# Houman Owhadi

# CSE15

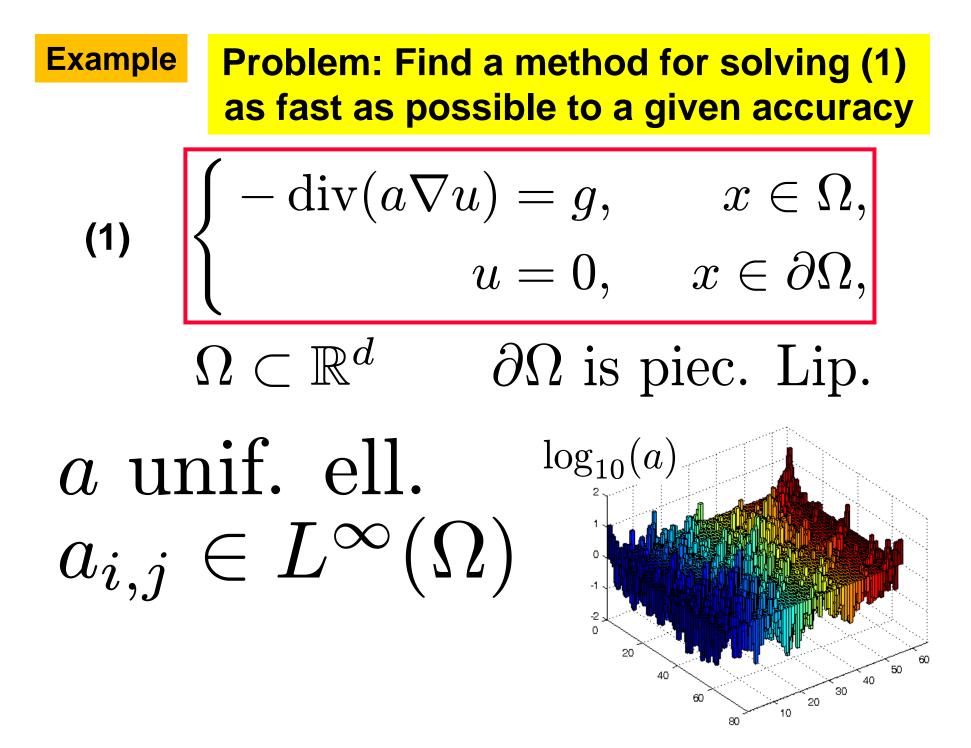






#### **Main Question**

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?



# **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!

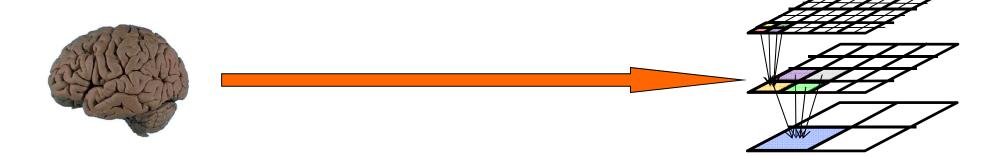
#### Low Rank Matrix Decomposition methods

Fast Multipole Method: [Greengard and Rokhlin, 1987]Hierarchical Matrix Method: [Hackbusch et al., 2002][Bebendorf, 2008]:

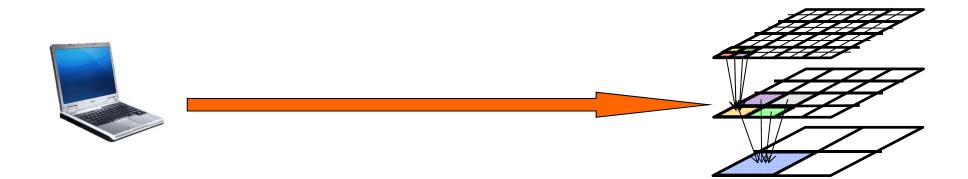
$$N \ln^{d+3} N$$
 complexity

#### **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

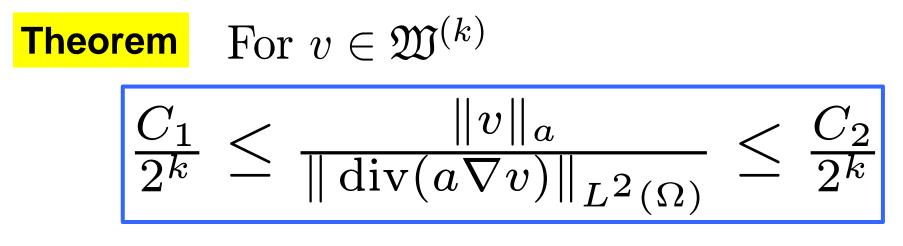
This is a theorem

#### **Resulting method:**

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

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

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



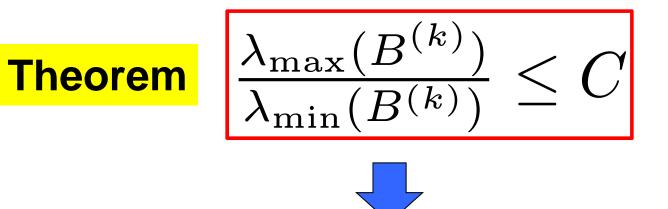
$$||v||_a^2 := \langle v, v \rangle_a = \int_{\Omega} (\nabla v)^T a \nabla v$$

