Bayesian Numerical Homogenization

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- H. Owhadi, Bayesian Numerical Homogenization (2014). arXiv:1406.6668

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Link between Bayesian Inference and Numerical Analysis

P. Diaconis (1988). Bayesian numerical analysis.

J. E. H. Shaw (1988). A quasirandom approach to integration in Bayesian statistics.

Henri Poincaré (1896). Calcul des probabilités.

$$f(x) = \exp\left(\cosh\left(\frac{x^2+\sin(x)}{3+\cos(x^3)}\right)\right)$$

Compute

$$\int_0^1 f(x)\,dx$$

Numerical Analysis Approach

Find a good quadrature rule for the numerical integration of f

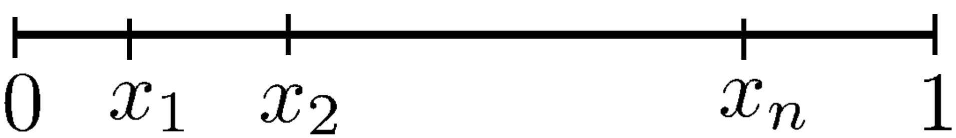
$$f(x) = \exp\left(\cosh\left(\frac{x^2 + \sin(x)}{3 + \cos(x^3)} \right) \right)$$

Compute

$$\int_0^1 f(x)\, dx$$

Bayesian Approach

- Put a prior in $\mathcal{C}([0,1])$
- Calculate f at $x_1, \ldots, x_n$



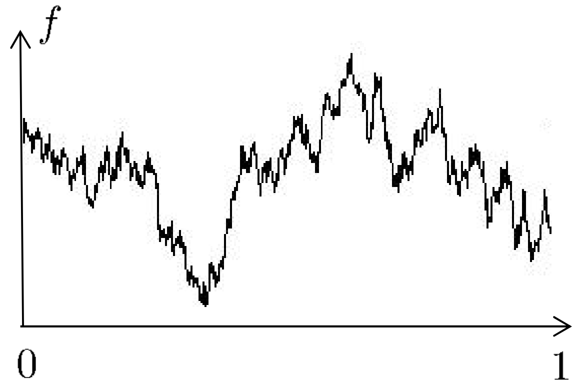
- Compute

$$\mathbb{E}\left[\int_0^1 f(x)\, dx \,\middle|\, f(x_1), \ldots, f(x_n) \right]$$

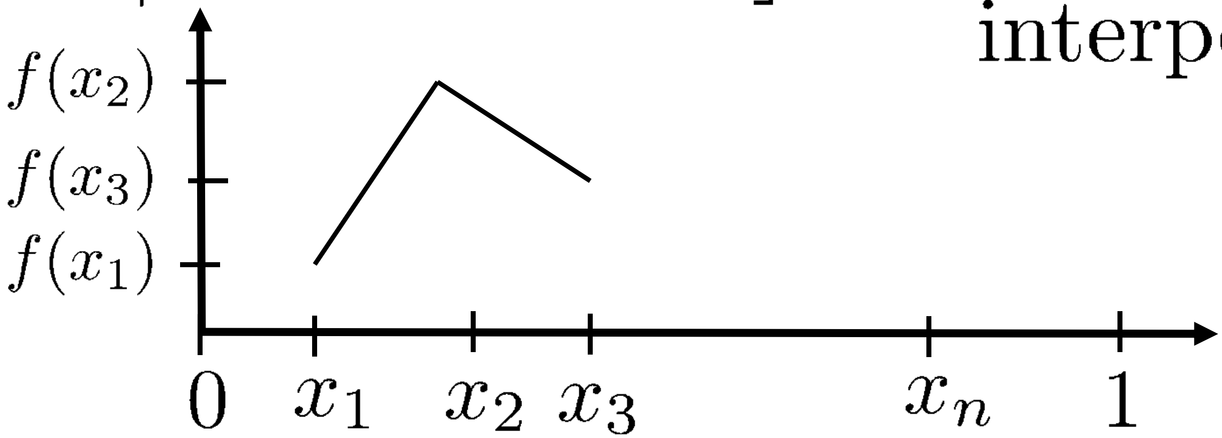
E.g.

Assume $f(t) = \xi + B_t$

$\xi \sim \mathcal{N}(0,1)$, B_t: B.M.



$\mathbb{E}\left[f(x) \,\middle|\, f(x_1), \ldots, f(x_n)\right]$ ➡ Piecewise linear interpolation of f

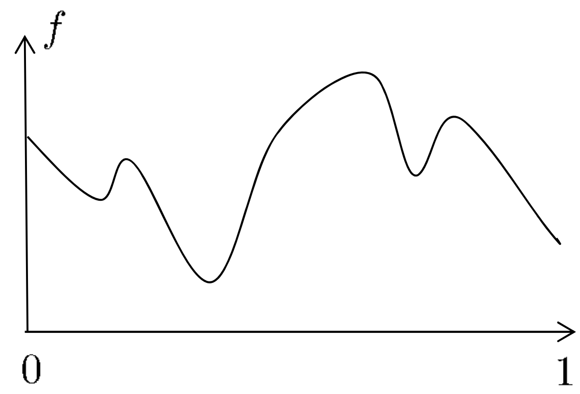


$\mathbb{E}\left[\int_0^1 f(x)\,dx \,\middle|\, f(x_1), \ldots, f(x_n)\right]$ ➡ Trapezoidal quadrature rule

E.g.

Assume $f(t) = \xi + \int_0^t B_s \, ds$

$\xi \sim \mathcal{N}(0,1)$ (↑ $\mathcal{N}(0,1)$), B_s ↑ B.M.



$$\mathbb{E}\Big[f(x)\Big|f(x_1),\ldots,f(x_n)\Big]$$ ➡ Cubic spline interpolant

E.g.

Integrate B.M. k times ➡ Splines of order $2k+1$

Hagan (1991). Bayes-Hermite quadrature

Q Similar link between numerical homogenization and Bayesian Inference?

Bayesian Numerical Homogenization

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

$\Omega \subset \mathbb{R}^d$ $\quad \partial\Omega$ is piec. Lip.

a unif. ell. $\quad a_{i,j} \in L^\infty(\Omega)$

$d \leq 3$

We want to homogenize (1)

We need $g \in L^2(\Omega)$

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

$$g \longrightarrow u$$

$$\mathcal{H}^{-1}(\Omega) \longrightarrow \mathcal{H}_0^1(\Omega)$$

$$L^2(\Omega) \longrightarrow V$$

$$V \subset\subset \mathcal{H}_0^1(\Omega) \qquad V \sim \mathcal{H}^2(\Omega)$$

Q: How to approximate V with a finite dimensional space?

Numerical Homogenization Approach

Work hard to find good basis functions

Harmonic Coordinates Babuska, Caloz, Osborn, 1994

Kozlov, 1979 Allaire Brizzi 2005; Owhadi, Zhang 2005

MsFEM [Hou, Wu: 1997]; [Efendiev, Hou, Wu: 1999]

[Fish - Wagiman, 1993] [Gloria 2010] Arbogast, 2011: Mixed MsFEM

Projection based method Nolen, Papanicolaou, Pironneau, 2008

HMM

Engquist, E, Abdulle, Runborg, Schwab, et Al. 2003-...

Flux norm Berlyand, Owhadi 2010; Symes 2012

Localization [Chu-Graham-Hou-2010] (limited inclusions)

[Efendiev-Galvis-Wu-2010] (limited inclusions or mask)

[Babuska-Lipton 2010] (local boundary eigenvectors)

[Owhadi-Zhang 2011] (localized transfer property)

[Malqvist-Peterseim 2012] Volume averaged interpolation

Bayesian Approach

Where do we put the prior?

$$-\operatorname{div}(a\nabla u) = g$$

On u ➡ The noise doesn't see the microstructure

On a ➡ PCA community, things get more complex

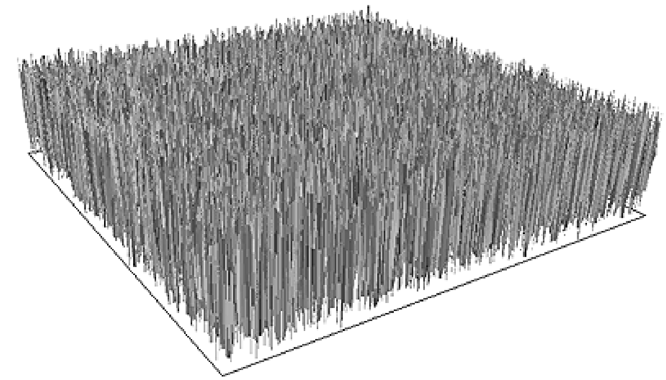
Proposition

➡ Put a prior on g

➡ Compute $\mathbb{E}\big[u(x)\big|\text{finite no of observations}\big]$

E.g. Replace g by ξ

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



ξ: White noise

Gaussian field with covariance function $\Lambda(x,y) = \delta(x-y)$

$\Leftrightarrow$ $\forall f \in L^2(\Omega)$, $\int_\Omega f(x)\xi(x)\,dx$ is $\mathcal{N}\left(0, \|f\|^2_{L^2(\Omega)}\right)$

Then a.s. (with proba 1)

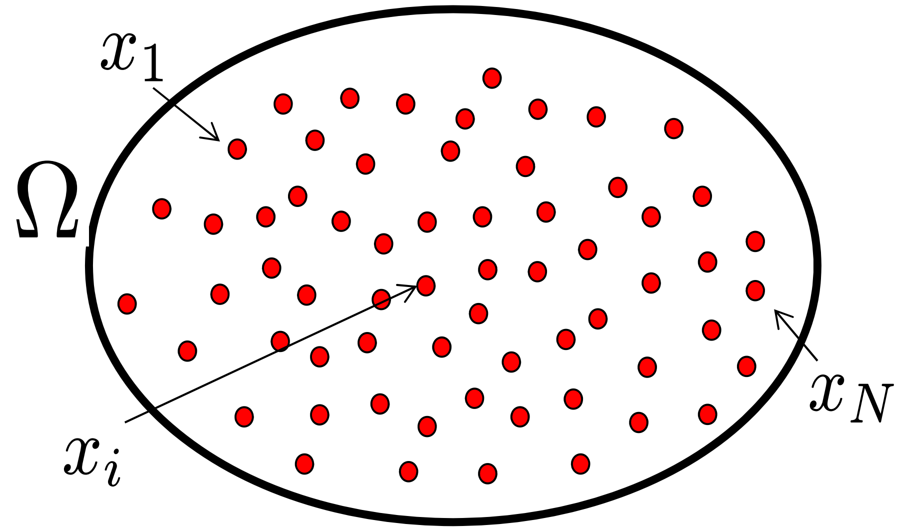
$\operatorname{div}(a\nabla u) \in L^2(\Omega)$ $\xRightarrow[\text{Stampacchia 1965}]{}$ $u \in C^\alpha(\Omega)$

$d \leq 3$

$\Longrightarrow$ u has well defined point values

Let

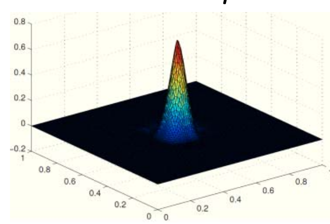
$x_1, \ldots, x_N \in \Omega$



Theorem

$$\mathbb{E}\Big[u(x)\Big|u(x_1),\ldots,u(x_N)\Big] = \sum_{i=1}^{N} u(x_i)\Phi_i(x)$$

$a = I_d$ ⟺ ϕ_i: Polyharmonic splines



[Harder-Desmarais, 1972]

[Duchon 1976, 1977,1978]

$a_{i,j} \in L^\infty(\Omega)$ ⟺ ϕ_i: Rough Polyharmonic splines

[Owhadi-Zhang-Berlyand 2013]

Link between Bayesian Inference & Numerical Homogenization

- Generic

- Guiding principle for coarse graining of multi-scale systems

1. Put a prior on deg. of freed. (source/force terms)
2. Select a finite no of coarse variables
3. Compute posterior value of state system conditionned on coarse variables

- Use it to indentify bases for arbitrary linear integro-differ. equations

General setup

(2) $$\begin{cases} \mathcal{L}u = g, & x \in \Omega, \\ \mathcal{B}u = 0, & x \in \partial\Omega, \end{cases}$$

$\mathcal{L}, \mathcal{B}$: Linear integro-differential operators on Ω & $\partial\Omega$

$$\mathcal{H}(\Omega) \longrightarrow \mathcal{H}_{\mathcal{L}}(\Omega) \times \mathcal{H}_{\mathcal{B}}(\Omega)$$

$$\mathcal{H}_{\mathcal{L}}(\Omega) \cup L^2(\Omega)$$

E.g.

$$\mathcal{L}u = -\operatorname{div}(a\nabla u) \qquad \mathcal{B}(u) = u$$

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

$$\mathcal{H}(\Omega) = \mathcal{H}^1(\Omega)$$
$$\mathcal{H}_{\mathcal{L}}(\Omega) = \mathcal{H}^{-1}(\Omega)$$

Bayesian Numerical Homogenization

Replace g by a stochastic field ξ

$$g \in L^2(\Omega) \Longleftrightarrow \xi\text{: white noise}$$

$$g \in H^{\pm s}(\Omega) \Longleftrightarrow \xi = \Delta^{\mp s/2}\text{white noise}$$

Consider

(3)

$$\begin{cases} \mathcal{L}u = \xi, & x \in \Omega, \\ \mathcal{B}u = 0, & x \in \partial\Omega, \end{cases}$$

$g \in L^2(\Omega)$ ⟷ ξ: white noise

Theorem The solution of (3) is a Gaussian field with covaraince function

$$\begin{aligned}\Gamma(x,y) &:= \mathbb{E}\big[u(x)u(y)\big] \\ &= \int_{\Omega^2} G(x,z)G(y,z)\,dz\end{aligned}$$

where
$$\begin{cases} \mathcal{L}G(x,z) = \delta(x-z), & x \in \Omega, \\ \mathcal{B}G(x,z) = 0, & x \in \partial\Omega, \end{cases}$$

Rk $\mathcal{L}^*\mathcal{L}\,\Gamma(x,y) = \delta(x-y)$

$$g \in L^2(\Omega) \quad \Longleftrightarrow \quad \xi\text{: white noise}$$

Theorem The solution of (3) is a Gaussian field with covaraince function

$$\begin{aligned}\Gamma(x,y) &:= \mathbb{E}\big[u(x)u(y)\big] \\ &= \int_{\Omega^2} G(x,z)G(y,z)\,dz\end{aligned}$$

where
$$\begin{cases} \mathcal{L}G(x,z) = \delta(x-z), & x \in \Omega, \\ \mathcal{B}G(x,z) = 0, & x \in \partial\Omega, \end{cases}$$

Rk $$\mathcal{L}^*\mathcal{L}\,\Gamma(x,y) = \delta(x-y)$$

We observe

$$\int_\Omega u(x)\Psi_i(x)\,dx \qquad\qquad i = 1,\ldots,N$$

$\Psi_1,\ldots,\Psi_N$: N linearly independent generalized functions on Ω.

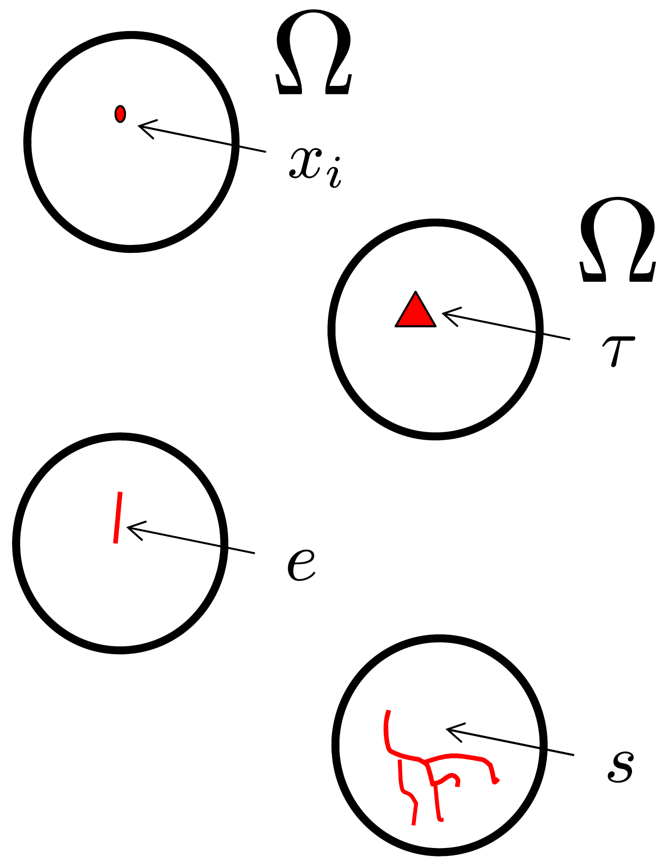
E.g.

$$\Psi_i(x) = \delta(x - x_i)$$

$$\Psi_i(x) = \mathcal{X}_\tau(x)$$

$$\Psi_i(x) = \mathcal{X}_e(x)$$

$$\Psi_i(x) = \mathcal{X}_s(x)$$



Assume $\forall i$

$$\int_{\Omega^2} \Psi_i(x)\Gamma(x,y)\Psi_i(y)\,dx\,dy < \infty$$

$$\Updownarrow$$

$$Z := \left(\int_\Omega u(x)\Psi_1(x)\,dx, \ldots, \int_\Omega u(x)\Psi_N(x)\,dx\right)$$

is a Gaussian vector with covariance matrix Θ

$$\Theta_{i,j} := \int_{\Omega^2} \Psi_i(x)\Gamma(x,y)\Psi_j(y)\,dx\,dy$$

Lemma Θ is symmetric,positive definite.

$$\forall l \in \mathbb{R}^N,\ l^T\Theta l = \|v\|^2_{L^2(\Omega)}$$

$$\mathcal{L}v = \sum_{j=1}^N l_j\Psi_j \text{ in } \Omega, \text{ and } \mathcal{B}v = 0 \text{ on } \partial\Omega$$

Theorem

$$\mathbb{E}\Big[u(x)\Big|Z\Big] = \sum_{i=1}^N Z_i \Phi_i(x)$$

with

$$Z_i = \int_\Omega u(y)\Psi_i(y)\,dy$$

and

$$\Phi_i(x) = \sum_{j=1}^N \Theta^{-1}_{i,j} \int_\Omega \Gamma(x,y)\Psi_j(y)\,dy$$

Furthermore

$$u(x) \text{ cond. on } Z \text{ is } \mathcal{N}\Big(\mathbb{E}\big[u(x)\big|Z\big], \sigma^2(x)\Big)$$

$$\sigma^2(x) = \Gamma(x,x) - \sum_{i,j=1}^N \Theta^{-1}_{i,j} \int_\Omega \Gamma(x,y)\Psi_i(y)\,dy \int_\Omega \Gamma(x,y)\Psi_j(y)\,dy$$

u sol. of **(2)** $\begin{cases} \mathcal{L}u = g, & x \in \Omega, \\ \mathcal{B}u = 0, & x \in \partial\Omega, \end{cases}$

Theorem Assume $\Gamma(x,x) < \infty$

$$\left| u(x) - \sum_{i=1}^{N} \Phi_i(x) \int_\Omega u(y)\Psi_i(y)\, dy \right| \leq \sigma(x) \|g\|_{L^2(\Omega)}$$

E.g. Assume $\Psi_i(x) = \delta(x - x_i)$

$$\Phi_i(x) = \sum_{j=1}^{N} \Theta^{-1}_{i,j} \int_\Omega \Gamma(x, x_j)$$

$$\Theta_{i,j} := \Gamma(x_i, x_j)$$

$$\left| u(x) - \sum_{i=1}^{N} u(x_i)\Phi_i(x) \right| \leq \sigma(x) \|g\|_{L^2(\Omega)}$$

Reproducing Kernel Hilbert Space

Define

$$V := \left\{ \Phi \in \mathcal{H}(\Omega) \middle| \mathcal{L}\Phi \in L^2(\Omega) \text{ and } \mathcal{B}\Phi = 0 \text{ on } \partial\Omega \right\}$$

$u, v \in V$

$$\langle u, v \rangle := \int_\Omega \big(\mathcal{L}u(x)\big)\big(\mathcal{L}v(x)\big)\, dx$$

$$\|v\|_V := \langle v, v \rangle^{\frac{1}{2}}$$

Theorem (V, Γ) forms a R.K.H.S.

