A calculus for the Optimal Quantification of Uncertainties

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CSE15

"Technology, in common with many other activities, tends toward avoidance of risks by investors. Uncertainty is ruled out if possible. People generally prefer the predictable. Few recognize how destructive this can be, how it imposes severe limits on variability and thus makes whole populations fatally vulnerable to the shocking ways our universe can throw the dice."

Frank Herbert (Heretics of Dune)

Main Question

Can we, to some degree, turn a scientific problem into a UQ problem and, to some degree, solve it as such in an automated fashion using techniques developed to deal with missing information in epistemic and model uncertainty?

Example

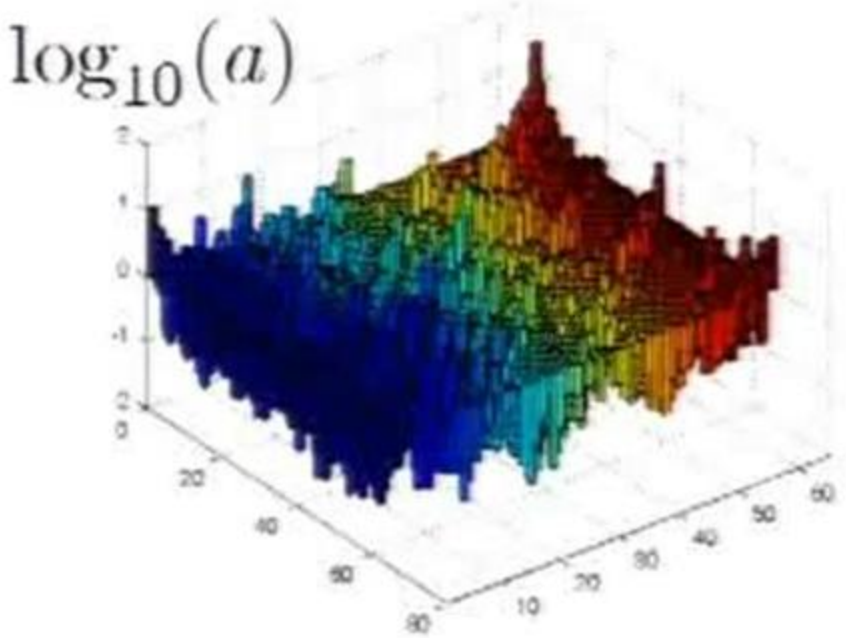
Problem: Find a method for solving (1) as fast as possible to a given accuracy

(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.

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



Multigrid Methods

Multigrid: [Fedorenko, 1961, Brandt, 1973, Hackbusch, 1978]

Multiresolution/Wavelet based methods

[Brewster and Beylkin, 1995, Beylkin and Coult, 1998, Averbuch et al., 1998]

- **Linear complexity with smooth coefficients**

Problem **Severely affected by lack of smoothness**

Robust/Algebraic multigrid

[Mandel et al., 1999,Wan-Chan-Smith, 1999, Xu and Zikatanov, 2004, Xu and Zhu, 2008], [Ruge-Stüben, 1987]

- Some degree of robustness but problem remains open with rough coefficients

Why? **Interpolation operators are unknown**

Don't know how to bridge scales with rough coefficients!

Low Rank Matrix Decomposition methods

Fast Multipole Method: [Greengard and Rokhlin, 1987]

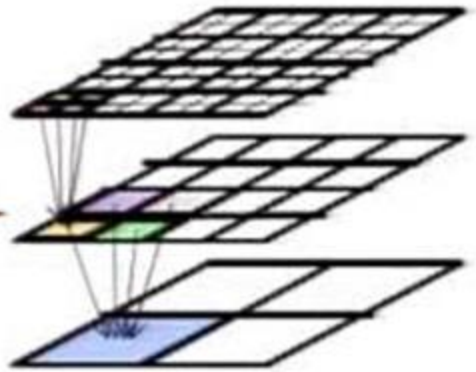
Hierarchical Matrix Method: [Hackbusch et al., 2002]

[Bebendorf, 2008]:

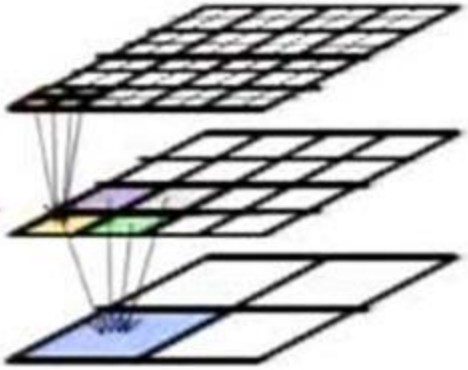
$$N \ln^{d+3} N \text{ complexity}$$

Common theme between these methods

Their process of discovery is based on intuition, brilliant insight, and guesswork



Can we turn this process of discovery into an algorithm?



Answer: Yes by identifying an underlying information game and finding an optimal strategy for playing the game

[Owhadi 2015, Multi-grid with rough coefficients and Multiresolution PDE decomposition from Hierarchical Information Games, arXiv:1503.03467]

Resulting method: $N \ln^2 N$ complexity

This is a theorem

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

Resulting method:

$$H_0^1(\Omega) = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)} \oplus_a \cdots$$

$$< \psi, \chi >_a := \int_\Omega (\nabla\psi)^T a \nabla\chi = 0 \text{ for } (\psi, \chi) \in \mathfrak{W}^{(i)} \times \mathfrak{W}^{(j)},\ i \neq j$$

Theorem For $v \in \mathfrak{W}^{(k)}$

$$\frac{C_1}{2^k} \leq \frac{\|v\|_a}{\|\operatorname{div}(a\nabla v)\|_{L^2(\Omega)}} \leq \frac{C_2}{2^k}$$

$$\|v\|_a^2 := < v, v >_a = \int_\Omega (\nabla v)^T a \nabla v$$

Looks like an eigenspace decomposition

$$u = w^{(1)} + w^{(2)} + \cdots + w^{(k)} + \cdots$$

$w^{(k)}$ = F.E. sol. of PDE in $\mathfrak{W}^{(k)}$

Can be computed independently

$B^{(k)}$: Stiffness matrix of PDE in $\mathfrak{W}^{(k)}$

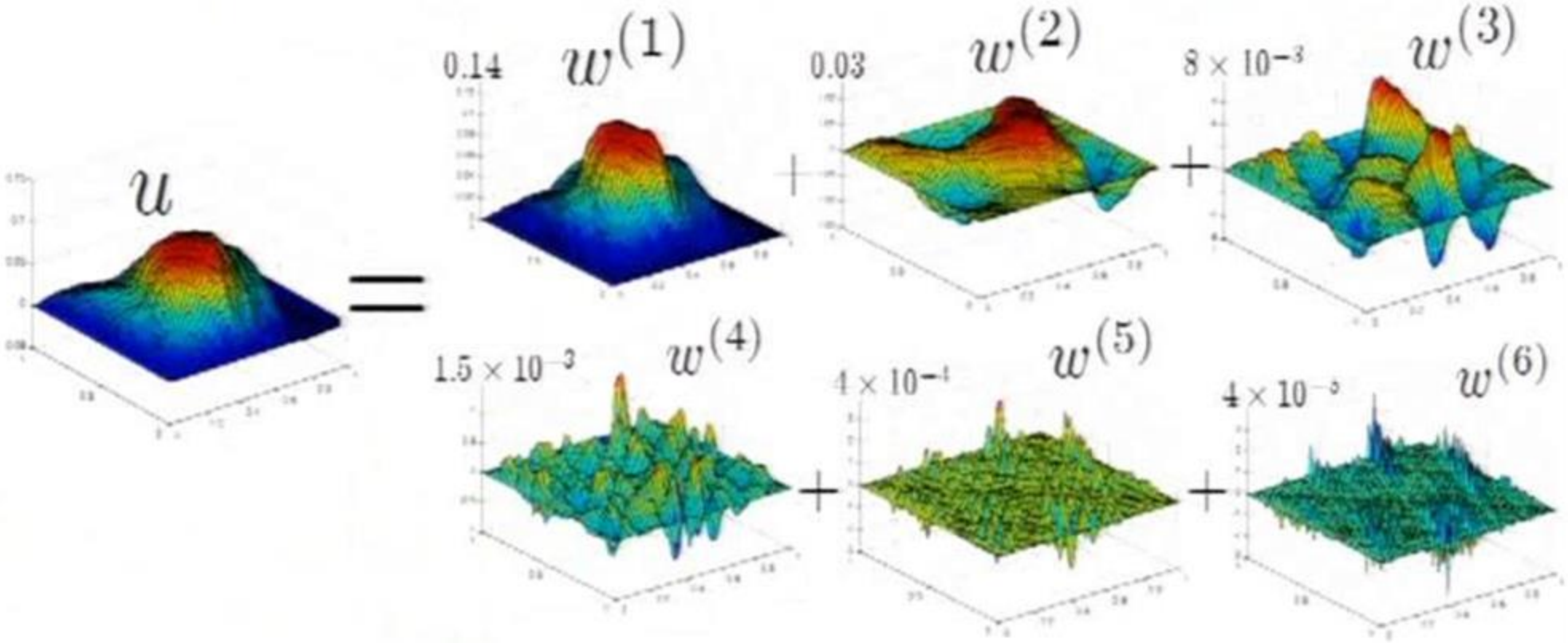
Theorem

$$\frac{\lambda_{\max}(B^{(k)})}{\lambda_{\min}(B^{(k)})} \leq C$$

Just relax in $\mathfrak{W}^{(k)}$ to find $w^{(k)}$

Quacks like an eigenspace decomposition

Multiresolution decomposition of solution space



Solve time-discretized wave equation (implicit time steps) with rough coefficients in $\mathcal{O}(N \ln^2 N)$-complexity

Swims like an eigenspace decomposition

$\mathfrak{V}$: F.E. space of $H_0^1(\Omega)$ of dim. N

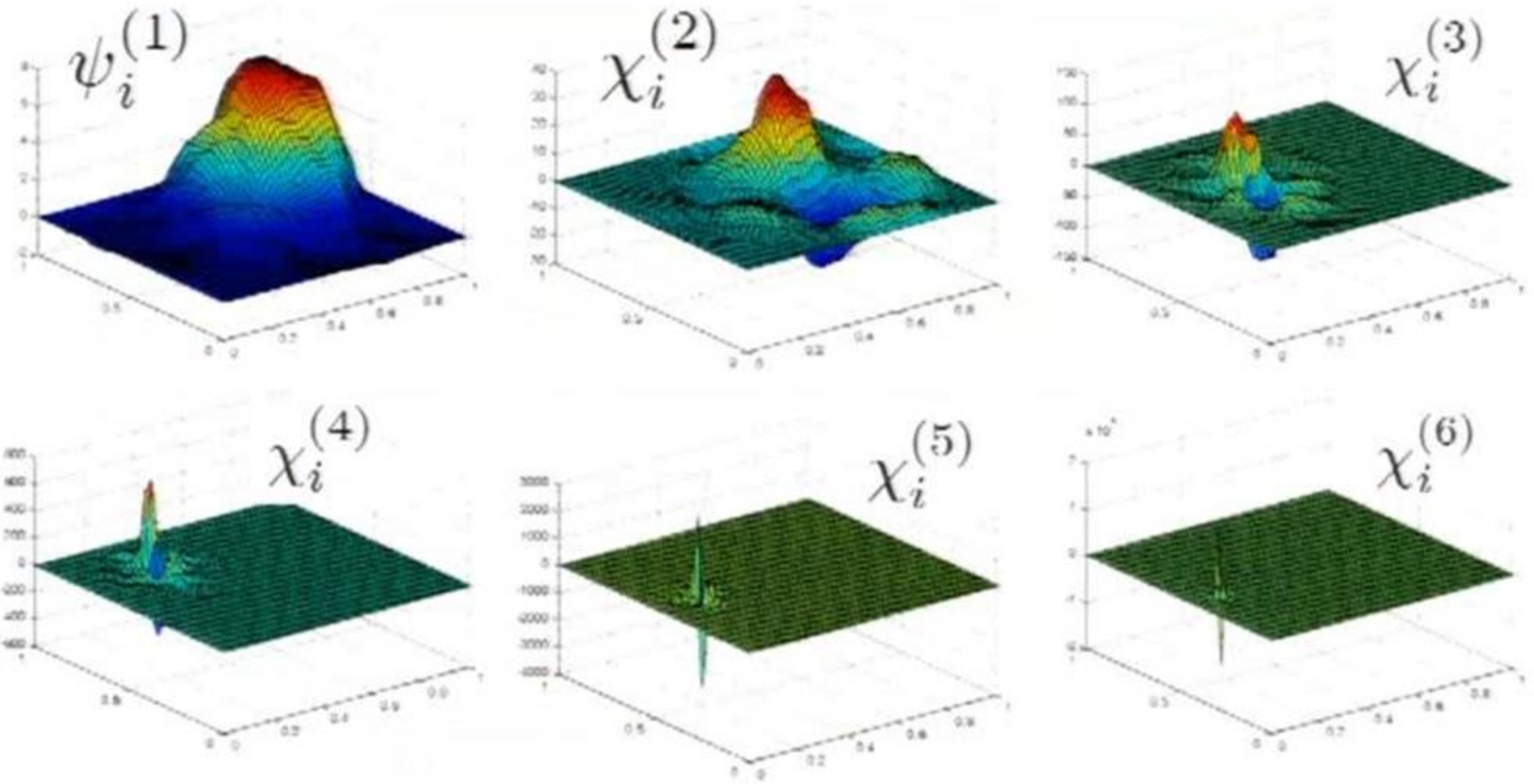
Theorem The decomposition

$$\mathfrak{V} = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)}$$

Can be performed and stored in

$$\mathcal{O}(N \ln^2 N) \text{ operations}$$

Doesn't have the complexity of an eigenspace decomposition



Basis functions look like and behave like wavelets: Localized and can be used to compress the operator and locally analyze the solution space