Looks like an eigenspace decomposition

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

# $w^{(k)} = F.E.$ sol. of PDE in $\mathfrak{W}^{(k)}$ Can be computed independently

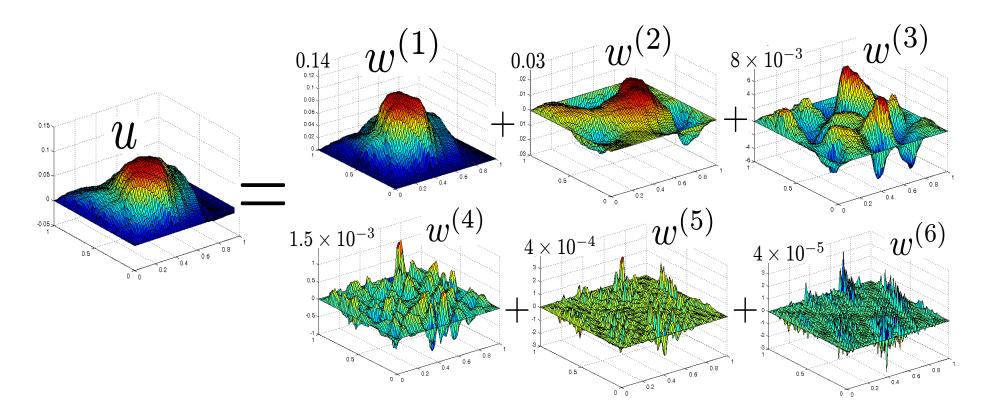
 $B^{(k)}$ : Stiffness matrix of PDE in  $\mathfrak{W}^{(k)}$ 



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

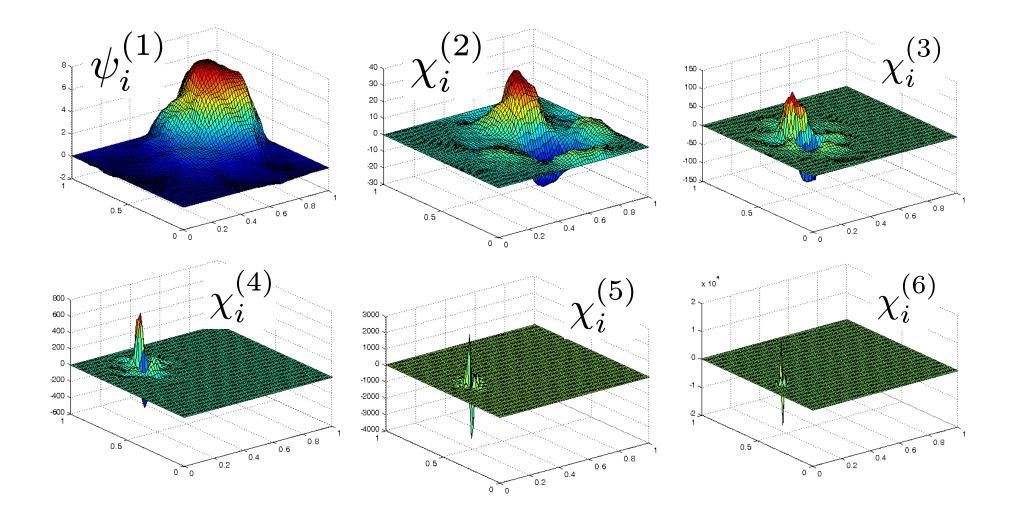
# $\mathfrak{V}$ : F.E. space of $H_0^1(\Omega)$ of dim. N