$$\big\langle v, \Gamma(\cdot, x) \big\rangle = v(x)$$

$$\big|v(x)\big| \leq \big(\Gamma(x, x)\big)^{\frac{1}{2}} \|v\|_V$$

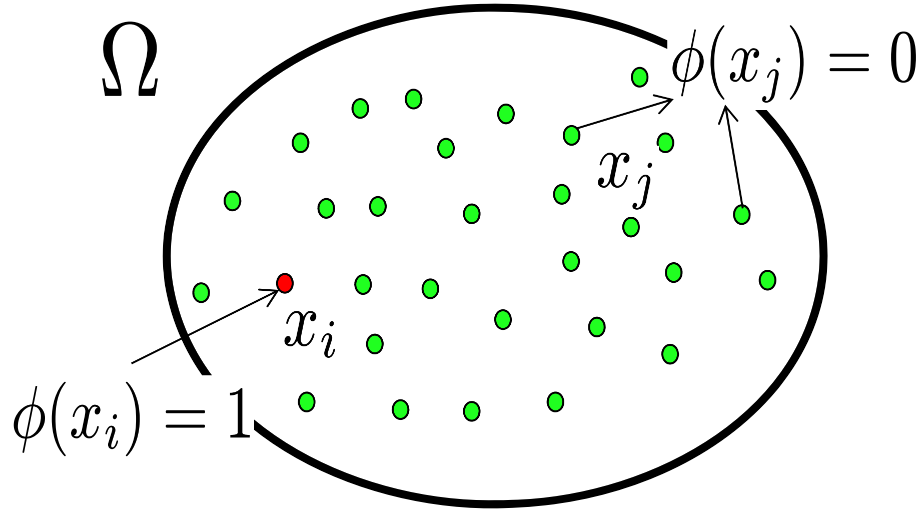
Optimal recovery properties of basis elements

Theorem Φ_i is the unique minimizer of the quadratic optimization problem

$$\begin{cases} \text{Minimize } \|\Phi\|_V \\ \text{Subject to } \Phi \in V \text{ and } \int_\Omega \Phi(x)\Psi_j(x)\,dx = \delta_{i,j} \end{cases}$$

E.g. $\mathcal{L}u = -\operatorname{div}(a\nabla u)$ $\quad \Psi_i(x) = \delta(x - x_i)$

$$\begin{cases} \text{Min } \int_\Omega \left|\operatorname{div}(a\nabla\phi)\right|^2 \\ \text{Subj to } \phi(x_j) = \delta_{i,j} \end{cases}$$

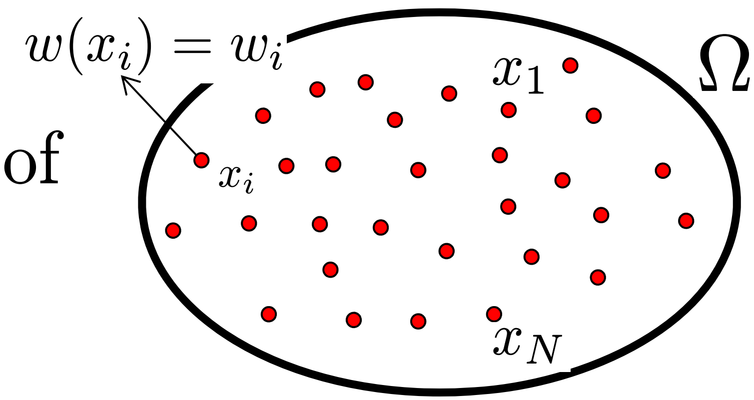


Optimal recovery properties of basis elements

Theorem $\sum_{i=1}^{N} w_i \Phi_i$ is the unique minimizer of the quadratic optimization problem

$$\begin{cases} \text{Minimize } \|\Phi\|_V \\ \text{Subject to } \Phi \in V \text{ and } \int_\Omega \Phi(x)\Psi_j(x)\,dx = w_j \end{cases}$$

E.g. $\mathcal{L}u = -\operatorname{div}(a\nabla u)$ $\quad \Psi_i(x) = \delta(x - x_i)$



$\sum_{i=1}^{N} w_i \phi_i$ is the unique minimizer of

$$\int_\Omega \big(\operatorname{div}(a\nabla\phi)\big)^2$$

over all $\phi \in V$ such that $\phi(x_i) = w_i$

Optimal recovery properties of basis elements

$$V_0 := \left\{ \Phi \in V \,\middle|\, \int_\Omega \Phi(x)\Psi_i(x)\,dx = 0, \quad \forall i \right\}$$

Theorem It holds true that

- $\Phi_i \perp V_0$

  $\forall i,\ \forall v \in V_0,\ \left\langle \Phi_i, v \right\rangle = 0$

- $\forall i, j,\ \left\langle \Phi_i, \Phi_j \right\rangle = \Theta_{i,j}$

- $\forall i,\ \forall v \in V$

  $\left\langle \Phi_i, v \right\rangle = \sum_{j=1}^{N} \Theta_{i,j}^{-1} \int_\Omega v(x)\Psi_j(x)\,dx$

$\mathcal{H}(\Omega)$-norm accuracy estimates

$$V_0 := \left\{\Phi \in V \,\middle|\, \int_\Omega \Phi(x)\Psi_i(x)\,dx = 0, \quad \forall i\right\}$$

$$\rho(V_0) := \sup_{v\in V_0} \frac{\|v\|_{\mathcal{H}(\Omega)}}{\|v\|_V}$$

u sol. of **(2)** $\begin{cases} \mathcal{L}u = g, & x \in \Omega, \\ \mathcal{B}u = 0, & x \in \partial\Omega, \end{cases}$

Theorem

$$\left\|u(x) - \sum_{i=1}^N \Phi_i(x) \int_\Omega u(y)\Psi_i(y)\,dy\right\|_{\mathcal{H}(\Omega)} \leq \rho(V_0)\|g\|_{L^2(\Omega)}$$

$\rho(V_0)$ is the smallest constant such that the inequality holds

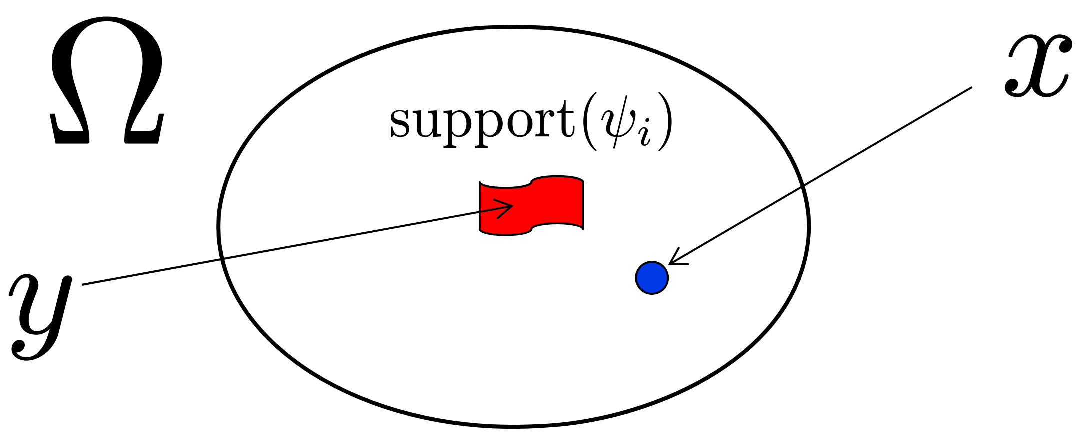
E.g. $\mathcal{L}u = -\operatorname{div}(a\nabla u) \qquad \mathcal{B}(u) = u$

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

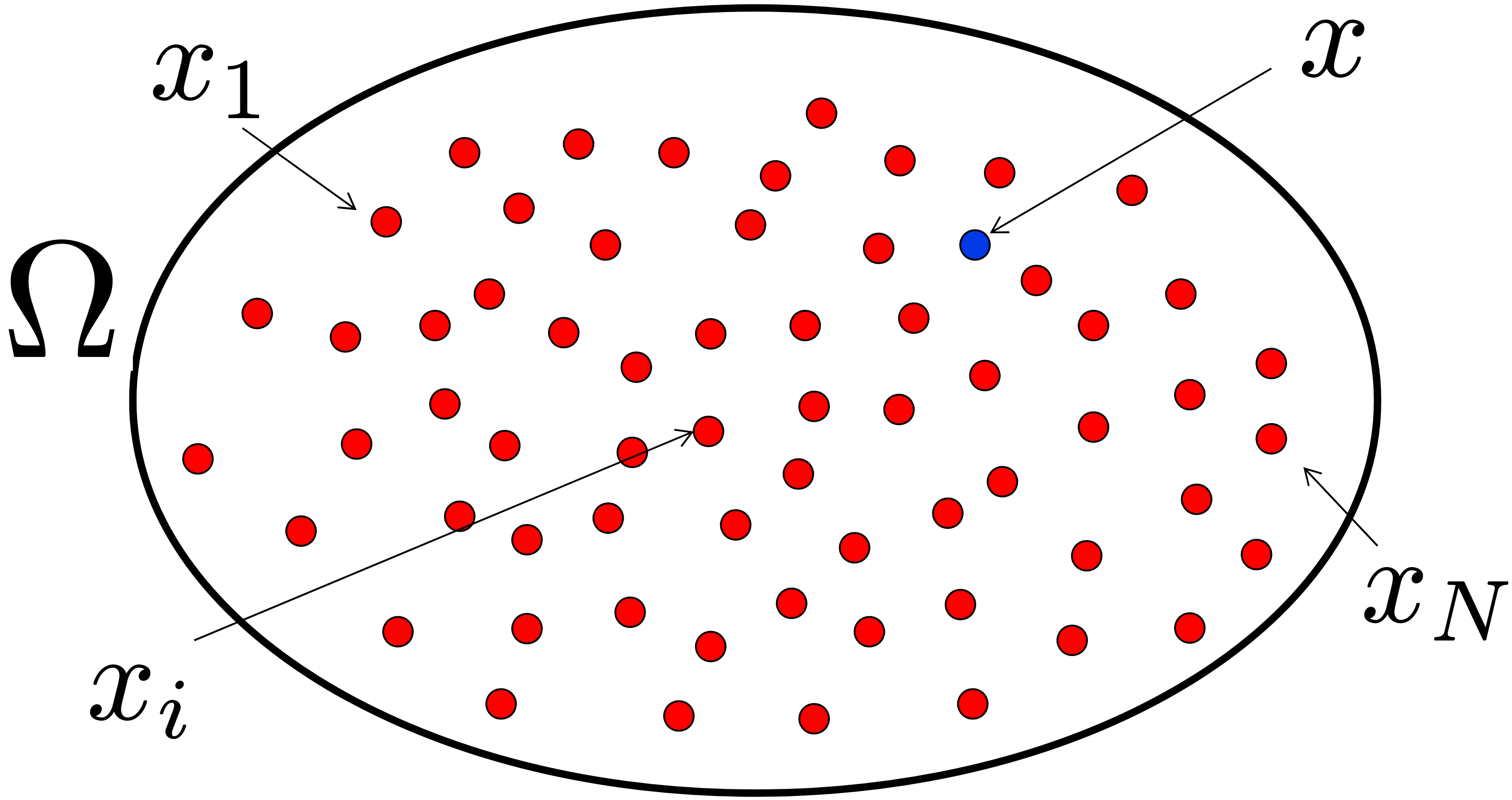
Theorem

$$\left\| u(x) - \sum_{i=1}^{N} \Phi_i(x) \int_\Omega u(y)\Psi_i(y)\,dy \right\|_{\mathcal{H}^1(\Omega)} \leq C\,H\,\|g\|_{L^2(\Omega)}$$

$$H := \sup_{x\in\Omega} \min_i \sup_{y\in \operatorname{support}(\psi_i)} \|x-y\|$$



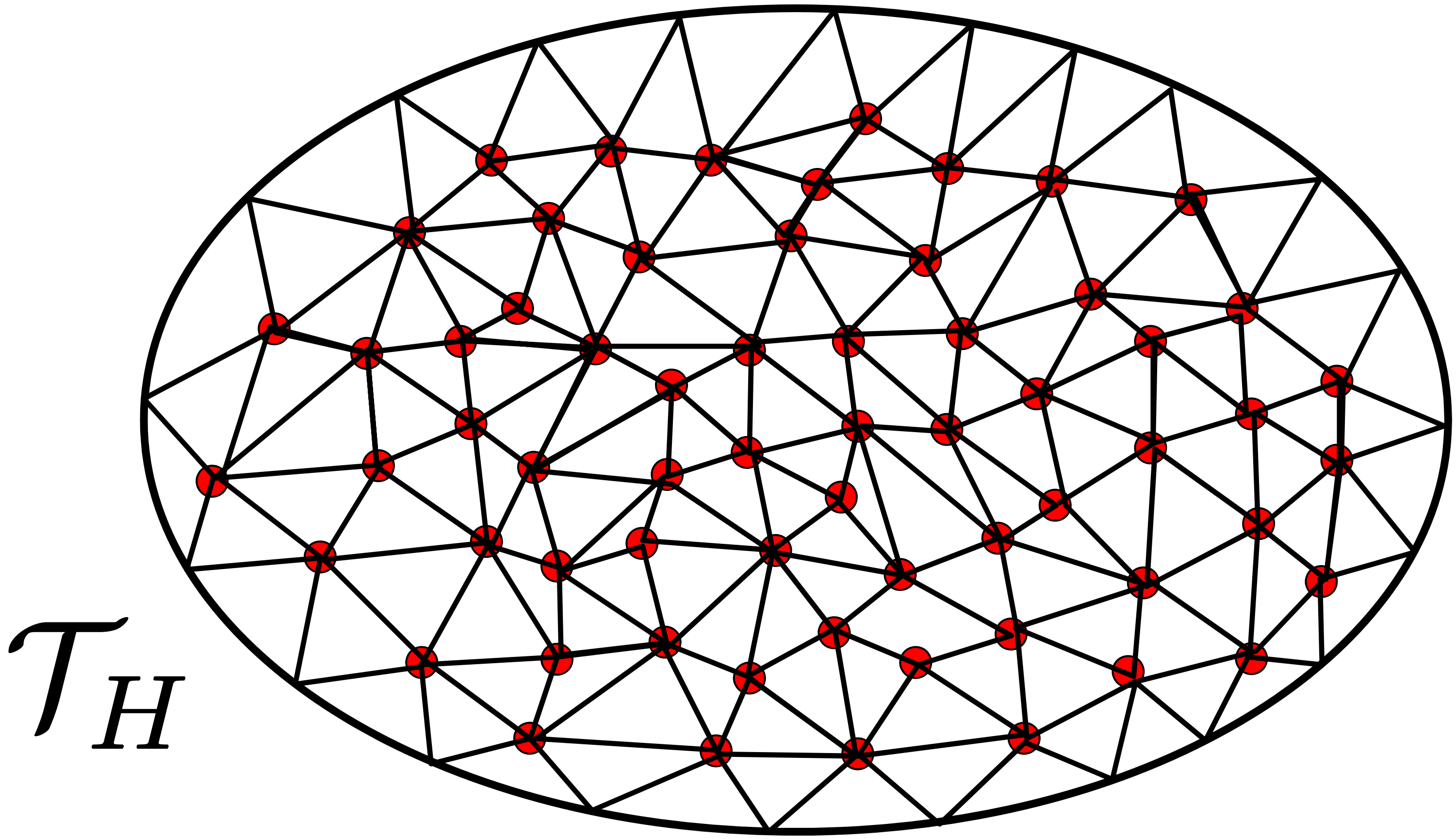
$$\Psi_i(x) = \delta(x - x_i)$$



The accuracy depends only on

$$H := \sup_{x \in \Omega} \min_i \|x - x_i\|$$

Accuracy of RPS as an interpolation basis

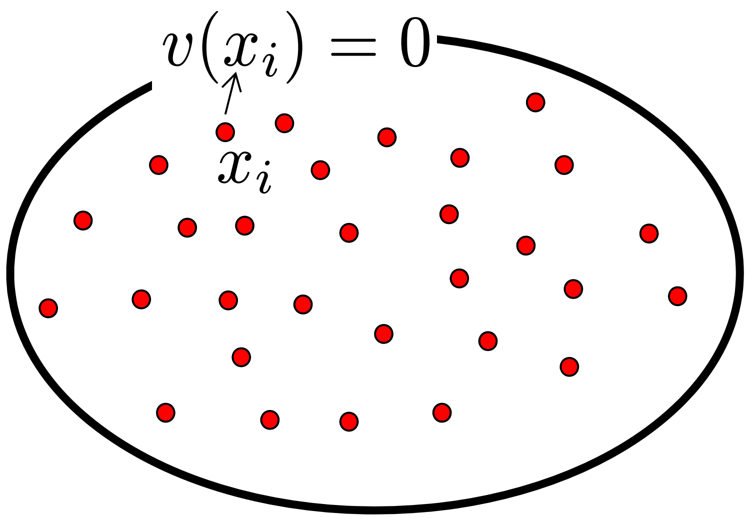


The accuracy is independent from aspect ratios

Higher order Poincare inequality

$$V := \{v \in \mathcal{H}_0^1(\Omega) \mid \operatorname{div}(a\nabla v) \in L^2(\Omega)\}$$

$$V_0 := \{v \in V \mid v(x_i) = 0 \text{ for all } i\}$$

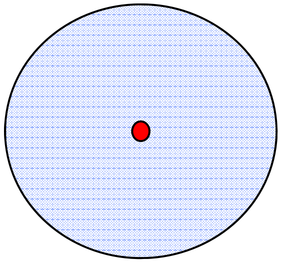


Theorem Let $f \in V_0$. It holds true that

$$\|\nabla f\|_{L^2(\Omega)} \leq CH \big\| \operatorname{div}(a\nabla f) \big\|_{L^2(\Omega)}$$

C depends on $\lambda_{\min}(a)$ and $\lambda_{\max}(a)$.

Proof

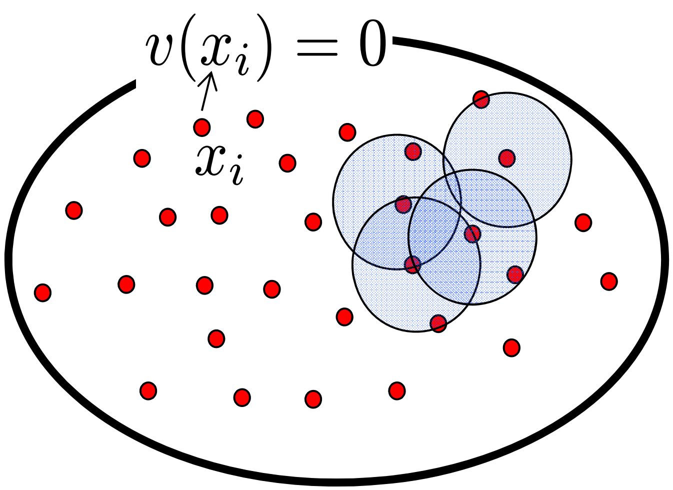


Lemma $d \le 3$. $B_1 := B(0,1)$.

If $v \in H^1(B_1)$ such that $\mathrm{div}(a\nabla v) \in L^2(B_1)$ then

$$\|v - v(0)\|_{L^2(B_1)}^2 \le C\Big(\|\nabla v\|_{L^2(B_1)}^2 + \big\|\mathrm{div}(a\nabla v)\big\|_{L^2(B_1)}^2 \Big)$$

C depends on $\lambda_{\min}(a)$ and $\lambda_{\max}(a)$.



Proof of the lemma per absurdum

There exists w_n, $w_n(0) = 0$, $\|w_n\|_{L^2(B_1)} = 1$ and

$$\|\nabla w_n\|^2_{L^2(B_1)} + \left\| \operatorname{div}(a \nabla w_n) \right\|^2_{L^2(B_1)} < \frac{1}{n}$$

Thus $\exists\ w_{n_j}$ and $w \in H^1(B_1)$ such that $w_{n_j} \rightharpoonup w$ weakly in $H^1(B_1)$ and $\nabla w_{n_j} \rightharpoonup \nabla w$ weakly in $L^2(B_1)$.

$\|\nabla w_n\|_{L^2(B_1)} \leq 1/n \Rightarrow \nabla w = 0 \Rightarrow w$ is a constant in B_1.

Rellich-Kondrachov theorem $\Rightarrow H^1(B_1) \subset\subset L^2(B_1)$
$\Rightarrow w_{n_j} \to w$ strongly in $L^2(B_1) \Rightarrow \|w\|_{L^2(B_1)} = 1$.