Discovery process

Identify underlying information game

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

Measurement functions: $\phi_1, \ldots, \phi_m \in L^2(\Omega)$

Player A

Chooses

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

$\|g\|_{L^2(\Omega)} \leq 1$

Player B

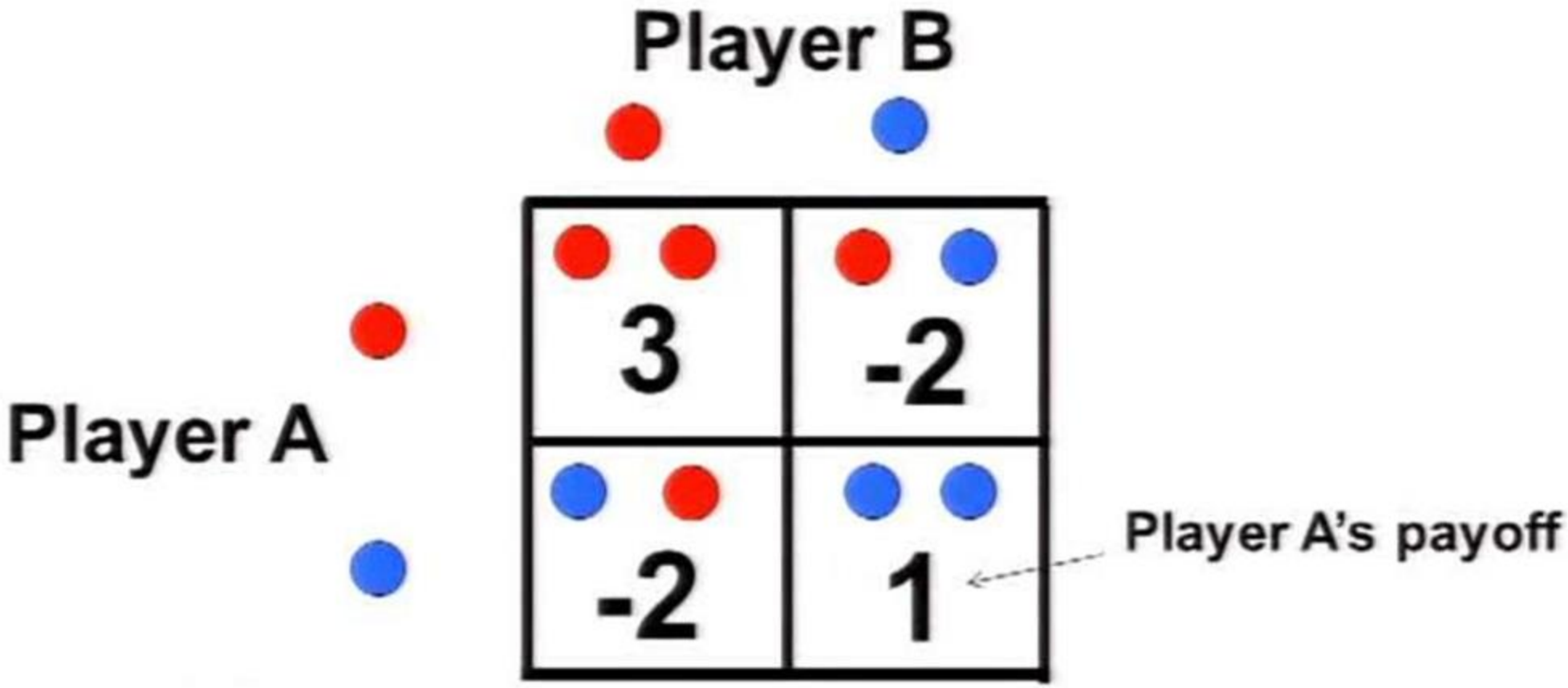
Sees $\int_\Omega u\phi_1, \ldots, \int_\Omega u\phi_m$

Chooses $u^* \in L^2(\Omega)$

$\mathcal{M}ax$ $\mathcal{M}in$

$$\|u - u^*\|_{L^2(\Omega)}$$

Deterministic zero sum game



Player A & B both have a blue and a red marble

At the same time, they show each other a marble

How should A & B play the (repeated) game?

Game theory

Optimal strategies are mixed strategies

Optimal way to play is at random

Player A \ Player B	q	$1-q$
p	3	-2
$1-p$	-2	1

John Von Neumann

John Nash

A's expected payoff

$$= 3pq + (1-p)(1-q) - 2p(1-q) - 2q(1-p)$$

$$= 1 - 3q + p(8q-3) = -\frac{1}{8} \quad \text{for } q = \frac{3}{8}$$

Player A

Chooses
$g \in L^2(\Omega)$
$\|g\|_{L^2(\Omega)} \leq 1$

Player B

Sees $\int_\Omega u\varphi_1, \ldots, \int_\Omega u\varphi_m$
Chooses $u^* \in L^2(\Omega)$

$$\left\| u - u^* \right\|_{L^2(\Omega)}$$

Continuous game but as in decision theory under compactness it can be approximated by a finite game

Abraham Wald

The best strategy for A is to play at random

Player's B best strategy live in the Bayesian class of estimators

Player B's class of mixed strategies

Pretend that player A is choosing g at random

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

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases} \quad \Longleftrightarrow \quad \begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ v = 0 \text{ on } \partial\Omega, \end{cases}$$

Player B's bet

$$u^*(x) := \mathbb{E}\left[v(x) \middle| \int_\Omega v(y)\phi_i(y)\,dy = \int_\Omega u(y)\phi_i(y)\,dy, \forall i\right]$$

Player's B optimal strategy?

Player B's best bet? $\Longleftrightarrow$ min max problem over distribution of ξ

Computational efficiency ➡ $\xi \sim \mathcal{N}(0, \Gamma)$

⬇

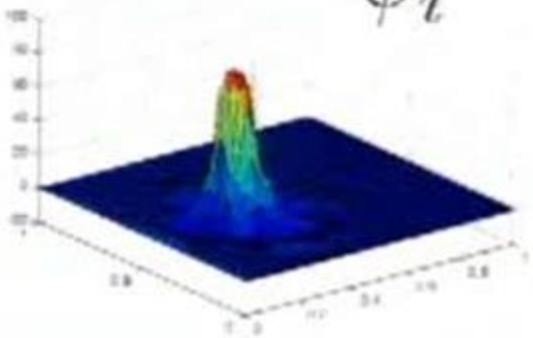
Elementary gambles form deterministic basis functions for player's B bet

⬇

Theorem

$$u^*(x) = \sum_{i=1}^{m} \psi_i(x) \int_\Omega u(y)\phi_i(y)\, dy$$

ψ_i



Gamblets

ψ_i: Elementary gambles/bets

Player B's bet if $\int_\Omega u\phi_j = \delta_{i,j},\ j = 1, \ldots, m$

$$\psi_i(x) := \mathbb{E}_{\xi \sim \mathcal{N}(0,\Gamma)}\left[v(x) \,\middle|\, \int_\Omega v(y)\phi_j(y)\, dy = \delta_{i,j},\ j \in \{1, \ldots, m\} \right]$$

What are these gamblets?

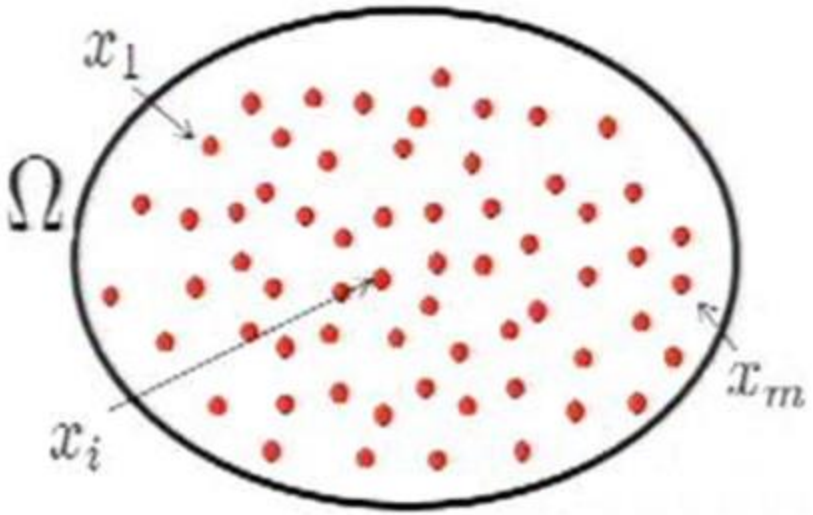
Depend on

- Γ: Covariance function of ξ (player's B decision)
- $(\phi_i)_{i=1}^m$: Measurements functions (rules of the game)

Example [Owhadi. 2014] arXiv:1406.6668

$$\Gamma(x,y) = \delta(x-y)$$

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



$$a = I_d \quad \Longleftrightarrow \quad \psi_i\text{: Polyharmonic splines}$$

[Harder-Desmarais, 1972] [Duchon 1976, 1977,1978]

$$a_{i,j} \in L^\infty(\Omega) \quad \Longleftrightarrow \quad \psi_i\text{: Rough Polyharmonic splines}$$

[Owhadi-Zhang-Berlyand 2013]

What is player's B best strategy?

What is player's B best choice for

$$\Gamma(x,y) = \mathbb{E}\big[\xi(x)\xi(y)\big] \quad ?$$

$$\boxed{\Gamma = \mathcal{L}} \longleftrightarrow \int_\Omega \xi(x) f(x)\, dx \sim \mathcal{N}(0, \|f\|_a^2)$$

$$\|f\|_a^2 := \int_\Omega (\nabla f)^T a \nabla f$$

$$\boxed{\mathcal{L} = -\operatorname{div}(a\nabla\cdot)}$$

Why? ⟷ **See algebraic generalization**

The recovery is optimal (Galerkin projection)

Theorem If $\Gamma = \mathcal{L}$ then

$u^*(x)$ is the F.E. solution of (1) in $\text{span}\{\mathcal{L}^{-1}\phi_i | i = 1, \ldots, m\}$

$$\|u - u^*\|_a = \inf_{\psi \in \text{span}\{\mathcal{L}^{-1}\phi_i : i \in \{1,\ldots,m\}\}} \|u - \psi\|_a$$

$$\mathcal{L} = -\operatorname{div}(a\nabla\cdot)$$

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

Optimal variational properties

Theorem

$\sum_{i=1}^{m} w_i \psi_i$ minimizes $\|\psi\|_a$
over all ψ such that $\int_\Omega \phi_j \psi = w_j$ for $j = 1, \ldots, m$

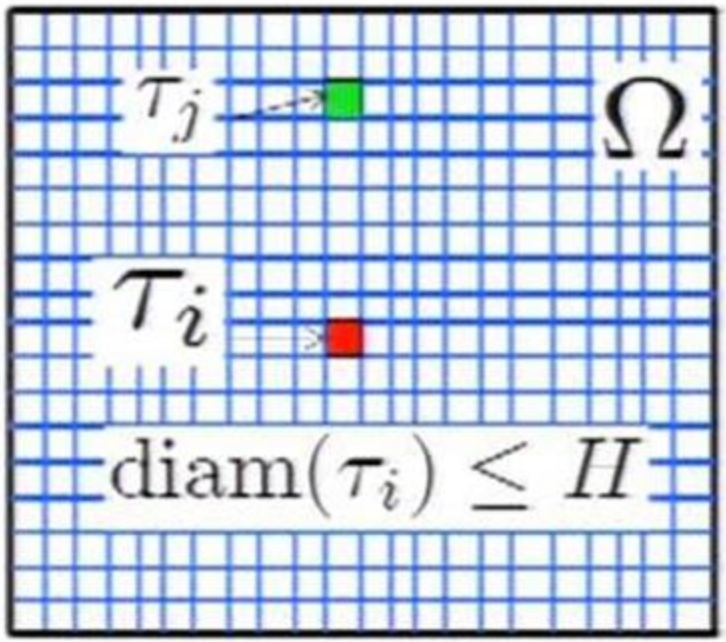
Variational characterization

Theorem ψ_i: Unique minimizer of

$$\begin{cases} \text{Minimize} & \|\psi\|_a \\ \text{Subject to} & \psi \in H_0^1(\Omega) \text{ and } \int_\Omega \phi_j \psi = \delta_{i,j}, \quad j = 1, \ldots, m \end{cases}$$

Selection of measurement functions

Example Indicator functions of a Partition of Ω of resolution H



$$\phi_i = 1_{\tau_i}$$

Theorem

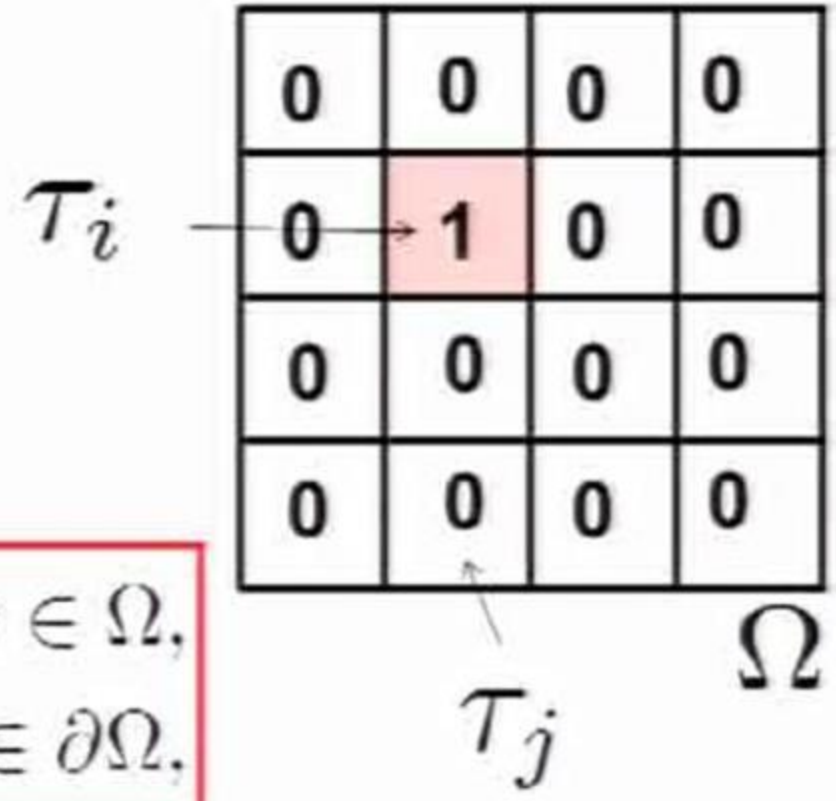
$$\|u - u^*\|_a \leq \frac{H}{\lambda_{\min}(a)} \|g\|_{L^2(\Omega)}$$

Elementary gamble

ψ_i

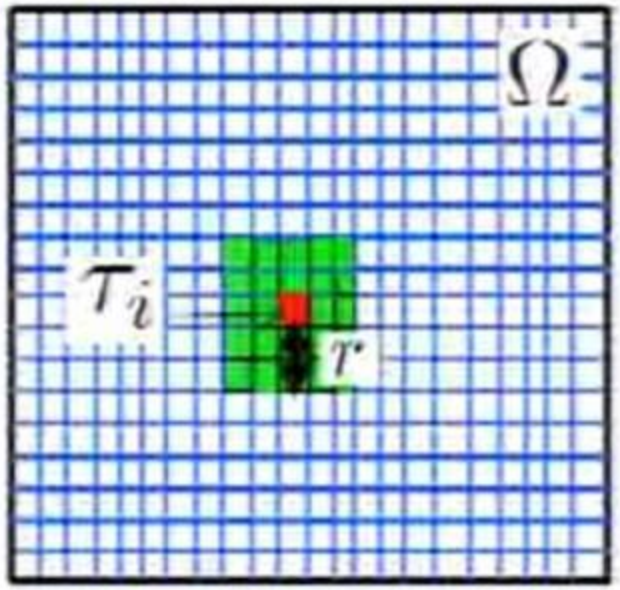
Your best bet on the value of u given the information that