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

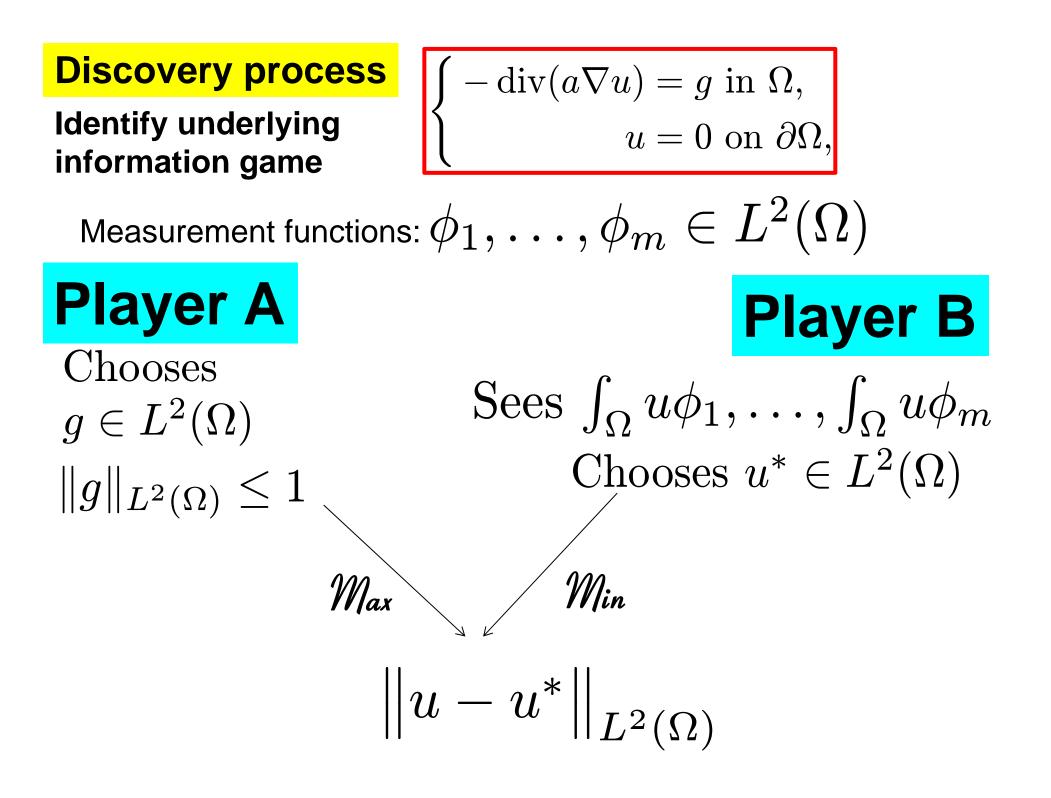
Can be performed and stored in

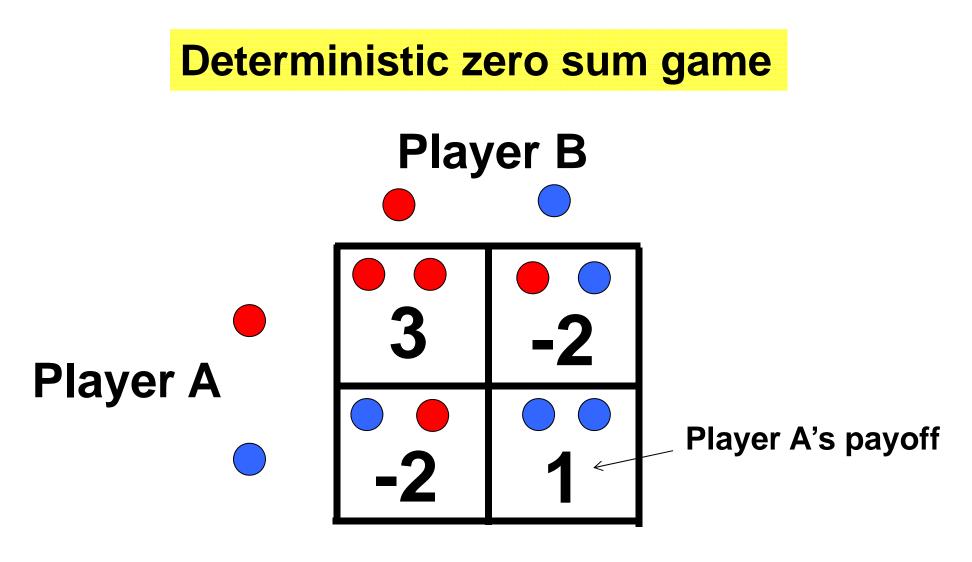
$$\mathcal{O}(N\ln^2 N)$$
 operations

Doesn't have the complexity of an eigenspace decomposition



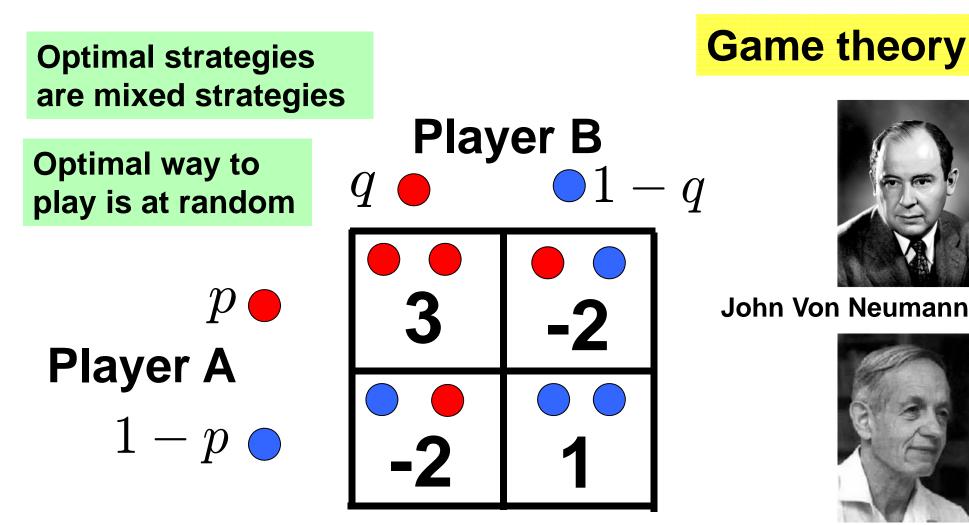
Basis functions look like and behave like wavelets: Localized and can be used to compress the operator and locally analyze the solution space



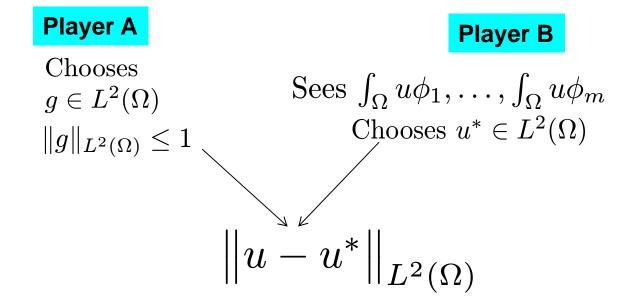


Player A & B both have a blue and a red marble At the same time, they show each other a marble

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



A's expected payoff John Nash = 3pq + (1-p)(1-q) - 2p(1-q) - 2q(1-p)= $1 - 3q + p(8q - 3) = -\frac{1}{8}$  for  $q = \frac{3}{8}$ 



