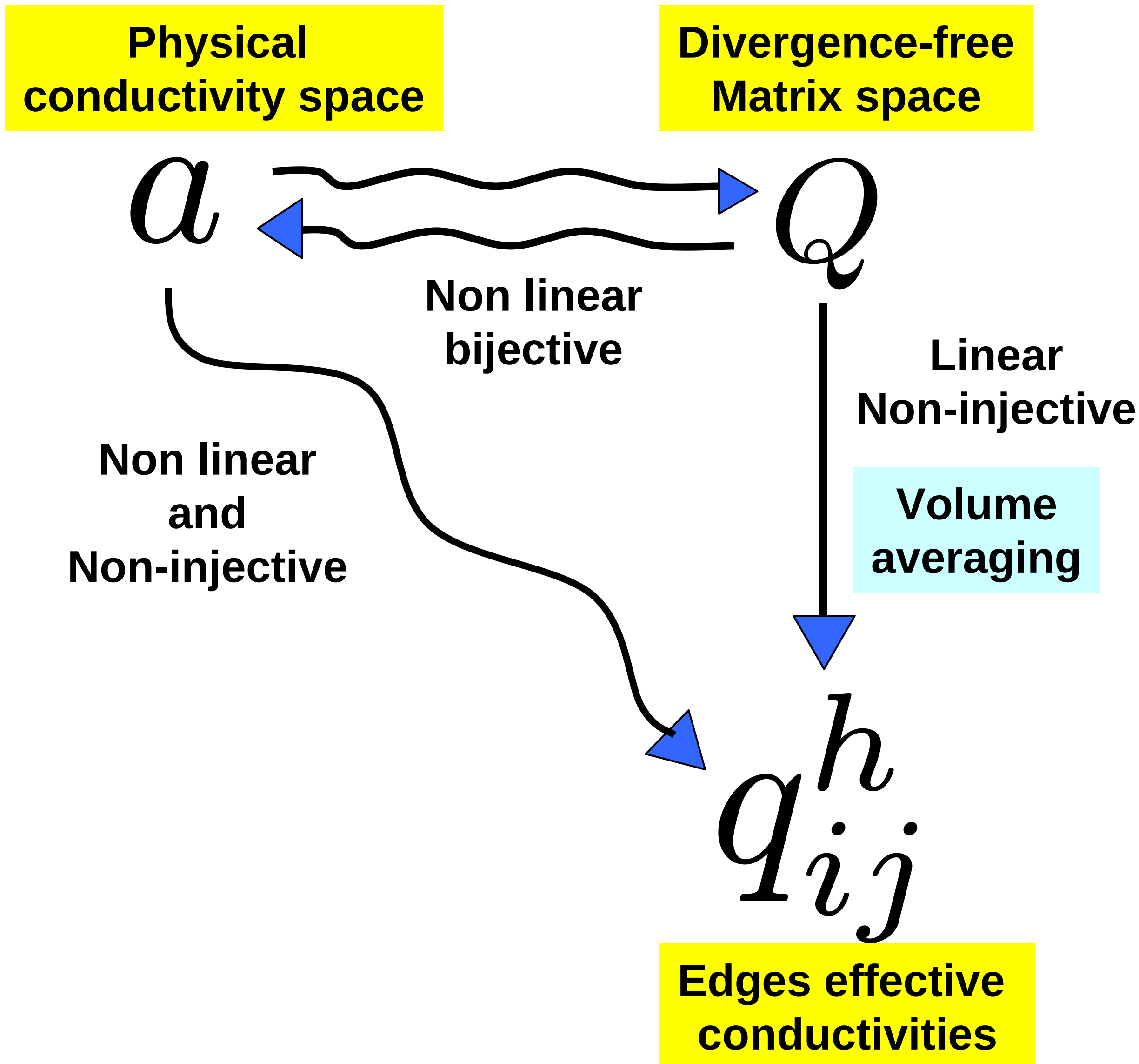
Inversion of the function $a \to Q$

Theorem If a is isotropic then

$$a = \sqrt{\det(Q) \circ G^{-1}}\, I_d$$

$$G := (G_1, G_2)$$

$$\begin{cases} \operatorname{div}\left(\dfrac{Q}{\sqrt{\det(Q)}} \nabla G_i\right) = 0 \quad \text{in} \quad \Omega \\ G_i(x) = x_i \quad \text{on} \quad \partial\Omega. \end{cases}$$



$$q_{ij}^h := -\int_\Omega (\nabla \varphi_i)^T Q(x) \nabla \varphi_j \, dx$$

Theorem

Convex functions

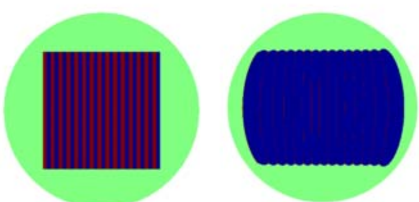
For each Q there exists a convex function s, unique up to affine functions, such that

$$\boxed{\mathrm{Hess}(s) = R^T Q R,}$$

where $\mathrm{Hess}(s)$ is the Hessian of s.

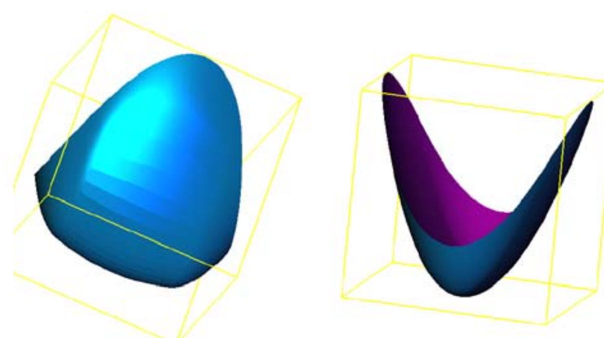
$$R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

a



1: The left-hand image shows the original scalar conductivity $\sigma(x) = a(x)\,\mathrm{Id}$. In blue regions a=0.05, in red regions a=1.95, and in green regions, a = 1.0. The right-hand image gives $\sqrt{\det Q} = \sigma(x) \circ F^{-1}$, showing how harmonic coordinates distort $\sigma(x)$.

s



Homogenization as a linear interpolation operator

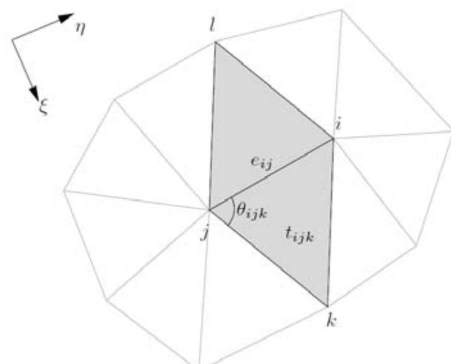
$$s^h(x) = \sum_i s(x_i)\varphi_i(x)$$

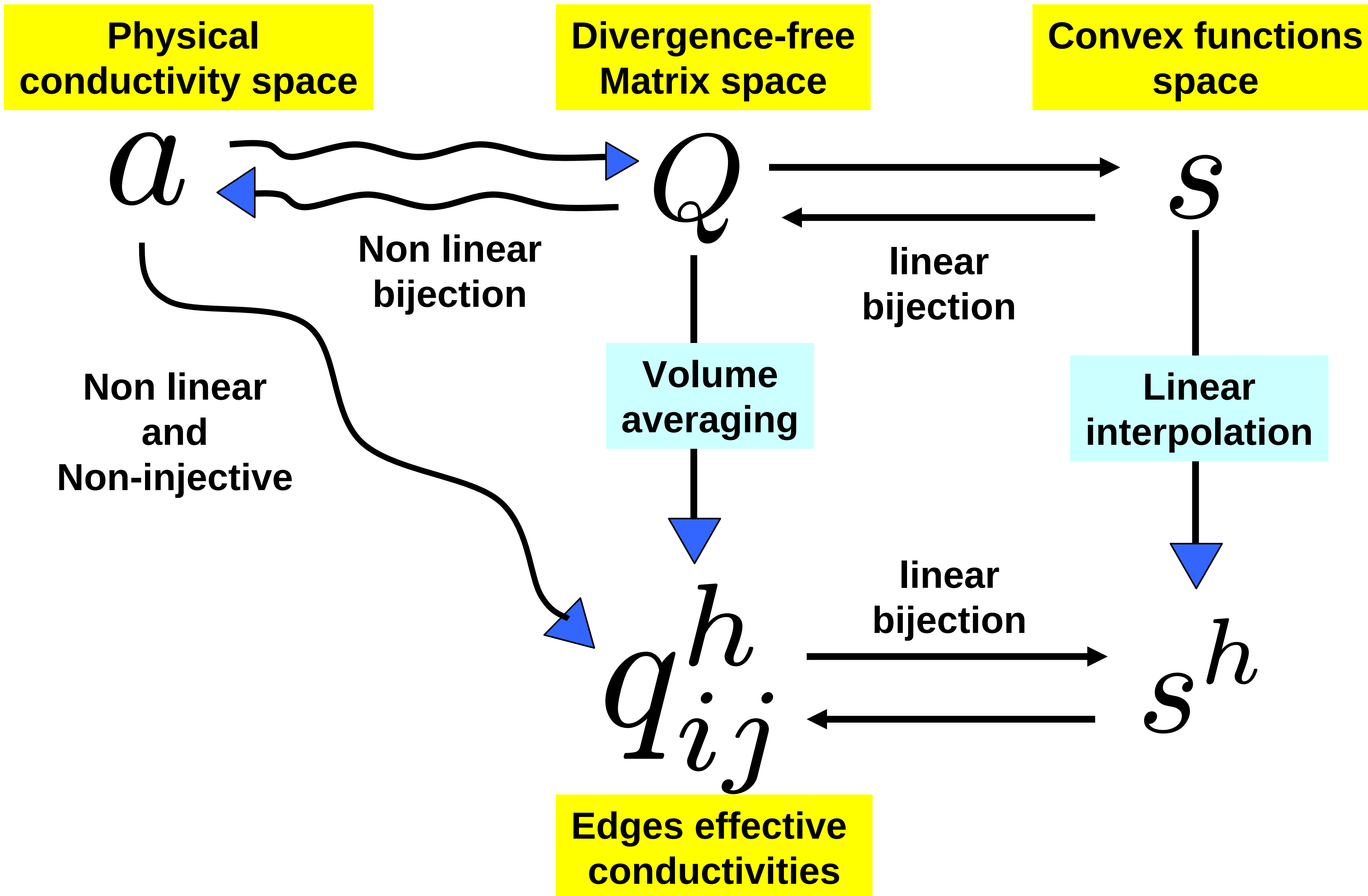
Theorem

$$q^h = R\,\mathrm{Hess}(s^h)R^T$$

where $\mathrm{Hess}(s)$ is the Hessian of s.

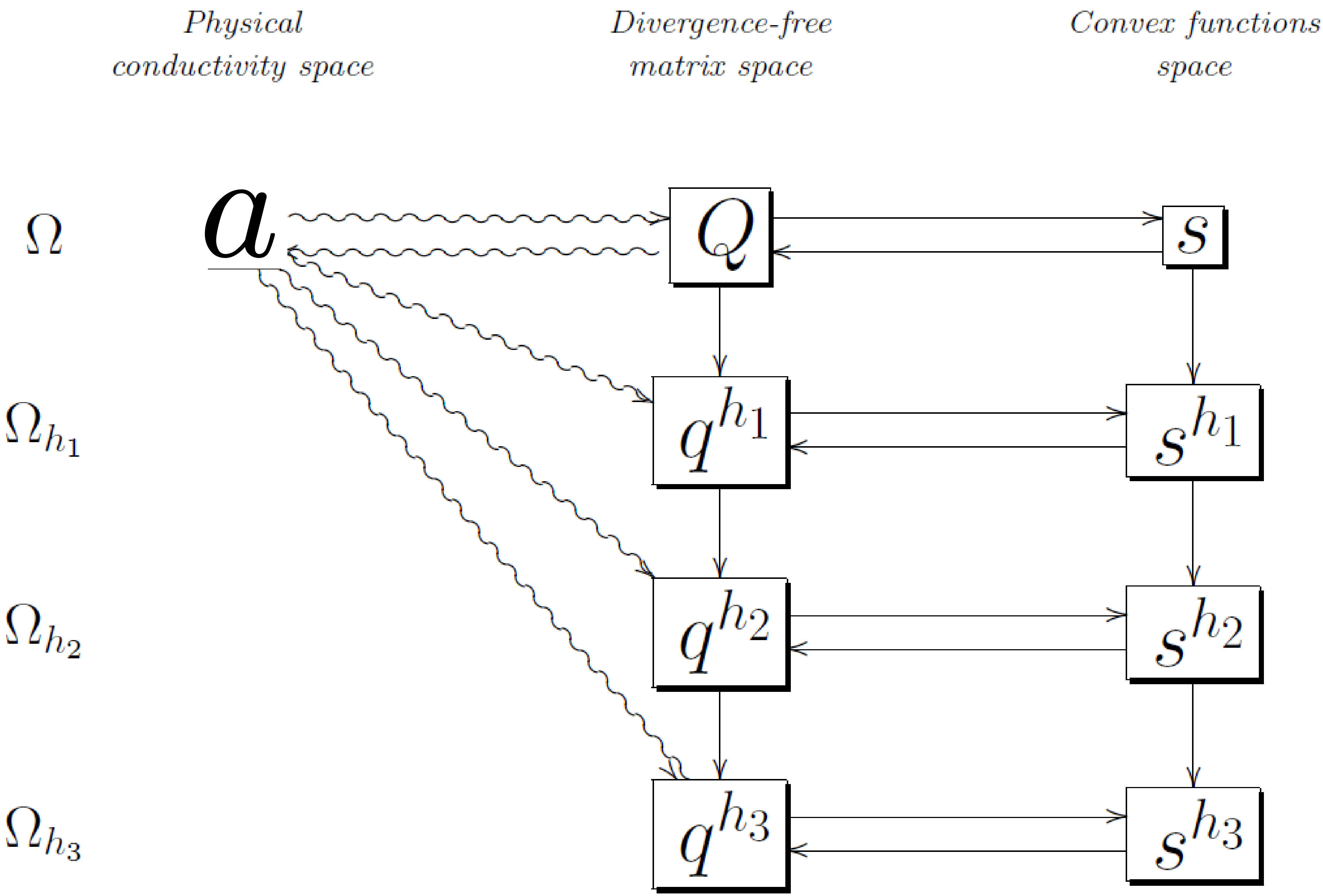
$$R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$





$$q^h = R\,\mathrm{Hess}(s^h)R^T$$

Semi-Group Property



Application to mesh optimization

Can we choose the mesh to minimize the constant in

$$\|u - u_h\|_{H_0^1(\Omega)} \leq Ch\|f\|_{L^\infty(\Omega)}$$

Discrete Dirichlet energy associated to the homogenized problem

$$E_Q(u) = \frac{1}{2}\sum_{i\sim j} q_{ij}^h \left(u_i - u_j\right)^2$$

Can we choose the mesh so that for all i,j $\forall i, j \ : \ q_{ij}^h > 0\,?$

Idea: Use optimal weighted Delauney triangulations for linearly interpolating convex functions