$\int_{\tau_i} u = 1$ and $\int_{\tau_j} u = 0$ for $j \neq i$



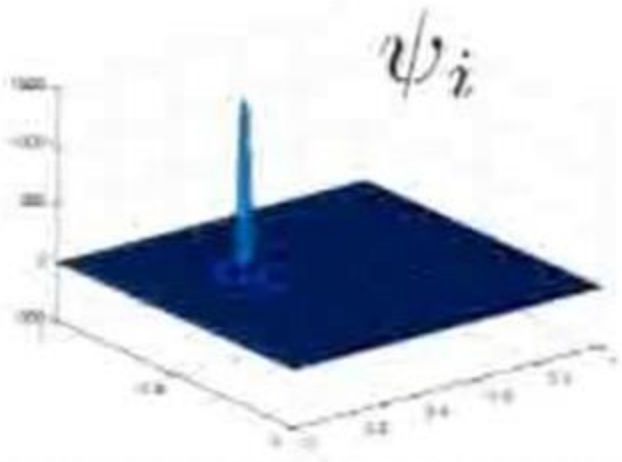
(1)
$$\begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

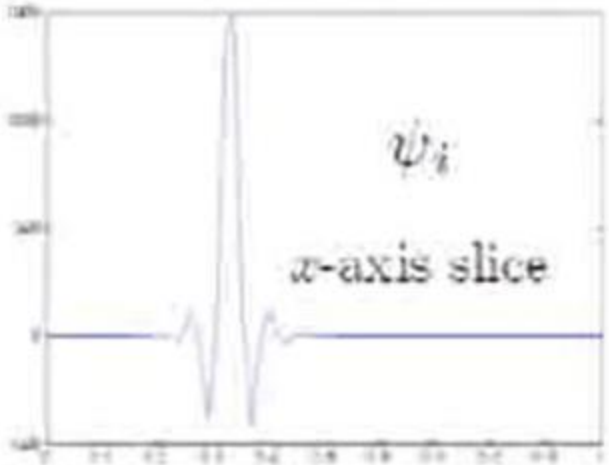
Exponential decay of gamblets

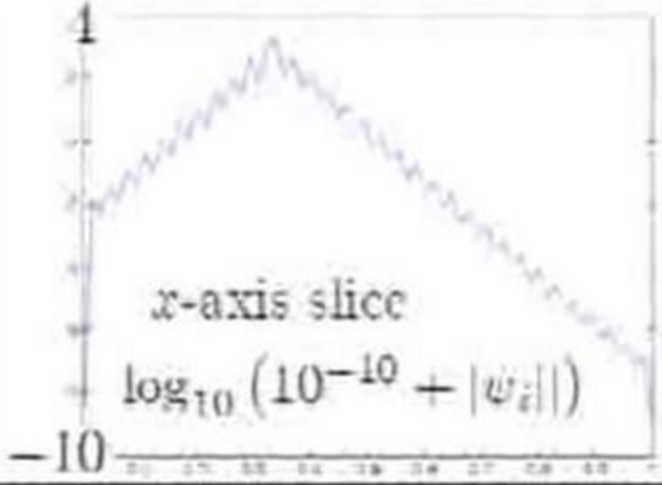


Theorem

$$\int_{\Omega \cap (B(\tau_i, r))^c} (\nabla \psi_i)^T a \nabla \psi_i \leq e^{-\frac{r}{\tau_H}} \|\psi_i\|_a^2$$



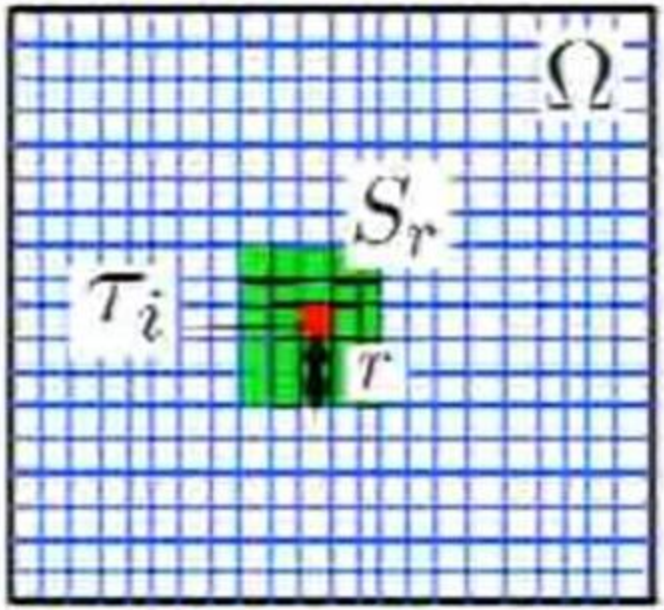




Localization of the computation of gamblets

$\psi_i^{\mathrm{loc},r}$: Minimizer of

$$\begin{cases} \text{Minimize} & \|w\|_a \\ \text{Subject to} & w \in \mathcal{W}_0^1(S_r) \text{ and } \int_{S_r} \omega_j w = \delta_{i,j} \\ & \text{for } \tau_j \in S_r \end{cases}$$



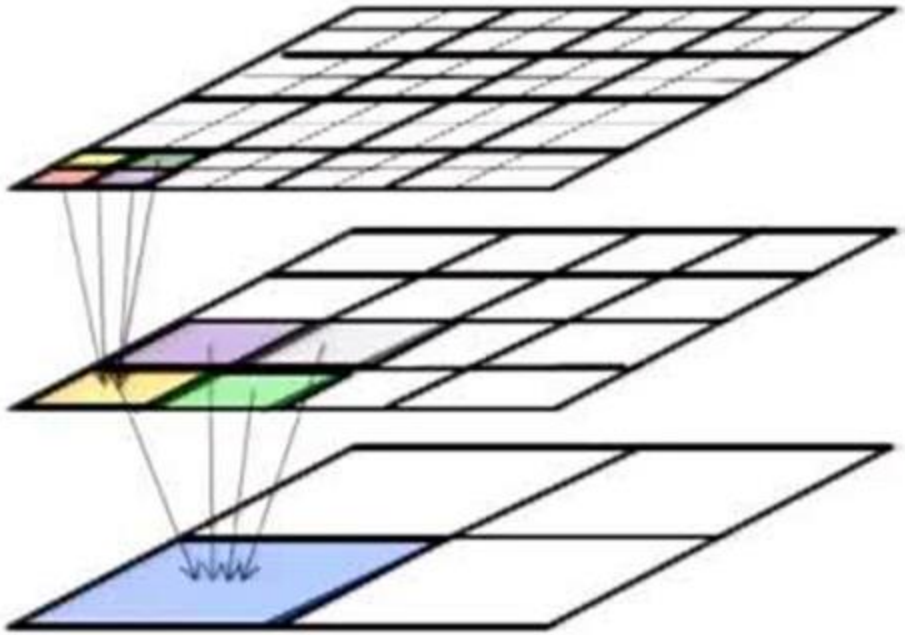
No loss of accuracy if localization $\sim H \ln \frac{1}{H}$

$$u^{*,\mathrm{loc}}(x) = \sum_{i=1}^{m} \psi_i^{\mathrm{loc,r}}(x) \int_\Omega u(y)\phi_i(y)\,dy$$

Theorem If $r \geq CH \ln \frac{1}{H}$

$$\|u - u^{*,\mathrm{loc}}\|_a \leq \frac{1}{\sqrt{\lambda_{\min}(a)}} H \|g\|_{L^2(\Omega)}$$

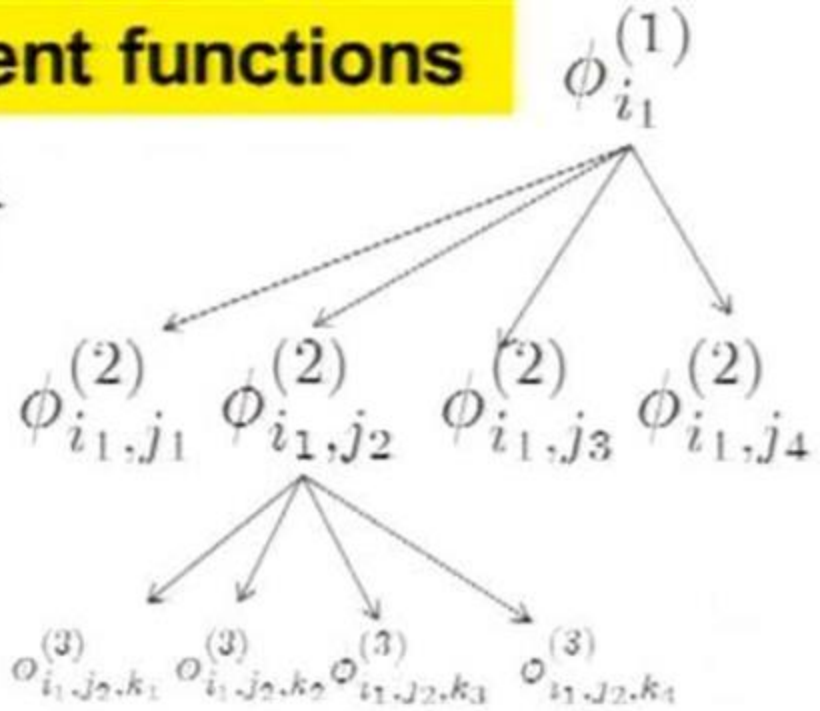
Formulation of the hierarchical game



Hierarchy of nested Measurement functions

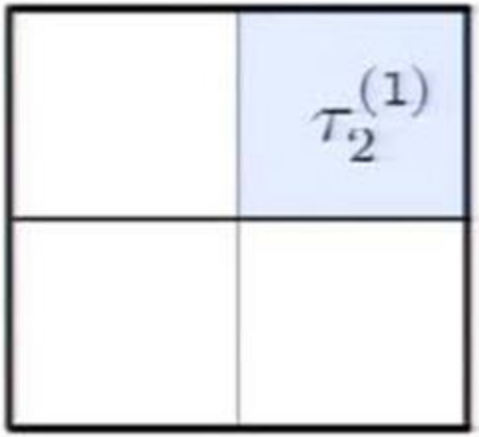
$$\phi^{(k)}_{i_1,\ldots,i_k} \text{ with } k \in \{1,\ldots,q\}$$

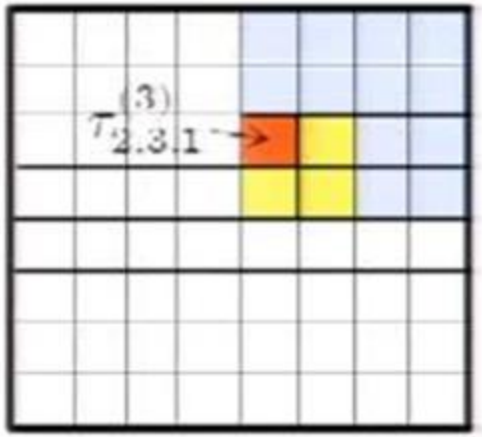
$$\phi^{(k)}_i = \sum_j c_{i,j}\phi^{(k+1)}_{i,j}$$



Example

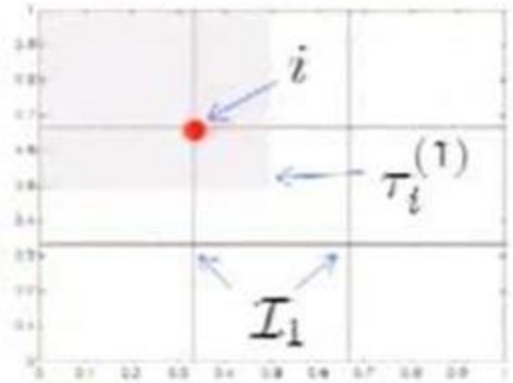
$\phi^{(k)}_i$: Indicator functions of a hierarchical nested partition of Ω of resolution $H_k = 2^{-k}$

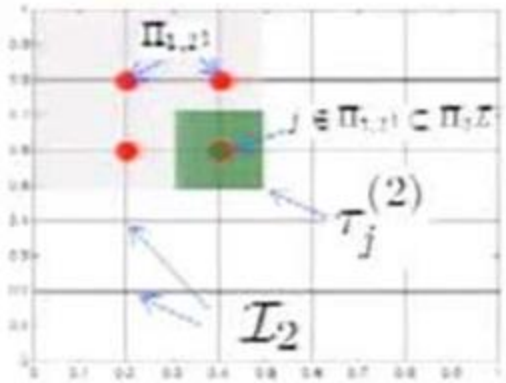


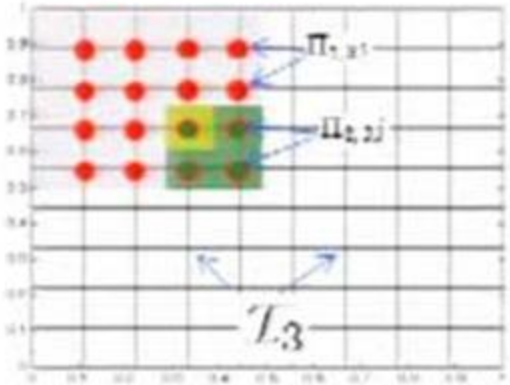


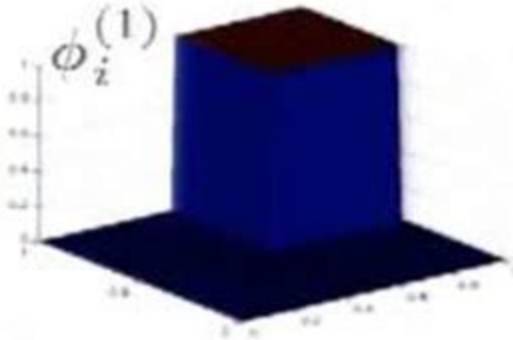
$$\phi^{(1)}_2 = 1_{\tau^{(1)}_2} \qquad \phi^{(2)}_{2,3} = 1_{\tau^{(2)}_{2,3}} \qquad \phi^{(3)}_{2,3,1} = 1_{\tau^{(3)}_{2,3,1}}$$