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**

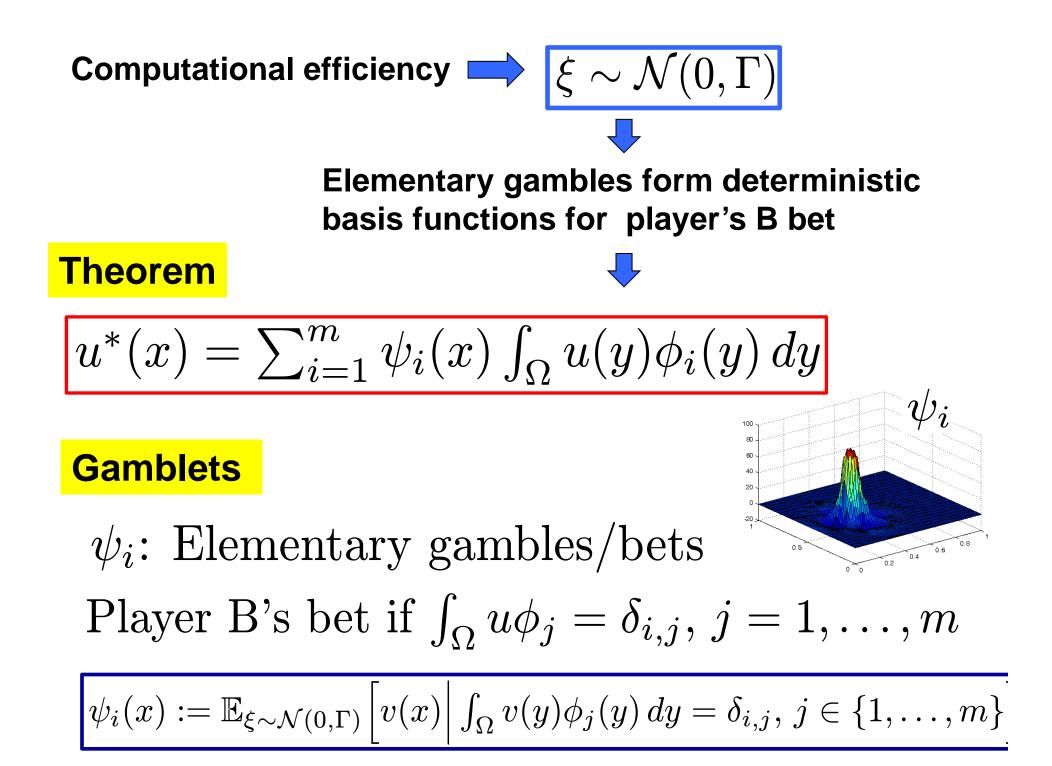
Pretend that player A is choosing g at random  $g \in L^2(\Omega)$   $\longleftrightarrow$   $\xi$ : Random field  $\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases}$   $\longleftrightarrow$   $\begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ v = 0 \text{ on } \partial\Omega, \end{cases}$ 

# **Player B's bet**

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

#### **Player's B optimal strategy?**

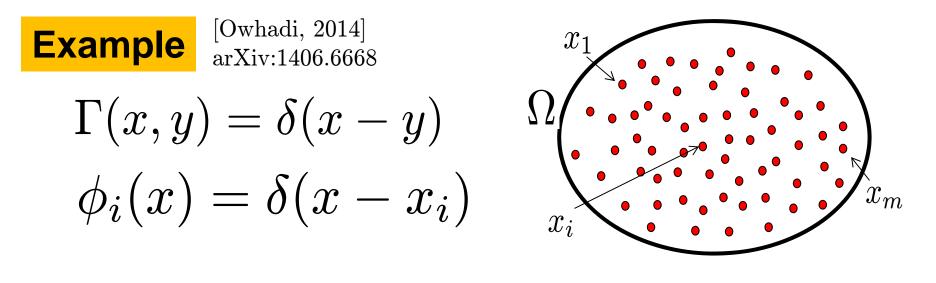
Player B's best bet?  $\longleftrightarrow$  min max problem over distribution of  $\xi$ 



#### What are these gamblets?

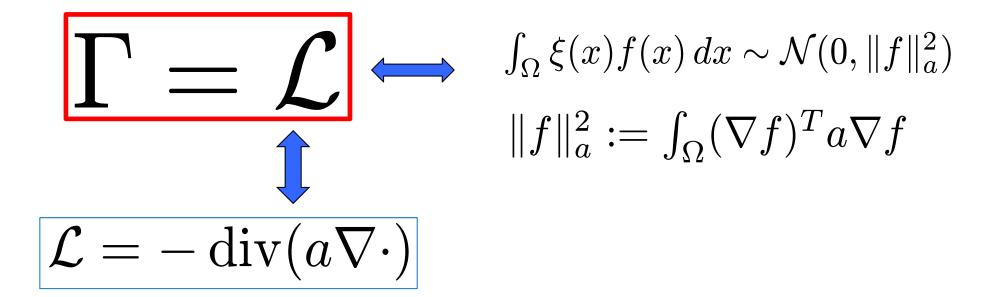
# Depend on

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



- $a = I_d \iff \psi_i$ : Polyharmonic splines [Harder-Desmarais, 1972][Duchon 1976, 1977, 1978]
- $a_{i,j} \in L^{\infty}(\Omega) \iff \psi_i$ : Rough Polyharmonic splines [Owhadi-Zhang-Berlyand 2013]

What is player's B best strategy? What is player's B best choice for  $\Gamma(x, y) = \mathbb{E}[\xi(x)\xi(y)]$  ?



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 span{ $\mathcal{L}^{-1}\phi_i | i = 1, ..., m$ }

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

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

#### **Optimal variational properties**

#### **Theorem**

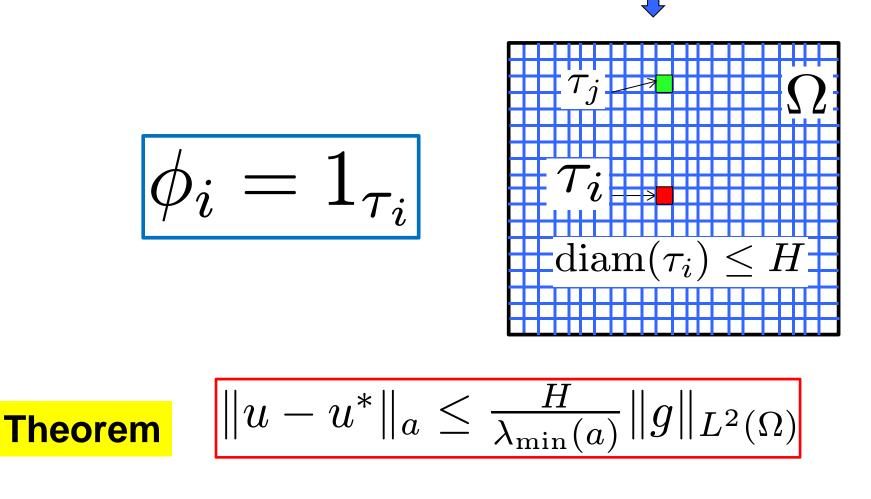
 $\sum_{i=1}^{m} w_i \psi_i \text{ minimizes } \|\psi\|_a$ over all  $\psi$  such that  $\int_{\Omega} \phi_j \psi = w_j$  for  $j = 1, \dots, m$ 