$$E_s = \int_\Omega |s(x,y) - s^h(x,y)|$$

Application to constant optimization

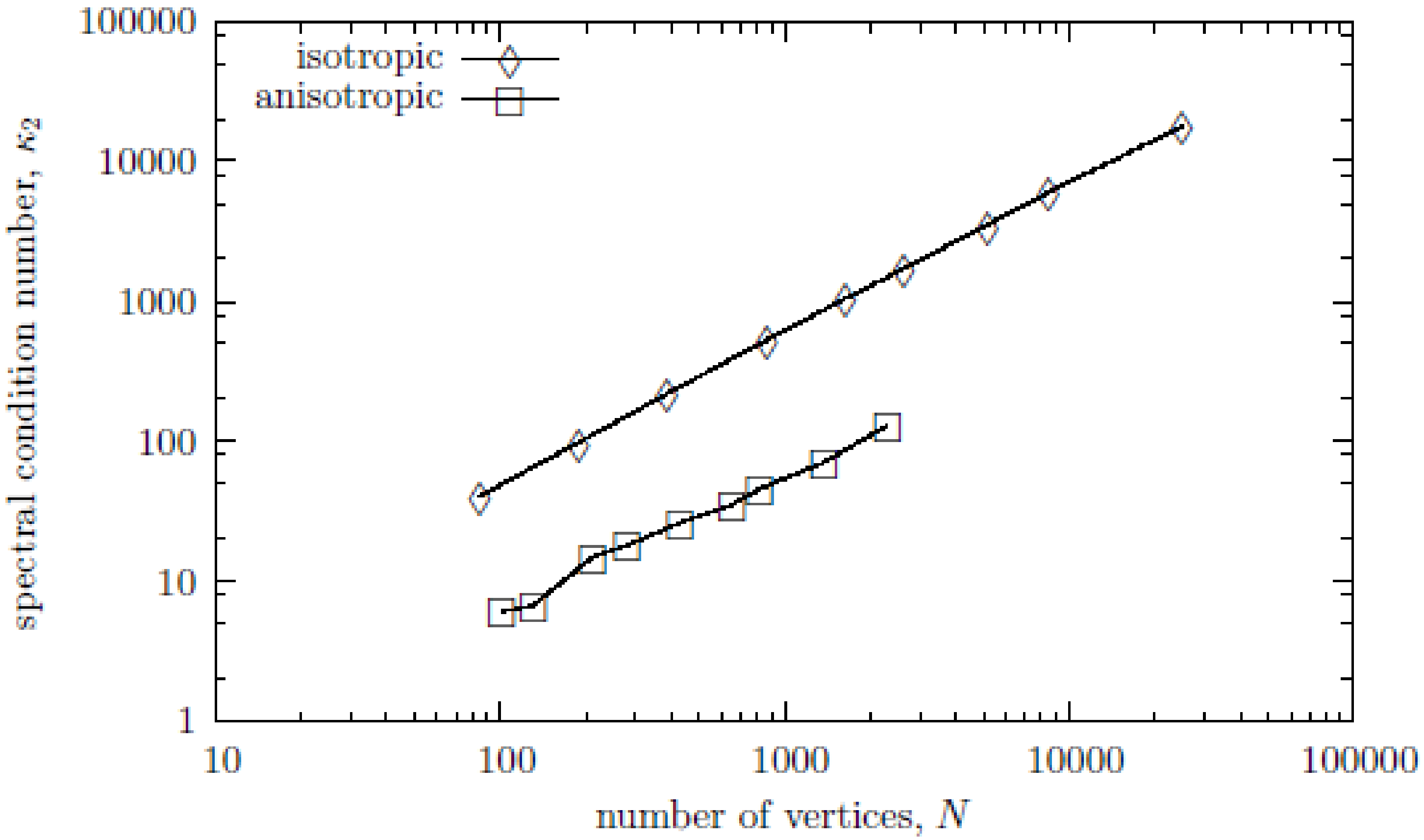
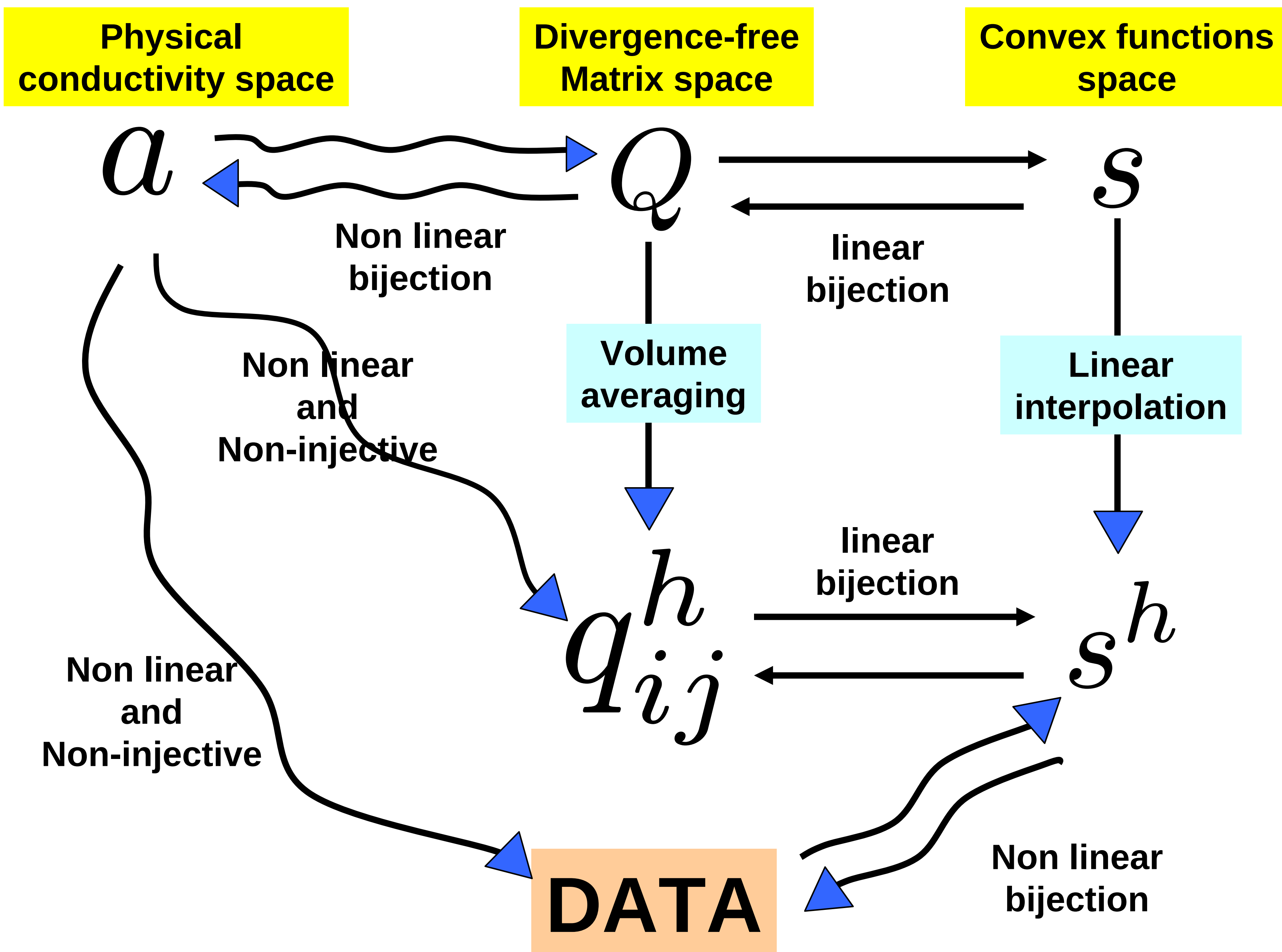
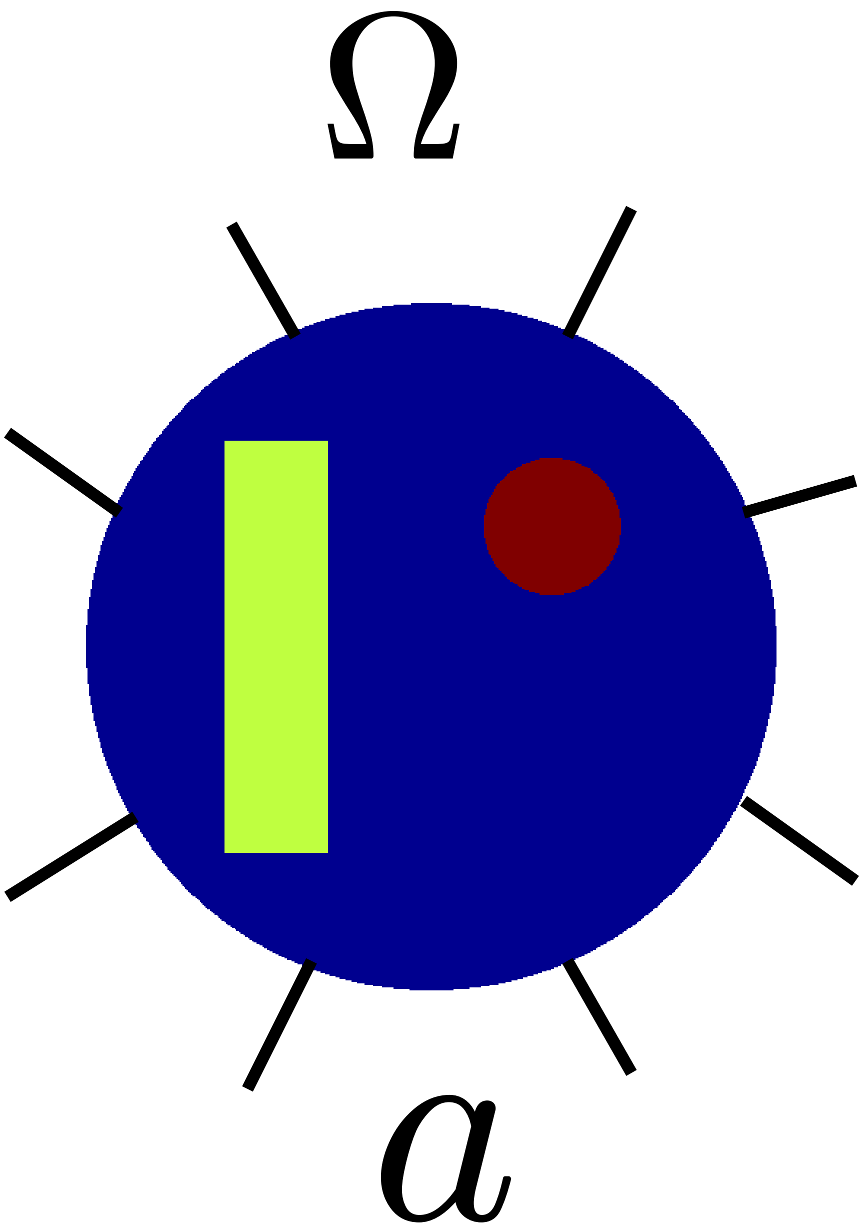


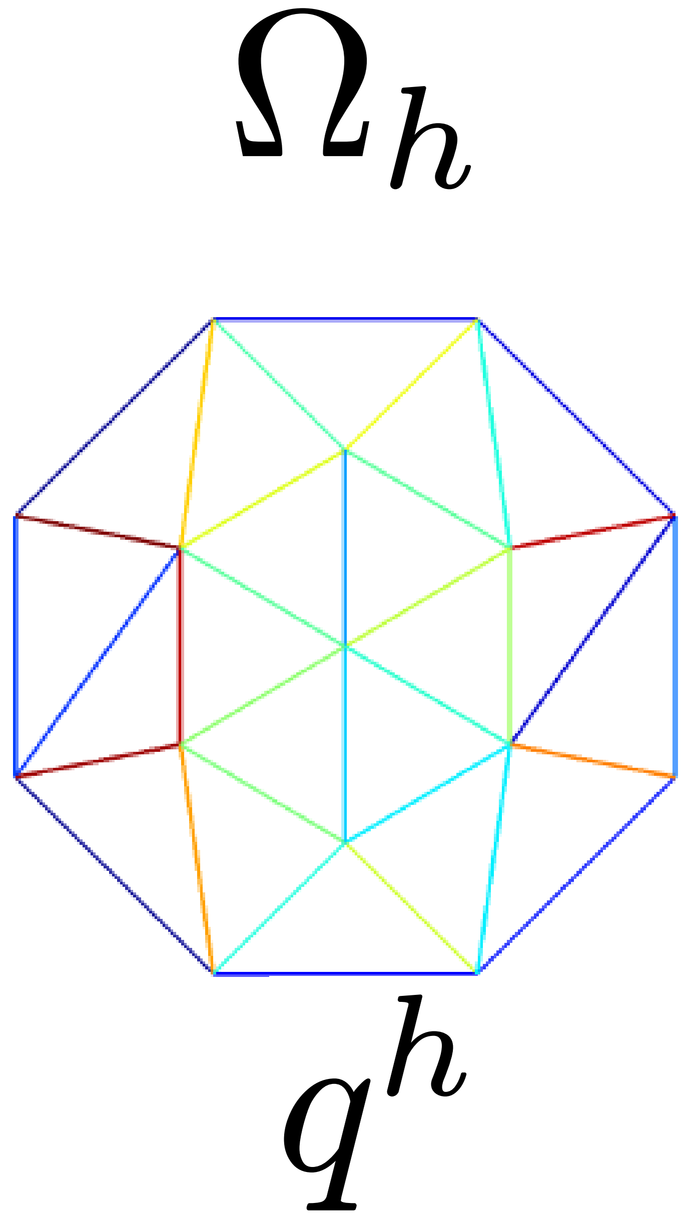
Figure 4.5: Matrix conditioning quality of adapted meshes measured by the spectral condition number κ_2 of the stiffness matrix. The condition number grows as $\mathcal{O}(N)$ in both cases, but is offset by a factor of about 5 in the adapted anisotropic meshes.