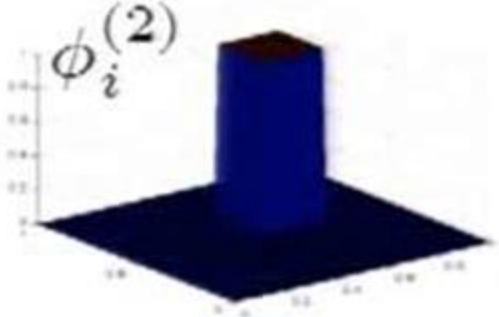
In the discrete setting simply aggregate elements (as in algebraic multigrid)

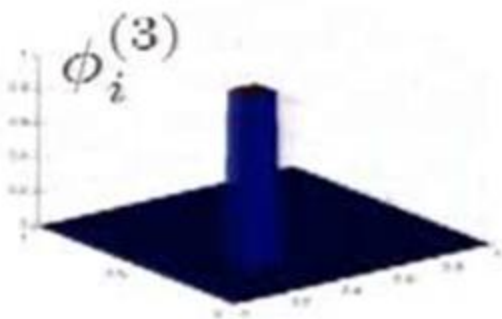


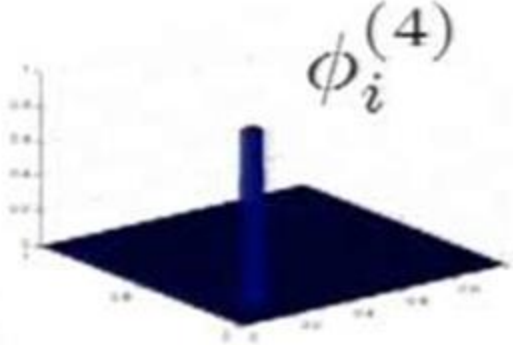


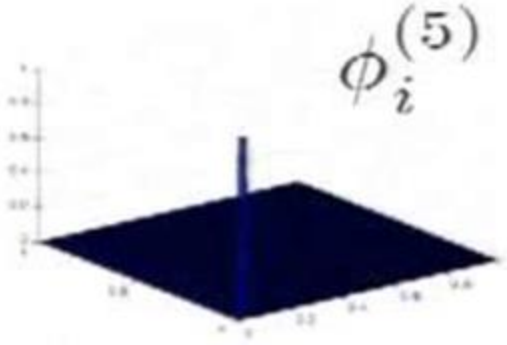


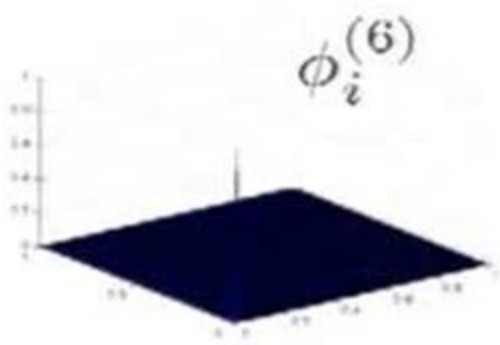












Formulation of the hierarchy of games

Player A

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

Player B

Chooses

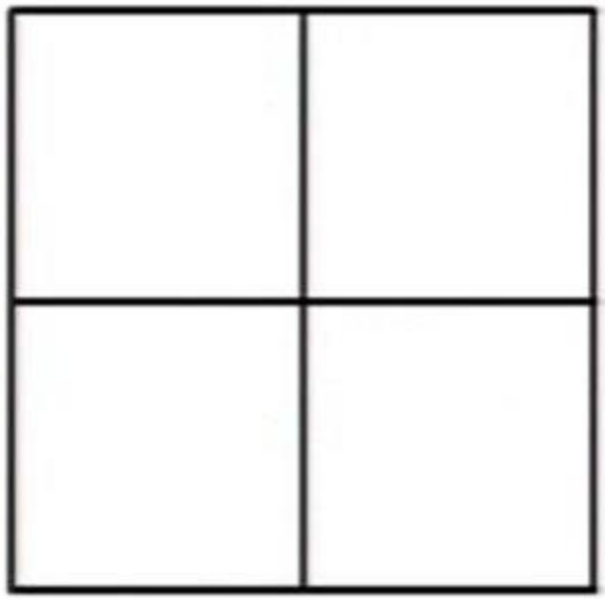
$g \in L^2(\Omega)$

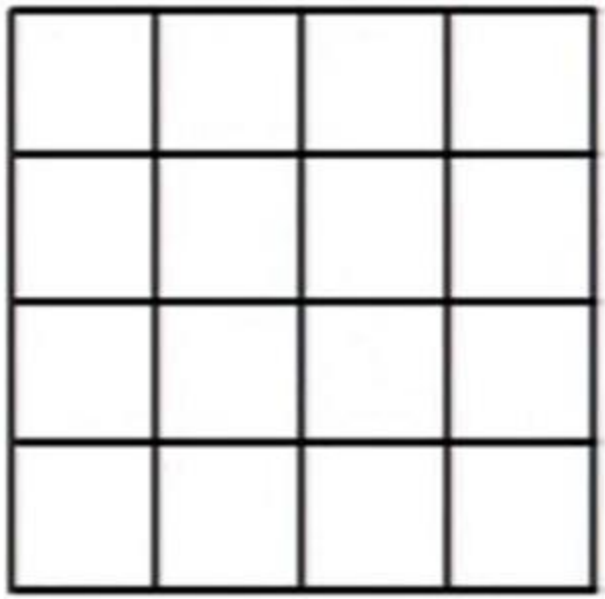
$\|g\|_{L^2(\Omega)} \leq 1$

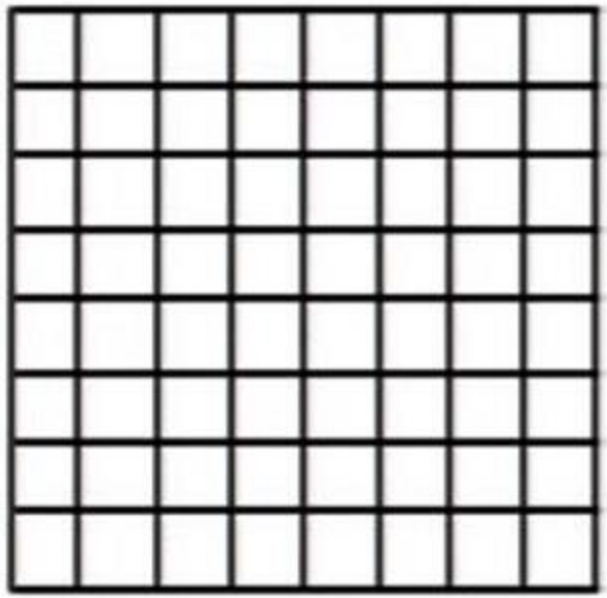
Sees $\{\int_\Omega u\phi_i^{(k)}, i \in \mathcal{I}_k\}$

Must predict

u and $\{\int_\Omega u\phi_j^{(k+1)}, j \in \mathcal{I}_{k+1}\}$







Player B's best strategy

$$\xi \sim \mathcal{N}(0, \mathcal{L})$$

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega. \\ u = 0 \text{ on } \partial\Omega, \end{cases} \quad \Longleftrightarrow \quad \begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega. \\ v = 0 \text{ on } \partial\Omega, \end{cases}$$

Player B's bets

$$u^{(k)}(x) := \mathbb{E}\Big[v(x)\Big| \int_\Omega v(y)\phi_i^{(k)}(y)\,dy - \int_\Omega u(y)\phi_i^{(k)}(y)\,dy.\ i \in \mathcal{I}_k\Big]$$

The sequence of approximations form a martingale under the mixed strategy emerging from the game

$$\mathcal{F}_k = \sigma\Big(\int_\Omega v\phi_i^{(k)},\ i \in \mathcal{I}_k\Big) \qquad v^{(k)}(x) := \mathbb{E}\Big[v(x)\Big|\mathcal{F}_k\Big]$$

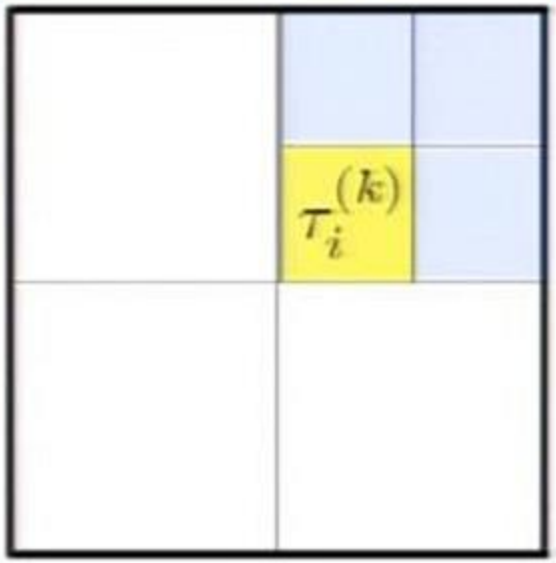
Theorem $\mathcal{F}_k \subset \mathcal{F}_{k+1}$

$$v^{(k)}(x) := \mathbb{E}\Big[v^{(k+1)}(x)\Big|\mathcal{F}_k\Big]$$

Accuracy of the recovery

Theorem

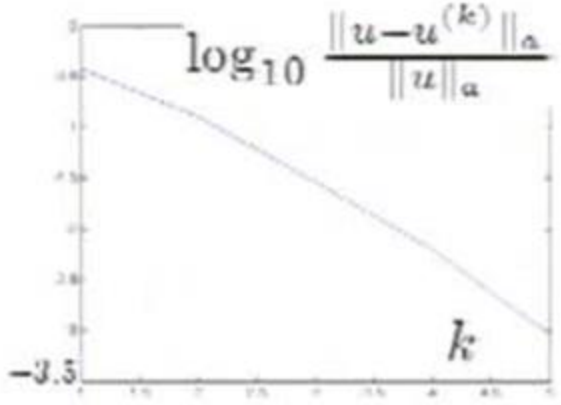
$$\|u - u^{(k)}\|_a \leq \frac{H_k}{\lambda_{\min}(a)} \|g\|_{L^2(\Omega)}$$

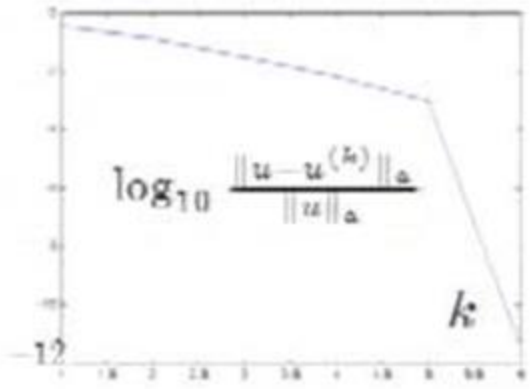


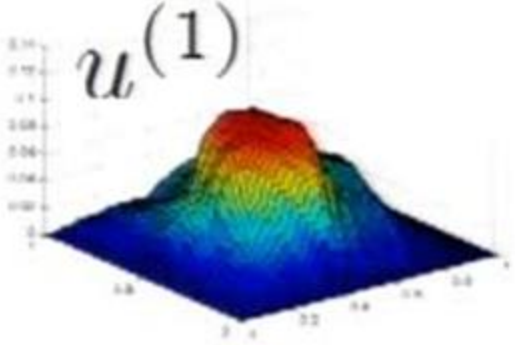
$$H_k := \max_i \operatorname{diam}(\tau_i^{(k)})$$

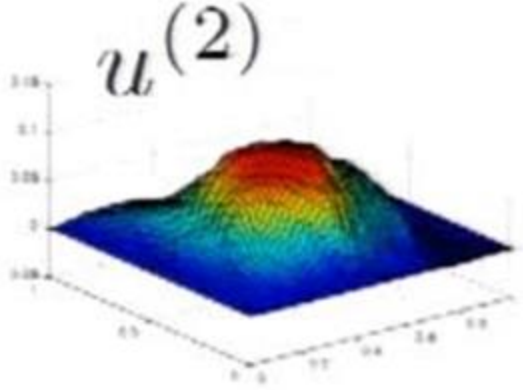
$$\phi_i^{(k)} = 1_{\tau_i^{(k)}} \qquad \operatorname{diam}(\tau_i^{(k)}) \leq H_k$$

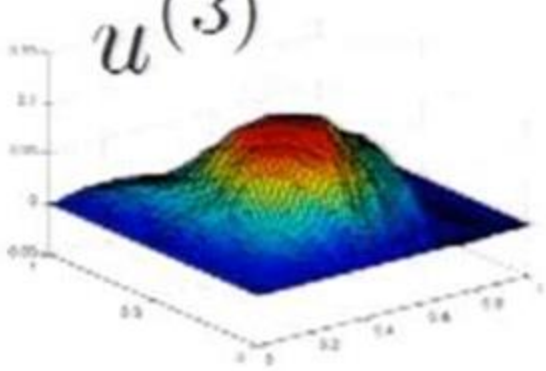
In a discrete setting the last step of the game recovers the solution to numerical precision