#### **Variational characterization**

**Theorem**
$$\psi_i$$
: Unique minimizer of $\begin{cases} \text{Minimize} & \|\psi\|_a \\ \text{Subject to} & \psi \in H^1_0(\Omega) \text{ and } \int_{\Omega} \phi_j \psi = \delta_{i,j}, \quad j = 1, \dots, m \end{cases}$ 

**Selection of measurement functions** 

# **Example** Indicator functions of a Partition of $\Omega$ of resolution H

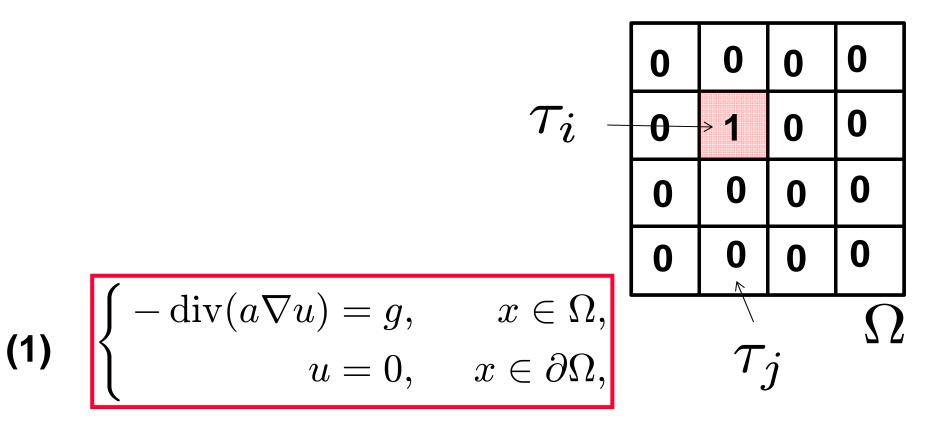


#### **Elementary gamble**



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

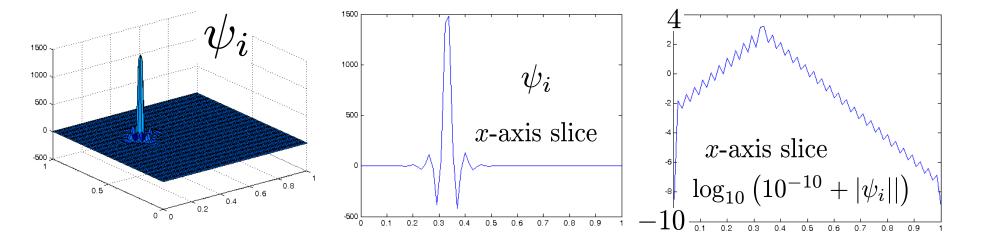
$$\int_{\tau_i} u = 1$$
 and  $\int_{\tau_j} u = 0$  for  $j \neq i$ 

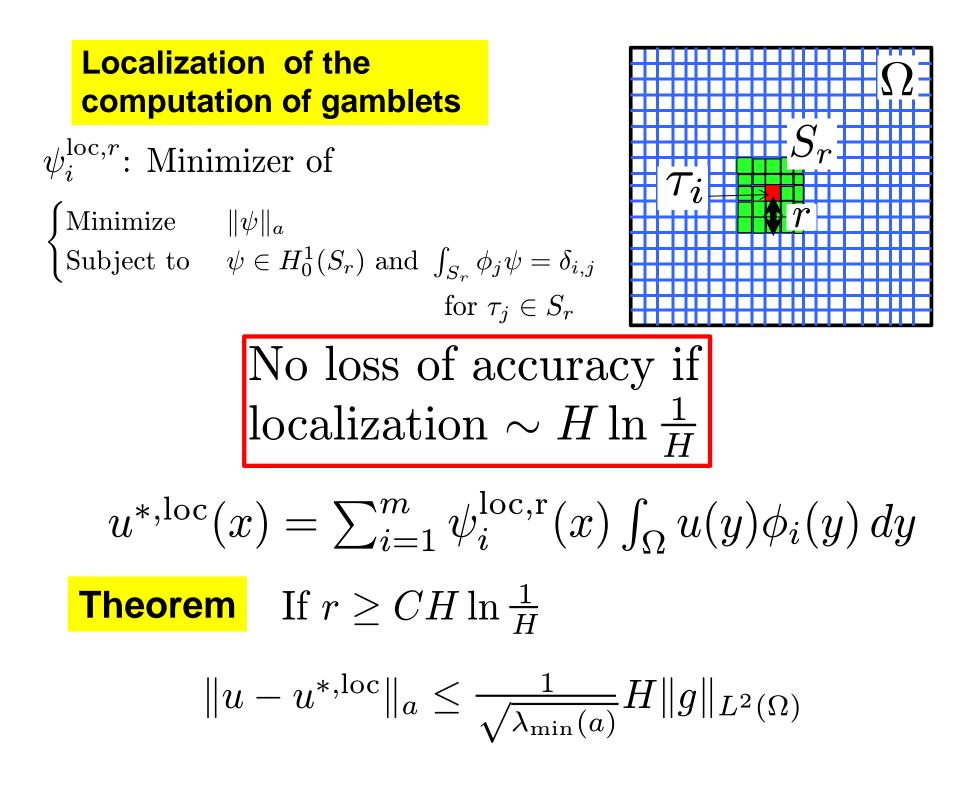




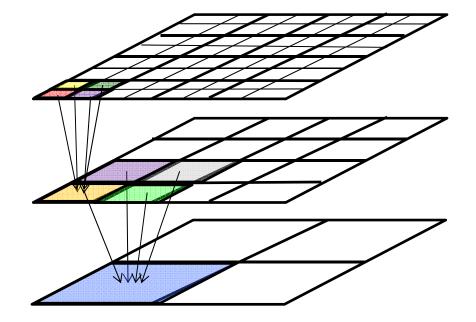
#### **Theorem**

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





#### **Formulation of the hierarchical game**



#### **Hierarchy of nested Measurement functions**

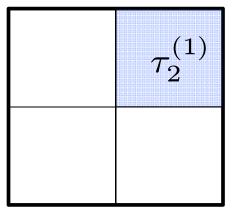
$$\phi_{i_1,...,i_k}^{(k)}$$
 with  $k \in \{1,..., \phi_{i_1,...,i_k}^{(k)} = \sum_j c_{i,j} \phi_{i,j}^{(k+1)}$ 