Application to ill posed inverse problems

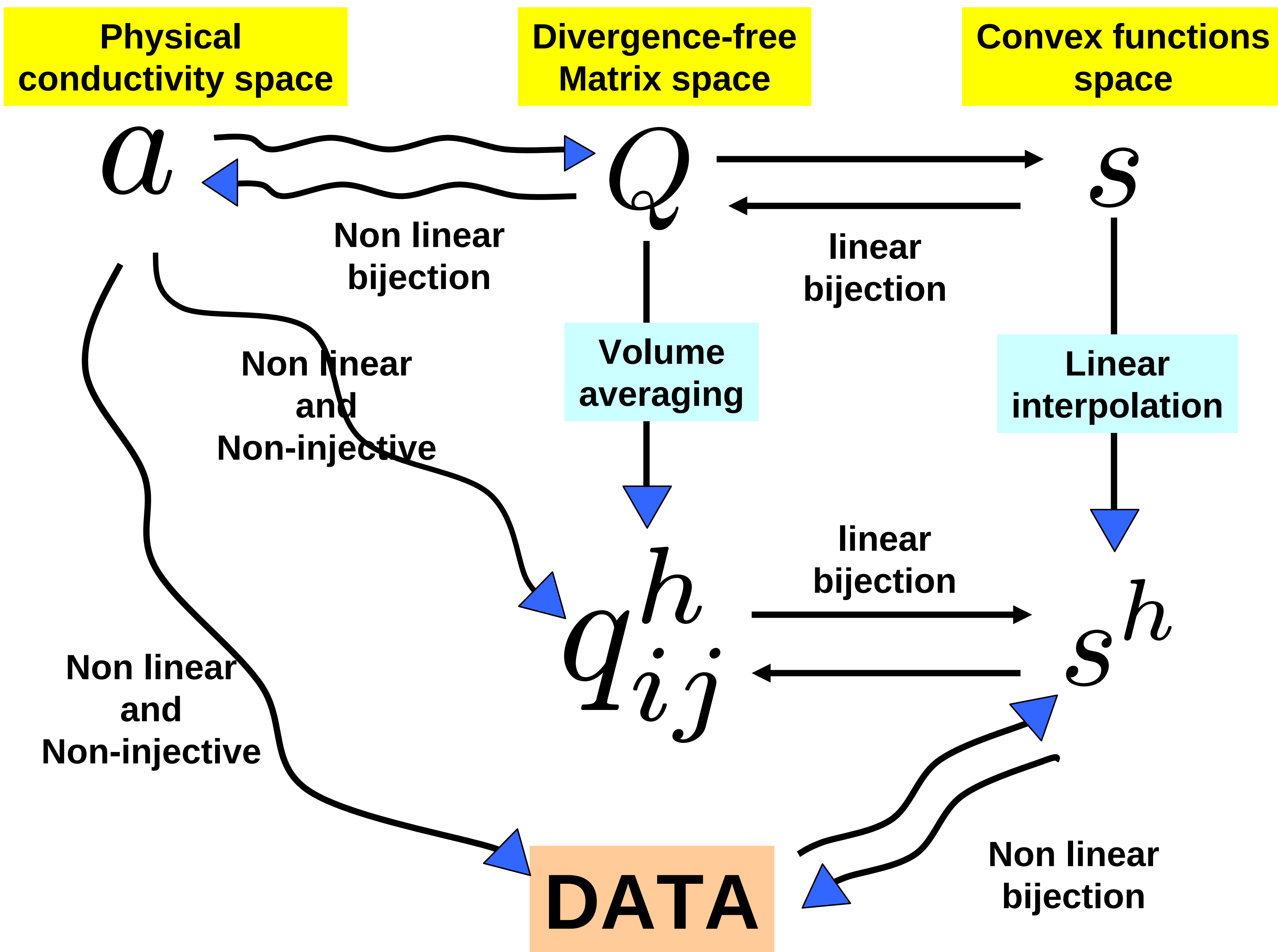


Application to EIT with incomplete measurements

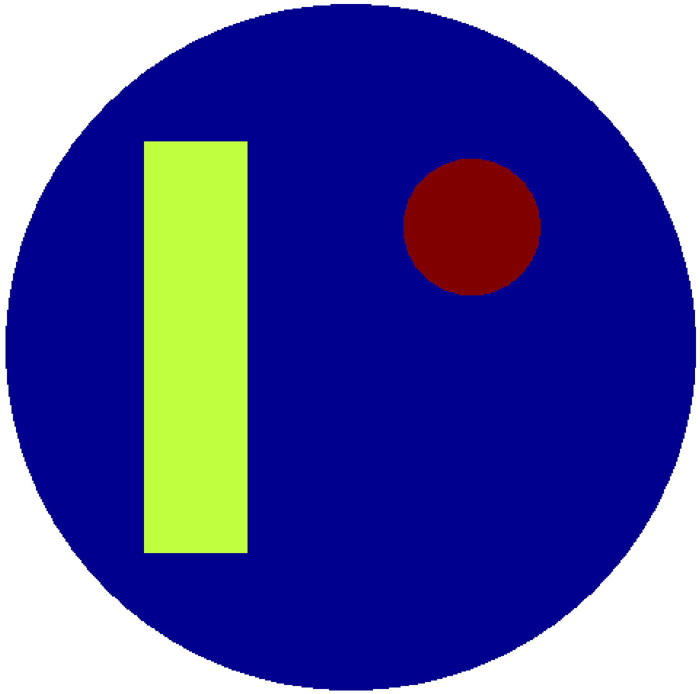


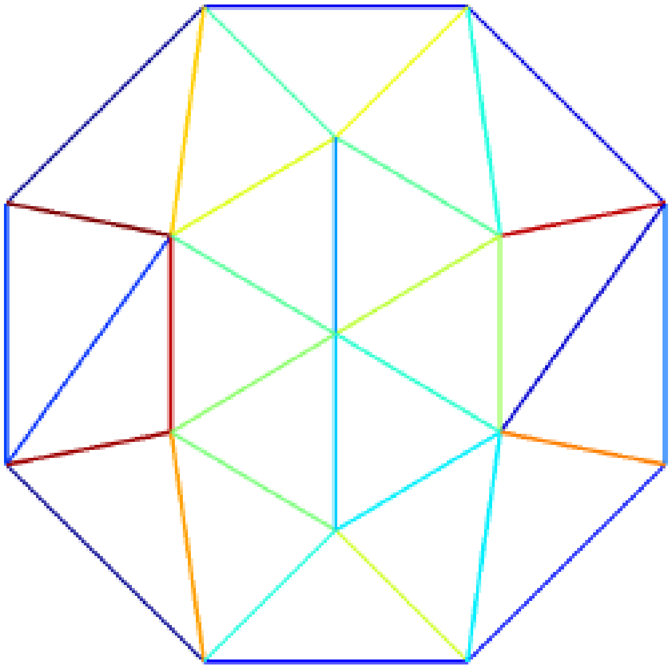


Application to ill posed inverse problems

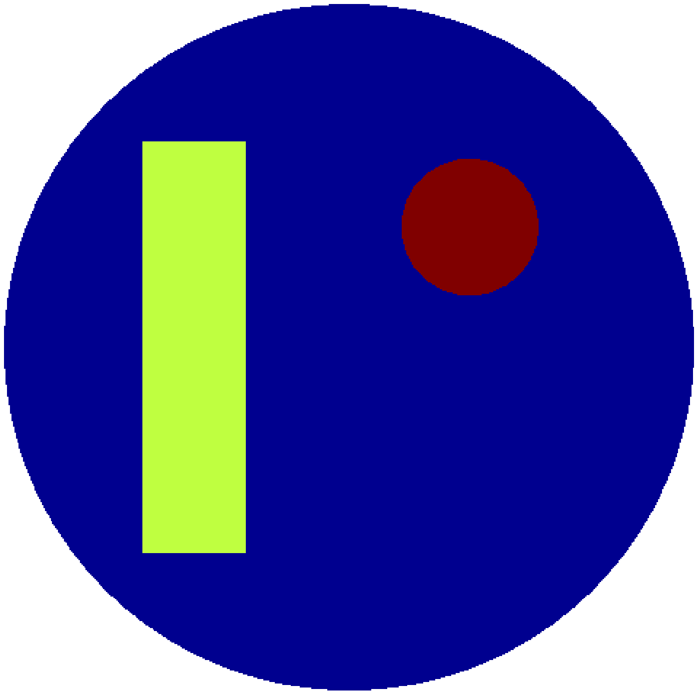


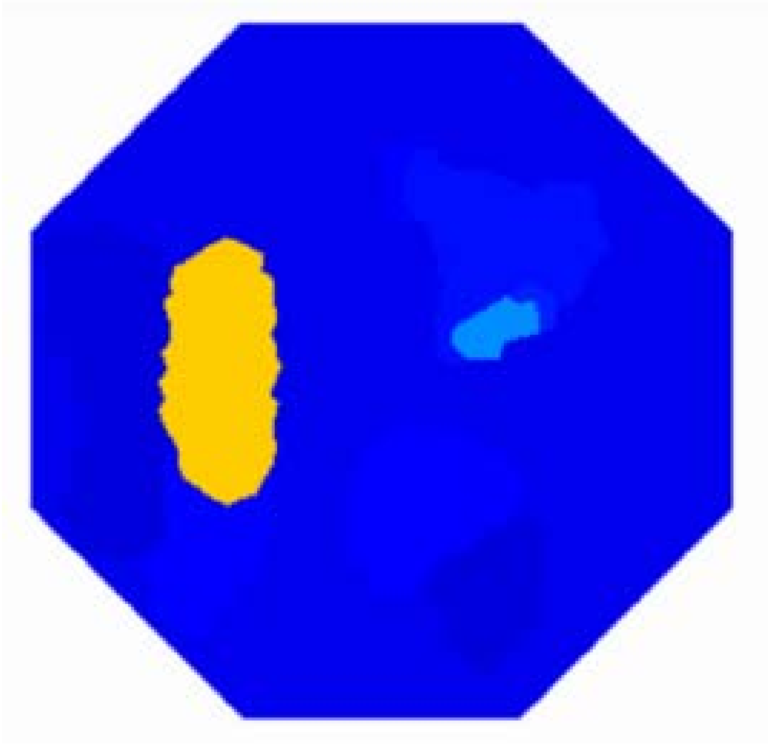
Application to EIT with incomplete measurements





Recovery with 8 boundary measurements

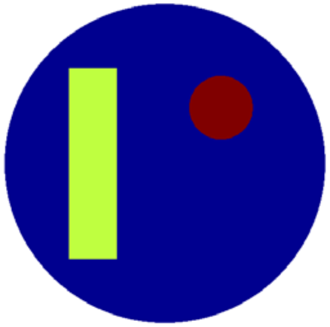




Achieve resolution below mesh size

EIT

σ



$$\begin{cases} -\operatorname{div}(a\nabla u) = 0, & x \in \Omega, \\ u = g, & x \in \partial\Omega, \end{cases}$$

$$\Lambda_a : H^{\frac{1}{2}}(\partial\Omega) \to H^{-\frac{1}{2}}(\partial\Omega)$$

$$g \to n.a\nabla u$$

Given Λ_a find a

EIT

For a given diffeomorphism Ψ from Ω onto Ω, write

$$\Psi_* a := \frac{(\nabla\Psi)^T a \nabla\Psi}{\det(\nabla\Psi)} \circ \Psi^{-1}$$

$$\Sigma(\Omega) = \{\sigma \in Ł^\infty(\Omega; \mathbb{R}^{2\times 2}) \mid \sigma = \sigma^T, 0 < \lambda_{\min}(\sigma) < \lambda_{\max}(\sigma) < \infty\}.$$

$$\begin{aligned} E_a = \{ & \sigma \in \Sigma(\Omega) \mid \sigma = \Psi_* a, \\ & \Psi : \Omega \to \Omega \\ & \text{is an } H^1\text{-diffeomorphism and } \Psi |_{\partial\Omega} = x\}. \end{aligned}$$

Isotropic solutions

Uhlmann, Sylvester, Kohn, Vogelius, Isakov and more recently, Alessandrini, Vessella, Lassas, Paivarinta

$$\Lambda_a \text{ uniquely determines } E_a$$

$$\text{There exists at most one}$$
$$\gamma \in E_\sigma \text{ such that } \gamma \text{ is isotropic.}$$

Let $\gamma \in E_\sigma$ such that γ is isotropic.

[Desbrun-Donaldson-Owhadi]

Theorem For any $M \in E_\sigma$,

$$\gamma = \sqrt{\det(M) \circ G^{-1}}\, I_d$$

$$\begin{cases} \operatorname{div}\left(\frac{M}{\sqrt{\det(M)}} \nabla G_i\right) = 0 \quad \text{in} \quad \Omega \\ G_i(x) = x_i \quad \text{on} \quad \partial\Omega. \end{cases}$$

Corollary γ is unique.

Theorem

If a is non isotropic and constant, then there exists no isotropic $\gamma \in E_a$

Theorem

There always exists a divergence free $Q \in E_a$ and it is unique

For any $M \in E_a$, $Q = F_* M$
where F: M-harmonic coordinates

$$\Lambda_a \to \gamma$$

Is not continuous with respect to the topology of G-convergence [Kohn-Vogelius-84]

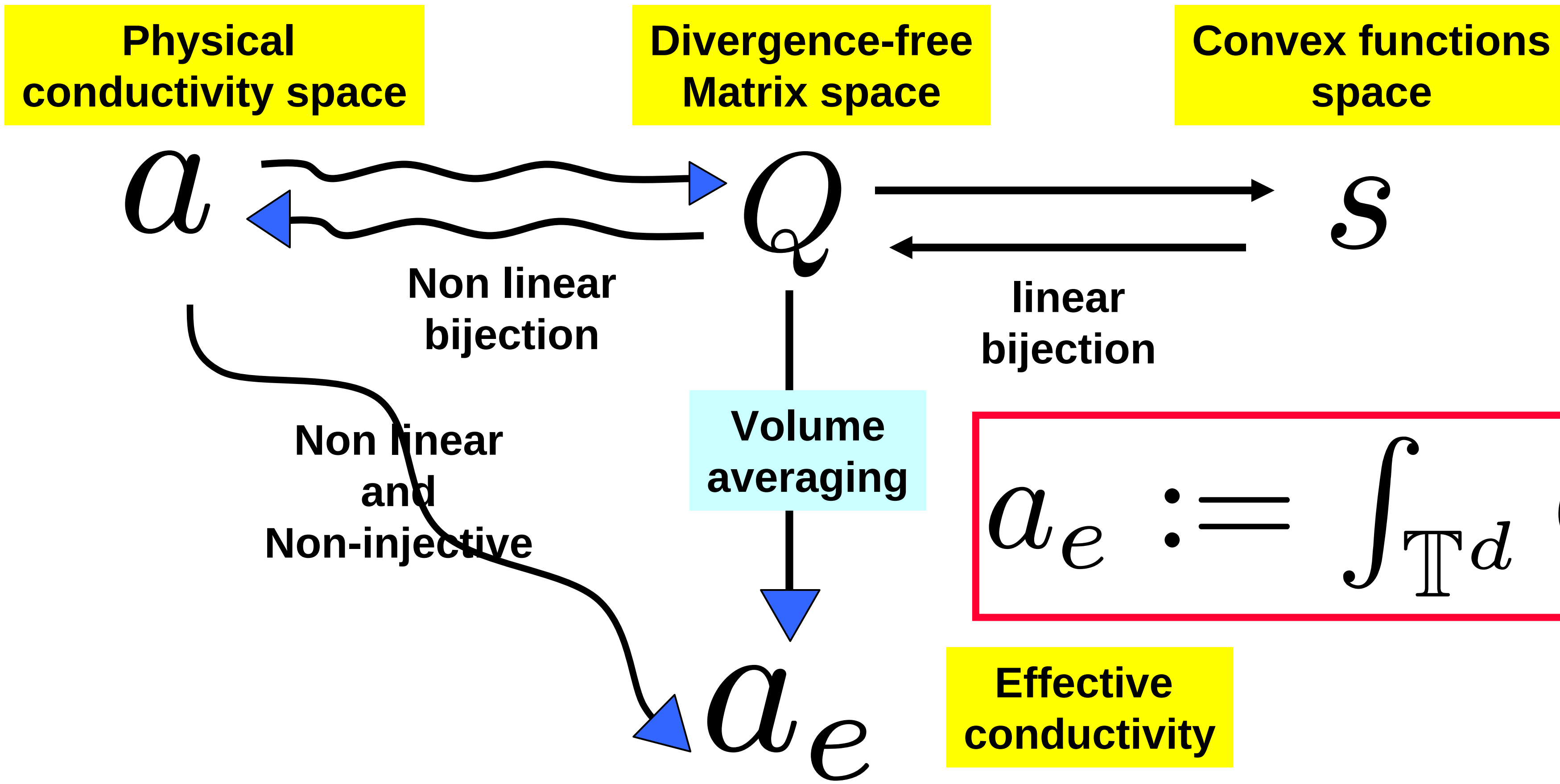
$$\Lambda_a \to Q$$

Is continuous with respect to the topology of G-convergence [Alessandrini-Cabib]

Convex functions form the natural parametrizing space for solutions of the EIT problem

[Desbrun-Donaldson-Owhadi-09]