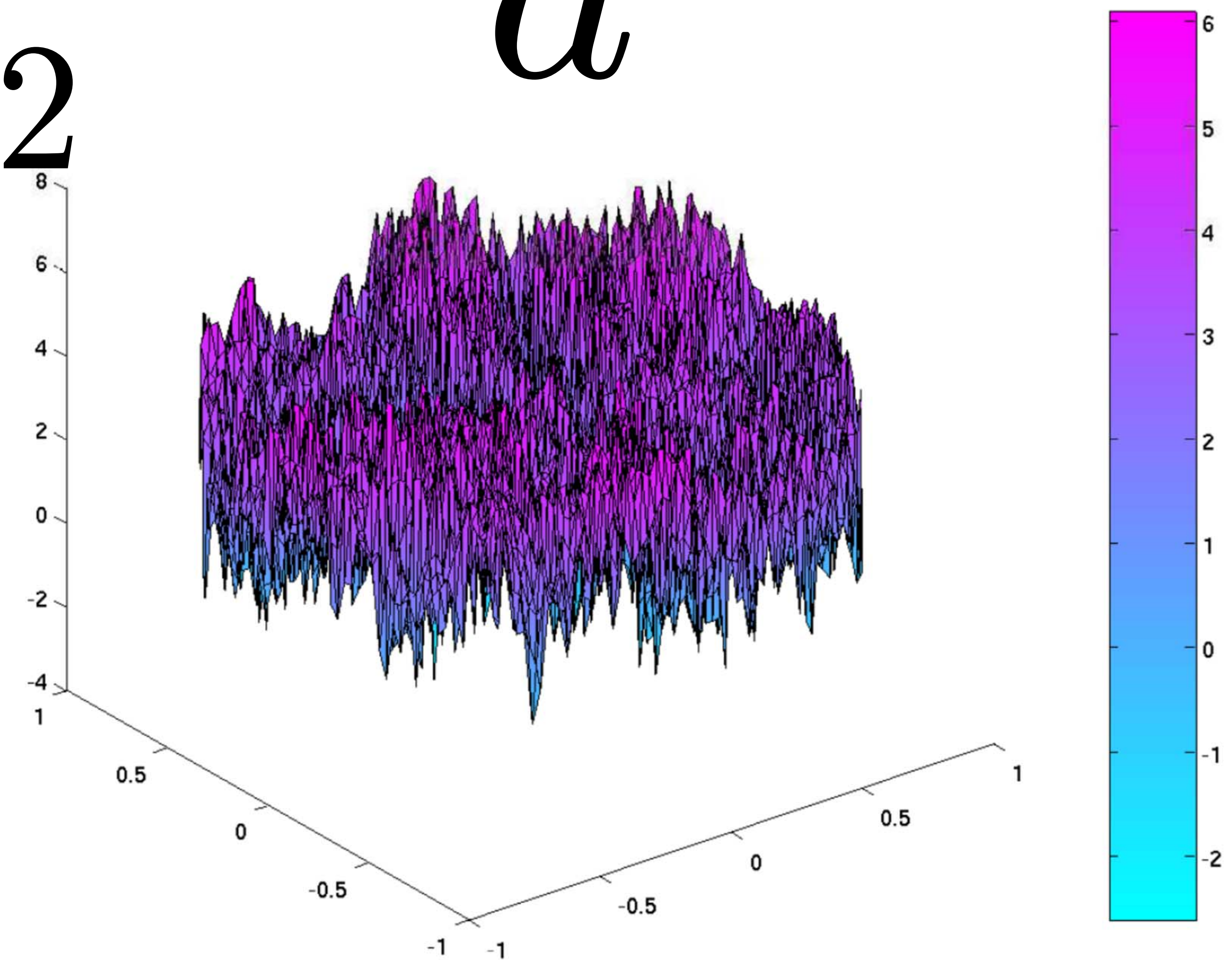
w_n uniformly Hölder cont. on $B(0, \frac{1}{2})$
$\Rightarrow w$ cont. in $B(0, \frac{1}{2})$ and $w(0) = 0$.

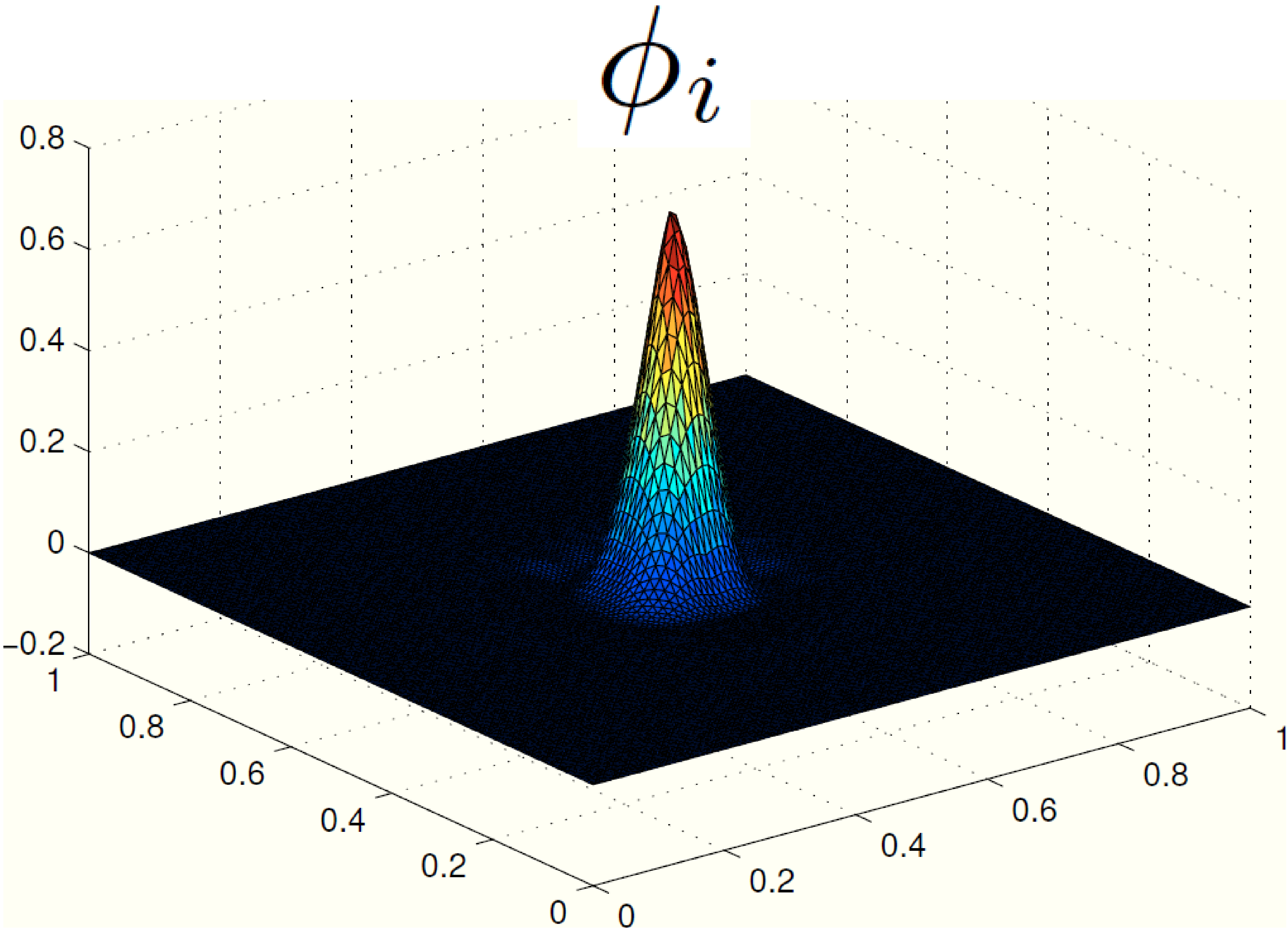
Contradicts w is a constant in B_1 with $\|w\|_{L^2(B_1)} = 1$.

What do rough polyharmonic splines look like?

$$a$$

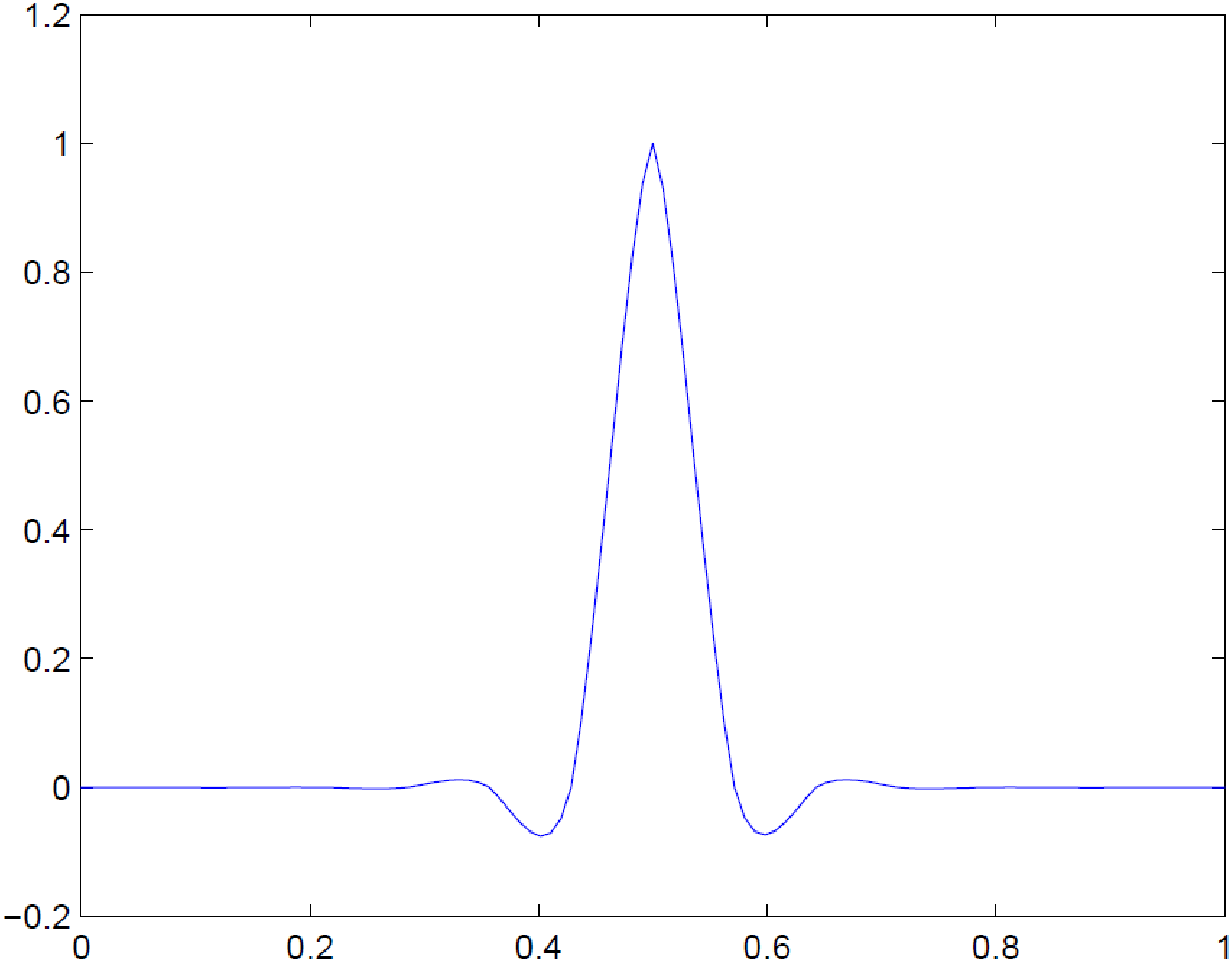
$$d = 2$$





ϕ_i
0.8
0.6
0.4
0.2
0
−0.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1

Slice of ϕ_i along the x-axis



1d example

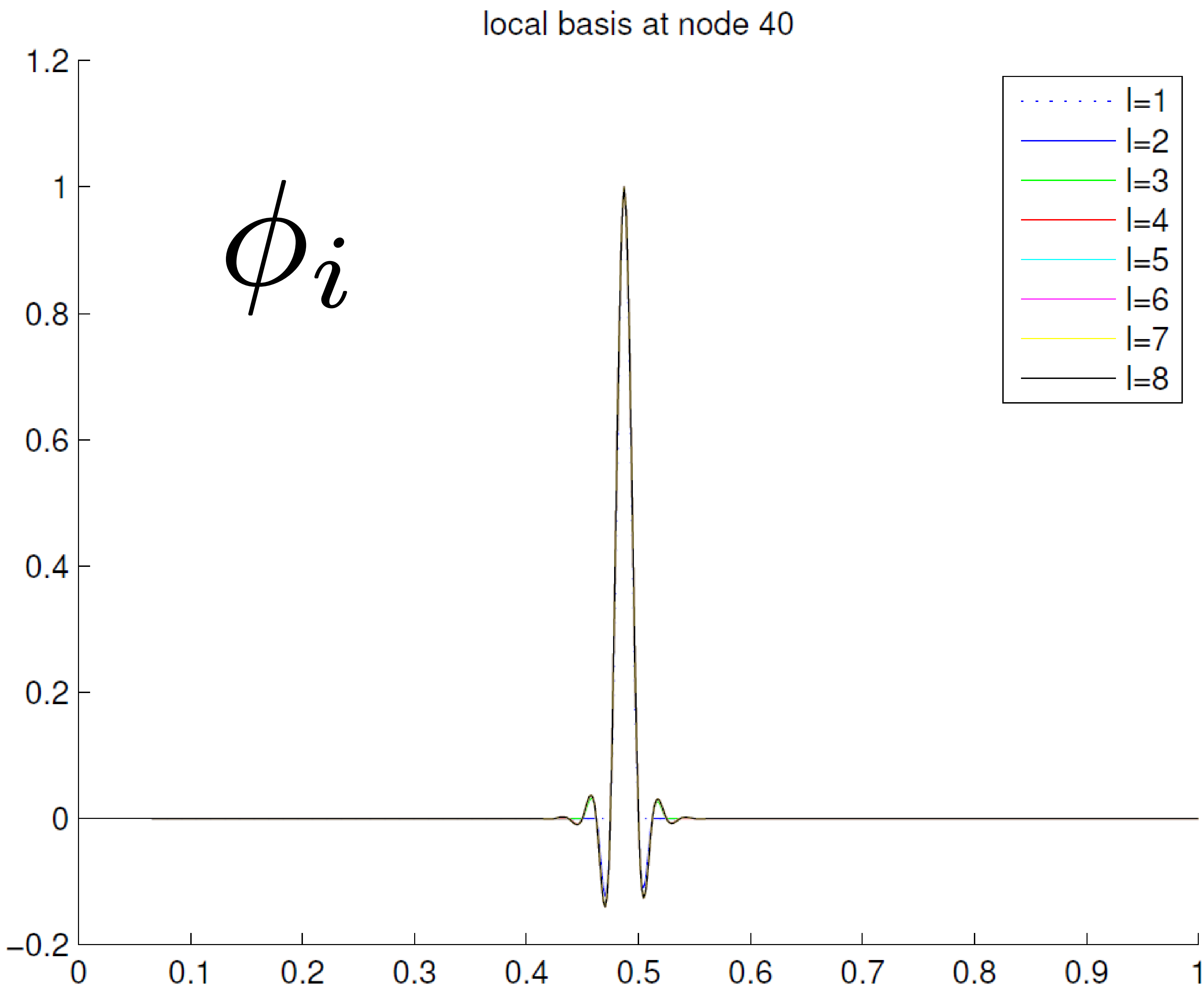
$$d = 1 \qquad \Omega = (0,1)$$

$$a(x) := 1 + \tfrac{1}{2}\sin\left(\sum_{k=1}^{K} k^{-\alpha}(\zeta_{1k}\sin(kx) + \zeta_{2k}\cos(kx))\right)$$

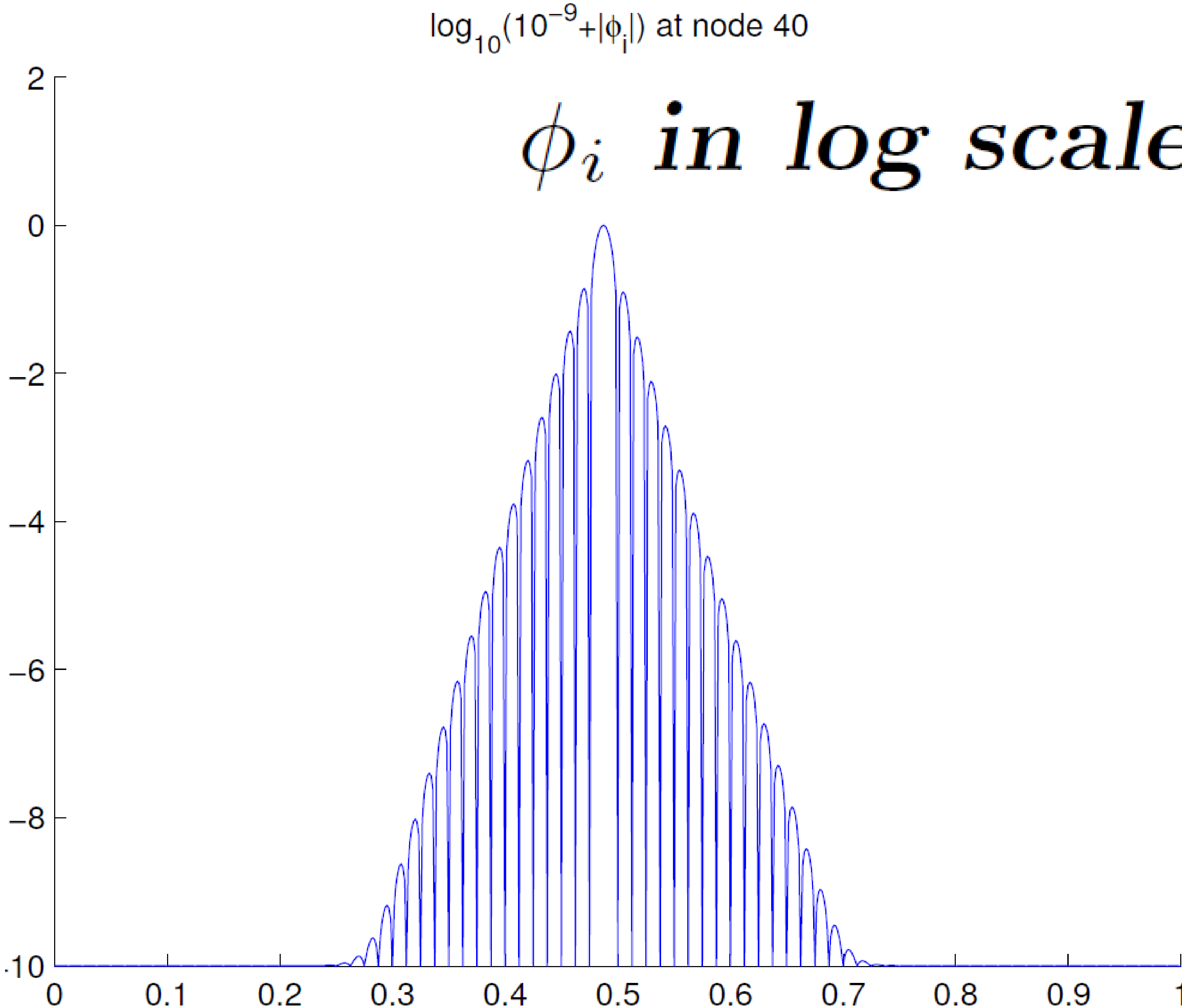
$\{\zeta_{1k}\}$, $\{\zeta_{2k}\}$: i.i.d. uniformly distributed in $[-\frac{1}{2}, \frac{1}{2}]$