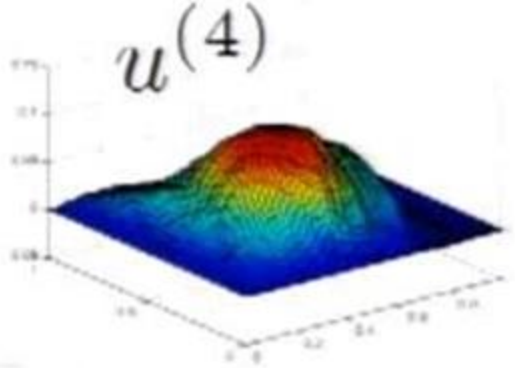


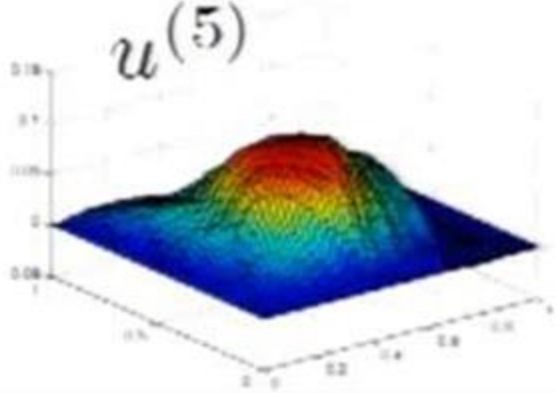


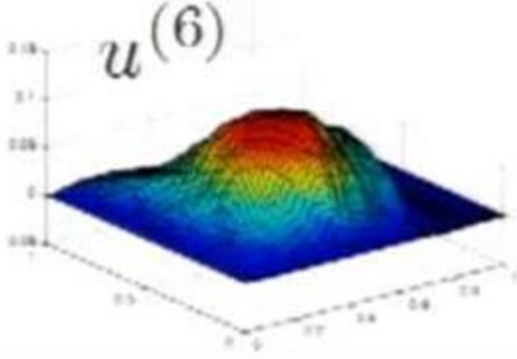












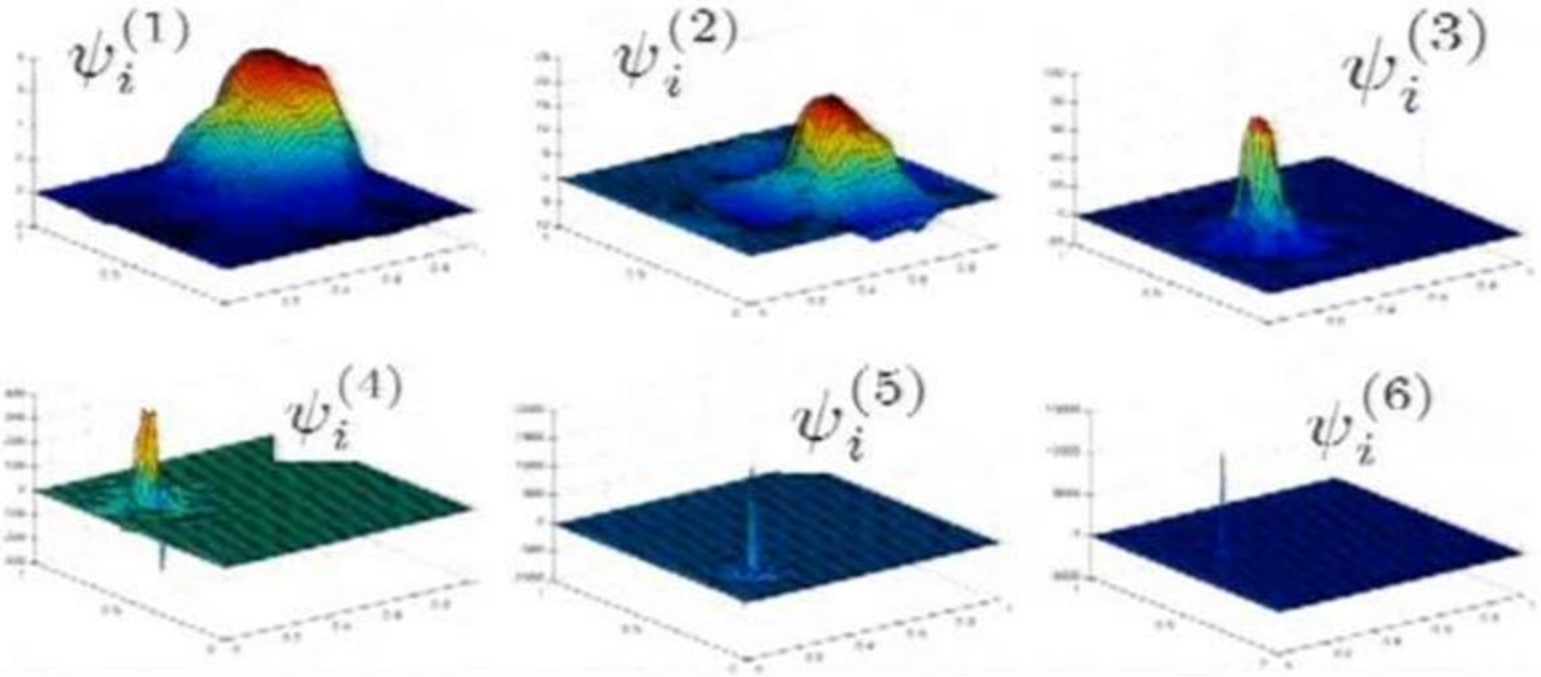
Gamblets Elementary gambles form a hierarchy of deterministic basis functions for player's B hierarchy of bets

Theorem

$$u^{(k)}(x) = \sum_i \psi_i^{(k)}(x) \int_\Omega u(y)\phi_i^{(k)}(y)\,dy$$

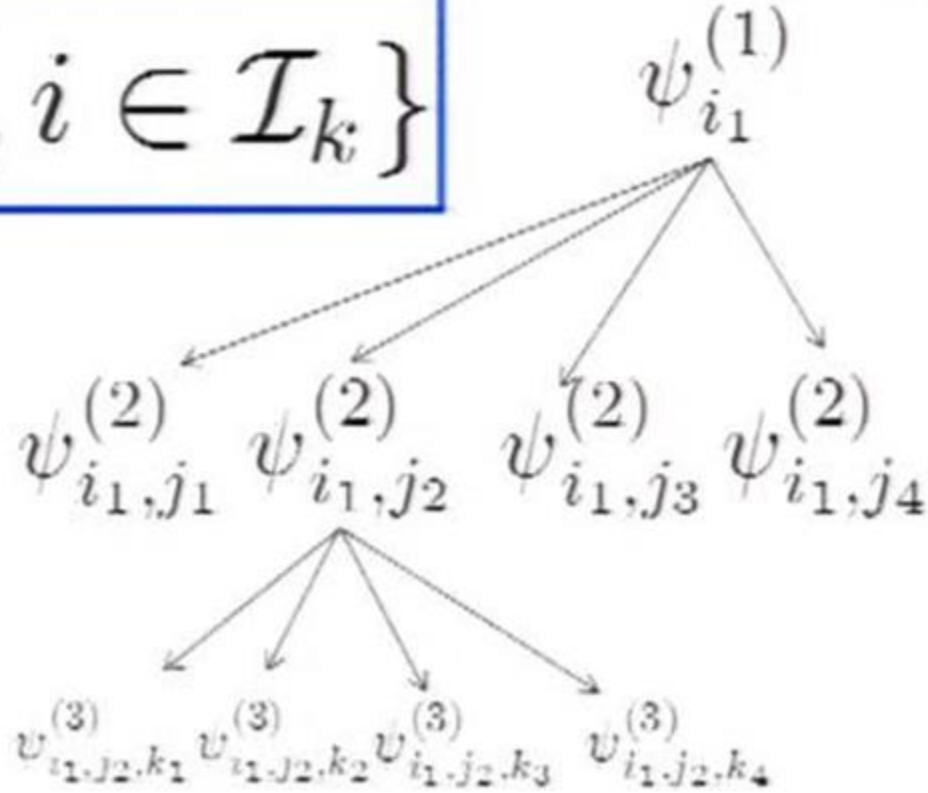
$\psi_i^{(k)}$: Elementary gambles/bets at resolution $H_k = 2^{-k}$

$$\psi_i^{(k)}(x) := \mathbb{E}\left[v(x) \,\middle|\, \int_\Omega v(y)\phi_j^{(k)}(y)\,dy = \delta_{i,j},\ j \in \mathcal{I}_k\right]$$



Gamblets are nested

$$\mathfrak{V}^{(k)} := \mathrm{span}\{\psi_i^{(k)}, i \in \mathcal{I}_k\}$$



Theorem

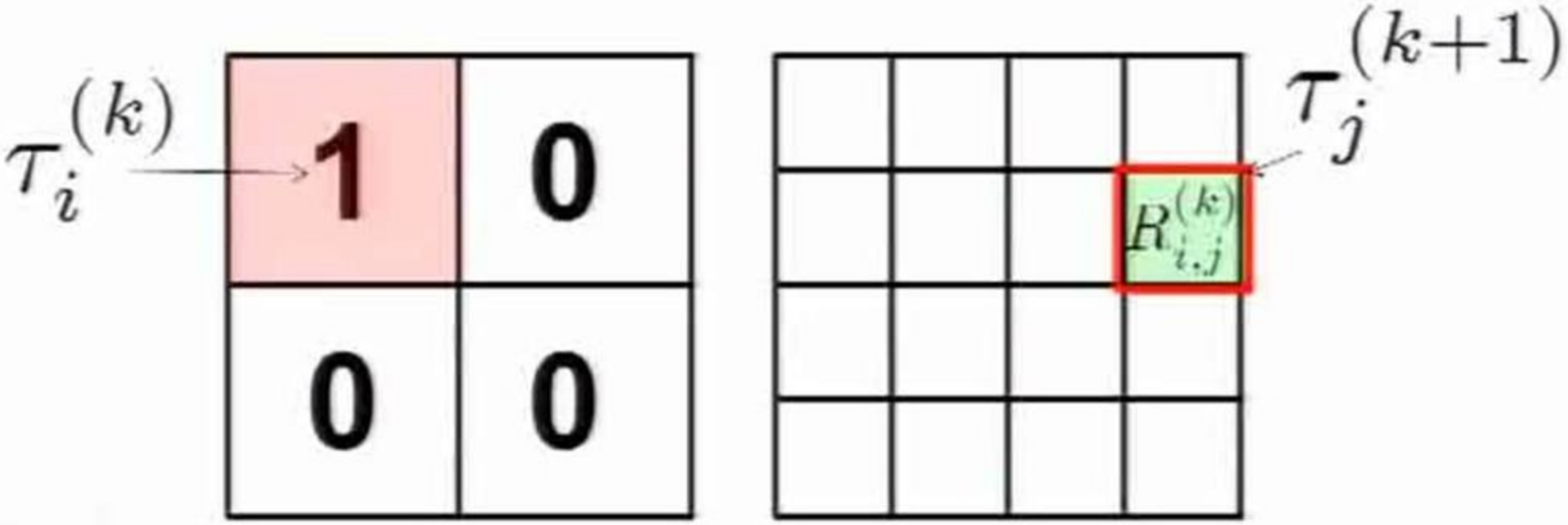
$$\mathfrak{V}^{(k)} \subset \mathfrak{V}^{(k+1)}$$

$$\psi_i^{(k)}(x) = \sum_{j \in I_{k+1}} R_{i,j}^{(k)} \psi_j^{(k+1)}(x)$$

Interpolation/Prolongation operator

$$R_{i,j}^{(k)} = \mathbb{E}\left| \int_\Omega v(y)\phi_j^{(k+1)}(y)\,dy \right| \int_\Omega v(y)\phi_l^{(k)}(y)\,dy = \delta_{i,l},\ l \in \mathcal{I}_k \Big|$$

$R_{i,j}^{(k)}$ Your best bet on the value of $\int_{\tau_j^{(k+1)}} u$ given the information that $\int_{\tau_i^{(k)}} u = 1$ and $\int_{\tau_l} u = 0$ for $l \neq i$



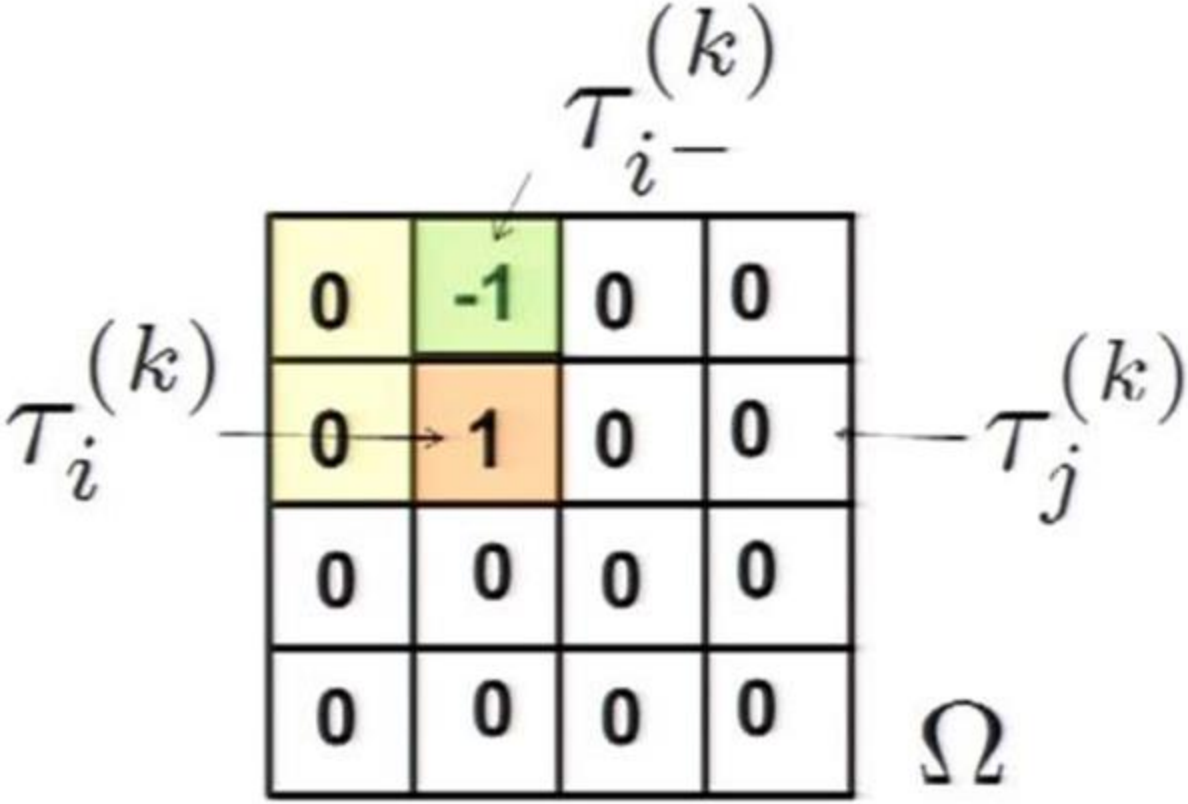
At this stage you can finish with classical multigrid