Periodic Microstructure



$$a_e := \int_{\mathbb{T}^d} Q$$

$$a_e = \int_{\mathbb{T}^d} a(I_d + \nabla \chi)$$

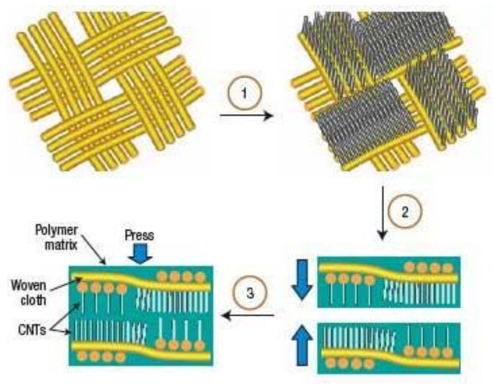
$$\begin{cases} \operatorname{div}\left(a(y)\nabla(y_i + \chi_i(y))\right) = 0 \\ \chi_i \quad \text{periodic} \end{cases}$$

Inverse homogenization

Given a_e find a

Optimal Shape Design / Structural Optimization

- **Murat, Tartar**
- **Milton**
- **Cherkaev**
- **Raitum**
- **Allaire**
- **Kohn**
- **Lurie**
- **Gibiansky, Glowinsky, Reyna, Lavrov, Kikuchi….**



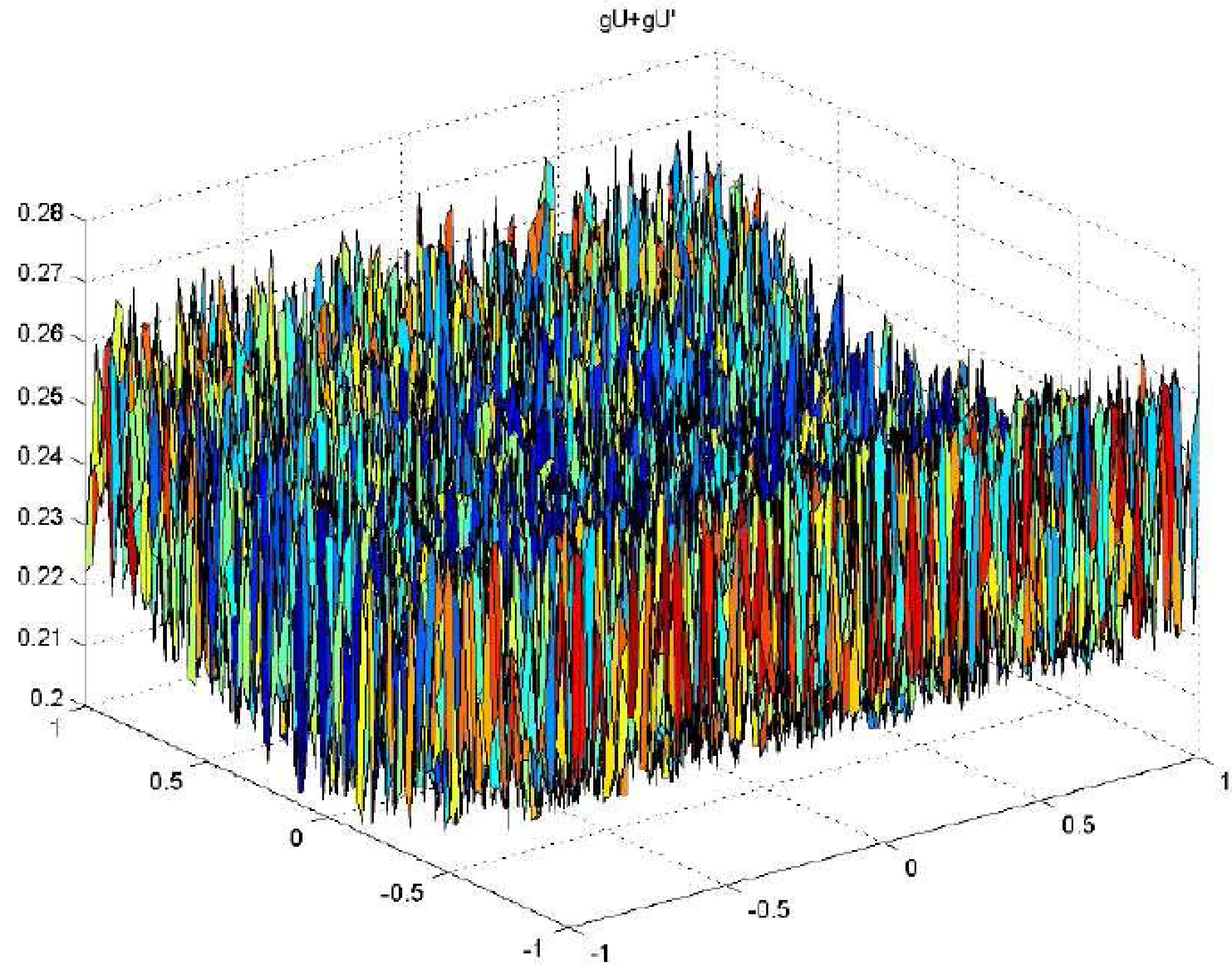
$$\text{Find } a \text{ that minimizes } J(a_e) \text{ or } J(a,u)$$

This problem is in general ill-posed,
i.e. it usually does not admit a solution in the class of admissible designs

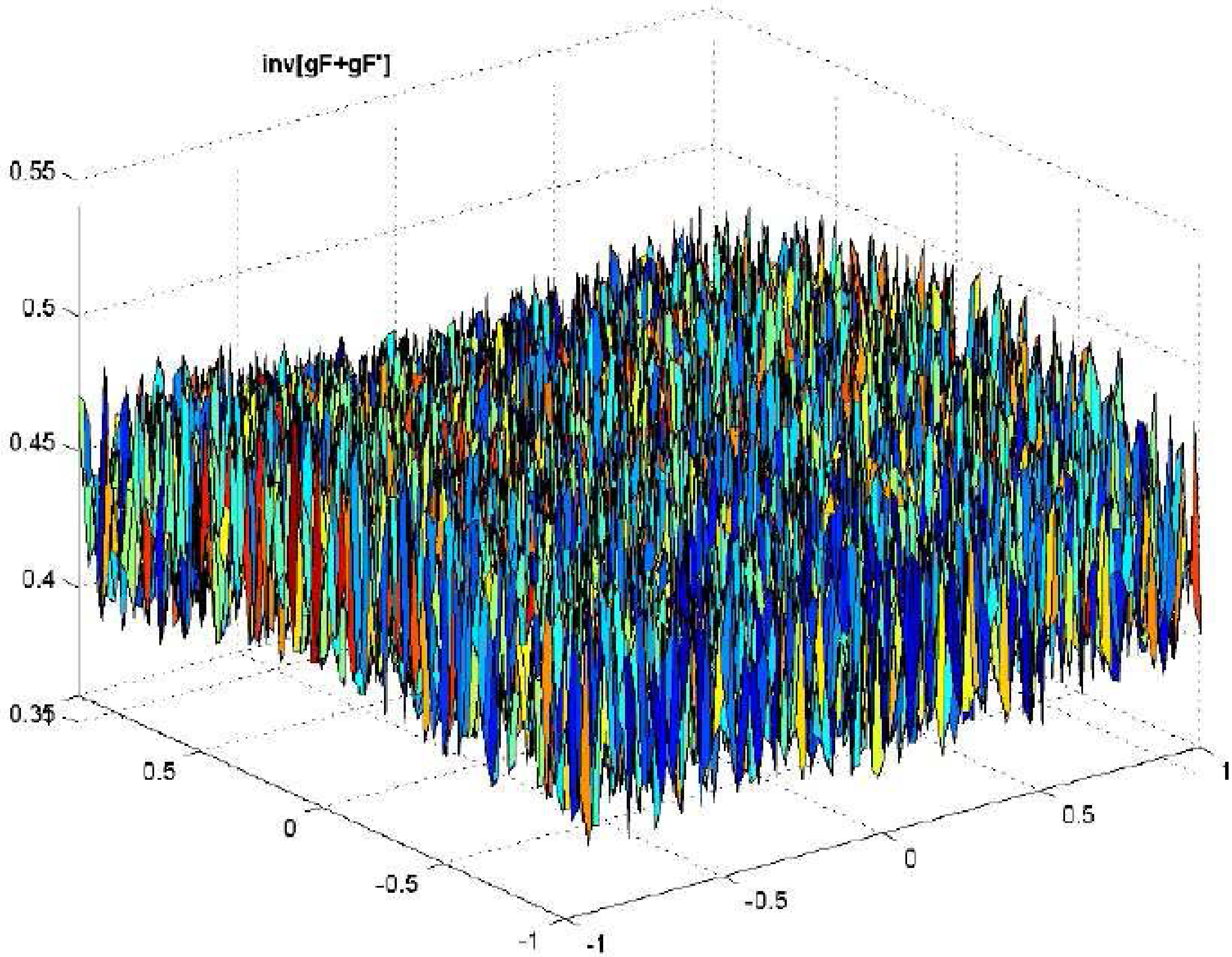
Relaxation method in calculus of variations

Transform an ill posed problem into a well posed one by defining generalized solutions

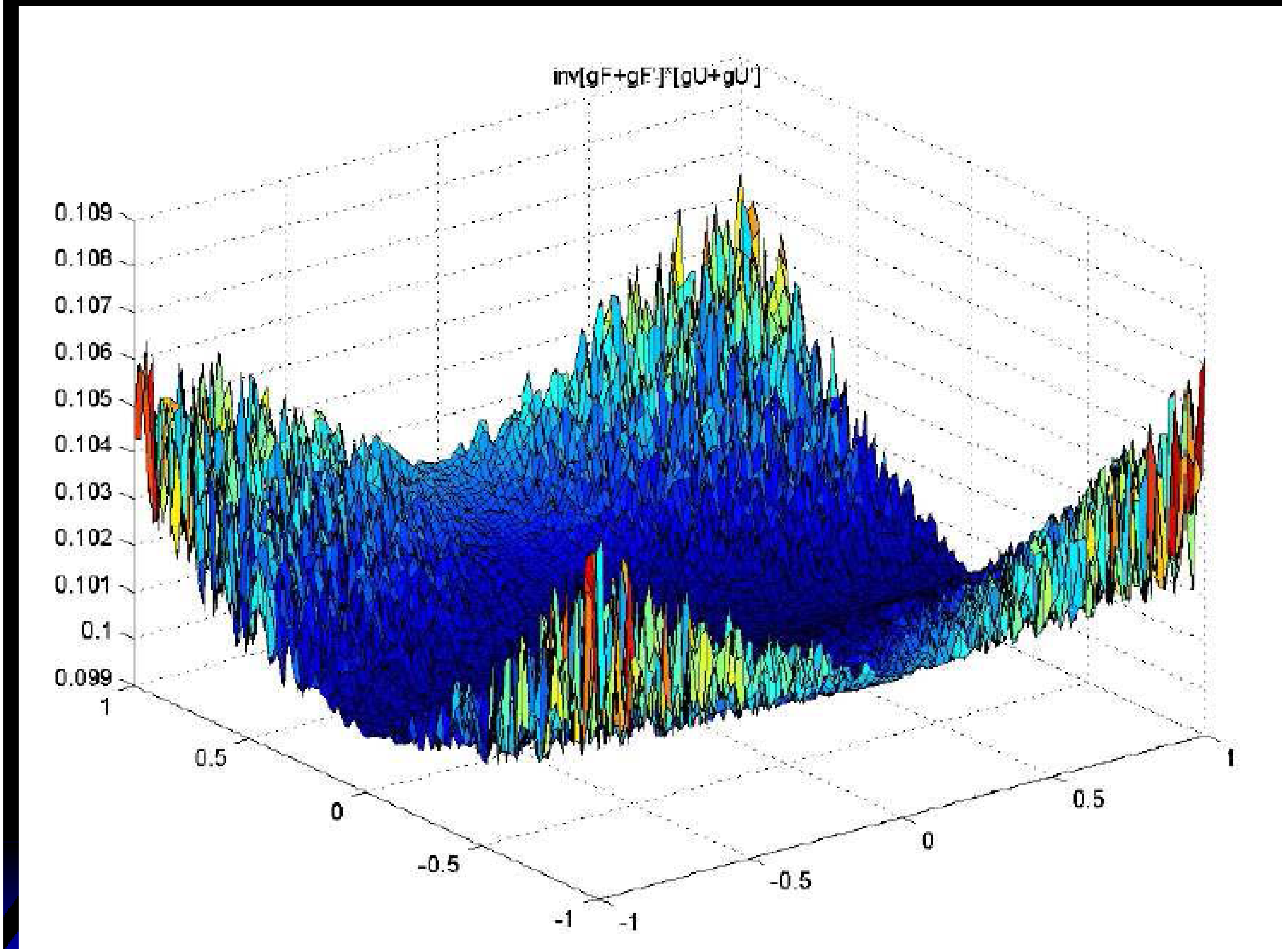
$$\nabla u + (\nabla u)^T$$



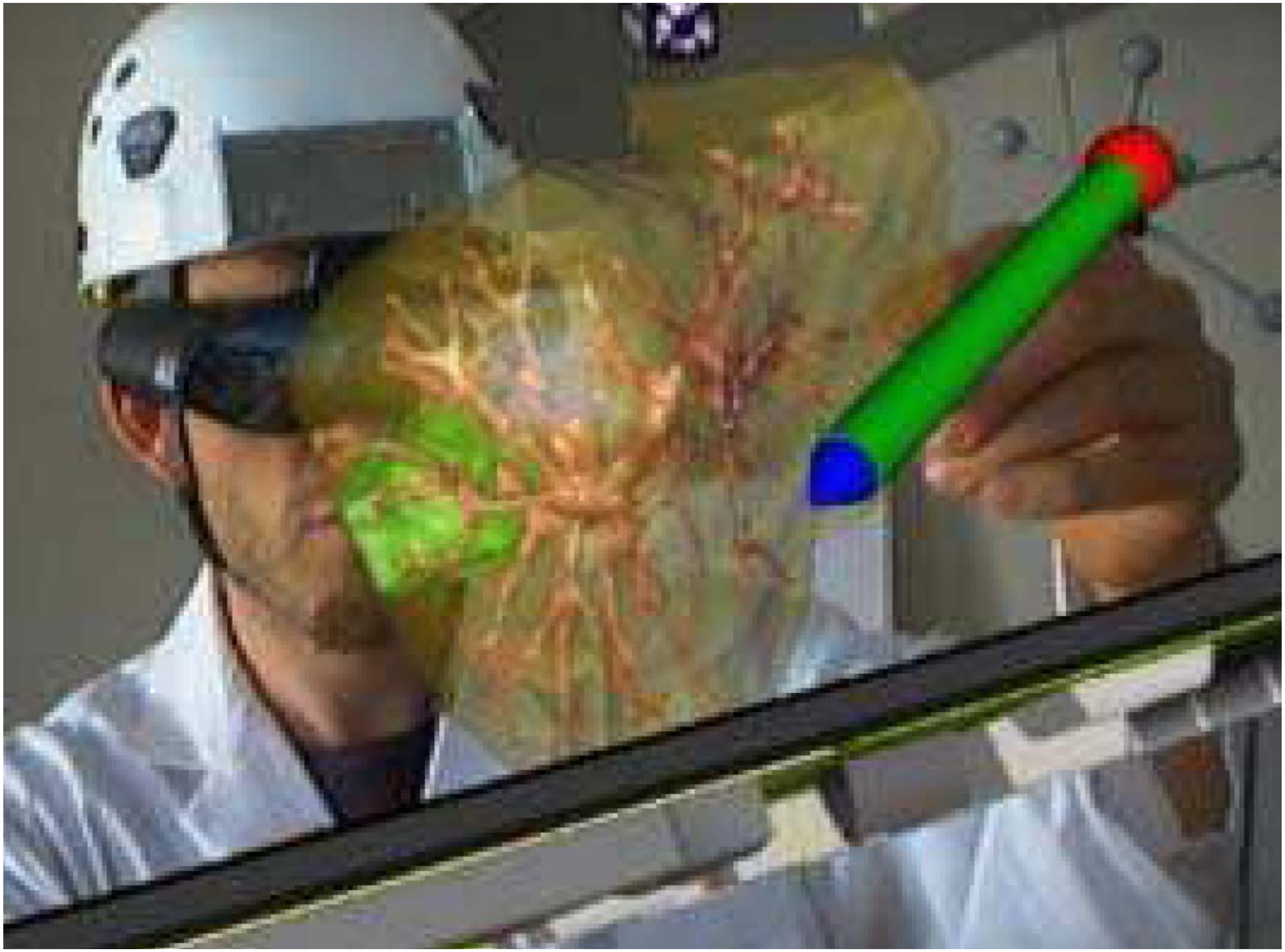
$$\left(\nabla F + (\nabla F)^T\right)^{-1}$$



$$\left(\nabla F+(\nabla F)^{T}\right)^{-1} : \left(\nabla u+(\nabla u)^{T}\right)$$