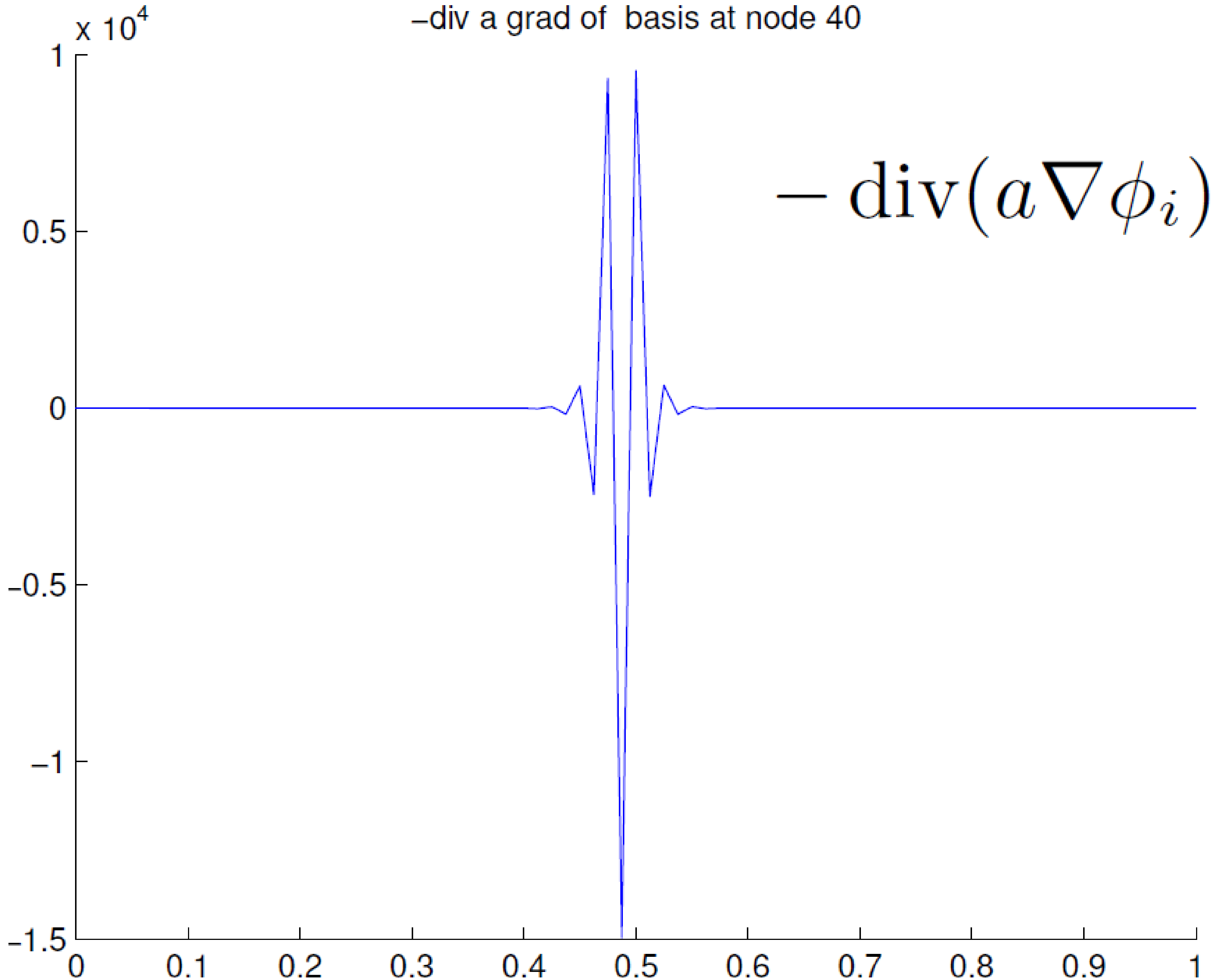
$$\left\langle |\hat{a}(k)|^2 \right\rangle \simeq |k|^{-\alpha}$$

Example taken out of [Hou-Wu 1997]
and [Ming-Yue 2006]

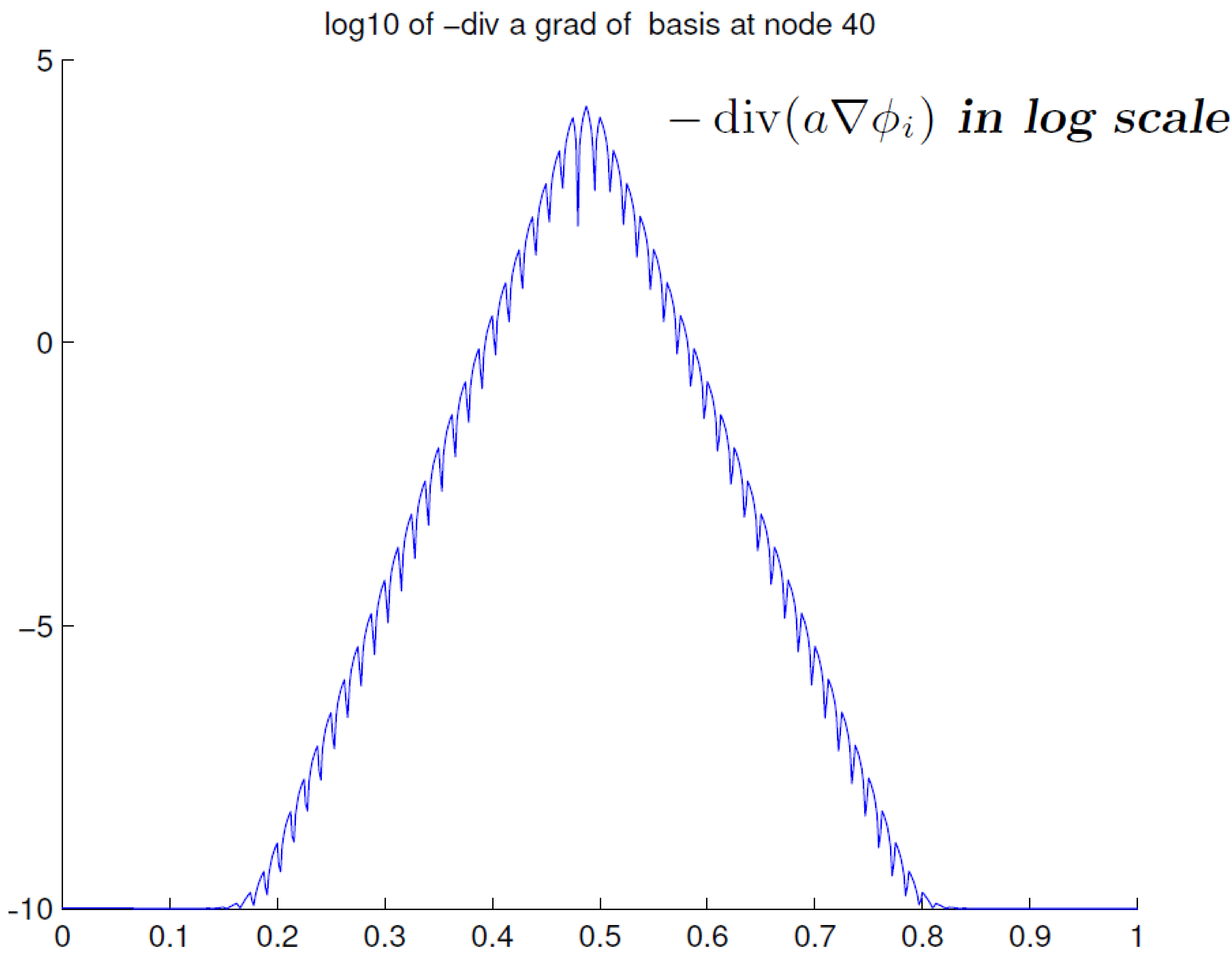

local basis at node 40
ϕ_i
l=1
l=2
l=3
l=4
l=5
l=6
l=7
l=8
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

ϕ_i in log scale



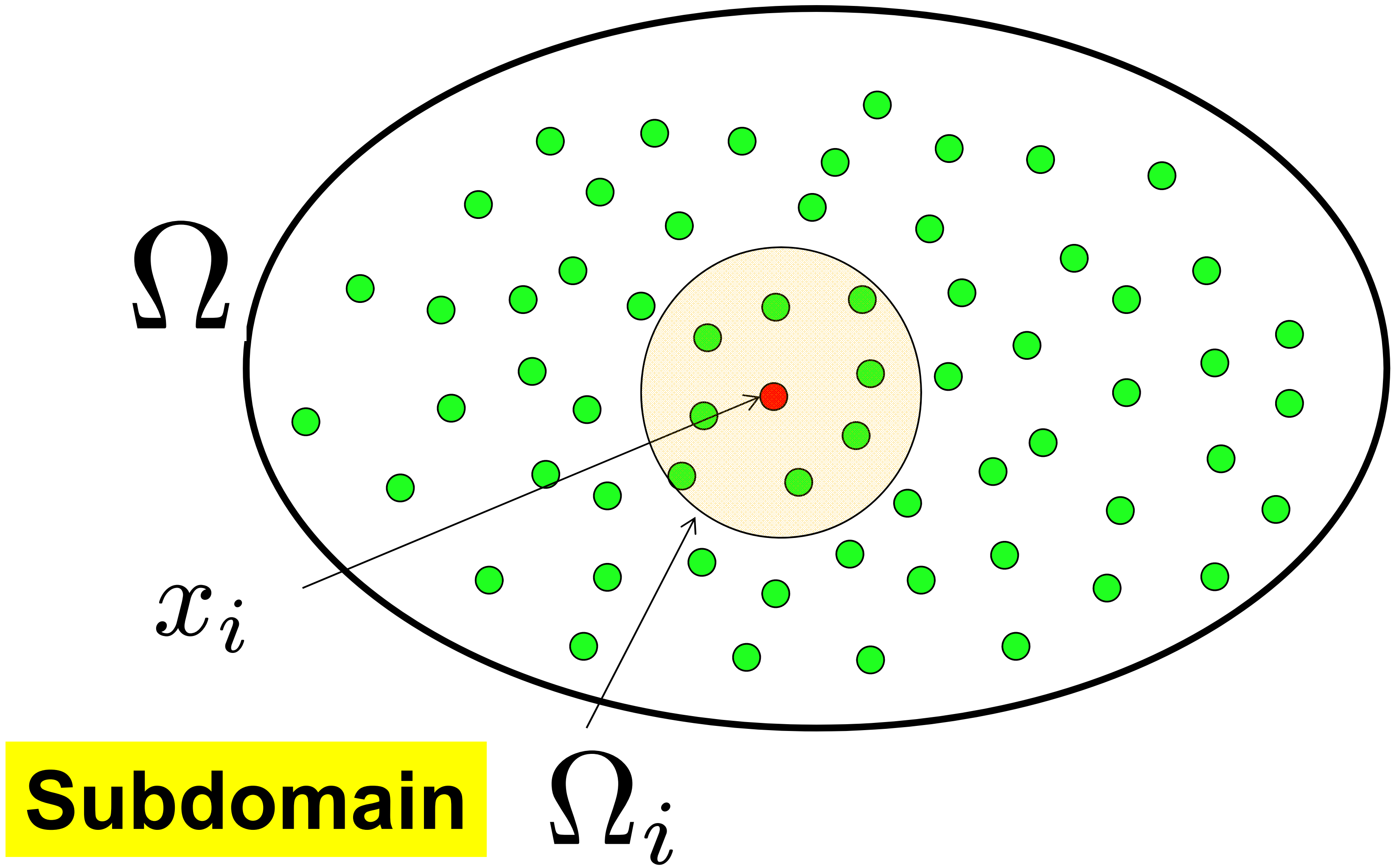


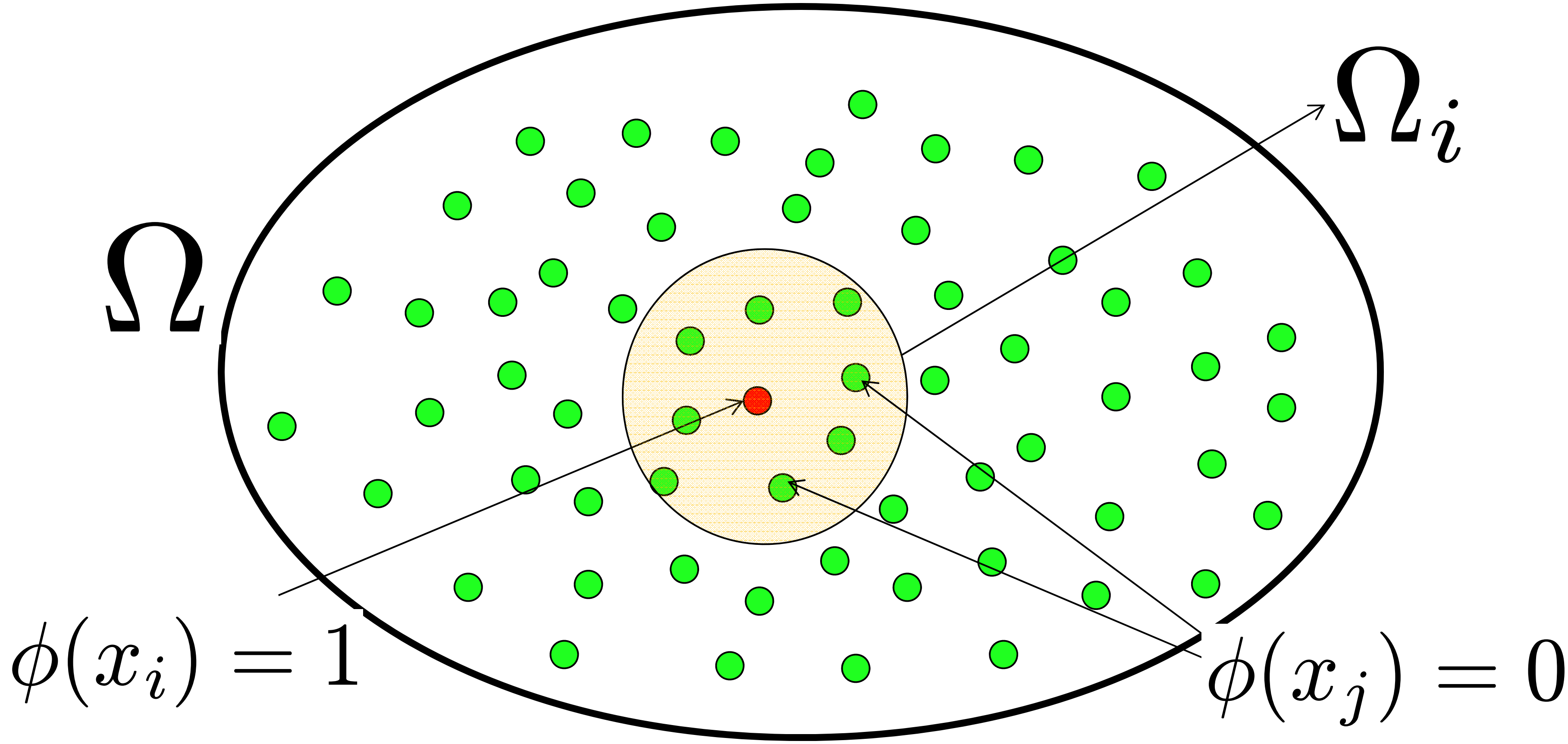
−div a grad of basis at node 40
x 10^4
1
0.5
0
−0.5
−1
−1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
$-\operatorname{div}(a\nabla\phi_i)$



log10 of −div a grad of basis at node 40
$-\operatorname{div}(a\nabla\phi_i)$ ***in log scale***
5
0
−5
-10
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Localization of the interpolation basis





ϕ_i^{loc} Minimizer of $\int_{\Omega_i} \big|\operatorname{div}(a\nabla\phi)\big|^2$

Subject to $\phi \in \mathcal{H}_0^1(\Omega_i)$

and $\phi(x_j)=\delta_{i,j}$

(1)

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

u: Solution of (1)

$u^{H,\mathrm{loc}}$: F.E. solution of (1) over $\mathrm{span}(\phi_i^{\mathrm{loc}})$

Theorem

$$\|u - u^{H,\mathrm{loc}}\|_{\mathcal{H}_0^1(\Omega)} \le C\,\|g\|_{L^2(\Omega)} \left(H + N \max_{i\in\mathcal{N}} \|\phi_i - \phi_i^{\mathrm{loc}}\|_{\mathcal{H}_0^1(\Omega)}\right)$$

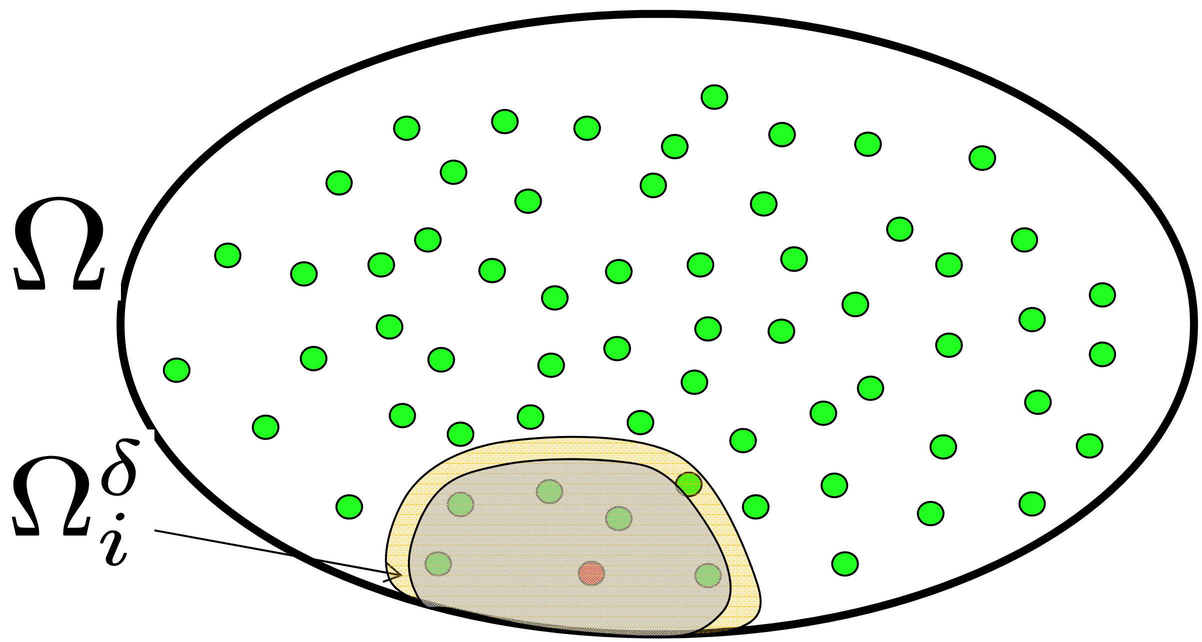
C depends on $\lambda_{\min}(a)$ and $\lambda_{\max}(a)$.