But we want multiresolution decomposition

Elementary gamble

$\chi_i^{(k)}$ Your best bet on the value of u given the information that

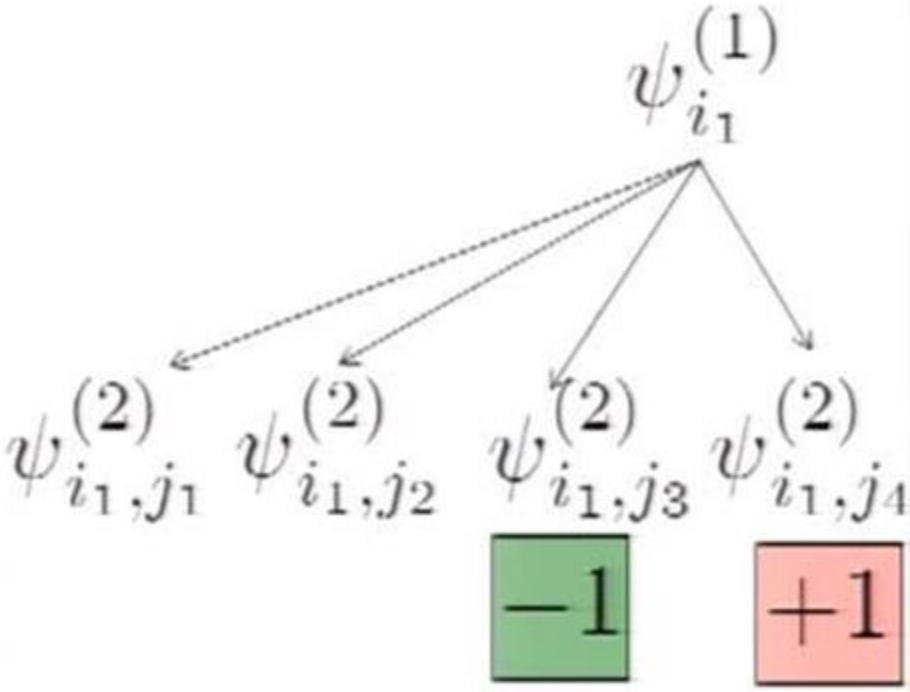
$\int_{\tau_i^{(k)}} u = 1$, $\int_{\tau_{i^-}^{(k)}} u = -1$ and $\int_{\tau_j^{(k)}} u = 0$ for $j \neq i$

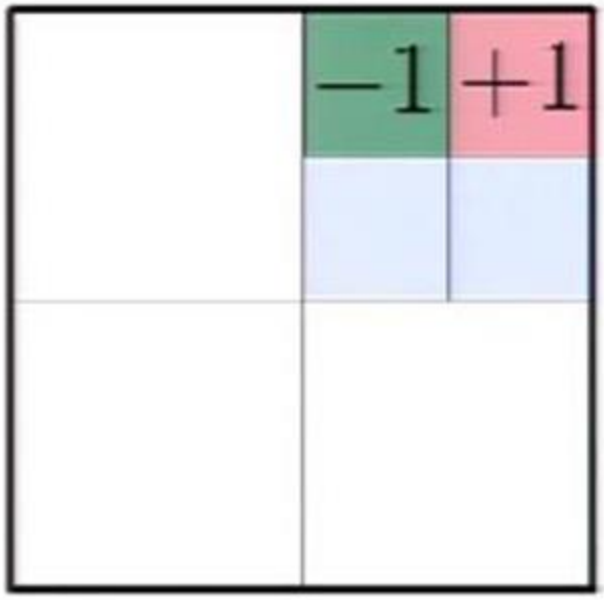


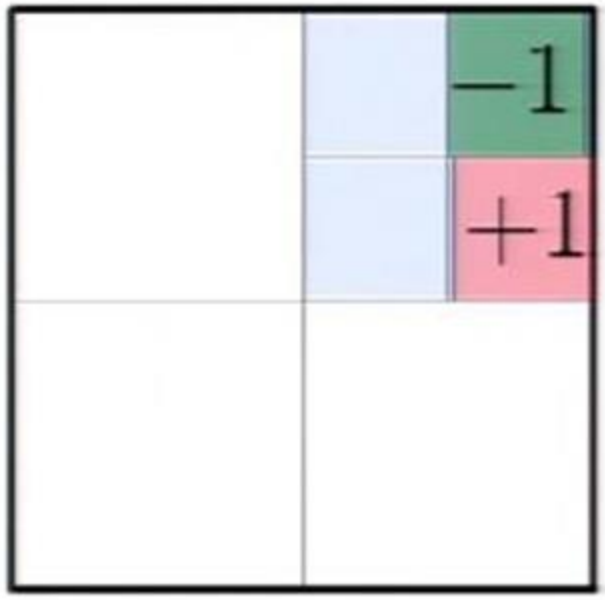
$$\chi_i^{(k)} = \psi_i^{(k)} - \psi_{i^-}^{(k)}$$

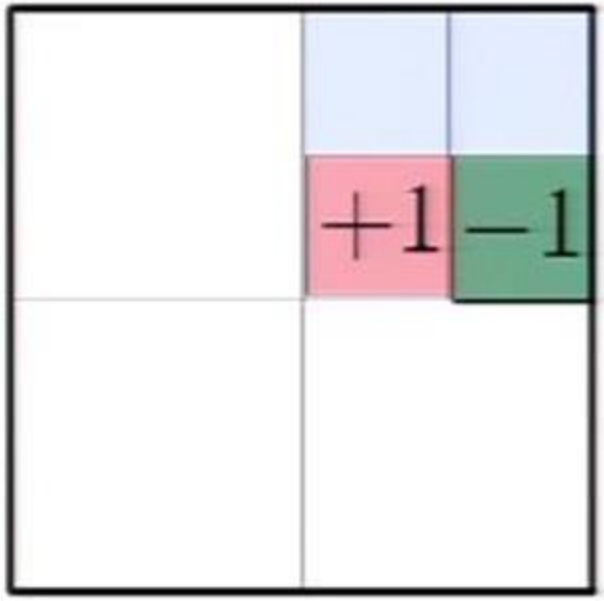
$$i = (i_1, \ldots, i_{k-1}, i_k)$$

$$i^- = (i_1, \ldots, i_{k-1}, i_k - 1)$$

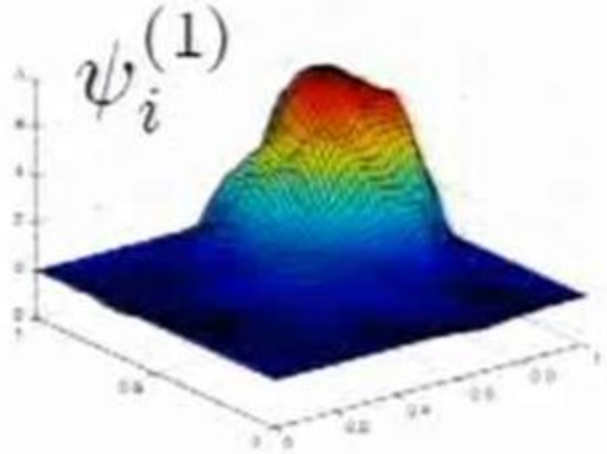


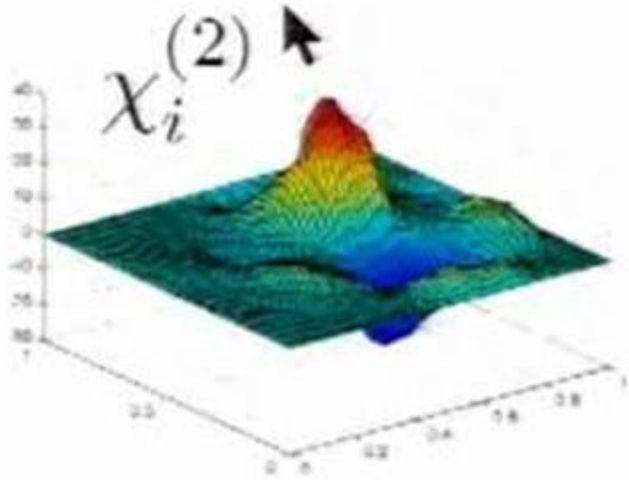


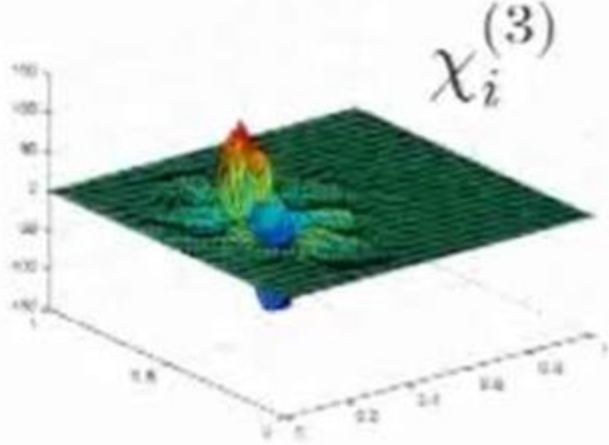


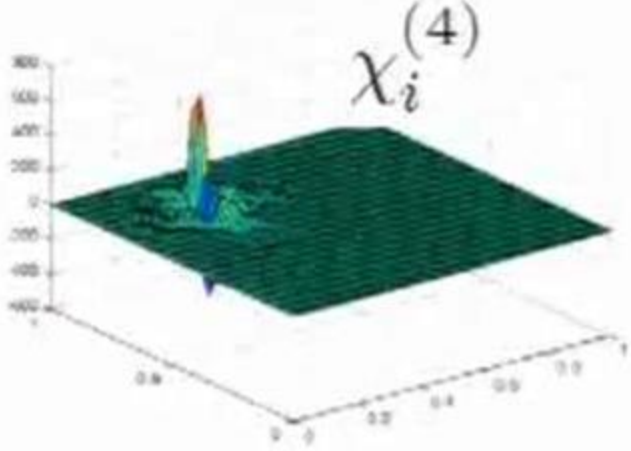


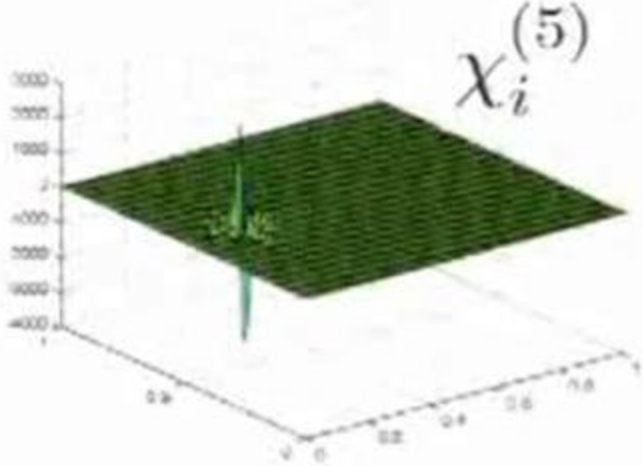
$$\chi_i^{(k)} = \psi_i^{(k)} - \psi_{i^-}^{(k)}$$

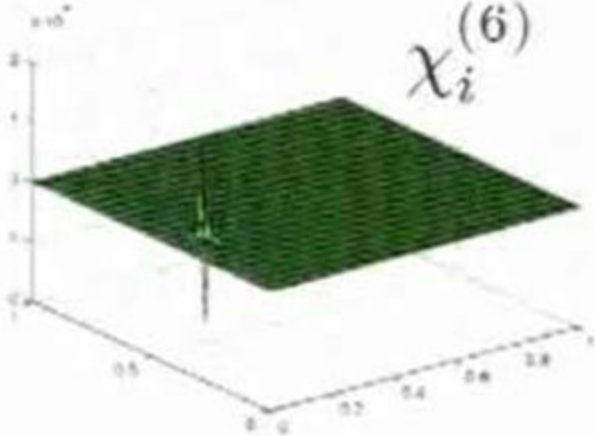












Multiresolution decomposition of the solution space

$$\mathfrak{V}^{(k)} := \mathrm{span}\{\psi_i^{(k)}, i \in \mathcal{I}_k\}$$

$$\mathfrak{W}^{(k)} := \mathrm{span}\{\chi_i^{(k)}, i\}$$

$\mathfrak{W}^{(k+1)}$: Orthogonal complement of $\mathfrak{V}^{(k)}$ in $\mathfrak{V}^{(k+1)}$ with respect to $<\psi,\chi>_a := \int_\Omega (\nabla\psi)^T a \nabla\chi$

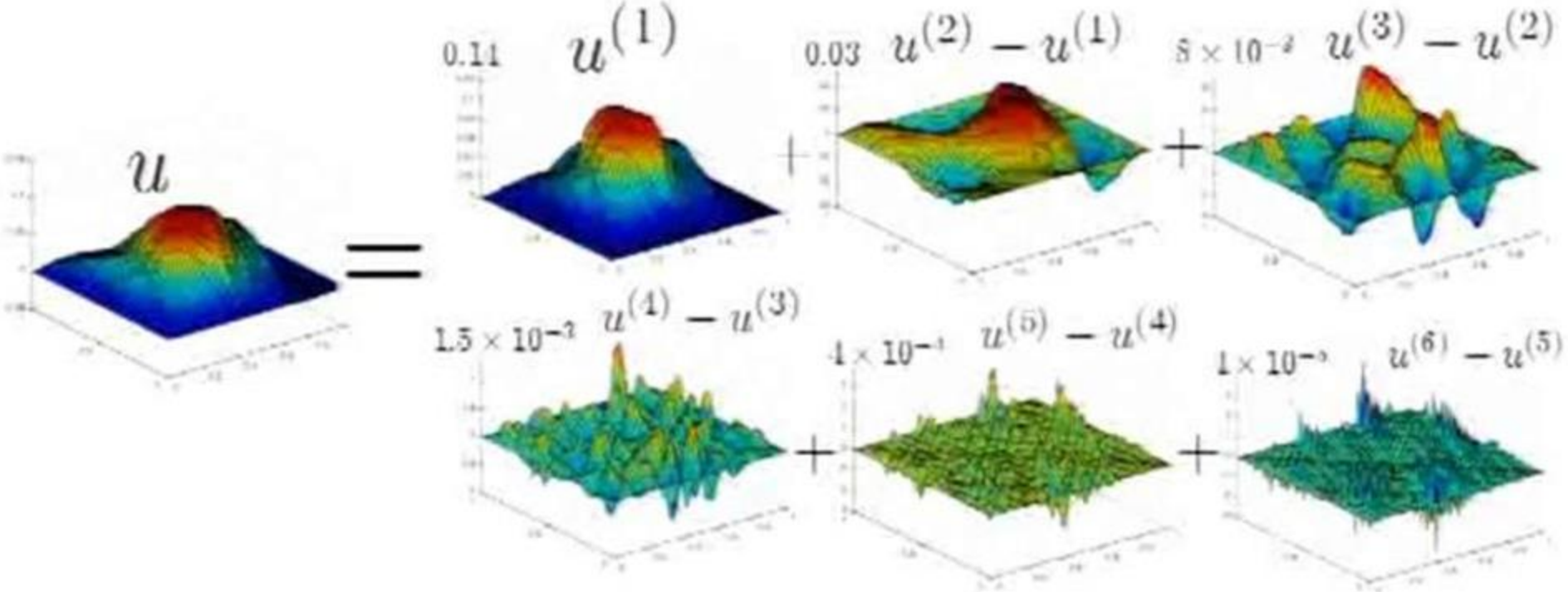
Theorem

$$H_0^1(\Omega) = \mathfrak{V}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)} \oplus_a \cdots$$