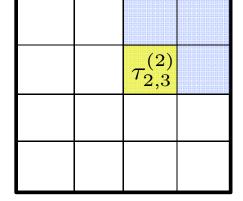
#### Example

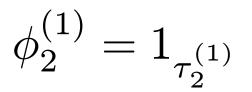
 $\phi_i^{(k)}$ : Indicator functions of a

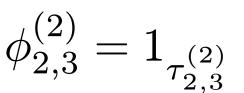
hierarchical nested partition of  $\Omega$  of resolution  $H_k = 2^{-k}$ 

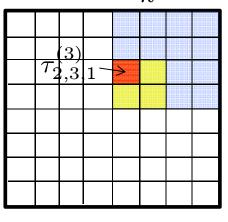
q







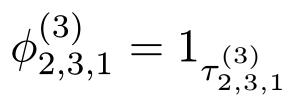




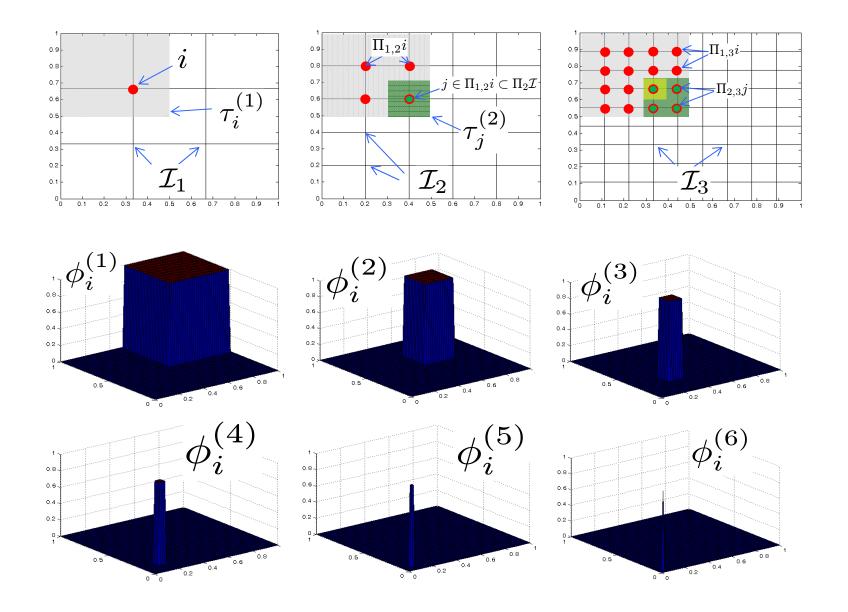
 $\phi_{i_1,j_1}^{(2)} \phi_{i_1,j_2}^{(2)} \phi_{i_1,j_3}^{(2)} \phi_{i_1,j_4}^{(2)}$ 

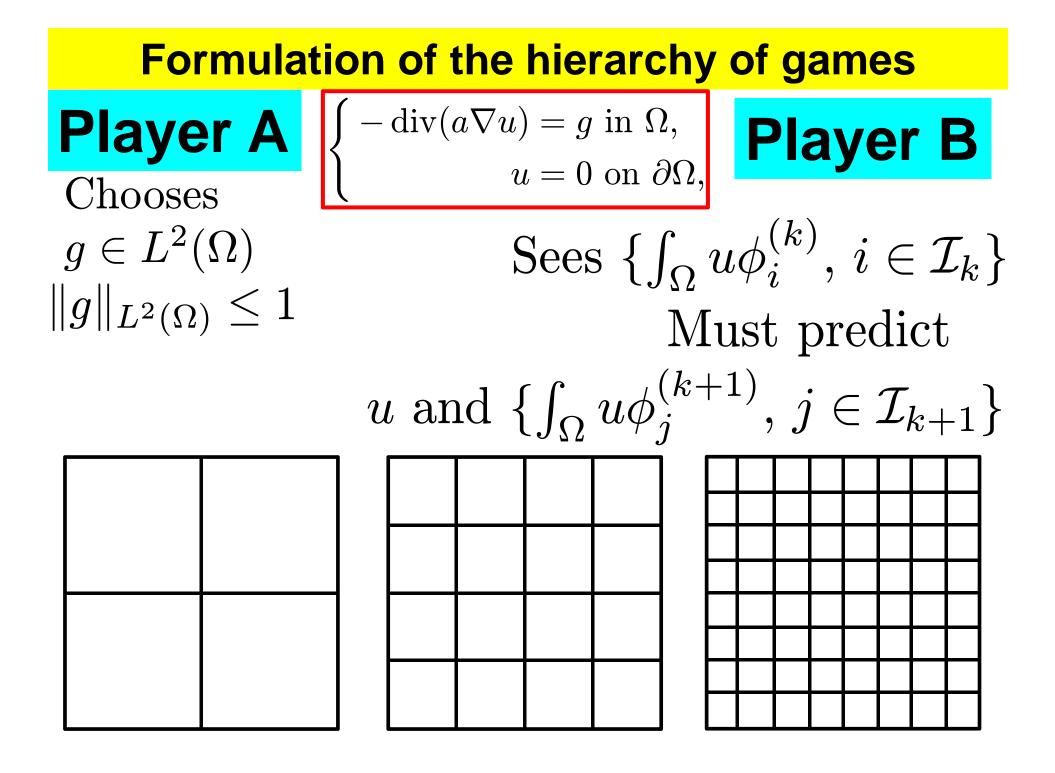
 $\phi_{i_1,j_2,k_1}^{(3)}\phi_{i_1,j_2,k_2}^{(3)}\phi_{i_1,j_2,k_3}^{(3)} \quad \phi_{i_1,j_2,k_4}^{(3)}$ 