Virtual Liver Surgery (it is ok to pre-compute Global solutions)
Lily Kharevych, Patrick Mullen, H. Owhadi, Mathieu Desbrun,



Elasto-dynamics

$$\rho\,\partial_t^2 u - \mathrm{div}(C(x) : \varepsilon(u)) = b(x,t)$$

$$C = (C_{ijkl}) \text{ rank-4 (elasticity) tensor}$$

$$\varepsilon(u)_{ij} = \frac{\partial_i u_j + \partial_j u_i}{2}$$

Potential energy (Hookean material)

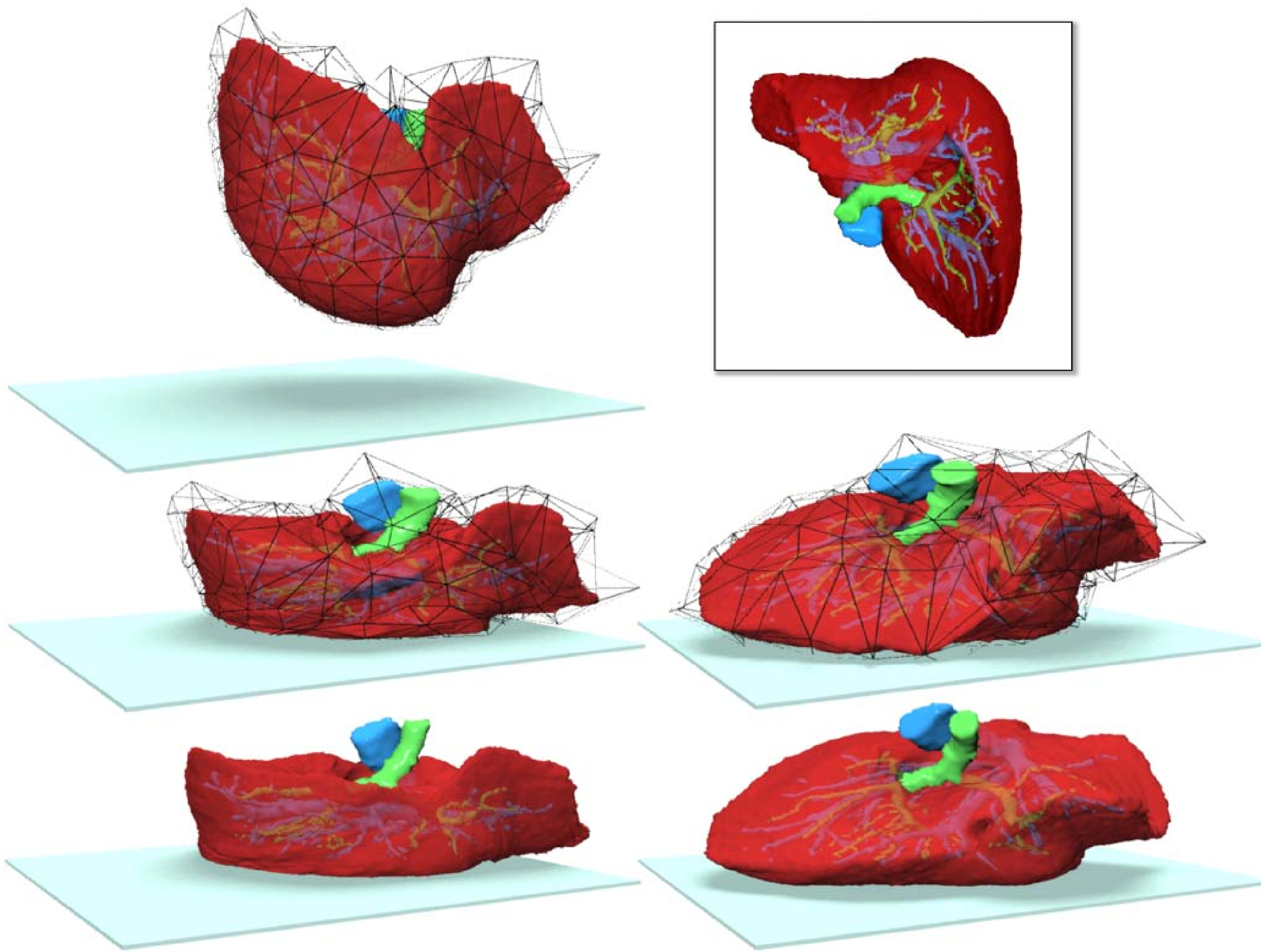
$$\mathcal{W}(u) := \frac{1}{2}\int_\Omega \varepsilon(u) : C : \varepsilon(u)$$

$$C_{ijkl} \in L^\infty(\Omega)$$

how to homogenize those equations?

Virtual Liver Surgery (it is ok to pre-compute Global solutions)

Lily Kharevych, Patrick Mullen, H. Owhadi, Mathieu Desbrun,



Numerical coarsening rationale [Kharevych-Muller-Owhadi-Desbrun-2009]

Introduce $\frac{d(d+1)}{2}$ characteristic displacements F_{ij}

$$\begin{cases} -\operatorname{div}(C : \varepsilon(F_{ij})) = 0 & \Omega \\ (C : F_{ij}).n = \big(C : \varepsilon(x_i e_j)\big).n & \partial\Omega \end{cases}$$

$C_{eff}(\tau)$: Effective elasticity tensor of tet τ

$\bar{F}$: linear interpolation of F over the coarse mesh

Derive $C_{eff}(\tau)$ so that $\forall l \in \mathbb{R}^{d\times d}$ $\quad F_l := \sum_{ij} F_{ij} l_{ij}$

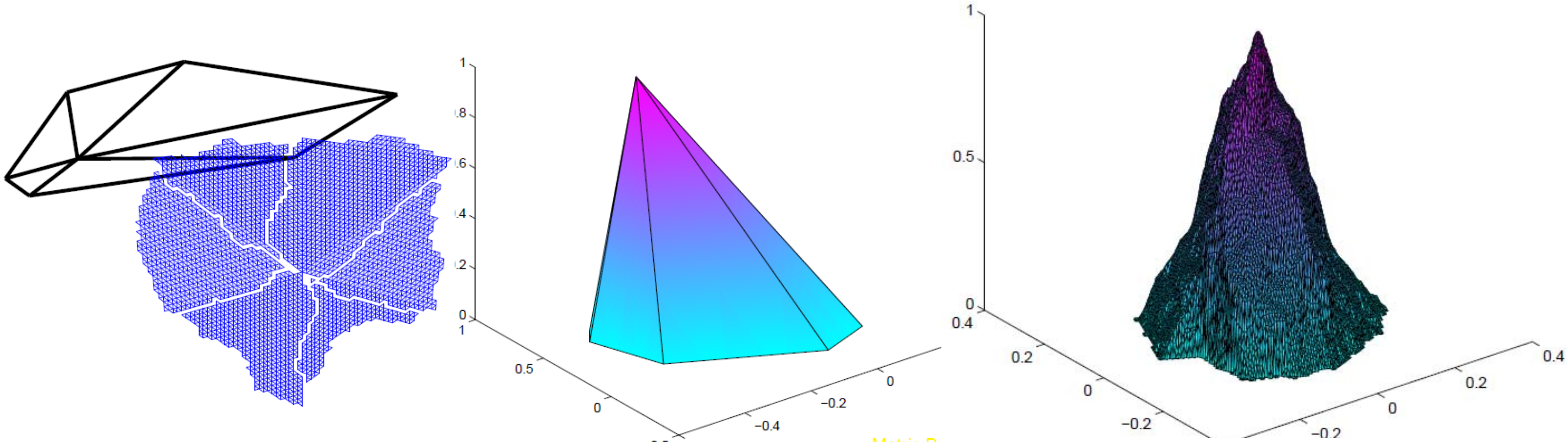
$$\int_\tau \varepsilon(F_l) : C : \varepsilon(F_l) = \int_\tau \varepsilon(\bar{F}_l) : C_{eff}(\tau) : \varepsilon(\bar{F}_l)$$

$$C_{eff}(\tau) := (\varepsilon_c(\bar{F}))^{-1} : \frac{1}{|\tau|} \int_\tau \varepsilon(F) : C : \varepsilon(F) : (\varepsilon_c(\bar{F}))^{-1}$$

[Kharevych-Muller-Owhadi-Desbrun-2009] **non-linear**

$$(1) \qquad \begin{cases} -\operatorname{div}(a\nabla u) = g & \Omega \\ u = 0 & \partial\Omega \end{cases}$$

$a_{i,j} \in L^{\infty}(\Omega)$



$\operatorname{support}(\psi_i) = F^{-1}(\operatorname{support}(\varphi_i))$

φ_i $\qquad$ $\psi_i = \varphi_i \circ F$

Can we localize the elements ψ_i to triangles of Ω_h?

[Owhadi-Zhang-2006]

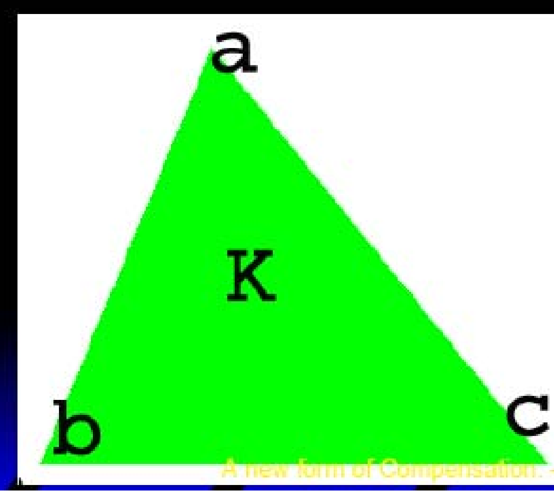
Generalization of the method II (SFEM) of [Babuška-Caloz-Osborn-1994]

If $d = 2$ and $g \in L^p(\Omega)$ then $(\nabla F)^{-1}\nabla u \in C^\alpha(\Omega)$
Because $(\nabla F)^{-1}\nabla u = (\nabla(u \circ F^{-1})) \circ F$
and $u \circ F^{-1} \in W^{2,p}(\omega)$, $F \in C^\alpha(\Omega)$, $W^{2,p} \subset C^{1,\alpha}$

$$\int_\Omega \nabla\varphi a \nabla u = \sum_{K \in \mathcal{T}_h} \int_K \nabla\varphi a \nabla F (\nabla F)^{-1} \nabla u$$

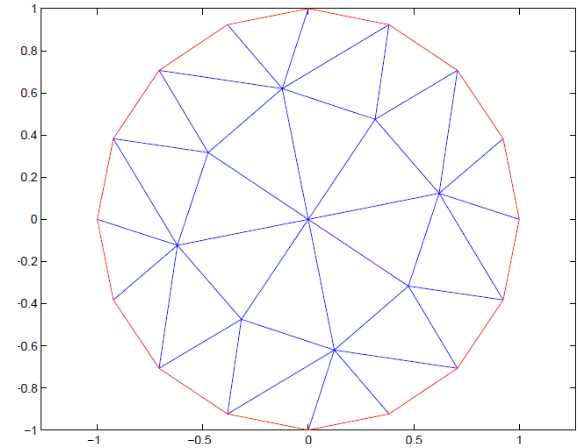
- $(\nabla F)^{-1}(x)\nabla u(x)$ almost constant within each triangle K and equal to $(\nabla F(K))^{-1}\nabla u(K)$

$$\begin{pmatrix} F(b) - F(a) \\ F(c) - F(a) \end{pmatrix}^{-1} \begin{pmatrix} u(b) - u(a) \\ u(c) - u(a) \end{pmatrix}$$



A new form of Compensation: -

Ω_h: Triangulation (tesselation of Ω) of resolution h



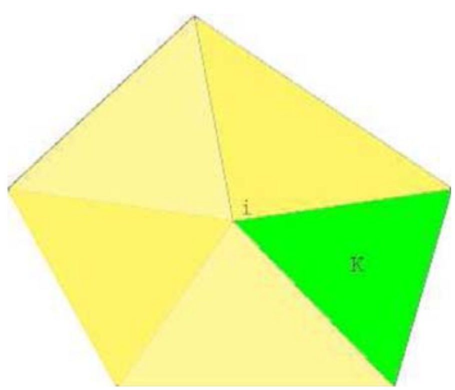
$$Z_h := \Big\{ v \in L^2(\Omega)$$

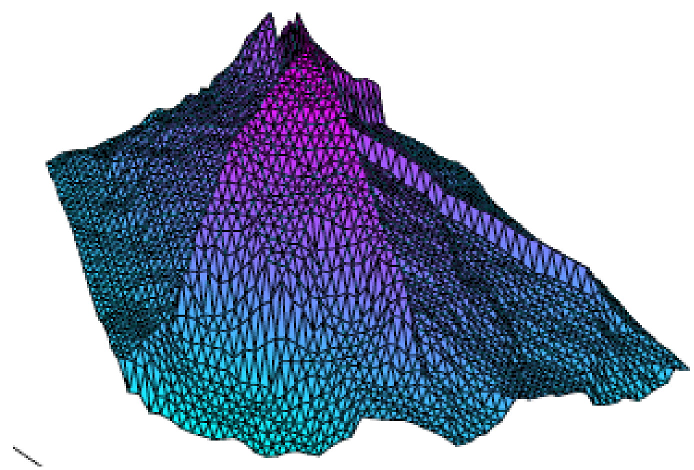
$$\forall \tau \in \Omega_h \ : \ v|_\tau \in \operatorname{span}\{1, F_1, \ldots, F_d\}$$

v is continuous at nodes of Ω_h

$v = 0$ at boundary nodes $\Big\}$

$\forall v \in Z_h$, $(\nabla F)^{-1} \nabla v$ is constant per triangle (tet)





$$B_h[v,w] := \sum_{\tau\in\Omega_h} \int_\tau (\nabla v)^T a \nabla w$$

SFEM Generalization of the method II (SFEM) of [Babuška-Caloz-Osborn-1994]

Look for $u_h \in Z_h \ : \ \forall v \in Z_h$

$$B_h[v,u_h] = \int_\Omega vg$$

Theorem [Owhadi-Zhang-2006]