Theorem

$$\|\phi_i - \phi_i^{\text{loc}}\|_{\mathcal{H}_0^1(\Omega)} \leq C H^{-7-2d} \Big(\| \operatorname{div}(a \nabla \phi_i^{\text{loc}}) \|_{L^2(\Omega_i^H)} + \|\phi_i^{\text{loc}}\|_{L^2(\Omega_i^H)} \Big)$$

C depends on $\lambda_{\min}(a)$ and $\lambda_{\max}(a)$.

$$\Omega_i^\delta := \{ x \in \Omega_i \mid \operatorname{dist}(x, \partial\Omega_i \cap \Omega) < \delta \}$$



(1)

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

u: Solution of (1)

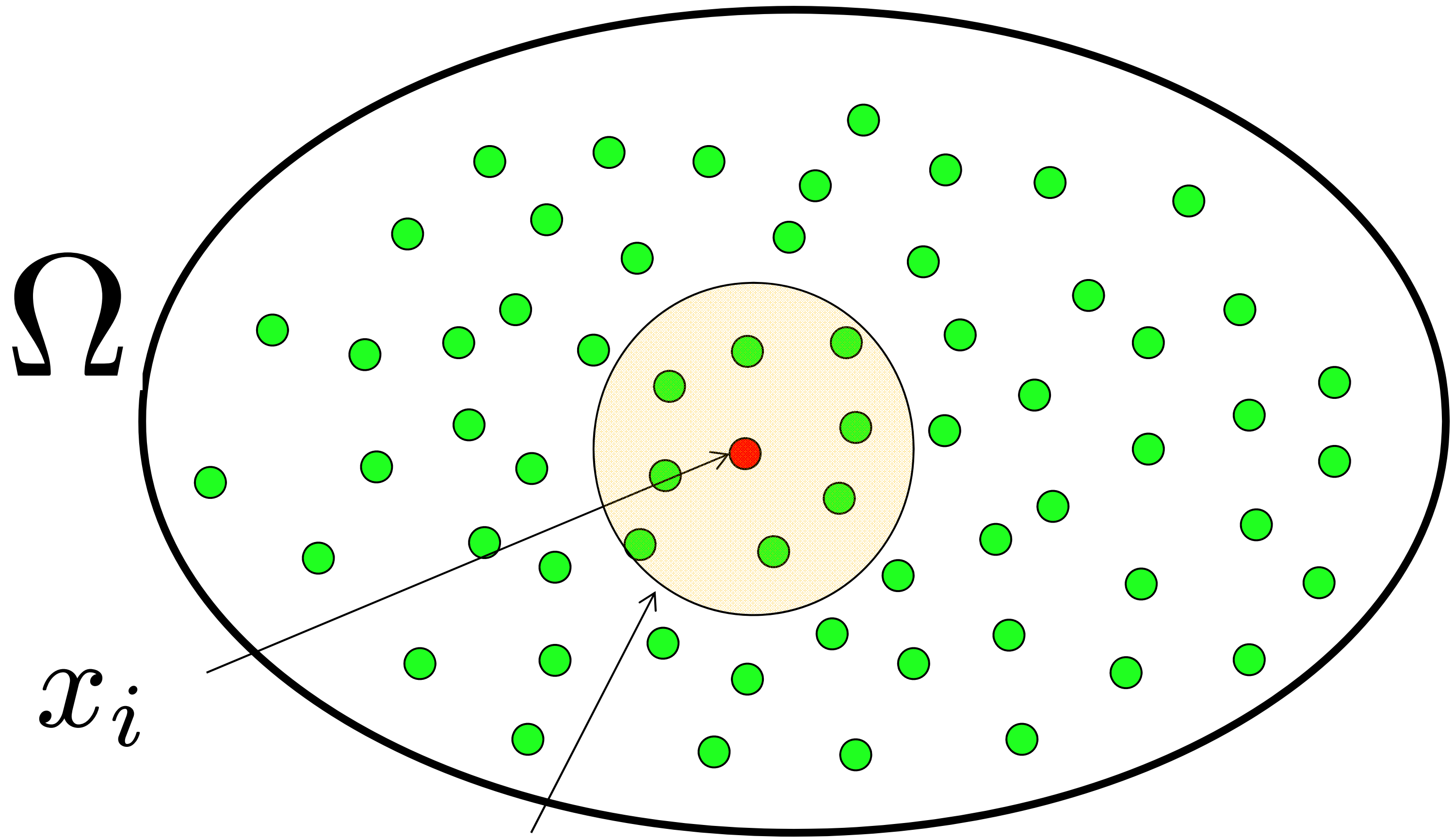
$u^{H,\text{loc}}$: F.E. solution of (1) over $\operatorname{span}(\phi_i^{\text{loc}})$

Theorem A posteriori error estimates

$$\|u - u^{H,\text{loc}}\|_{\mathcal{H}_0^1(\Omega)} \leq C \,\|g\|_{L^2(\Omega)} (H + E)$$

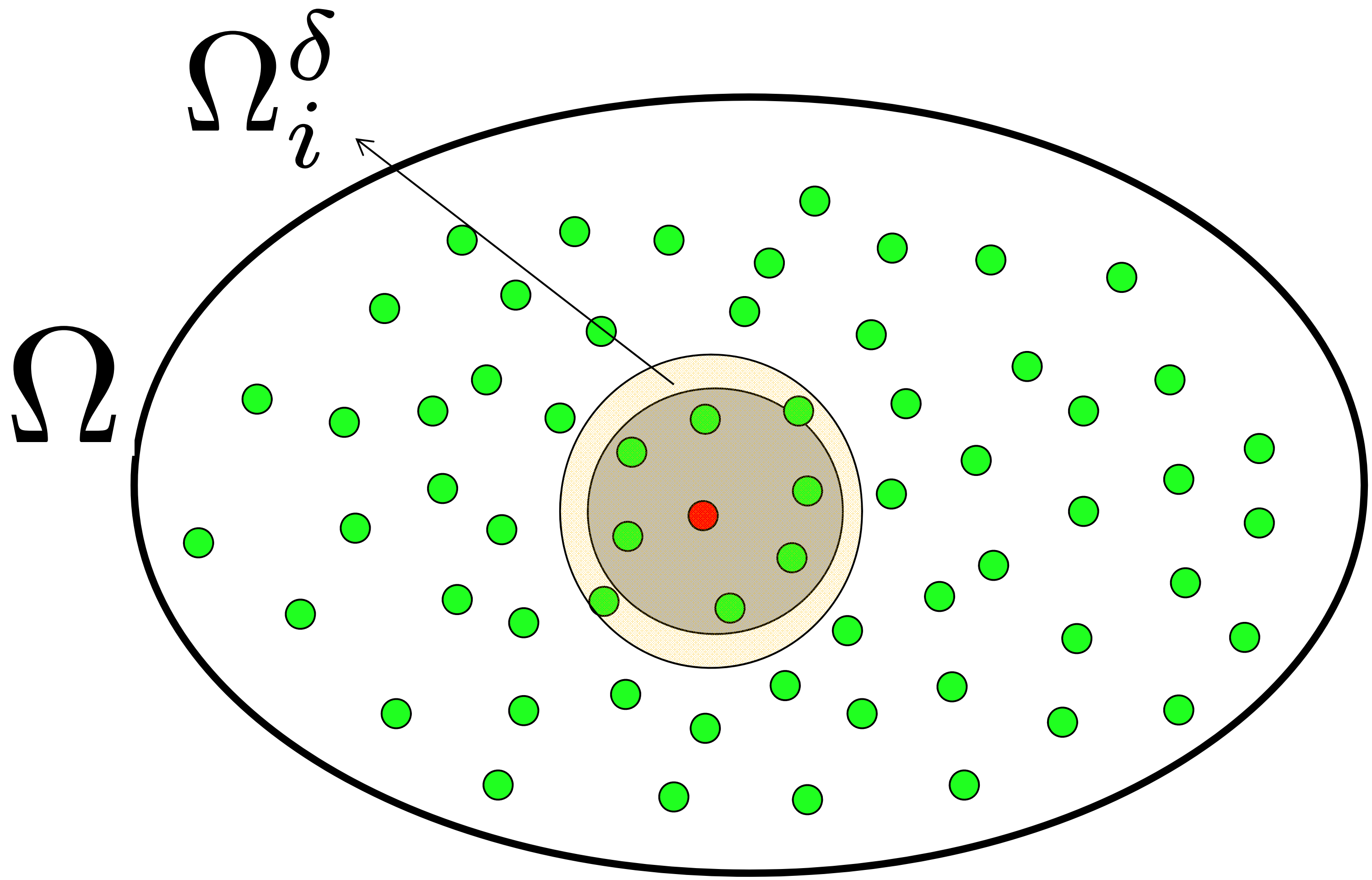
$$E = H^{-7-3d} \max_{i \in \mathcal{N}} \left(\|\operatorname{div}(a\nabla\phi_i^{\text{loc}})\|_{L^2(\Omega_i^H)} + \|\phi_i^{\text{loc}}\|_{L^2(\Omega_i^H)} \right)$$

C depends on $\lambda_{\min}(a)$ and $\lambda_{\max}(a)$.

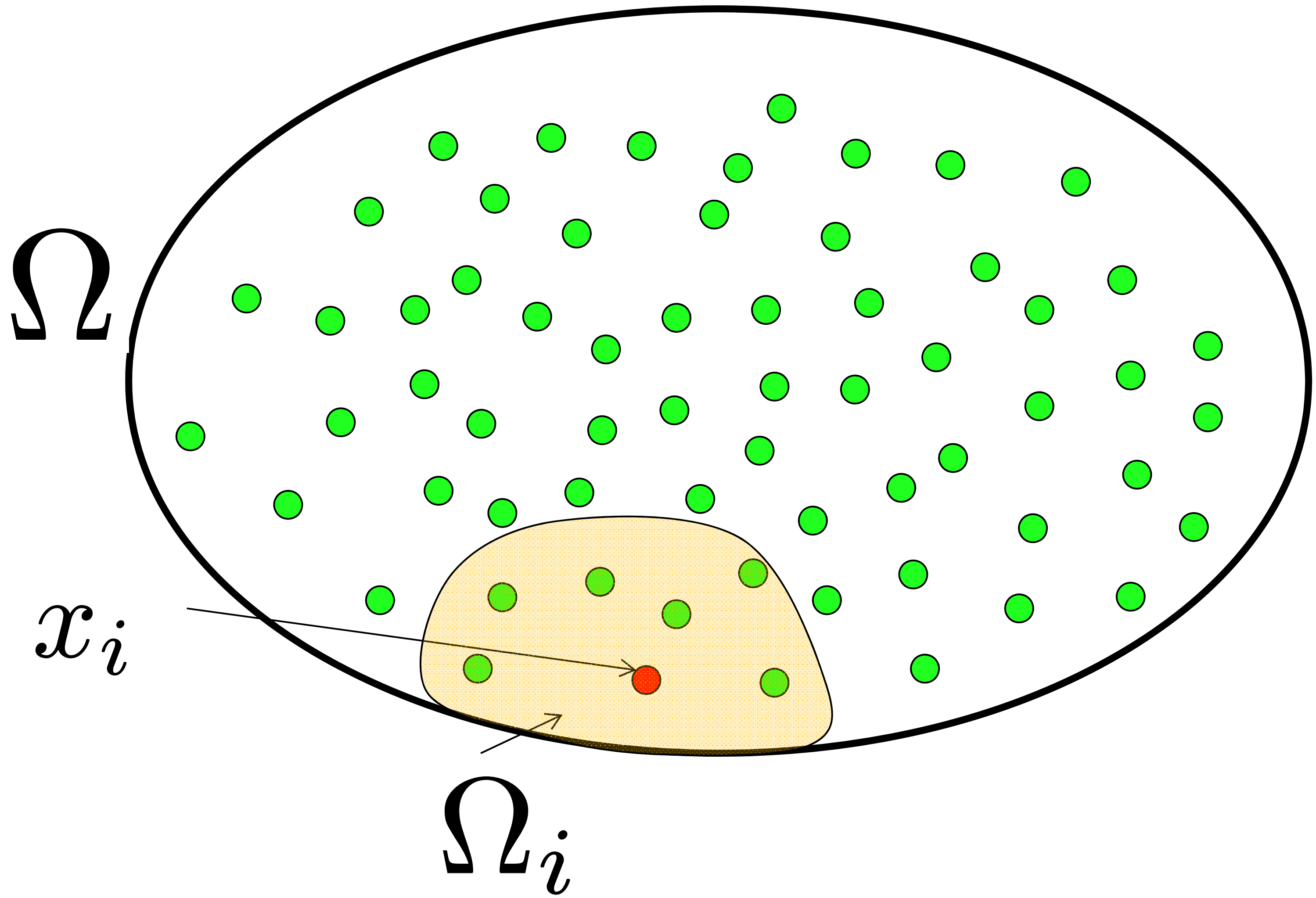


Subdomain Ω_i

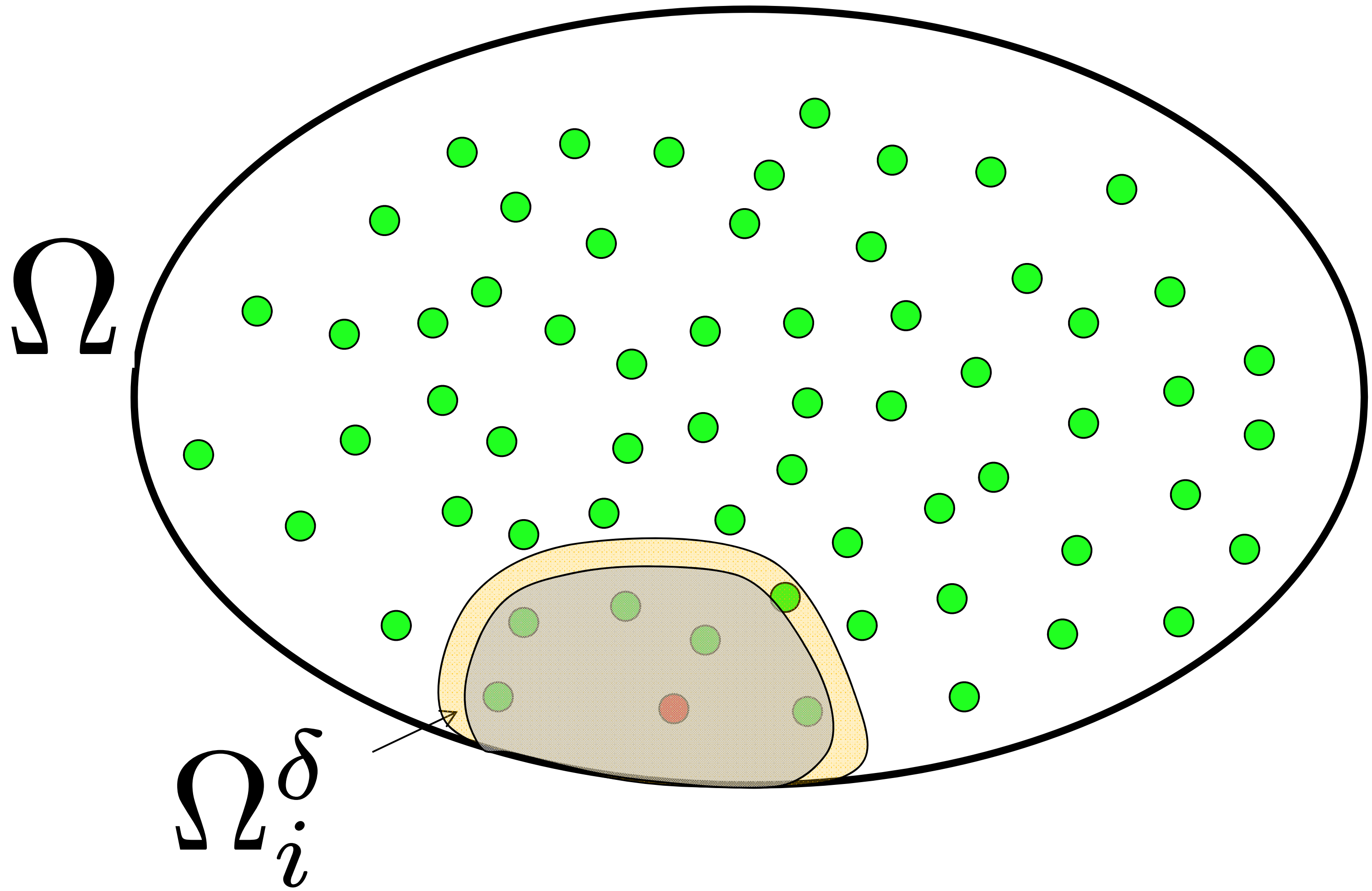
$$\Omega_i^\delta := \{x \in \Omega_i \mid \mathrm{dist}(x, \partial\Omega_i \cap \Omega) < \delta\}$$



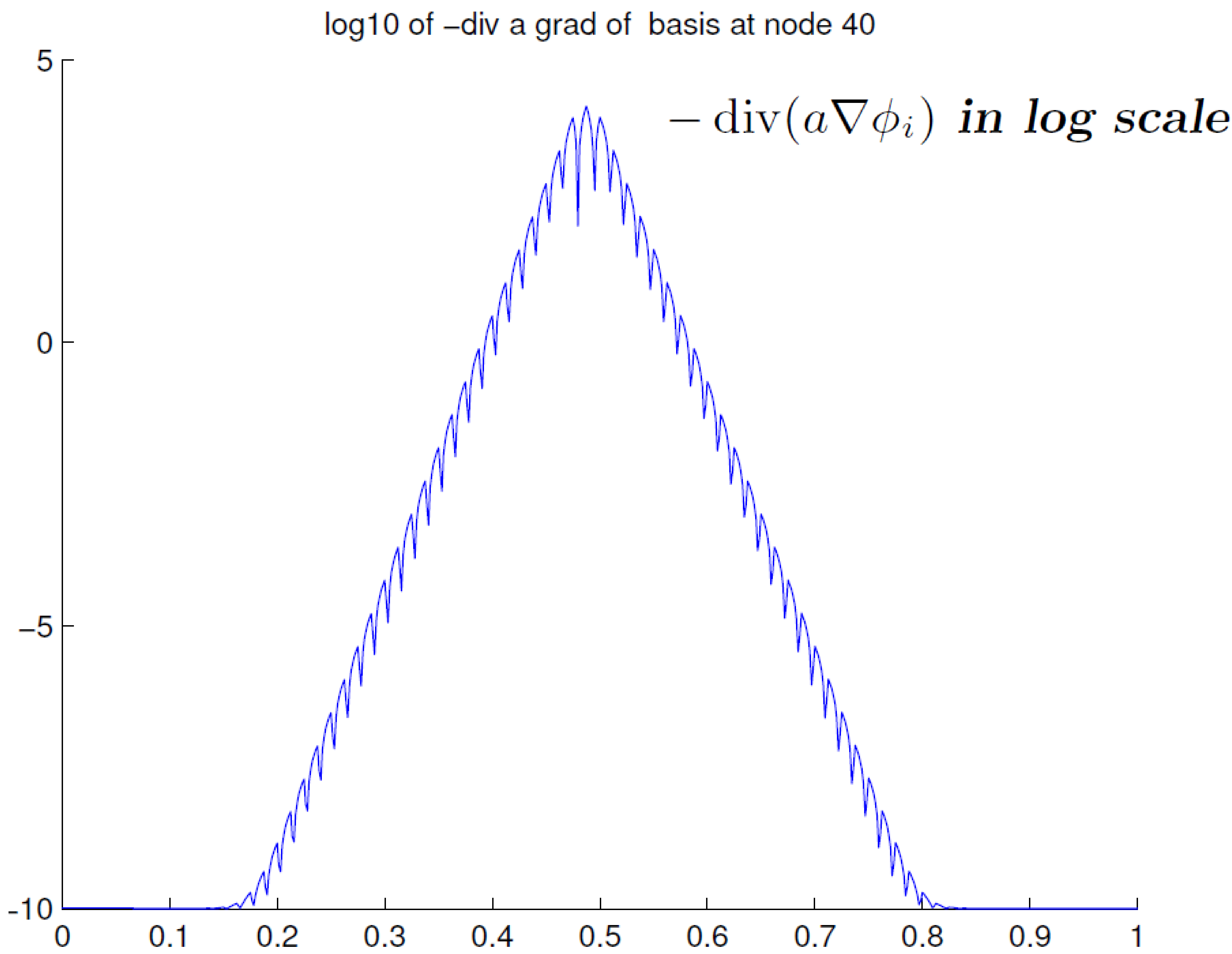
$$\Omega_i^\delta := \{x \in \Omega_i \mid \mathrm{dist}(x, \partial\Omega_i \cap \Omega) < \delta\}$$