 $\phi_{i_1}^{(1)}$ 



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





Player B's best strategy
$$\xi \sim \mathcal{N}(0, \mathcal{L})$$
 $\left\{ -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{array} \right\}$  $\left\{ -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ v = 0 \text{ on } \partial\Omega, \end{array} \right.$ 

#### **Player B's bets**

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

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

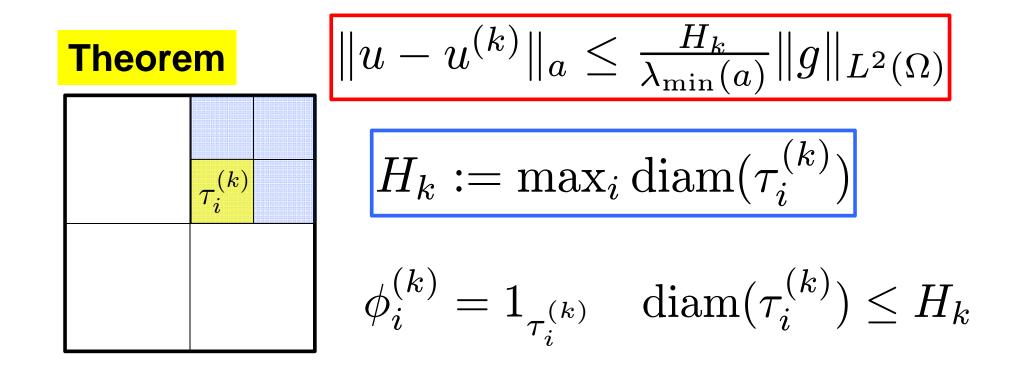
$$\mathcal{F}_k = \sigma(\int_{\Omega} v \phi_i^{(k)}, i \in \mathcal{I}_k) \quad v^{(k)}(x) := \mathbb{E}[v(x) | \mathcal{F}_k]$$

**Theorem** 

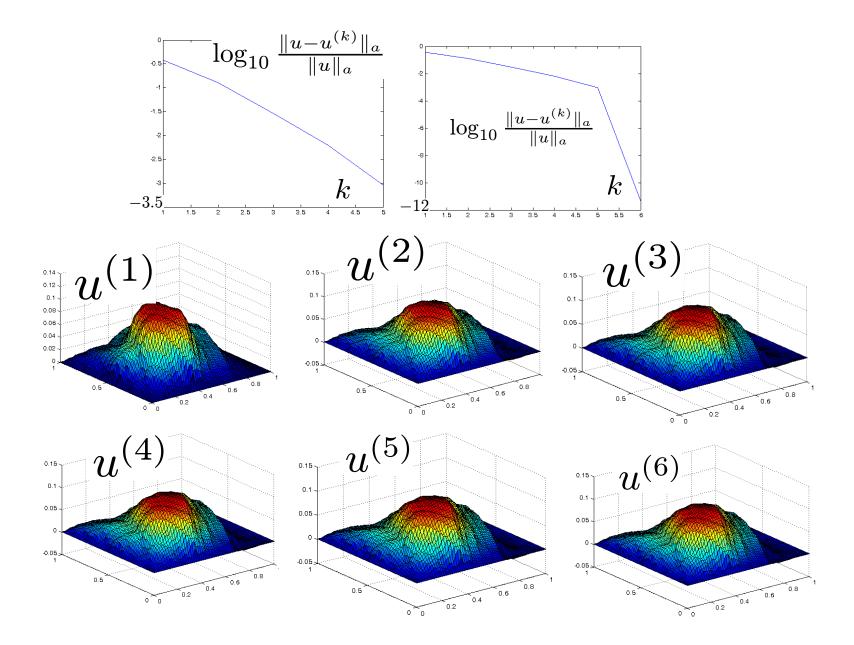
$$\mathcal{F}_k \subset \mathcal{F}_{k+1}$$