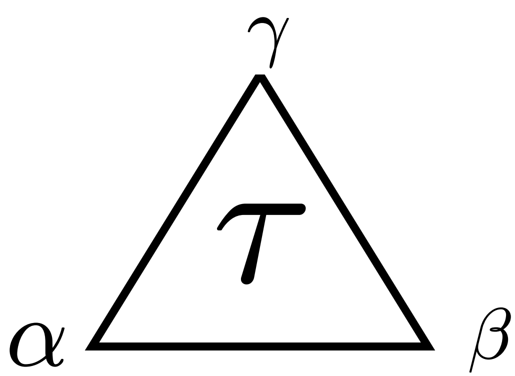
$(d=2)$ If M satisfies (CTC) the $\exists \alpha > 0$

$$\Big[B_h[u-u_h, u-u_h]\Big]^{\frac{1}{2}} \leq C h^\alpha \|g\|_{L^\infty(\Omega)}$$

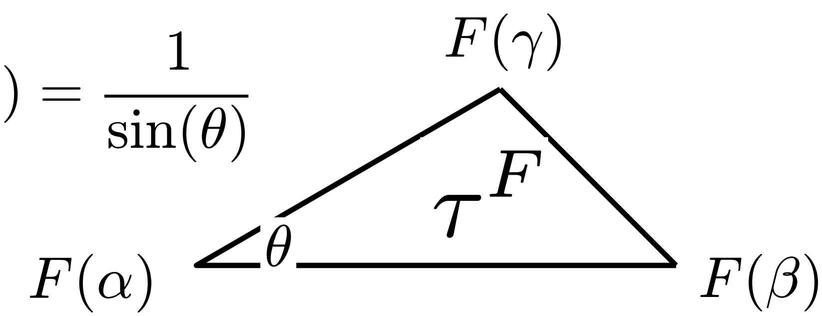
Theorem [Owhadi-Zhang-2006]

$(d=2)$ If M satisfies (CTC) the $\exists \alpha > 0$

$$\Big[B_h[u-u_h, u-u_h]\Big]^{\frac{1}{2}} \leq C h^{\alpha} \|g\|_{L^\infty(\Omega)}$$

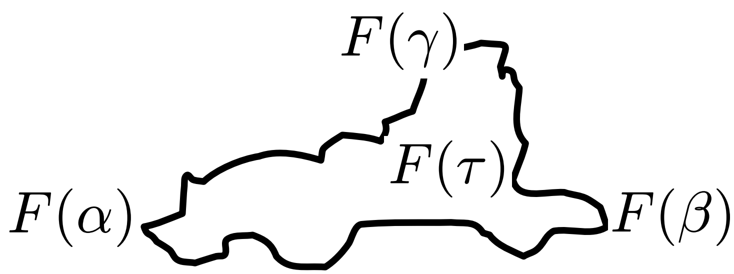


$$\eta(\tau^F) = \frac{1}{\sin(\theta)}$$



C depends on

$\eta(\tau^F)$
and $\chi^F(\tau)$



$$\chi(\tau^F) = \frac{area(\tau^F \cup F(\tau) - \tau^F \cap F(\tau))}{area(\tau^F)}$$

$\forall v \in Z_h$ $\bar{v}$: Linear interpolation of v over Ω_h

Theorem [Owhadi-Zhang-2006]

$(d=2)$ If M satisfies (CDC) the $\exists \alpha > 0$

$$\|\bar{u} - \bar{u}_h\|_{H_0^1(\Omega)} \leq C h^{\alpha} \|g\|_{L^\infty(\Omega)}$$

$\forall v \in Z_h$ $\qquad U_h[\bar{v}, \bar{u}_h] = \int_\Omega v g$

$\forall v \in Z_h \quad \bar{v}$: Linear interpolation of v over Ω_h

$$\forall v, w \in Z_h \quad B_h[v, w] = U_h[\bar{v}, \bar{w}]$$

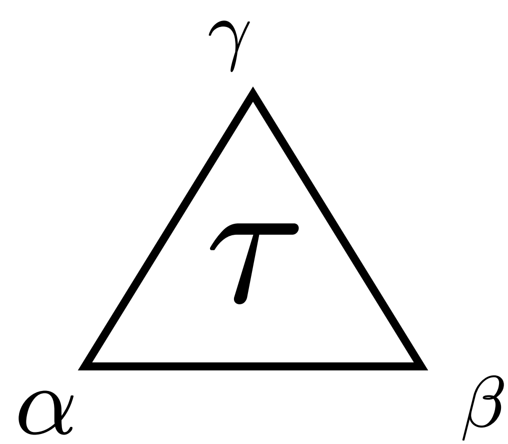
$$U_h[\bar{v}, \bar{w}] = \sum_{\tau \in \Omega_h} (\nabla \bar{v})^T(\tau) a^*(\tau) \nabla \bar{w}(\tau)$$

$$a^*(\tau) = \big(\nabla_c F(\tau)\big)^{-1,T} \big\langle (\nabla F)^T a \nabla F \big\rangle_\tau \big(\nabla_c F(\tau)\big)^{-1}$$

$a^*(\tau)$: Effective conductivity of τ

$$a^*(\tau) = \left(\nabla_c F(\tau)\right)^{-1,T} \left\langle (\nabla F)^T a \nabla F \right\rangle_\tau \left(\nabla_c F(\tau)\right)^{-1}$$

$$< M >_\tau = \frac{1}{|\tau|} \int_\tau M$$



$$\nabla_c F(\tau) := \begin{pmatrix} \beta - \alpha \\ \gamma - \alpha \end{pmatrix}^{-1} \begin{pmatrix} F(\beta) - F(\alpha) \\ F(\gamma) - F(\alpha) \end{pmatrix}.$$

$$a^*(\tau) = \big(\nabla_c F(\tau)\big)^{-1,T} \big\langle (\nabla F)^T a \nabla F \big\rangle_\tau \big(\nabla_c F(\tau)\big)^{-1}$$

If $a = a(\frac{x}{\epsilon})$ and $a(y)$ is periodic or ergodic, then

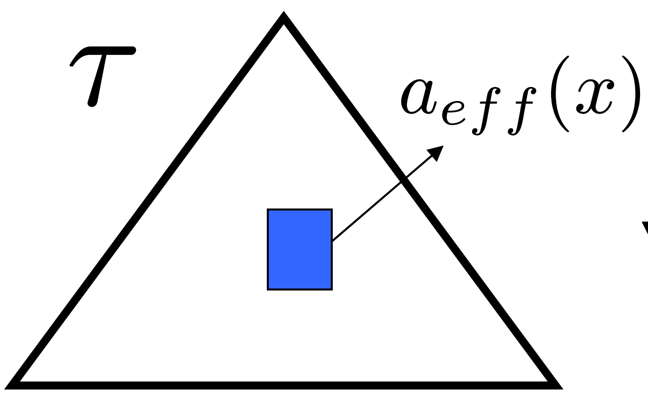
$$\nabla_c F(\tau) \xrightarrow[\epsilon \to 0]{} I_d \qquad a^*(\tau) \xrightarrow[\epsilon \to 0]{} a_{eff}$$

$a(x, y)$, slow/smooth in x, periodicin y (or ergodic +mixing)

$$a = a(x, \frac{x}{\epsilon})$$

$a(x, y)$, slow/smooth in x,

periodic in y (or ergodic +mixing)



$$u_\epsilon \xrightarrow[\epsilon \to 0]{\text{weakly in} H_0^1(\Omega)} u_0$$

$$\nabla u_\epsilon \xrightarrow[\text{two scale conv}]{} \nabla F(y) \nabla u_0(x)$$

Two scale convergence (Nguetseng and Allaire)

HMM (Heterogeneous Multiscale Method) (E-Engquist-Al...)

$a^*(\tau)$: can be recovered from a "local energy principle"

[Babuška-Sauter-2004/2008] ("recovery method")

[Shu-Babuška-Xiao-Xu-Zikatanov-2008]

Efficient solvers for high-dimensional lattice equations:
Key idea: Define a bilinear form on the continuous level which has equivaent energy as the original lattice equations.

Define $a_{eff}(\tau)$ so for a given set of "representative solutions"

a_{eff}-(coarse scale) Dirichlet energy on τ
= a-(fine scale) Dirichlet energy on τ

Define $a_{eff}(\tau)$ so that $\forall l \in \mathbb{R}^d$

$$\underbrace{(\nabla_c F_l(\tau))^T a_{eff}(\tau) \nabla_c F_l(\tau)}_{\text{Coarse Dirichlet energy of } \bar{F}_l \text{ on } \tau} = \underbrace{\frac{1}{|\tau|} \int_\tau (\nabla F_l)^T a \nabla F_l}_{\text{Dirichlet energy of } F_l \text{ on } \tau}$$

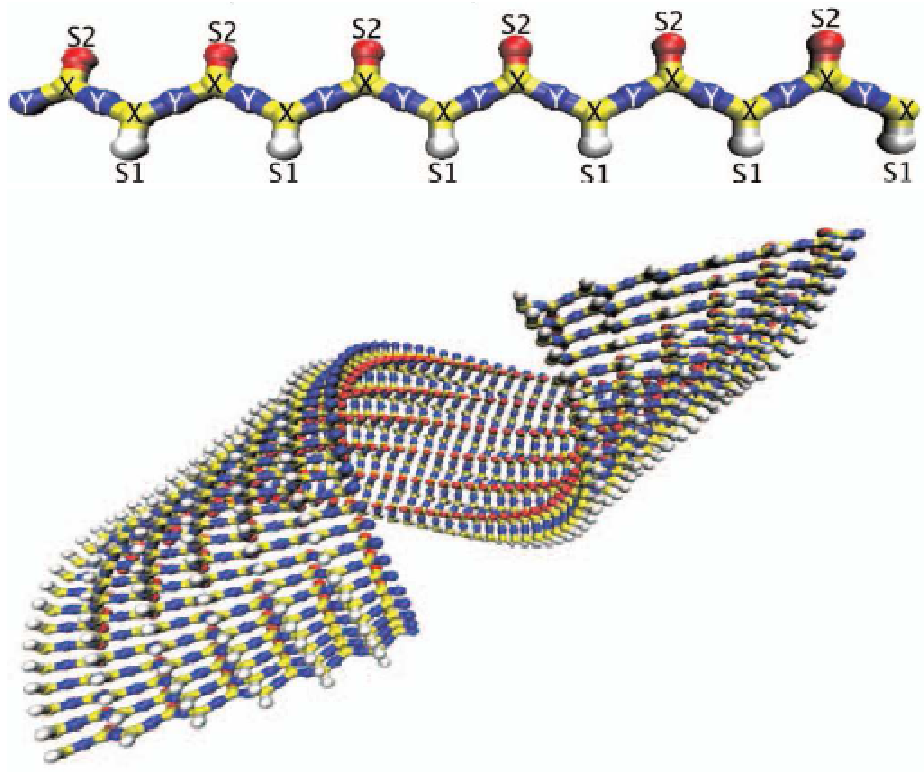
$$F_l = \sum_{i=1}^d l_i F_i(x)$$

$$\boxed{a_{eff}(\tau) = \big(\nabla_c F(\tau)\big)^{-1,T} \big\langle (\nabla F)^T a \nabla F \big\rangle_\tau \big(\nabla_c F(\tau)\big)^{-1}}$$

$$\boxed{a_{eff}(\tau) = a^*(\tau)}$$

Atomistic to continuum
Zhang-Berlyand-Federov-Owhadi

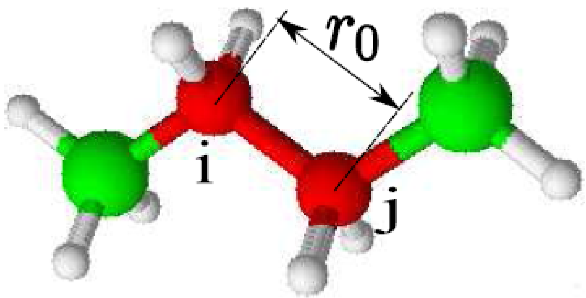
Many nanostructures and biomaterials can be achieved through molecular self-assembly characterized by



- main building block: short chain biomolecules, e.g. peptides.
- formation of a hierarchy of higher-order structures via non-covalent interactions,
- the intrinsic chirality of peptides has a major impact on their self-assembly behavior.

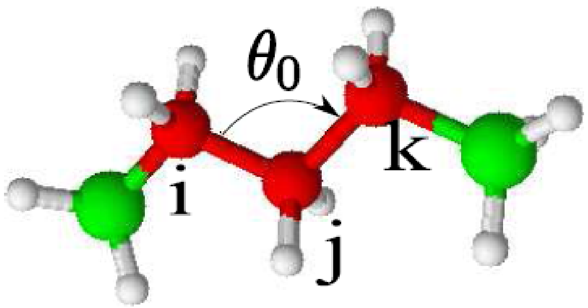
Bonded Interactions

Constrain configuration of the backbones.



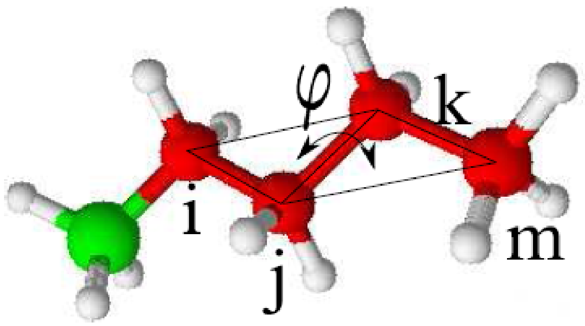
Bond Length Potential

$$U_{bond} = \frac{K_b}{2}(r - r_0)^2$$



Bond Angle Potential,

$$U_{angle} = \frac{K_\theta}{2}(\theta - \theta_{eq})^2$$



Dihedral Angle Potential

$$U_{tors} = \sum_{n=1}^{3} \{ \frac{V_n}{2}[1+(-1)^{n+1} \cos n\varphi] \}$$

quantify twist of the backbone

Non Bonded Interactions

Driving force for the self-assembly.

Lennard-Jones potentials:
model hydrophobic/hydrophilic interaction.

$$U_{LJ}(r_{ij}) = 4\varepsilon_{ij}[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}]$$

$$\begin{aligned} E &= \sum_{bonds} \frac{1}{2} K_b (r - r_0)^2 + \sum_{angles} \frac{1}{2} K_q (\theta - \theta_0)^2 \\ &+ \sum_{dihedrals} \sum_{n=1}^{3} \{ \frac{V_n}{2} [1 + (-1)^{n+1} \cos n\varphi] \} \\ &+ \sum_{i} \sum_{j>i} \{ 4\epsilon_{ij} [(\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}] \} \end{aligned}$$

Coulomb potentials:
long range interaction

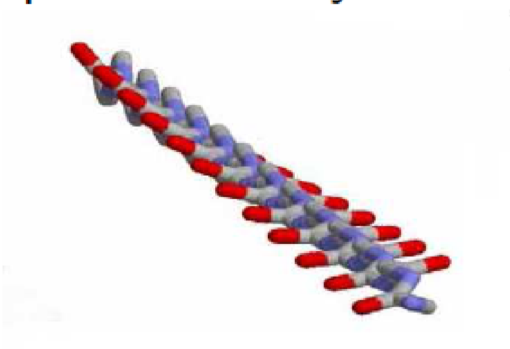
$$U_{(}r) = \frac{1}{4\pi\epsilon\epsilon_0} \frac{q_i q_j}{r_{ij}}$$

Molecular simulation can be done with the knowledge of potential function.