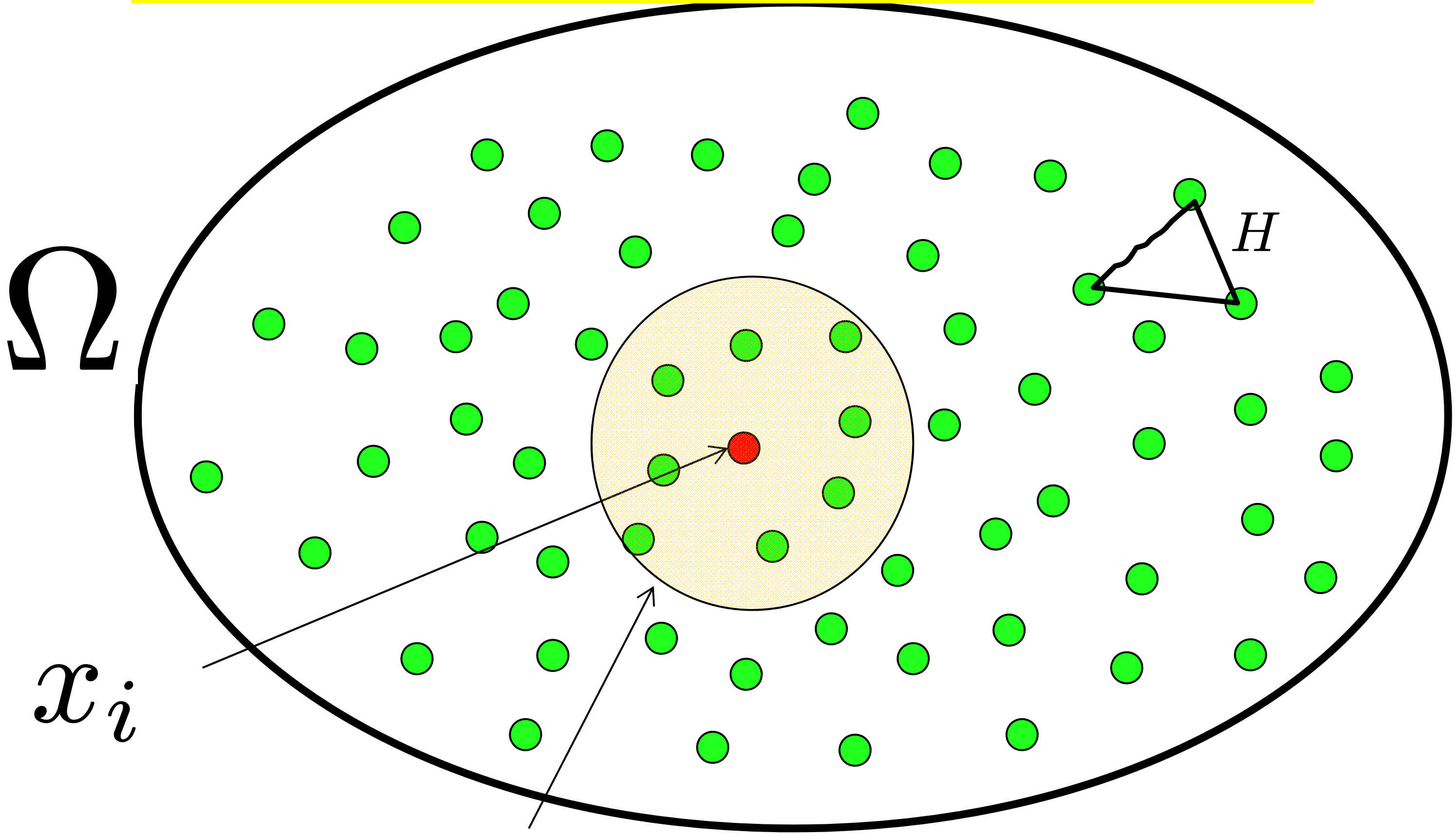
$$\Omega_i^\delta := \{x \in \Omega_i \mid \mathrm{dist}(x, \partial\Omega_i \cap \Omega) < \delta\}$$



$$\Omega_i^\delta := \{x \in \Omega_i \mid \mathrm{dist}(x, \partial\Omega_i \cap \Omega) < \delta\}$$


log10 of –div a grad of basis at node 40
$-\operatorname{div}(a\nabla\phi_i)$ ***in log scale***
5
0
–5
-10
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Sparse super-localization



Subdomain Ω_i of size $C^* H \ln \frac{1}{H}$

$$\left(B(x_i, C^* H \ln \frac{1}{H}) \cap \Omega\right) \subset \Omega_i$$

Sparse super-localization

u: Solution of (1)

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

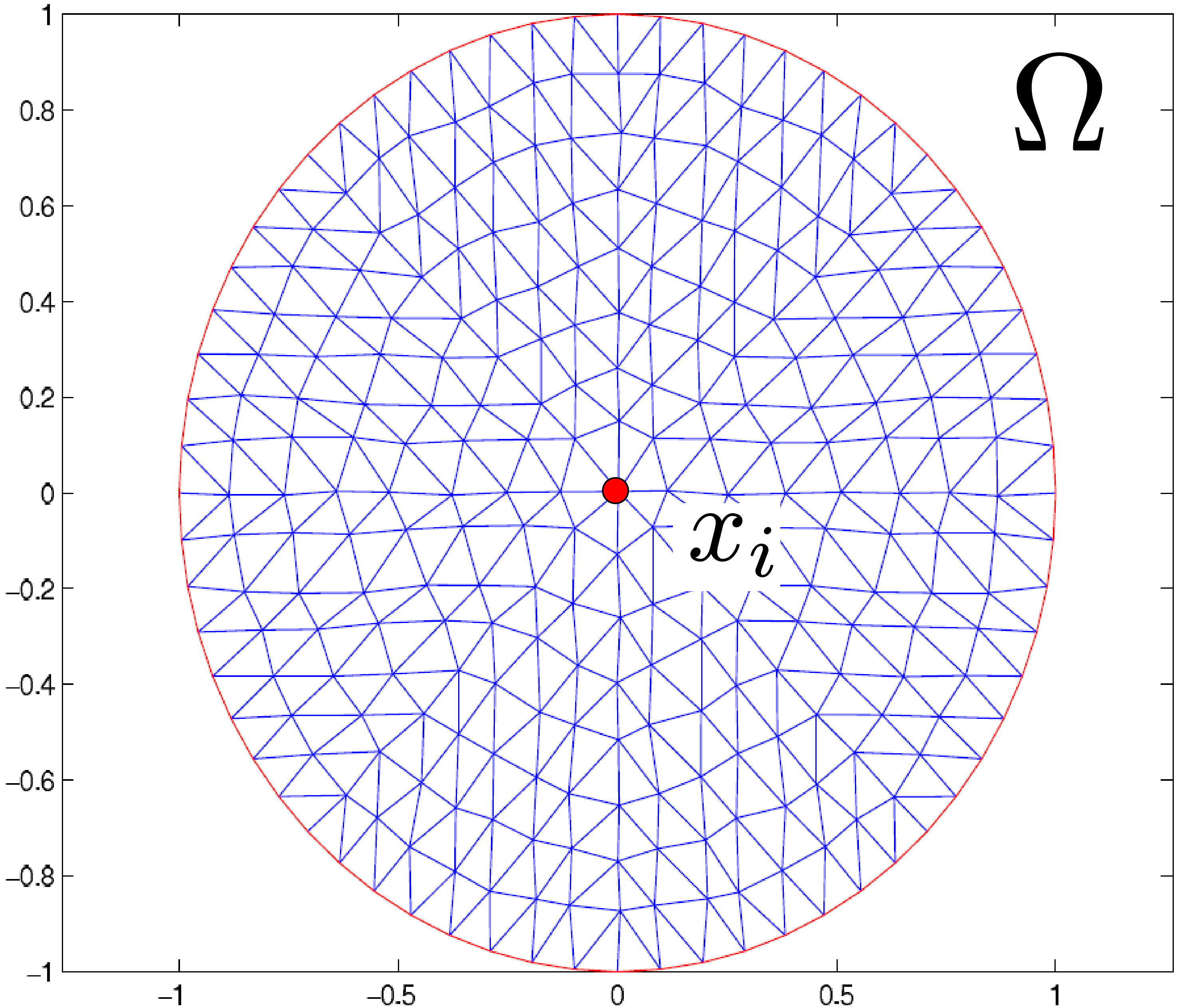
$u^{H,\mathrm{loc}}$: F.E. solution of (1) over $\operatorname{span}(\phi_i^{\mathrm{loc}})$

Theorem

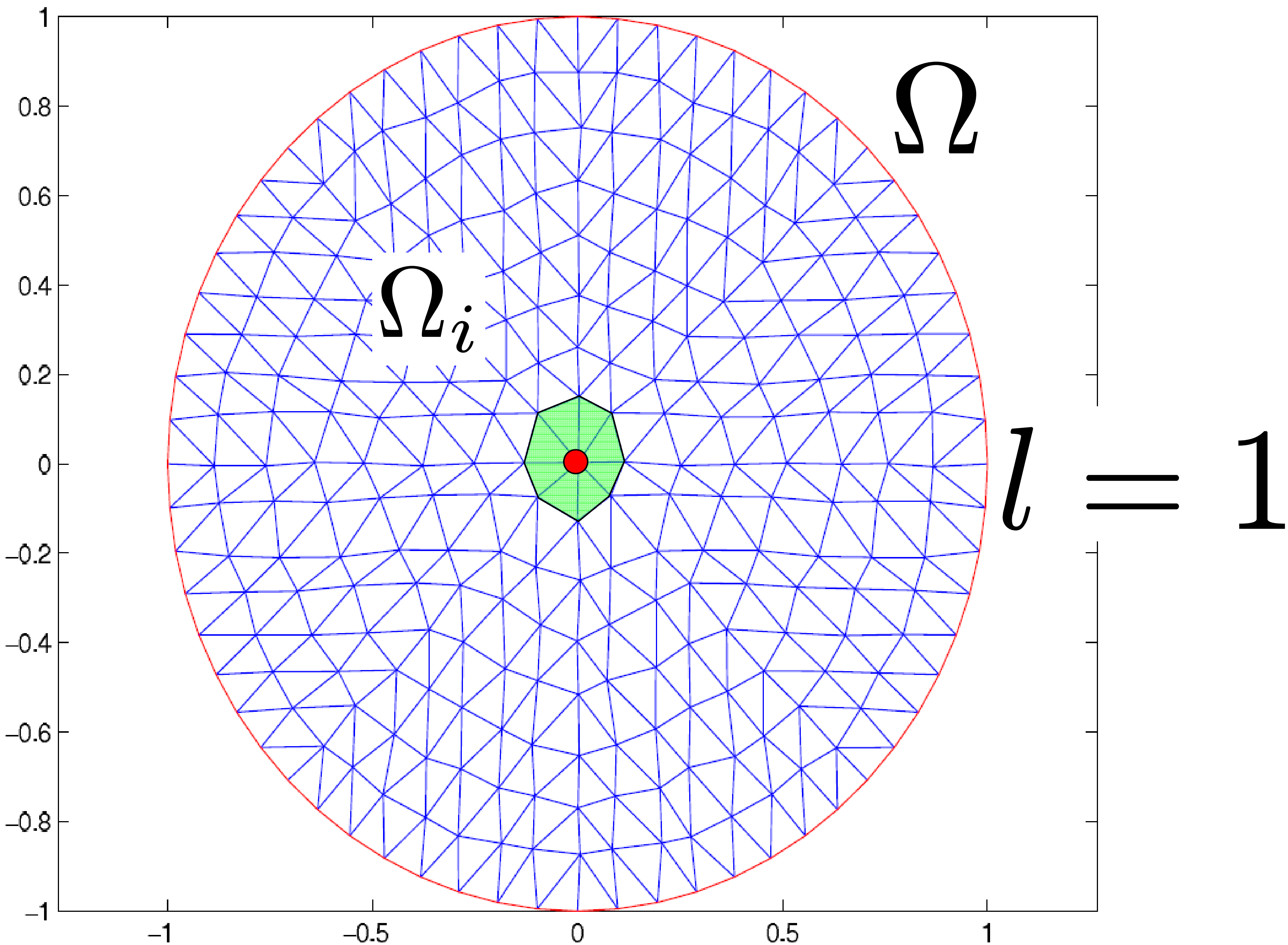
If $\left(B(x_i, C^* H \ln \frac{1}{H}) \cap \Omega\right) \subset \Omega_i$, then

$$\|u - u^{H,\mathrm{loc}}\|_{\mathcal{H}_0^1(\Omega)} \leq C\, H \|g\|_{L^2(\Omega)}$$

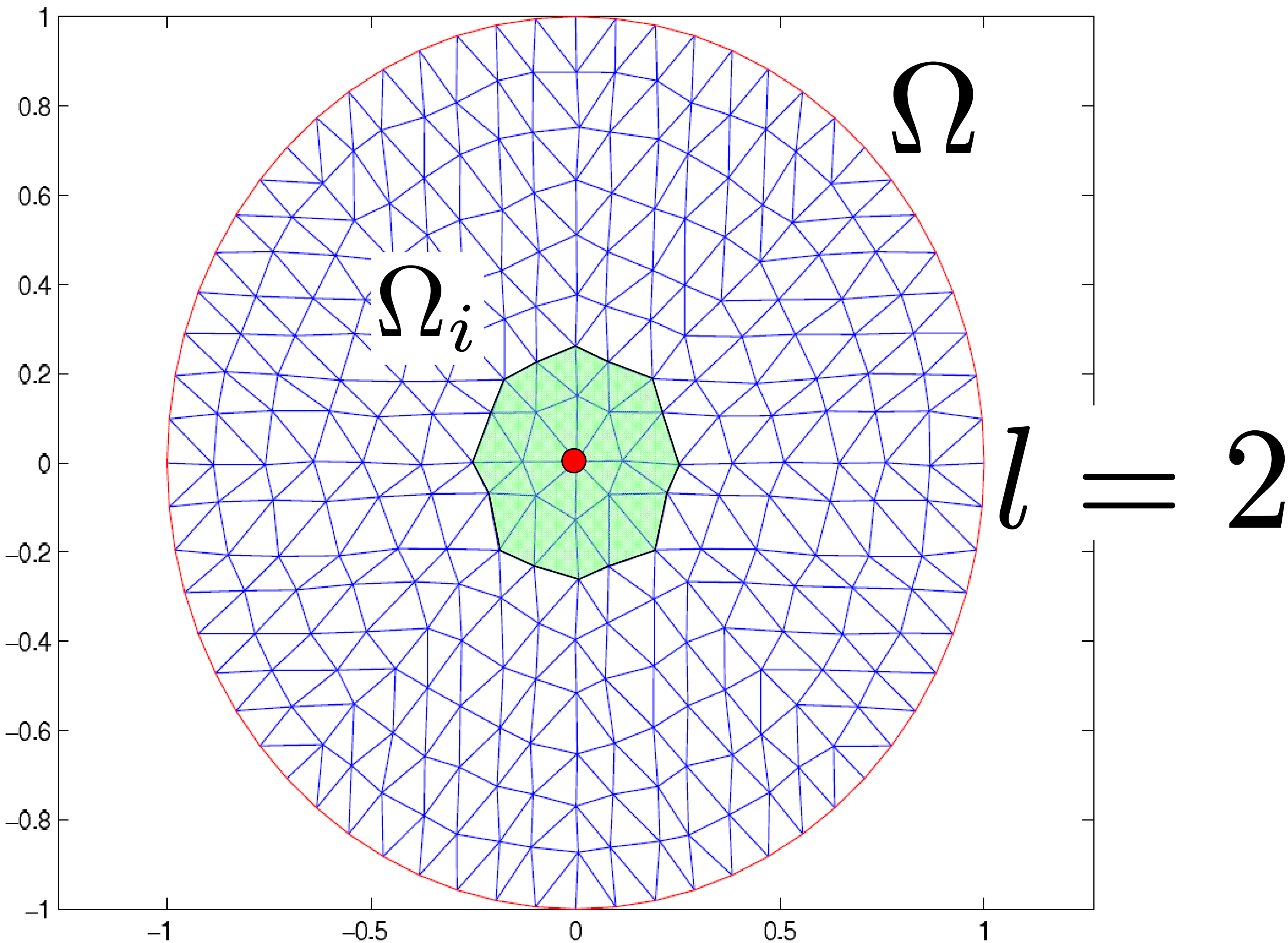
C depends on $\lambda_{\min}(a)$ and $\lambda_{\max}(a)$.



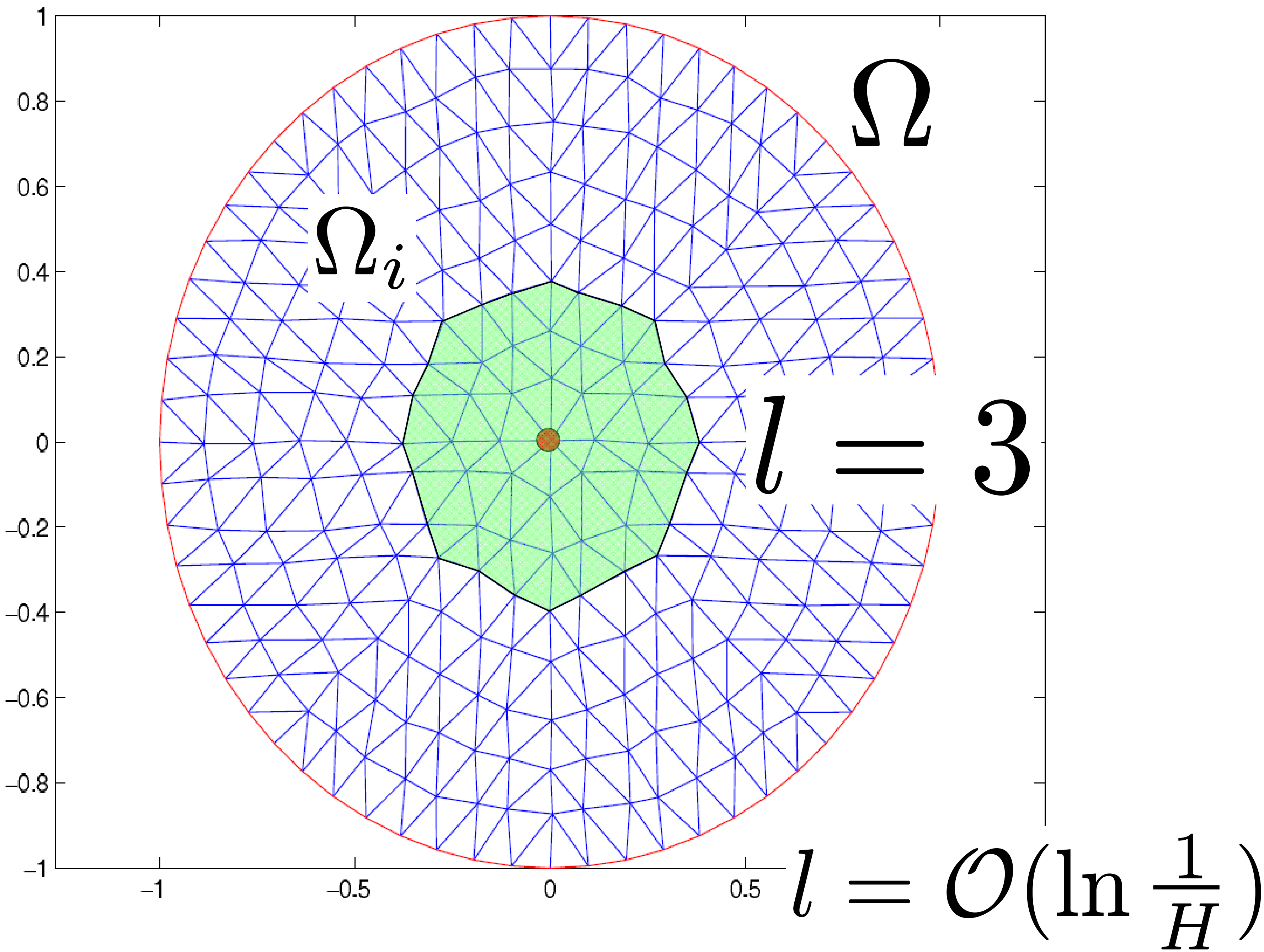
Ω
x_i
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1



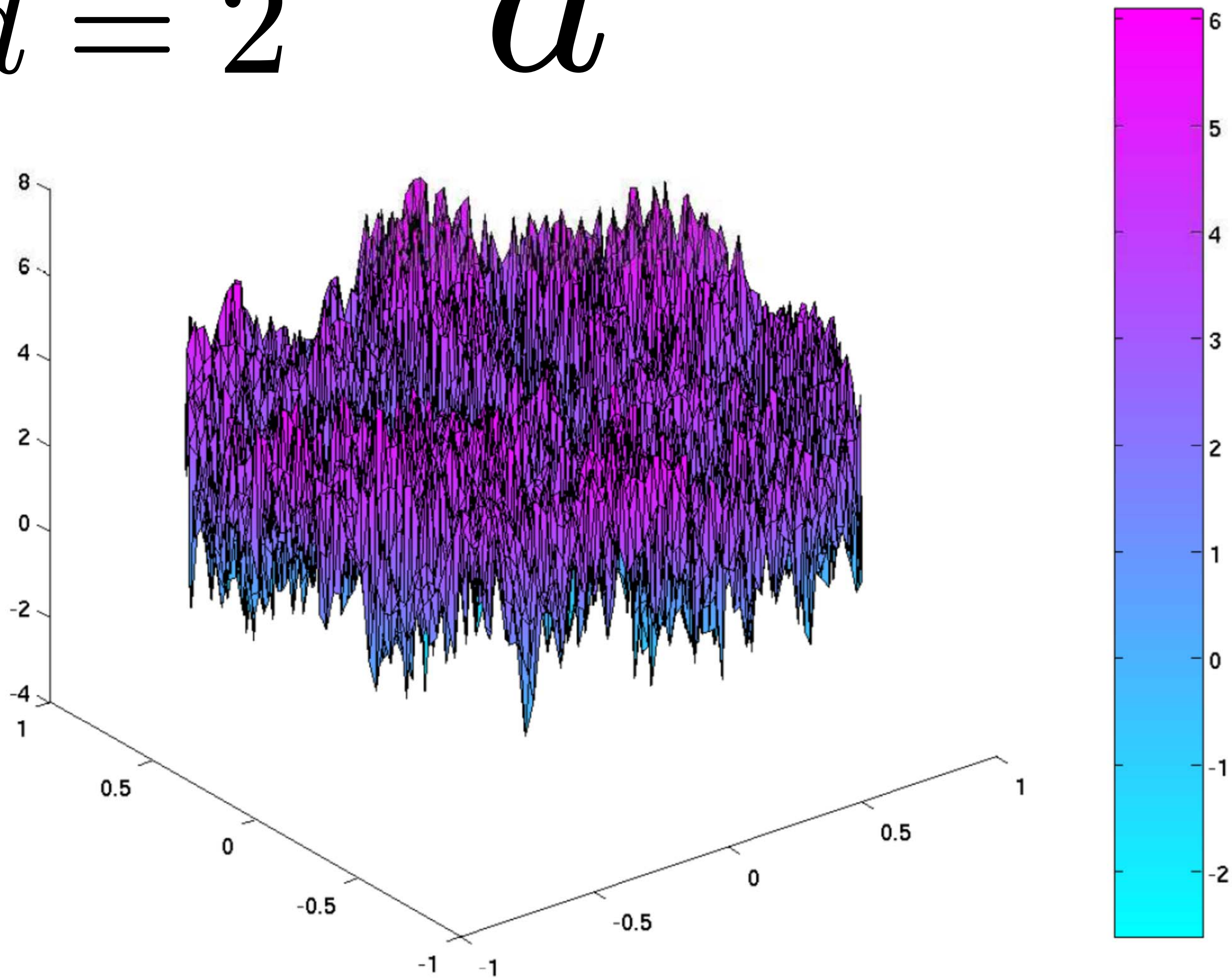
Ω
Ω_i
l = 1
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1