Multiresolution decomposition of the solution

Theorem

$$u^{(k+1)} - u^{(k)} = \text{F.E. sol. of PDE in } \mathfrak{W}^{(k+1)}$$



Subband solutions $u^{(k+1)} - u^{(k)}$
can be computed independently

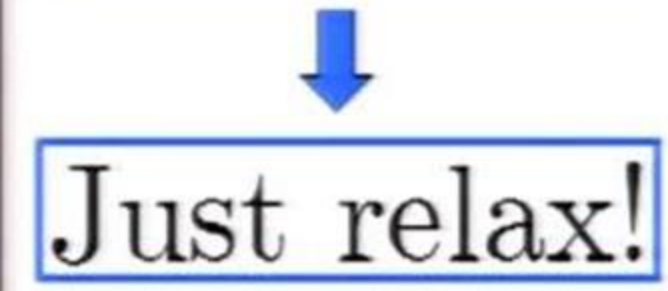
Uniformly bounded condition numbers

$$A_{i,j}^{(k)} := \left\langle \psi_i^{(k)}, \psi_j^{(k)} \right\rangle_a$$

$$B_{i,j}^{(k)} := \left\langle \chi_i^{(k)}, \chi_j^{(k)} \right\rangle_a$$

Theorem

$$\frac{\lambda_{\max}(B^{(k)})}{\lambda_{\min}(B^{(k)})} \leq C$$

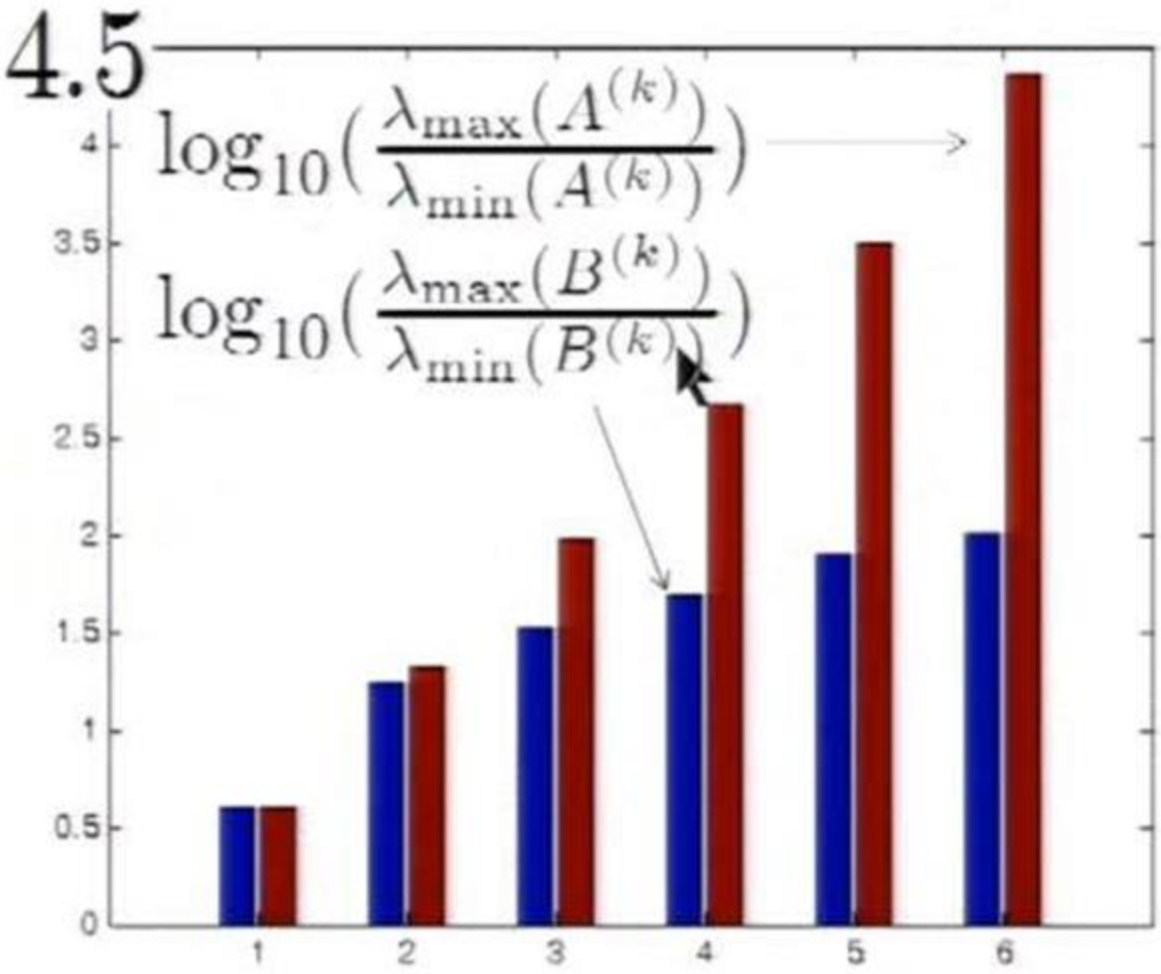


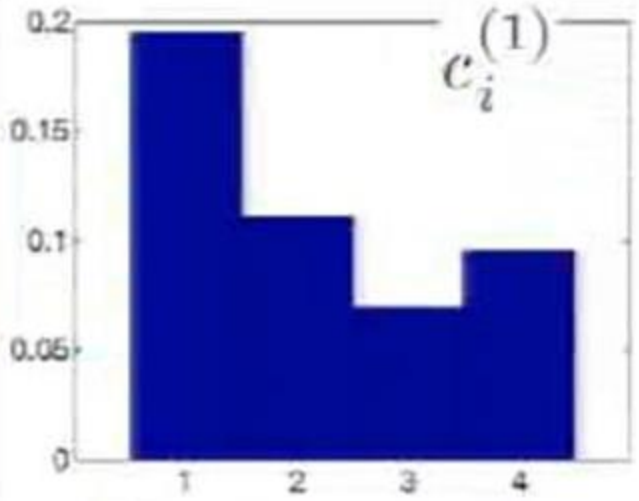
Just relax!

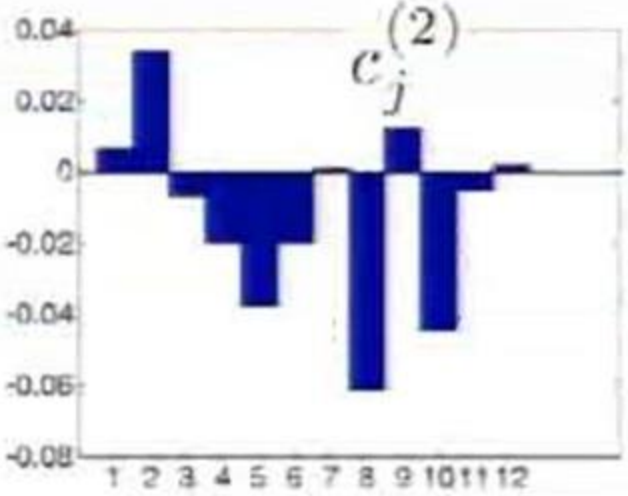
In $v \in \mathfrak{W}^{(k)}$

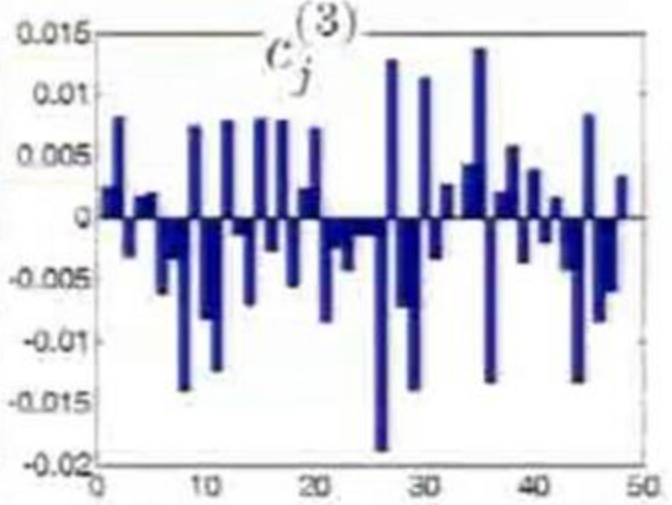
to get

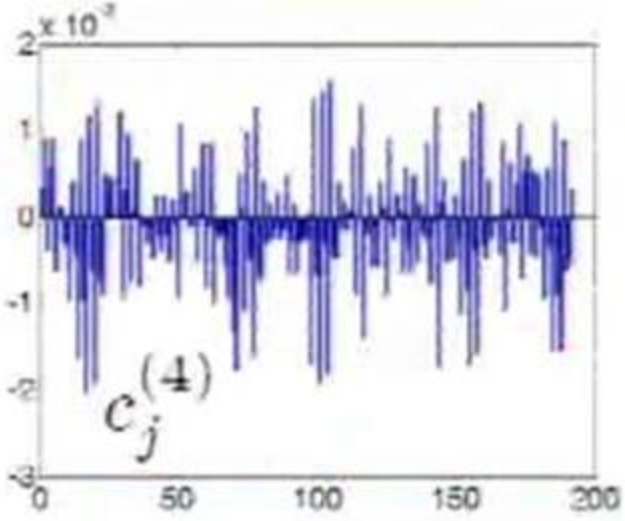
$u^{(k)} - u^{(k-1)}$

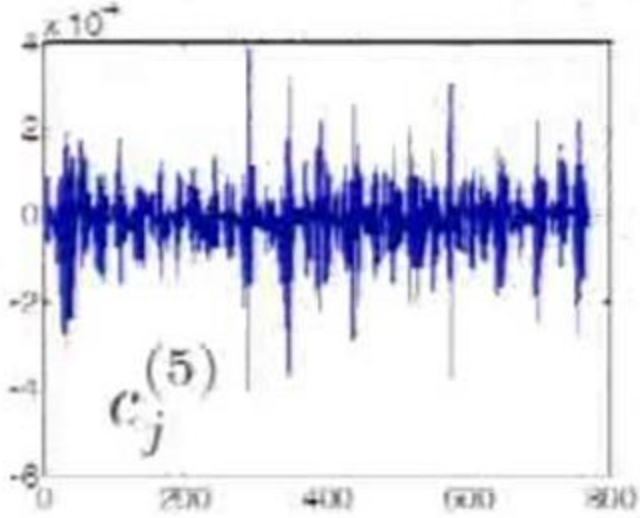


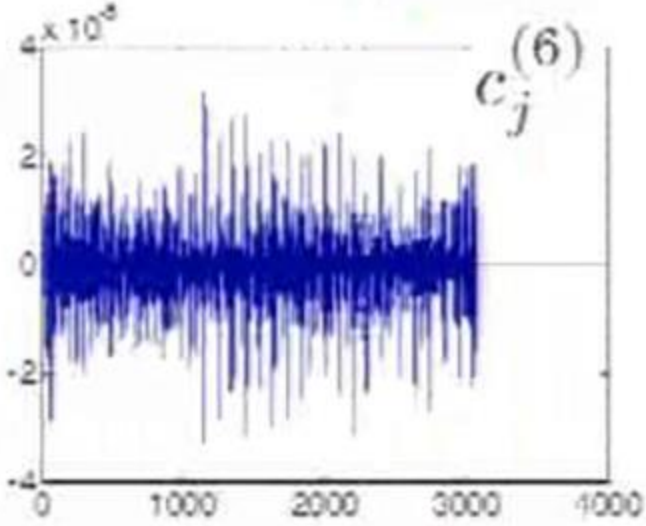










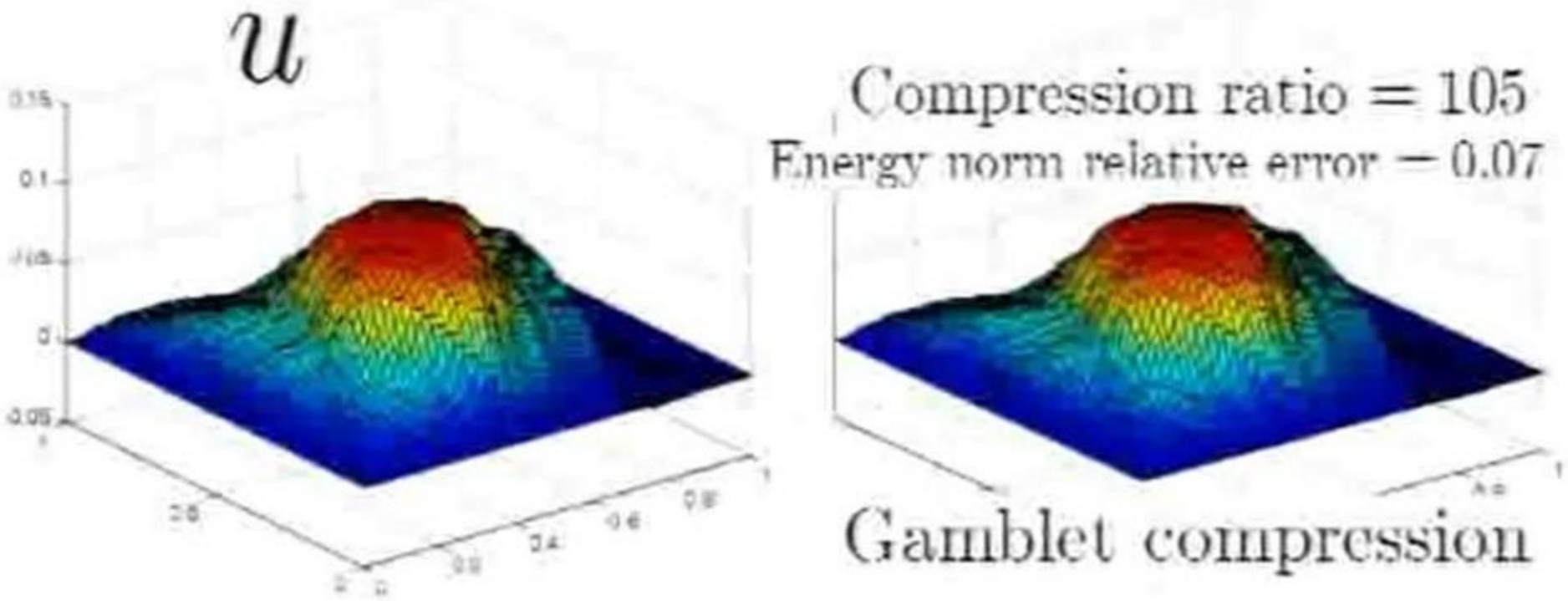


$$u = \sum_i c_i^{(1)} \frac{\psi_i^{(1)}}{\|\psi_i^{(1)}\|_a} + \sum_{k=2}^{q} \sum_j c_j^{(k)} \frac{\chi_j^{(k)}}{\|\chi_j^{(k)}\|_a}$$