Atomistic origin of chirality

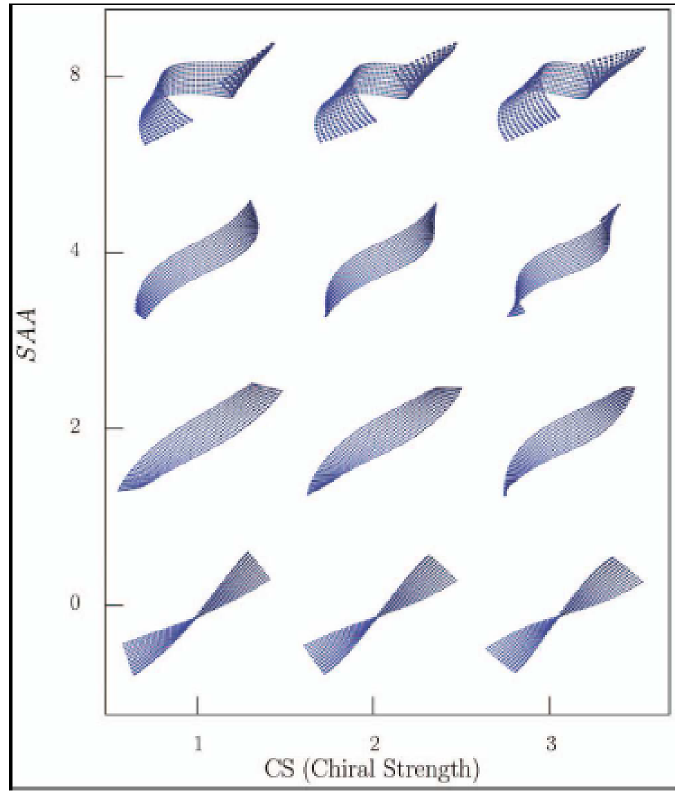
The chirality of the β-sheet self-assembly can be attributed to the interplay between chirality and chemical assymetry.

- CS: twist in the backbone, quantified by the dihedral angle.



- SAA: assymetry of solute-solvent interaction for different side chains, quantified by the interaction stength ε of Lennard-Jones interaction.

From helicoid to cylindrical



G. BellesiaG, M.V. Fedorov, Y.A. Kuznetsov, E.G. Timoshenko, J. Chem. Phys. 128, 195105, 2008

Atomistic to continuum approach

Existing approach for thin elastic structures
– film, sheet, tape, membrane, shell...

- Friesecke and James (2000): derive Cosserat membrane theory from multiple atomistic layers.
- Bernd Schmidt (2006): rigorous justification of Friesecke and James' result using Γ-convergence.
- Arroyo and Belyschko (2003): exponential Cauchy-Born rule for one-atom thick crystalline sheets.
- Yang and Weinan E (2006): local Cauchy Born rule, incorporates curvature effect to derive continuum model with finite deformation.

Fully nonlinear, membrane and bending modes tightly coupled.
Crystalline order, evaluation requires inner displacement relaxation.

Atomistic to continuum modeling: Energy Matching

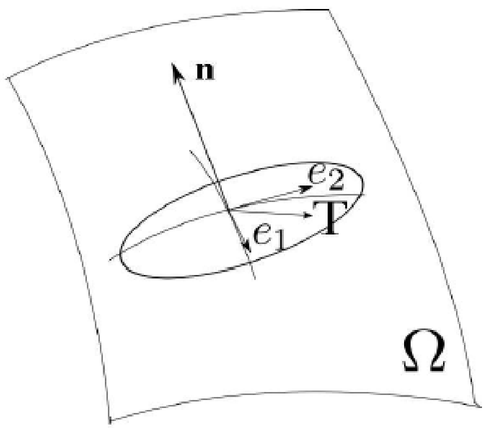
Enforce that the elastic energy of the continuum model matches the total energy of the atomistic model for all possible displacement fields.

$$E_{el} = E_{atom}$$

If the continuum model is inhomogeneous, subdivide the domain into subdomains which the material parameters are homogeneous, and enforce the equality within each subdomain,

Continuum Elastic Energy

Thin Shell Theory:



Assumption:

- Kirchhoff-Love
- (Quasi-)Inextensible.

n: a unit normal to Ω,
T: a unit tangent to Ω,
$S(\mathbf{T}) = -\partial_{\mathbf{T}}\mathbf{n}$: the shape operator of **n** acting on **T** .

Bending energy for a **Kirchhoff-Love inextensible** shell of thickness $2h$:

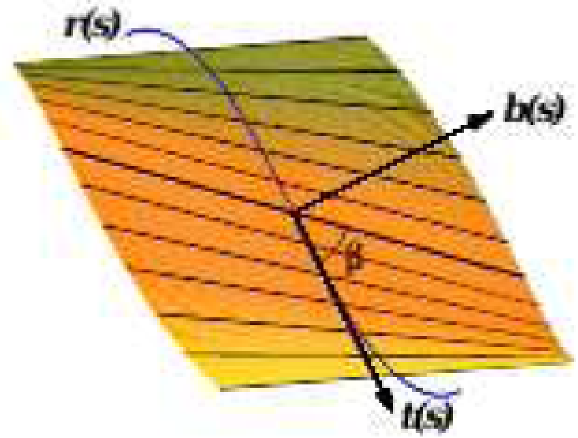
$$\begin{aligned} U &= \frac{D}{2}\int\int_{\Omega}[\nu(\mathrm{tr}(\Delta S))^2 + (1-\nu)\mathrm{tr}((\Delta S)^2)]d\sigma \\ &= D\int\int_{\Omega}[(1+\nu)(H-H_0)^2 + (1-\nu)((\Delta A)^2 + 4AA_0\sin^2\theta)]d\sigma \end{aligned}$$

$A = \sqrt{H^2 - G}$, H mean curvature, G Gaussian curvature, θ is the angle between deformed and undeformed principal axes,

$\boxed{D = 2h^3E/[3(1-\nu^2)]}$, E Young's modulus, ν Poisson's ratio.

Continuum Elastic Energy

For developable surfaces,
$H = A = \kappa_1/2$, $G = 0$, κ is the curvature of the centerline, η is the torsion,



$$U = Dw \int_0^L g(k, \eta, \eta')ds + \text{const}$$

If the centerline has intrinsic curvature κ_0 and intrisic torsion τ_0,

$$U_F = \int_0^L [\frac{B}{2}(\kappa - \kappa_0)^2 + \frac{C}{2}(\tau - \tau_0)^2]ds$$

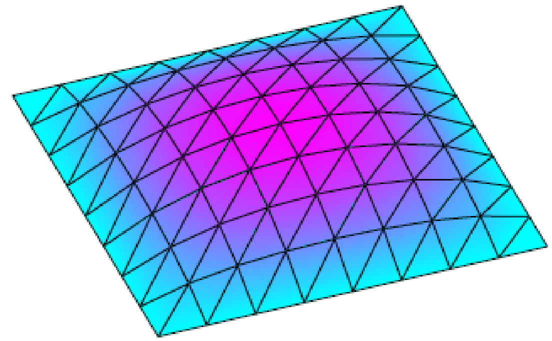
Another variation of the shell energy functional, is known in membrane physics as Canham-Helfrich energy

$$\int k(H - H_0)^2 dS$$

Discrete Elastic Energy

To simplify, we focus on the energy functional $\int_{\Omega} k(H - H_0)^2 dS$.

The atomistic lattice $\longrightarrow$ a triangulated piecewise linear surface.
Problem: Define geometric quantities, curvatures, normal, ... for triangulated surface.



Use Discrete geometry operator (Schröder, Desbrun, Zorin et.al)
For example, the normal mean curvature vector $H\mathbf{n}$ at a vertex P can be defined as

$$H(P)\mathbf{n}(P) = \frac{1}{\mathcal{A}_{\mathcal{P}}} \int_{\mathcal{A}_{\mathcal{P}}} H\mathbf{n}dS = -\frac{1}{2\mathcal{A}_{\mathcal{P}}} \int_{\mathcal{A}_{\mathcal{P}}} \Delta \mathbf{x} dS$$

where $\mathcal{A}_{\mathcal{P}}$ is a properly chosen nonoverlap area around P.
The discrete bending energy can therefore expressed as a summation over verticies

$$E_B = \sum (H(P) - H_0(P))^2 \text{area}(\mathcal{A}(P))$$

Discrete Elastic Energy

Problem: finding the minimizer of the elastic energy with the **inextensible** constrain and proper boundary conditions.
Total elastic energy = membrane energy + bending energy

$$E_{el} = E_M + k_B E_B$$

The constrain is enforced by penalize on the membrane energy.
Membrane energy E_M is composed of stretching and shear mode

$$E_M = k_L E_L + K_A E_A$$

stretching energy measures local change in length

$$E_L = \sum_e (1 - \|e\|/\|e_0\|)^2 \|e_0\|$$

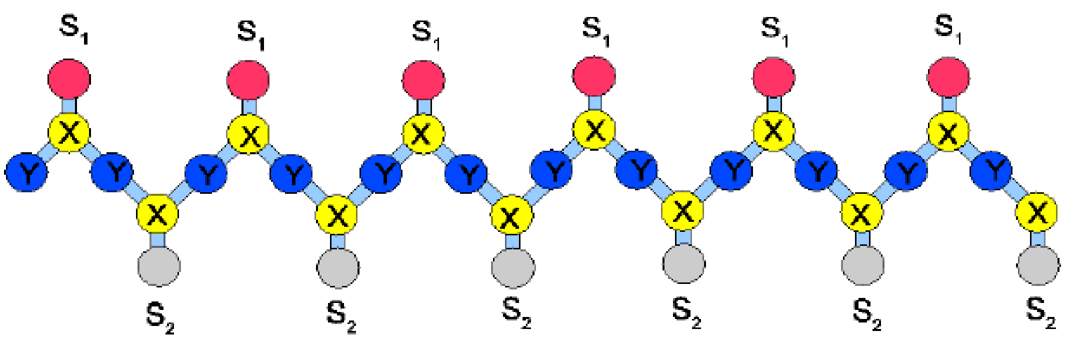
Shearing energy measures local change in area

$$E_A = \sum_A (1 - \|A\|/\|A_0\|)^2 \|A_0\|$$

In the implementation, we choose larger and larger stiffness constant k_L and k_A to enforce the **quasi-inextensible** constrain.

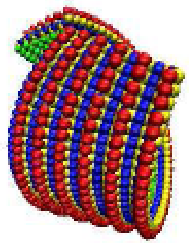
Set Up of the Problem

$M = 60$ $\beta-$peptides are placed into a planar, parallel arrangement, forming a flat tape.
We run atomistic simulation with respect to both the **chiral strength** (CS) and the **side chain asymmetry** (SAA) for the Lennard-Jones interaction of side chain pairs $S_2 - S_2$ and $S_1 - S1$, $\boxed{\text{SAA} = \frac{\varepsilon_{S_1}}{\varepsilon_{S_2}}}$.

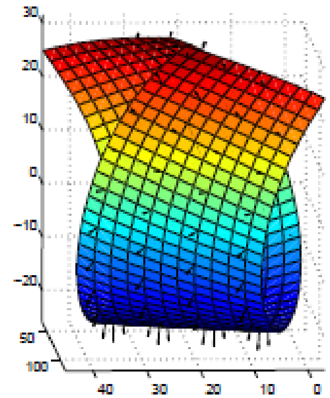


A single amino acid is represented by three beads (X and Y for the backbone and S_1 or S_2 as the side chain).
Bead X: $C_\alpha H - C'O$ (Carboxyl) group   Bead Y: NH (amino) group.

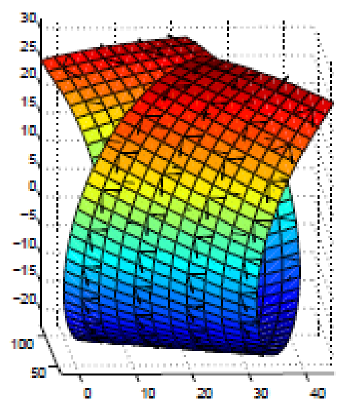
Results



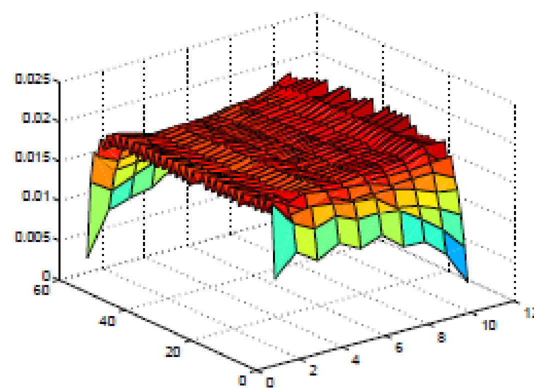
(a) Atomistic configuration, SAA=5, CS=1



(b) Mean curvature vector $\mathsf{K}(x)$

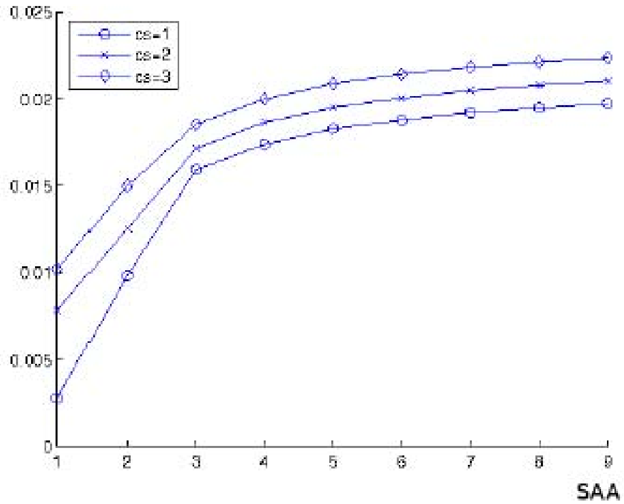


(c) Principal directions e_1 and e_2

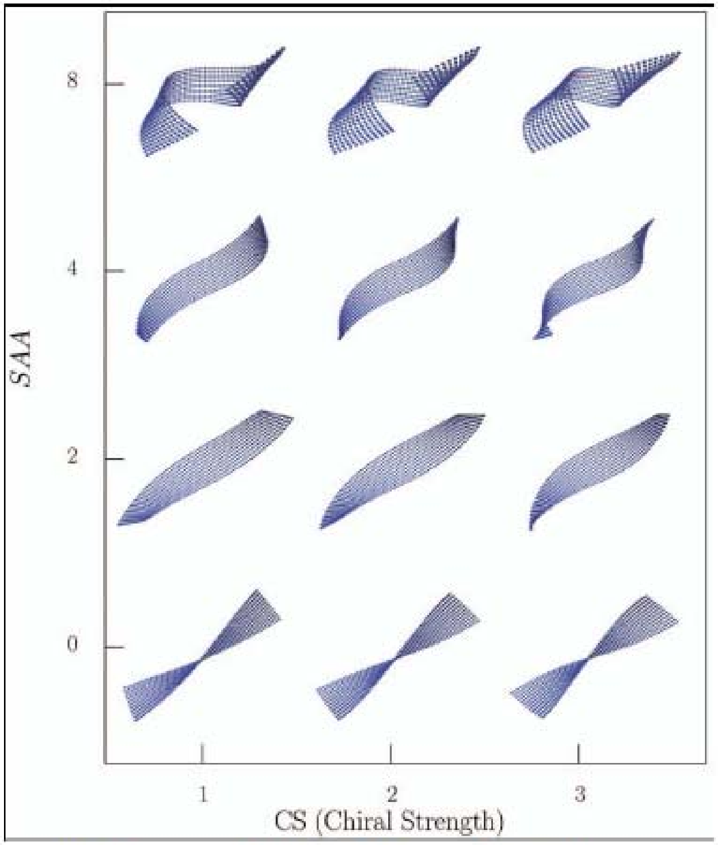


(d) mean curvature of the atomistic tape

Mean Curvature vs atomistic parameters

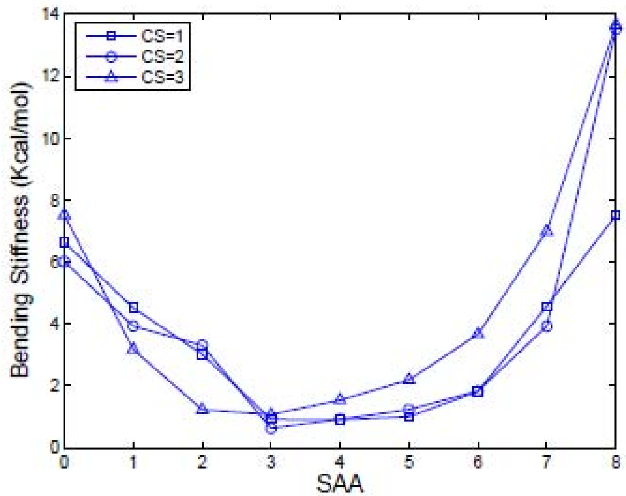


averaged mean curvature with respect to side chain assymetry (SAA) and backbone twist (CS).