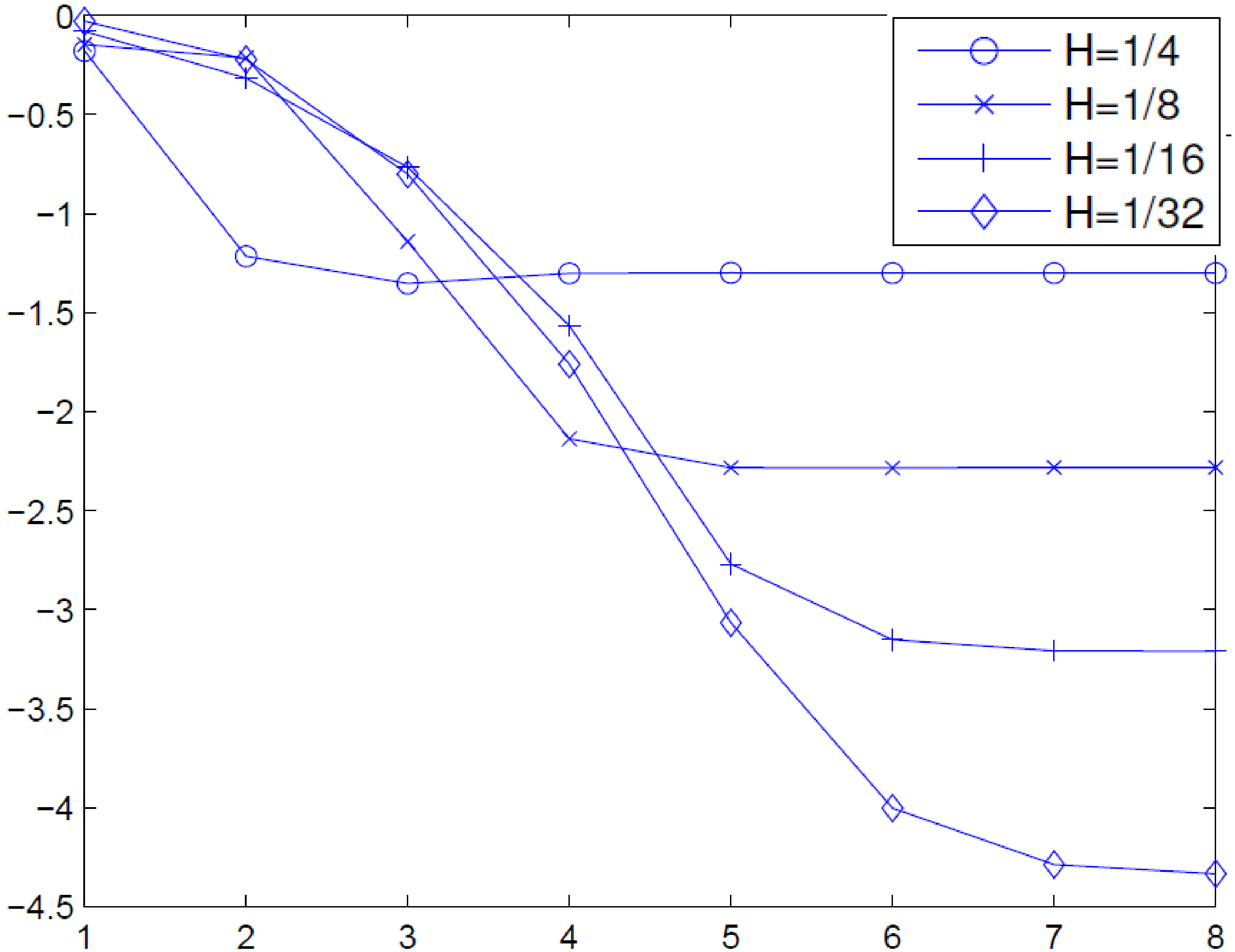


Ω
Ω_i
$l = 2$
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1

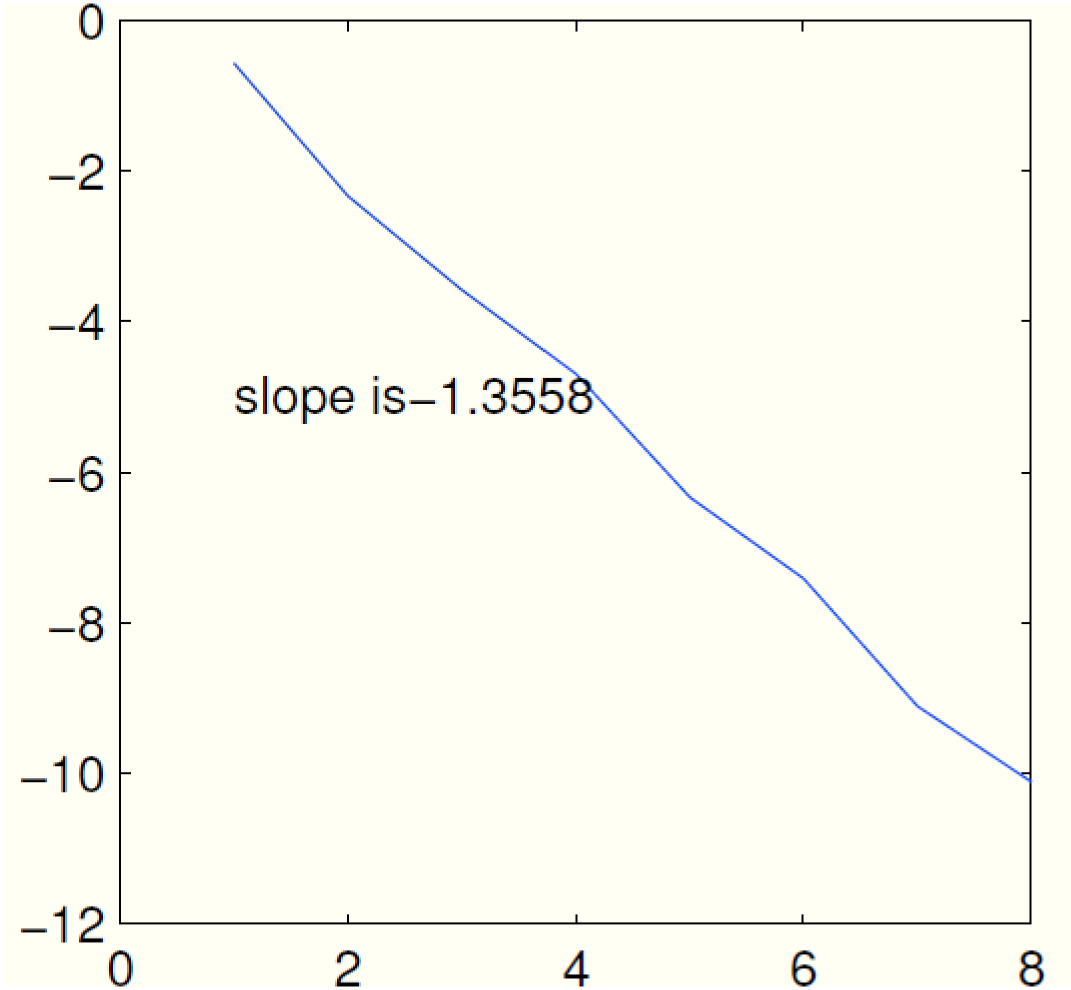

Ω
Ω_i
$l = 3$
$l = \mathcal{O}(\ln \frac{1}{H})$
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5

$d = 2$ a





$\|u - u^{H,\mathrm{loc}}\|_{\mathcal{H}^1(\Omega)}$ vs number of layers l in $\log_{10}$ scale



$\|u - u^{H,\mathrm{loc}}\|_{\mathcal{H}^1(\Omega)}$ vs number of layers l in log scale

1d example

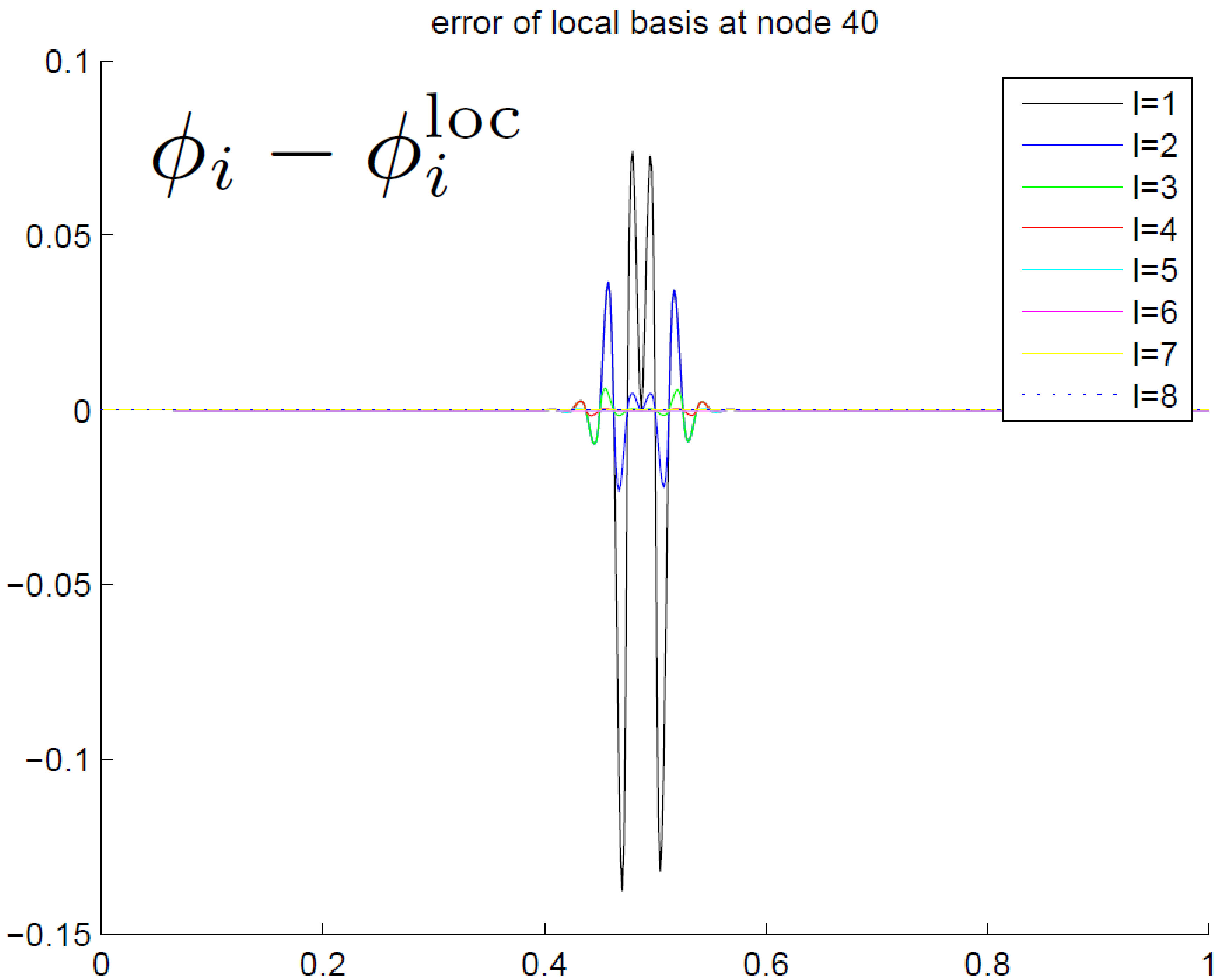
$$d = 1 \qquad \Omega = (0,1)$$

$$a(x) := 1 + \tfrac{1}{2}\sin\left(\textstyle\sum_{k=1}^{K} k^{-\alpha}(\zeta_{1k}\sin(kx) + \zeta_{2k}\cos(kx))\right)$$

$\{\zeta_{1k}\}$, $\{\zeta_{2k}\}$: i.i.d. uniformly distributed in $[-\frac{1}{2}, \frac{1}{2}]$

$$\left\langle |\hat{a}(k)|^2 \right\rangle \simeq |k|^{-\alpha}$$

Example taken out of [Hou-Wu 1997]
and [Ming-Yue 2006]


error of local basis at node 40
$\phi_i - \phi_i^{\mathrm{loc}}$
0.1
0.05
0
−0.05
−0.1
−0.15
0
0.2
0.4
0.6
0.8
1
l=1
l=2
l=3
l=4
l=5
l=6
l=7
l=8

H: Size of the coarse mesh.

h: Size of the fine mesh.

Computational cost | **Localization**

Offline

RPS:

Owhadi-Zhang-Berlyand-12

$$\left(\frac{\log(1/H)}{h}\right)^d$$

$$H \ln \frac{1}{H}$$

Online

$$H^{-d}$$

The basis remains accurate for hyperbolic PDEs

$$\begin{cases} \rho(x)\partial_t^2 u(x,t) - \operatorname{div}\big(a(x)\nabla u(x,t)\big) = g(x,t) & x \in \Omega_T, \\ u = 0 & x \in \partial\Omega_T, \\ \partial_t u = 0 & x \in \Omega \times \{t = 0\} \end{cases}$$

(1) $\Omega_T = \Omega \times (0, T)$

$\rho \in L^\infty(\Omega)$ $\rho(x) \geq \rho_{\min} > 0$

$\partial_t g \in L^2(\Omega_T)$

$u^{H,\mathrm{loc}}$: F.E. solution of (1) over $\mathrm{span}(\phi_i^{\mathrm{loc}})$

$$\boxed{u^{H,\mathrm{loc}}(x,t) = \sum_i c_i(t)\phi_i^{\mathrm{loc}}(x)}$$

The basis remains accurate for hyperbolic PDEs

$$\int \rho \phi_j^{\mathrm{loc}} \partial_t^2 u^{H,\mathrm{loc}} = \int_\Omega \nabla \phi_j^{\mathrm{loc}} a \nabla u^{H,\mathrm{loc}} + \int \phi_j^{\mathrm{loc}} g$$

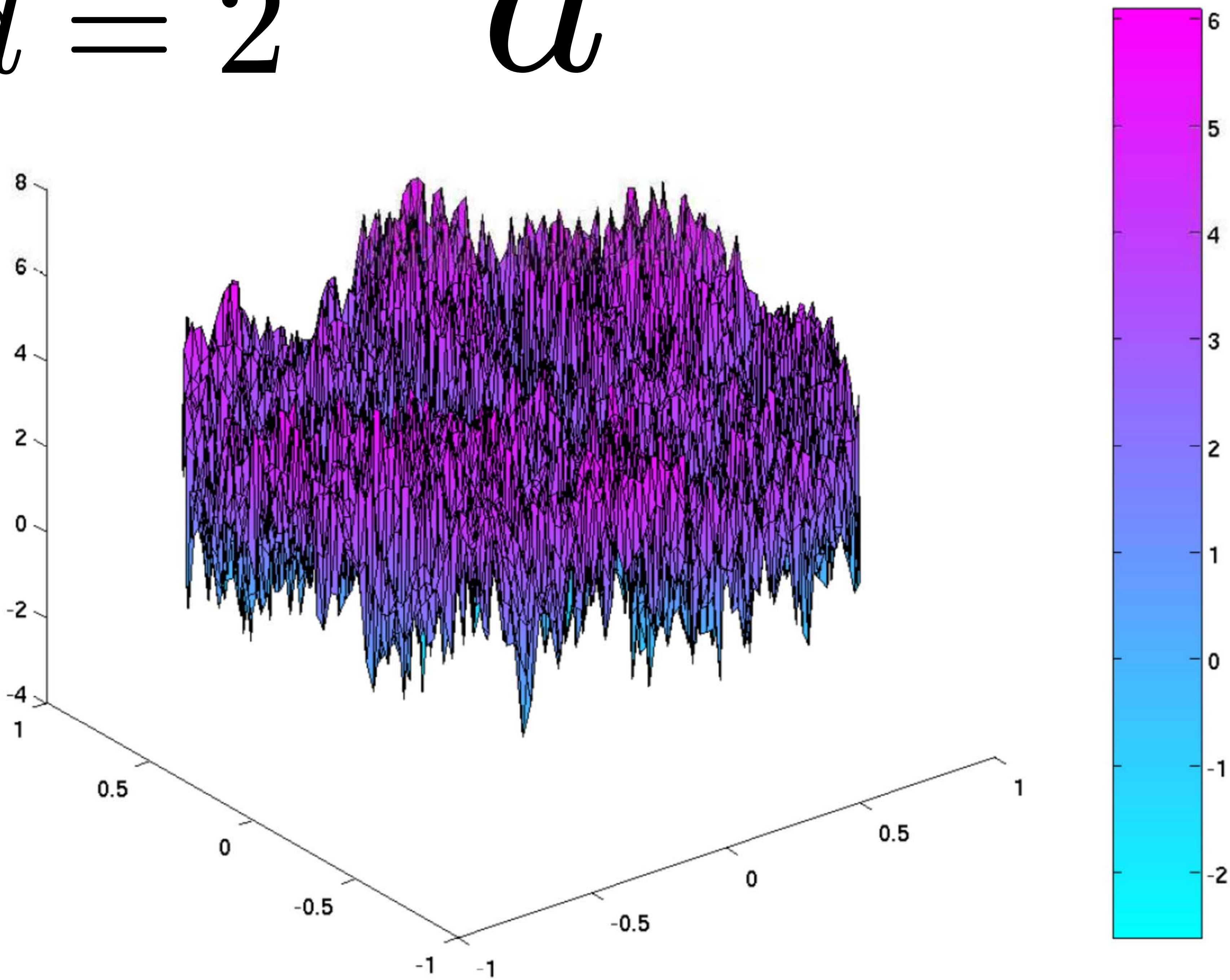
Theorem

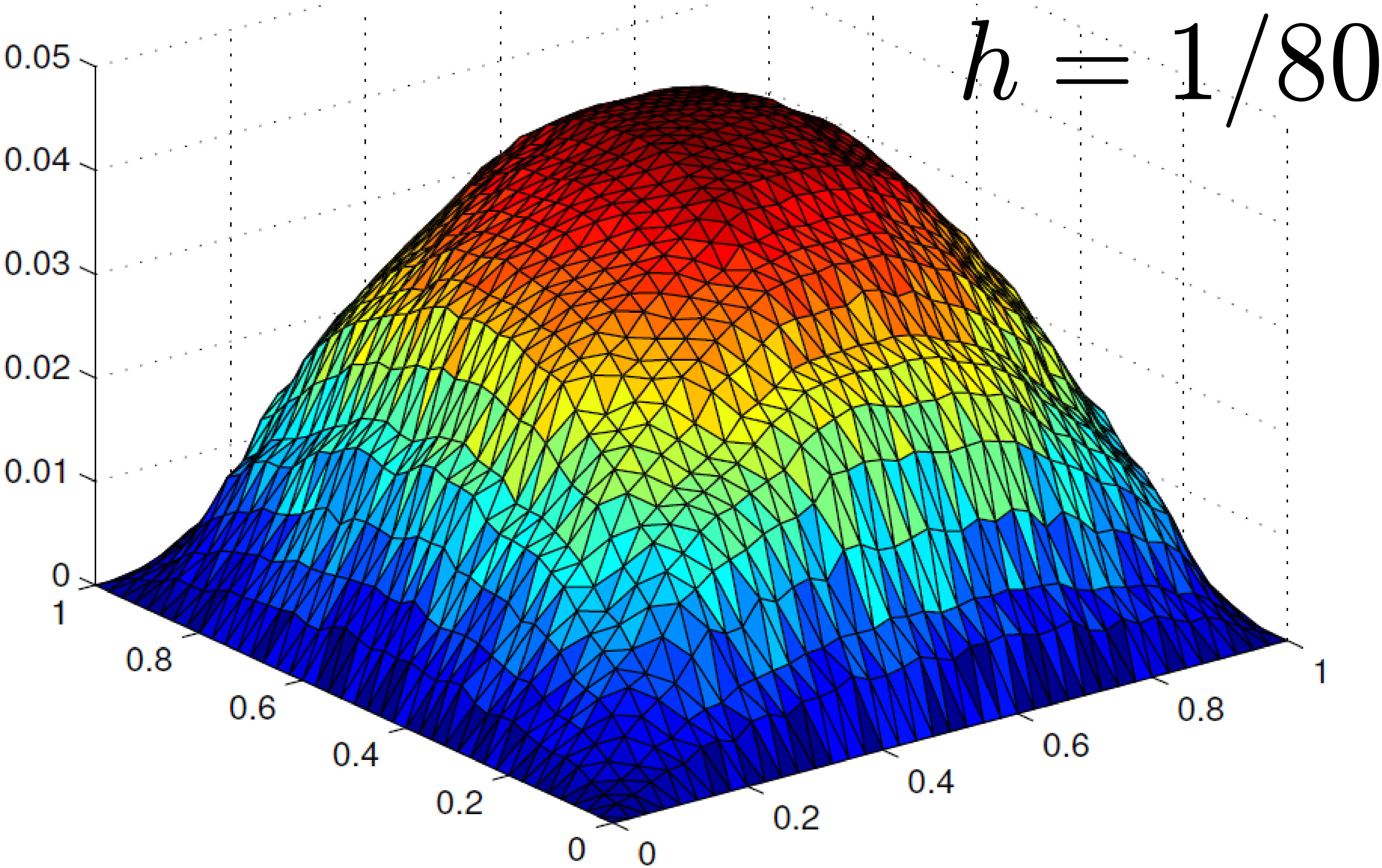
$$\|\partial_t (u - u^{H,\mathrm{loc}})(.,T)\|_{L^2(\Omega)} + \|u - u^{H,\mathrm{loc}}\|_{L^2(0,T,\mathcal{H}_0^1(\Omega))}$$
$$\leq C\Big(\|\partial_t g\|_{L^2(\Omega_T)} + \|g(x,0)\|_{L^2(\Omega)}\Big) H$$