Coefficients of the solution in the gamblet basis

Operator Compression

Gamblets behave like wavelets but they are adapted to the PDE and can compress its solution space



Throw 99% of the coefficients

Fast gamblet transform

$$\mathcal{O}(N \ln^2 N) \text{ complexity}$$

Nesting

$$A^{(k)} = (R^{(k,k+1)})^T A^{(k+1)} R^{(k,k+1)}$$

Level(k) gamblets and stiffness matrices can be computed from level(k+1) gamblets and stiffness matrices

Well conditioned linear systems

Underlying linear systems have uniformly bounded condition numbers

$$\psi_i^{(k)} = \psi_{(i,1)}^{(k+1)} + \sum_j C_{i,j}^{(k+1),\chi} \chi_j^{(k+1)}$$

$$C^{(k+1),\chi} = (B^{(k+1)})^{-1} Z^{(k+1)}$$

$$Z_{j,i}^{(k+1)} := -(e_j^{(k+1)} - e_{j-}^{(k+1)})^T A^{(k+1)} e_{(i,1)}^{(k+1)}$$

Localization

The nested computation can be localized without compromising accuracy or condition numbers

Theorem

Localizing $(\psi_i^{(k)})_{i \subset \mathcal{I}_k}$ and $(\chi_i^{(k)})_i$ to subdomains of size

$\geq C\Pi_k \ln^2 \frac{1}{\Pi_k}$ ➡ Cond. No $(B^{(k),\mathrm{loc}}) \leq C$

$\geq C\Pi_k(\ln^2 \frac{1}{\Pi_k} + \ln \frac{1}{\epsilon})$ ➡

$$\left\| u - u^{(1),\mathrm{loc}} - \sum_{k=1}^{q-1} (u^{(k+1),\mathrm{loc}} - u^{(k),\mathrm{loc}}) \right\|_a \leq \epsilon$$

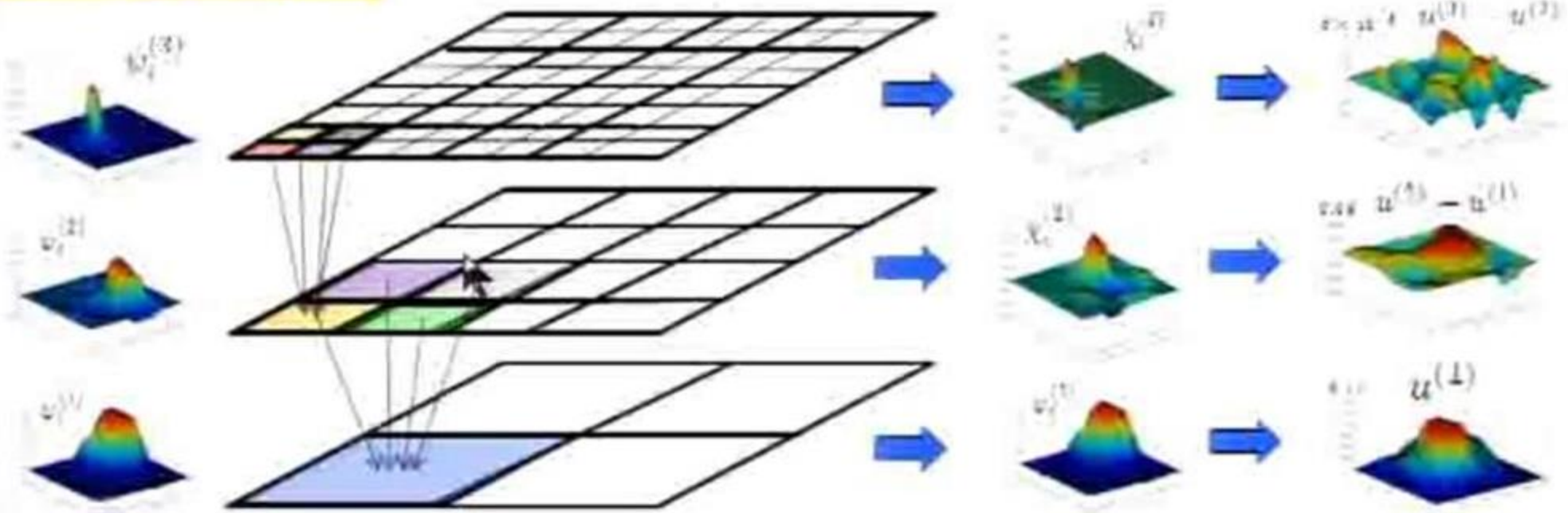
Theorem

The number of operations to achieve accuracy ϵ is $\sim N\left(\ln^2 N + \ln \frac{1}{\epsilon}\right) \ln \frac{1}{\epsilon}$

Complexity

$$\mathcal{O}(N \ln^2 N)$$

Parallel operating diagram both in space and in frequency



Generalization to linear systems of equations

Identification of the optimal prior/mixed strategy in that setting

Approximate solution x of

$$Ax = b$$

A: Known $n \times n$ symmetric positive definite matrix

b: Unknown element of $\mathbb{R}^n$

Based on the information that

$$\Phi x = y$$

Φ: Known $m \times n$ rank m matrix $(m < n)$

$$b^T b \leq 1$$

y: Known element of $\mathbb{R}^m$

Game theoretic formulation

$$Ax = b$$

Player A

Chooses

$b \in \mathbb{R}^n$

$b^T b \leq 1$

Player B

Sees

$y = \Phi x$

Chooses x^*

$\mathcal{M}ax$ $\mathcal{M}in$

$$\left\| x - x^* \right\|_2$$

Zero sum game

Best way to play: Mixed strategy

Player B's mixed strategy

$$Ax = b \iff AX = \xi$$

$$\xi \sim \mathcal{N}(0, Q)$$

Player's B bet

$$x^* = \mathbb{E}\left[X | \Phi X = y\right] = \Psi y$$

Perspectives

How is this related to model uncertainty?

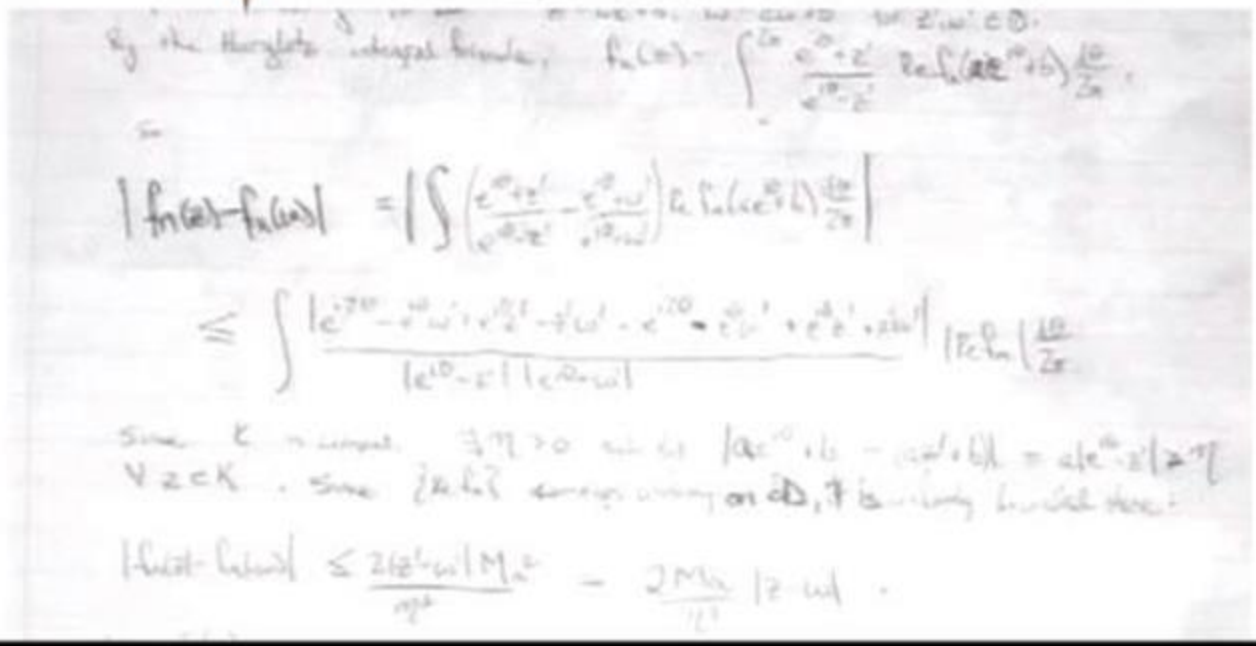
Motivations for developing this kind of framework

Solving PDEs: Two centuries ago

$$\Delta u = f$$

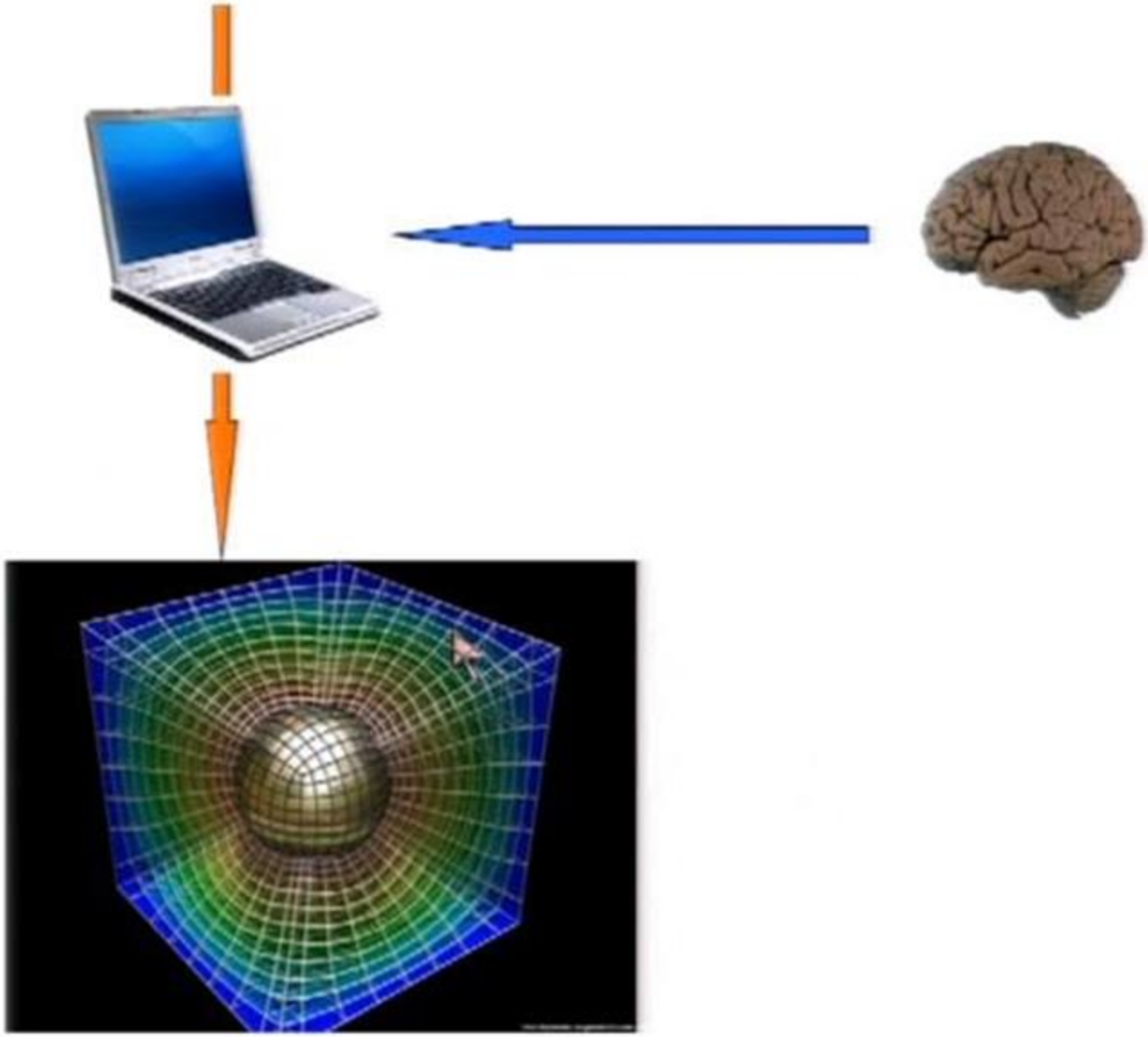
A. L. Cauchy
(1789-1857)

S. D. Poisson
(1781-1840)

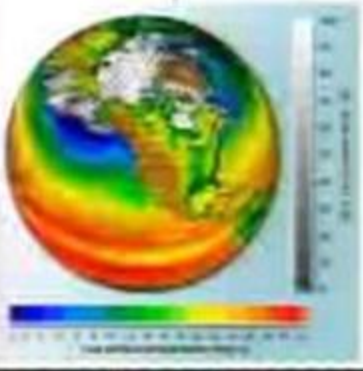


Solving PDEs: Now.

$$\Delta u = f$$



Find the best climate model now

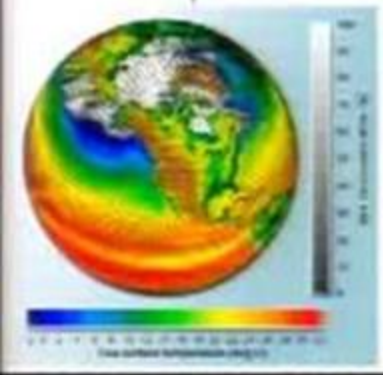


Find a 95% interval of confidence on average global temperatures in 50 years

Problem

- Incomplete information on underlying processes
- Limited computation capability
- You don't know $\mathbb{P}$
- You have limited data

Can a machine compute the best climate model?



2 Major problems

- **Even if you have access to the most powerful computer in the universe, what do you compute?**
- **The space of models is infinite and calculus on a computer is discrete and finite.**

Need a framework to turn this problem into a well posed one.

Need a calculus to manipulate infinite dimensional information structures

Framework: Game/Decision Theory

Player A

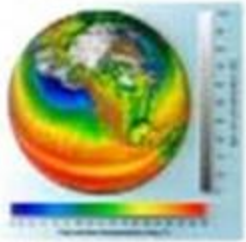
Chooses candidate

Player B

Sees data

Chooses model

$$\mathcal{E}(\text{candidate}, \text{model}(\text{data}))$$



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

Leads to optimization problems over measures over spaces of measures and functions

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