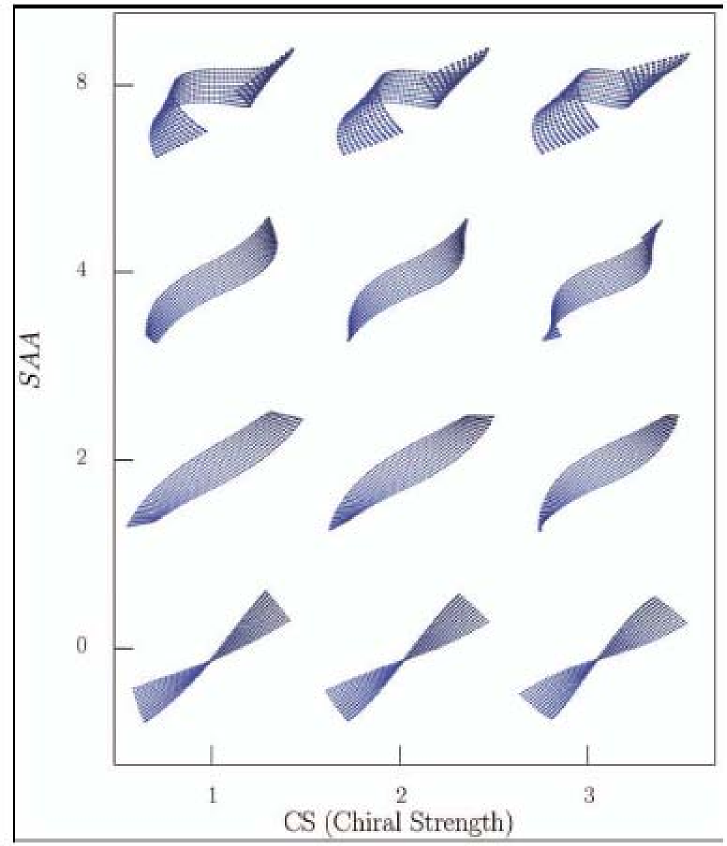


G. BellesiaG, M.V. Fedorov, Y.A. Kuznetsov, E.G. Timoshenko, J. Chem. Phys. 128, 195105, 2008

Mean Curvature vs atomistic parameters

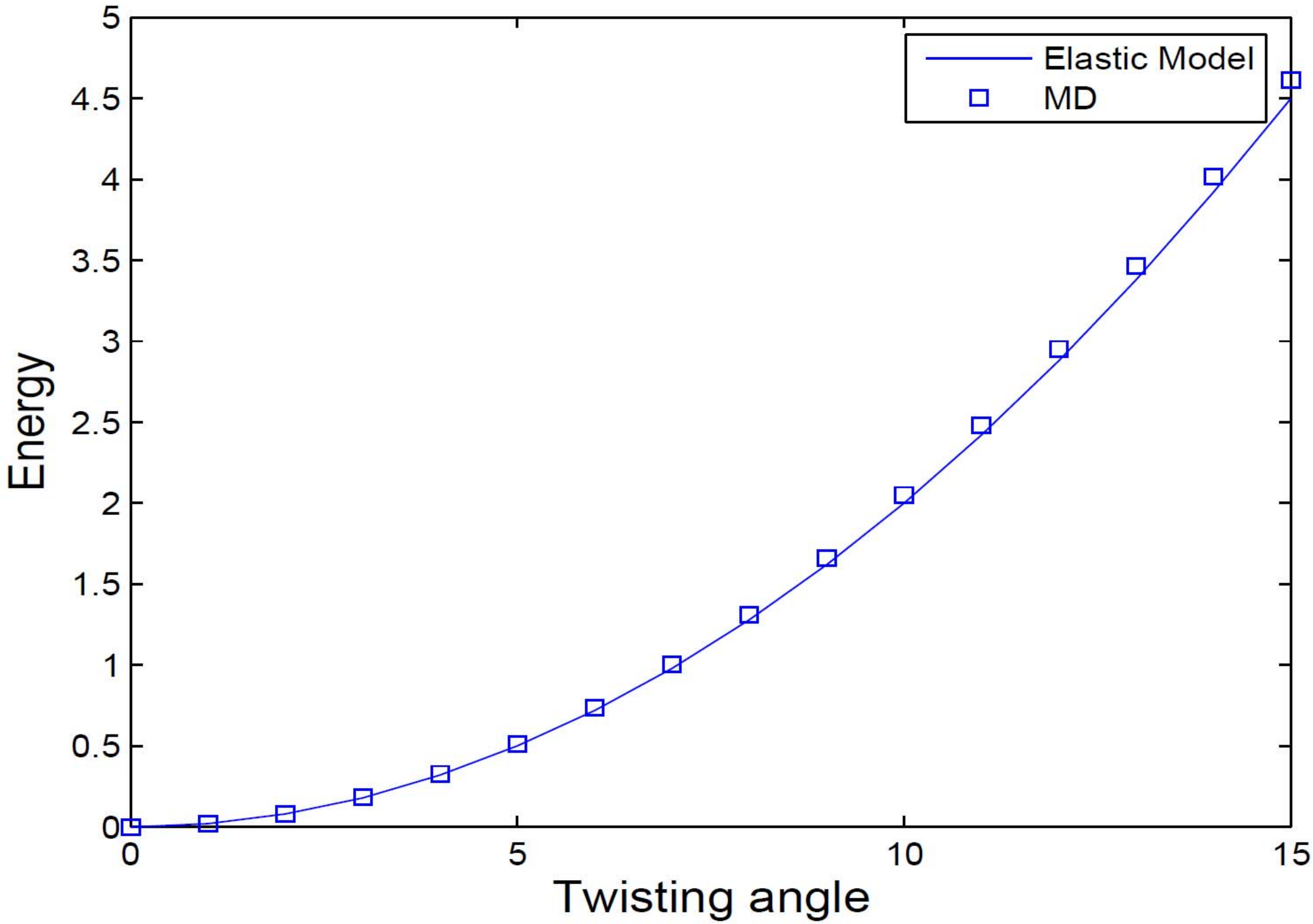


bending stiffness with respect to side chain assymetry (SAA) and backbone twist (CS).



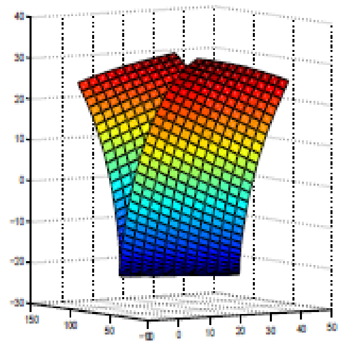
G. BellesiaG, M.V. Fedorov, Y.A. Kuznetsov, E.G. Timoshenko, J. Chem. Phys. 128, 195105, 2008

Energy vs Twist

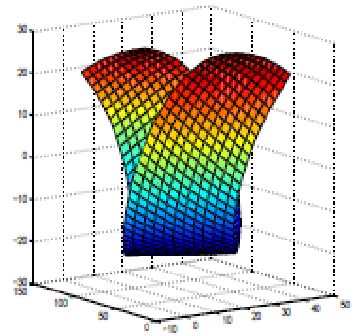


Energy vs Twist

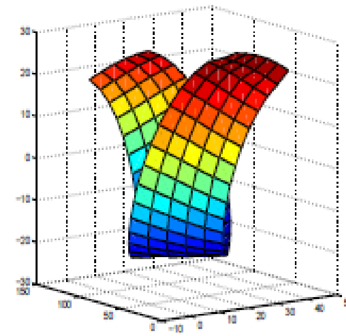
Two shorter sides are twisted from the equilibrium configuration.



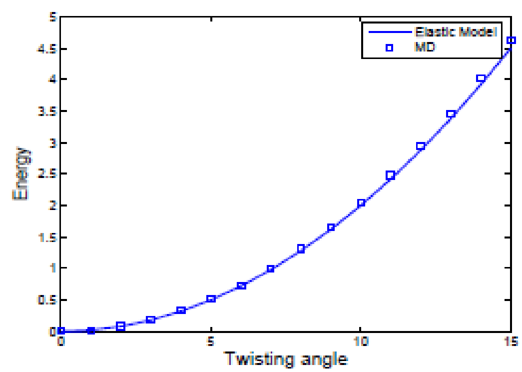
(a) reference configuration, MD



(b) deformed configuration, MD



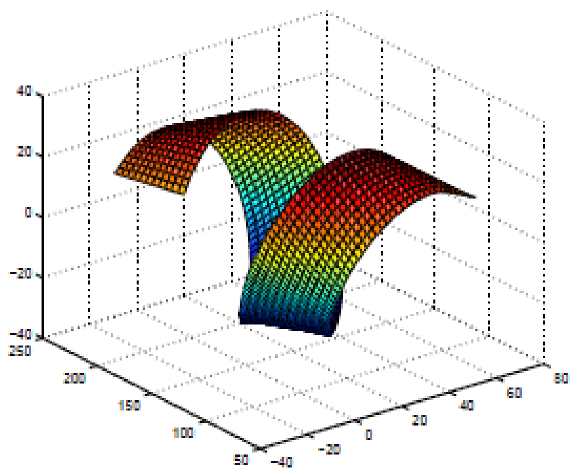
(c) deformed configuration, elastic



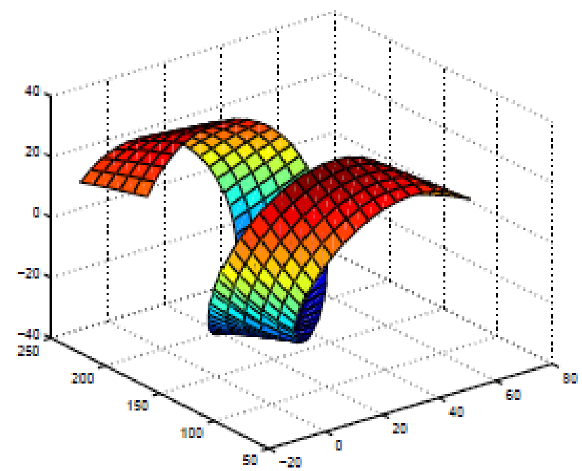
(d) Energy vs. Twist Angle

Configuration of Elongated Tape

Using the parameters of $M = 60$ peptides to calculate the equilibrium configuration for $M = 120$ peptides.

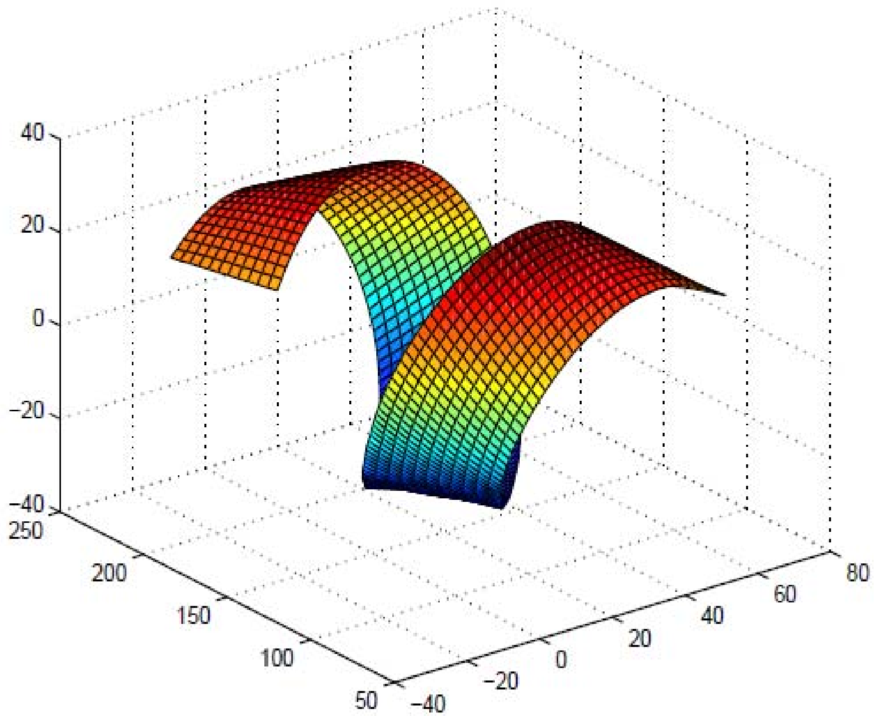


(e) MD simulation

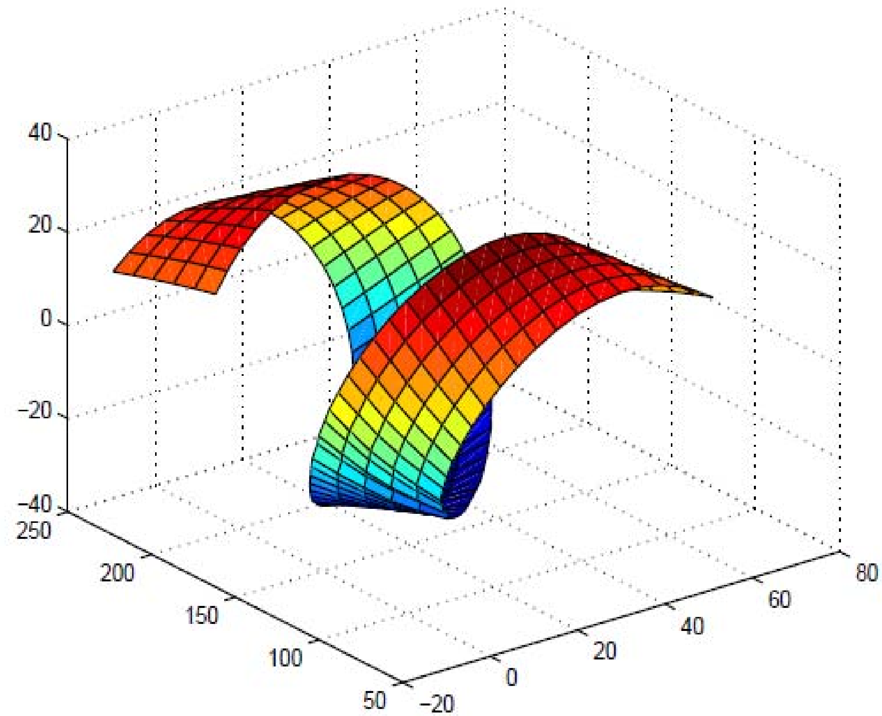


(f) Elastic model

Configuration of Elongated Tape



(e) MD simulation



(f) Elastic model