Further (implicit) discretization of $[0,T]$ with time steps Δt

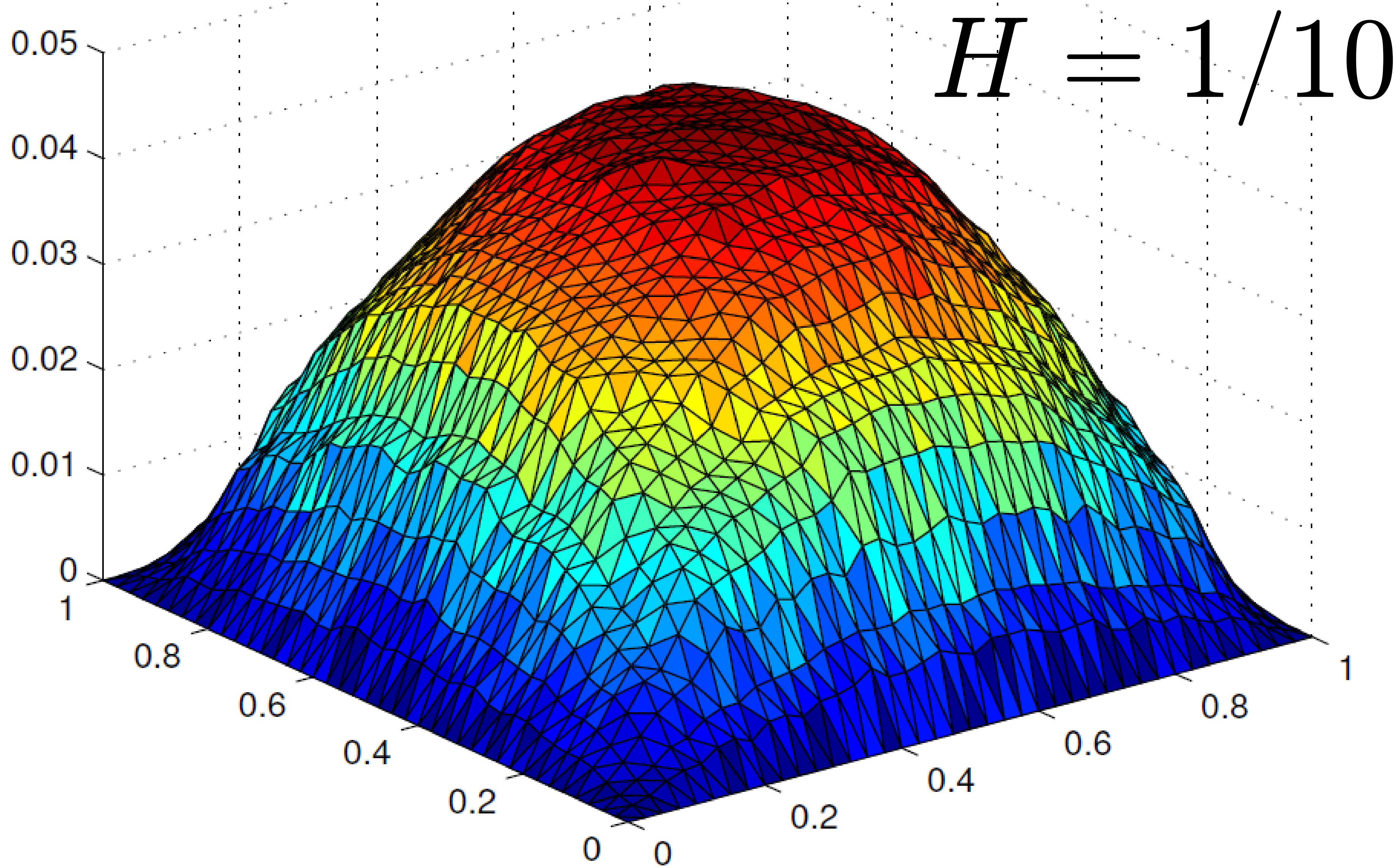
$$\mathrm{Error} \sim (\Delta t + H)$$

$d = 2$ $\quad a$

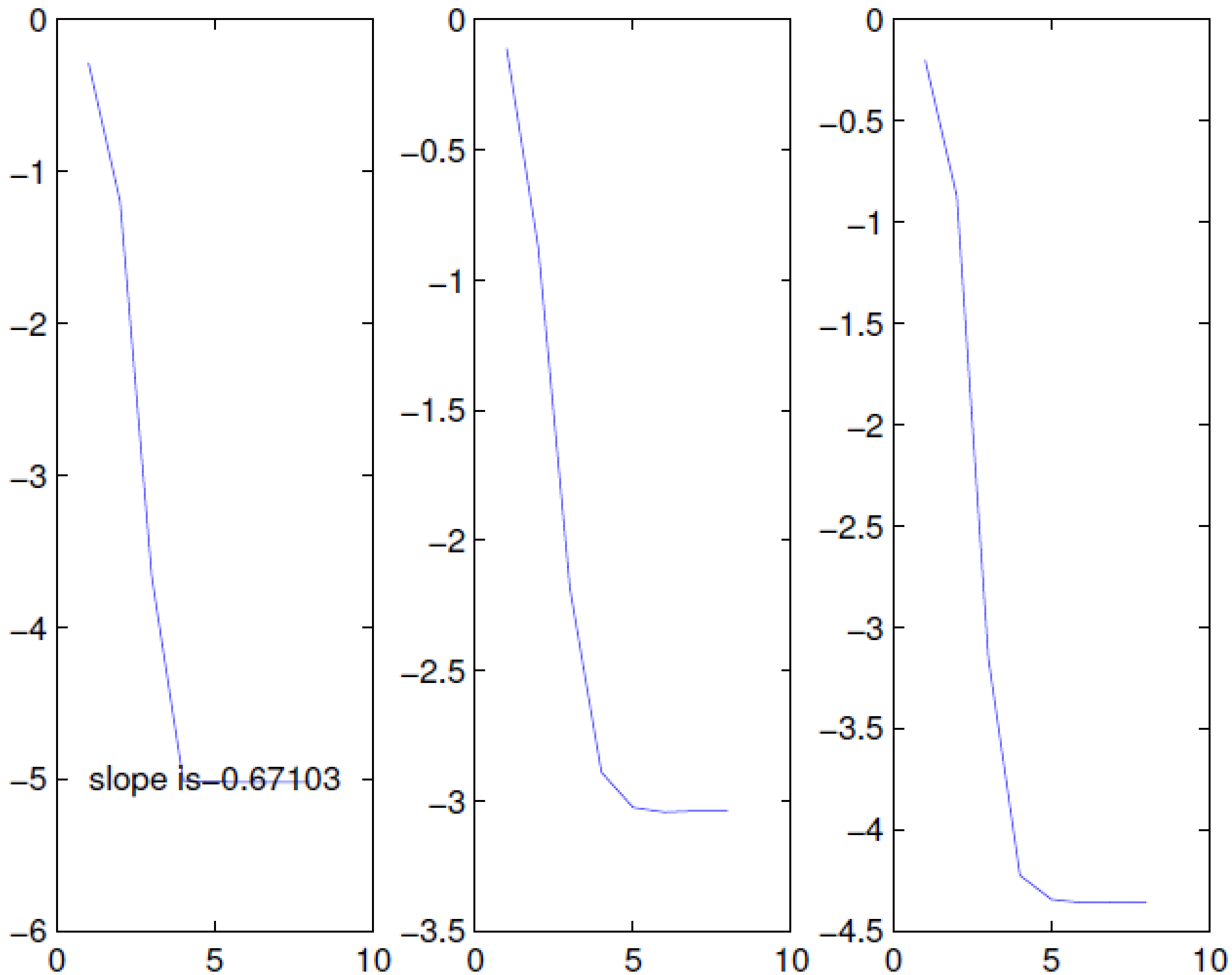




$u(x, T)$ for $T = 1$



$u^{H,\mathrm{loc}}(x, T)$ for $T = 1$



$\|u - u^{H,\text{loc}}\|$ in L^2, $\mathcal{H}^1$ and L^∞ norm

vs number of layers l, in log scale

Quantity of Interest $\Phi(\mu^\dagger) = \mu^\dagger[X \geq a]$

$\mu^\dagger$: Unknown or partially known measure of probability on $\mathbb{R}$

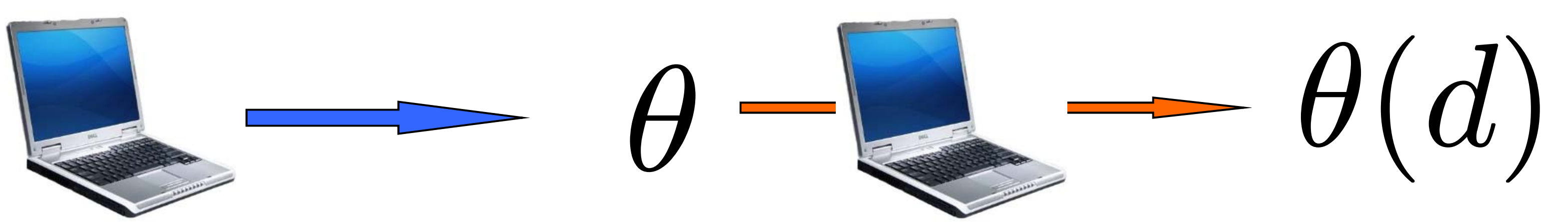
You know $\mu^\dagger \in \mathcal{A}$

You observe $d = (d_1, \ldots, d_n) \in \mathbb{R}^n$

n i.i.d samples from $\mu^\dagger$

Problem:

Compute the best estimate of $\Phi(\mu^\dagger)$



Player A

Chooses $\mu^\dagger \in \mathcal{A}$

Player B

Chooses θ

$$\mathcal{E}(\mu^\dagger, \theta)$$

Mean squared error

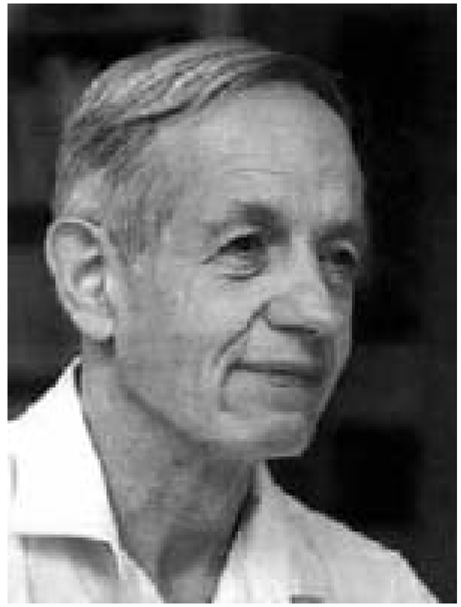
$$\mathcal{E}(\mu^\dagger, \theta) = \mathbb{E}_{d \sim (\mu^\dagger)^n}\Big[\big[\theta(d) - \Phi(\mu^\dagger)\big]^2\Big]$$

Confidence error

$$\mathcal{E}(\mu^\dagger, \theta) = \mathbb{P}_{d \sim (\mu^\dagger)^n}\Big[\big|\theta(d) - \Phi(\mu^\dagger)\big| \geq r\Big]$$

Game theory and statistical decision theory

John Von Neumann



John Nash

Abraham Wald

The best strategy is to play at random

Obtained by finding the worst prior in the Bayesian class of estimators

Player A

Chooses $\mu^\dagger \in \mathcal{A}$

Player B

Chooses θ

$$\mathcal{E}(\mu^\dagger, \theta)$$

Best strategy for A $\quad \mu^\dagger \sim \pi_A \in \mathcal{M}(\mathcal{A})$

The best strategy for B

$$\theta_{\pi_B}(d) = \mathbb{E}_{\mu \sim \pi_B,\, d' \sim \mu^n}\Big[\Phi(\mu) \Big| d' = d\Big]$$

The best strategy for A and B = worst prior for B

$$\max_{\pi \in \mathcal{M}(\mathcal{A})} \mathbb{E}_{\mu \sim \pi}\Big[\mathcal{E}(\mu, \theta_\pi)\Big]$$

Can this form of calculus in infinite dimensional spaces and framework facilitate the process of scientific discovery?

Identification of accurate bases for numerical homogenization with optimal recovery properties

Bayesian Numerical Homogenization

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

$\Omega \subset \mathbb{R}^d$ $\partial\Omega$ is piec. Lip.

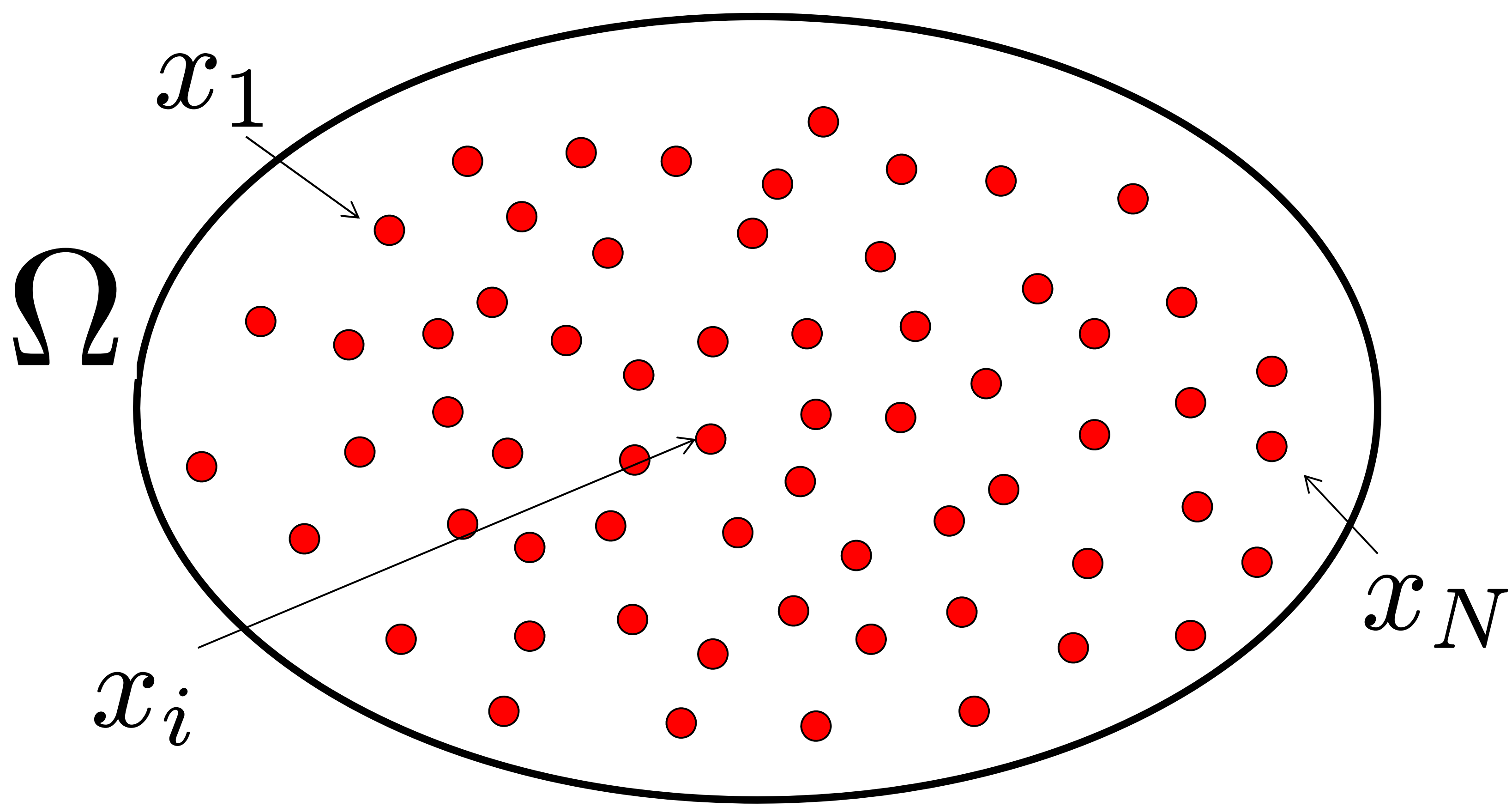
a unif. ell. $a_{i,j} \in L^\infty(\Omega)$

$d \leq 3$

We want to homogenize (1)

Alternative Approach

$$\text{Select } \{x_1, \ldots, x_N\} \subset \Omega$$



Player A

Chooses

$g \in L^2(\Omega)$

Player B

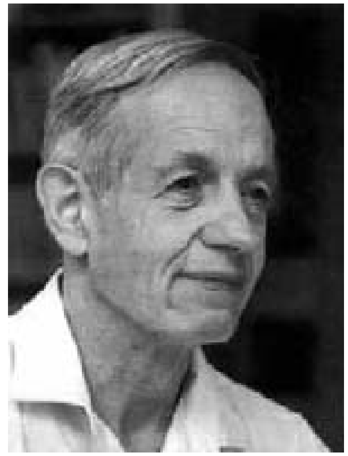
Sees

$u(x_1), \ldots, u(x_N)$

Chooses θ

$$\mathcal{E}(g,\theta) = \Big| u(x) - \theta\big(u(x_1), \ldots, u(x_N)\big) \Big|^2$$

Game theory and statistical decision theory



John Nash

John Von Neumann

Abraham Wald

The best strategy is to play at random

Obtained by finding the worst prior in the Bayesian class of estimators

Replace g by a stochastic field ξ

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

$g \in L^2(\Omega)$ ⟺ ξ: white noise

$g \in H^{\pm s}(\Omega)$ ⟺ $\xi = \Delta^{\mp s/2}$white noise

Best strategy

$$\theta = \mathbb{E}\left[u(x) \middle| u(x_1), \ldots, u(x_N)\right]$$