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

#### **Accuracy of the recovery**



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

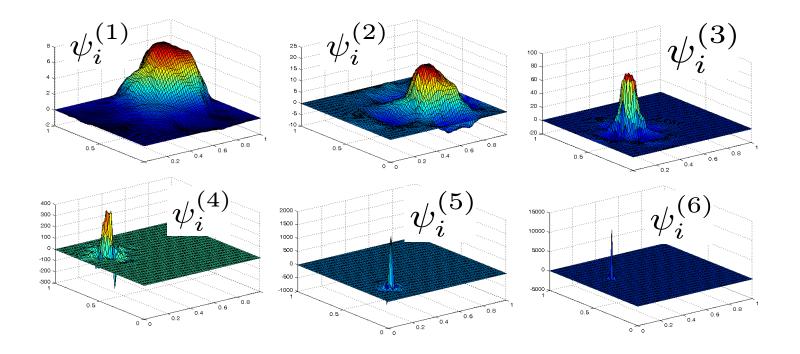


**Gamblets** Elementary gambles form a hierarchy of deterministic basis functions for player's B hierarchy of bets

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  $H_k = 2^{-k}$ 

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



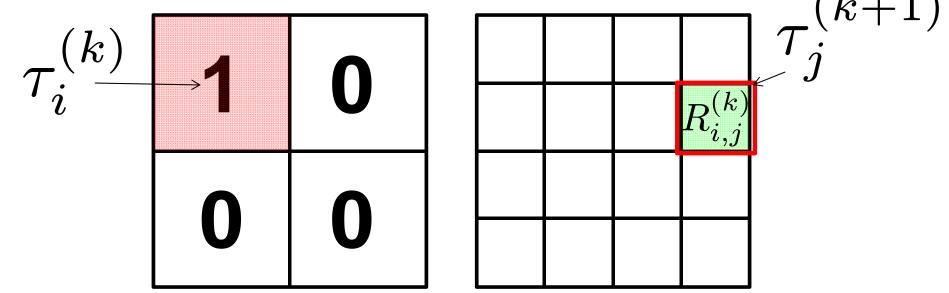
#### **Gamblets are nested**

$$\begin{split} \mathfrak{V}^{(k)} &:= \operatorname{span}\{\psi_{i}^{(k)}, i \in \mathcal{I}_{k}\} \begin{array}{c} \psi_{i_{1}}^{(1)} \\ \psi_{i_{1}}^{(1)} \\ \psi_{i_{1},j_{1}}^{(2)} & \psi_{i_{1},j_{2}}^{(2)} & \psi_{i_{1},j_{3}}^{(2)} \\ \psi_{i_{1},j_{1}}^{(2)} & \psi_{i_{1},j_{2}}^{(2)} & \psi_{i_{1},j_{3}}^{(2)} \\ \psi_{i_{1},j_{1}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2},k_{1}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2},k_{1}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2},k_{3}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2$$

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

#### **Interpolation/Prolongation operator**

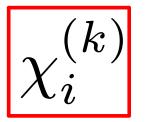
$$\begin{split} R_{i,j}^{(k)} &= \mathbb{E} \left[ \int_{\Omega} v(y) \phi_{j}^{(k+1)}(y) \, dy \right| \int_{\Omega} v(y) \phi_{l}^{(k)}(y) \, dy = \delta_{i,l}, \, l \in \mathcal{I}_{k} \right] \\ \hline R_{i,j}^{(k)} \text{ Your best bet on the value of } \int_{\tau_{j}^{(k+1)}} u \\ \text{given the information that} \\ \int_{\tau_{i}^{(k)}} u = 1 \text{ and } \int_{\tau_{l}} u = 0 \text{ for } l \neq i \end{split}$$



#### At this stage you can finish with classical multigrid

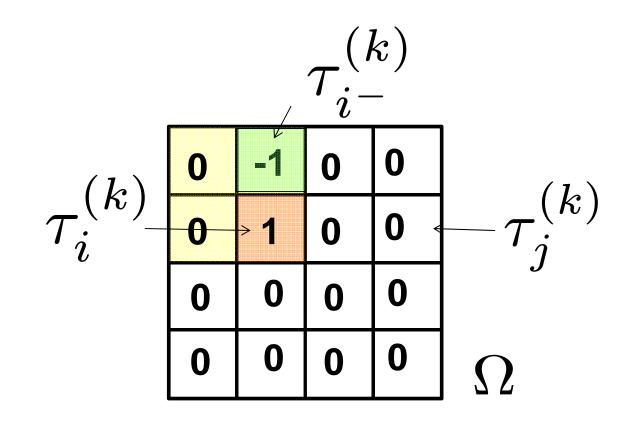
**But we want multiresolution decomposition** 

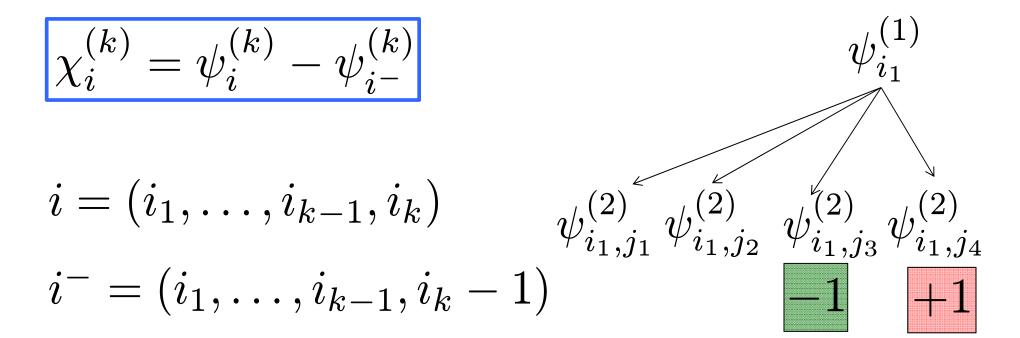
#### **Elementary gamble**

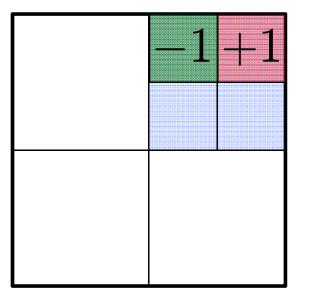


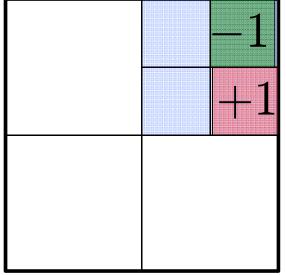
Your best bet on the value of u given the information that

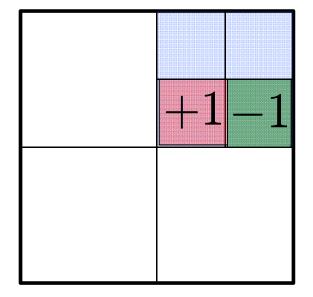
 $\int_{\tau_i^{(k)}} u = 1, \int_{\tau_i^{(k)}} u = -1 \text{ and } \int_{\tau_j^{(k)}} u = 0 \text{ for } j \neq i$ 



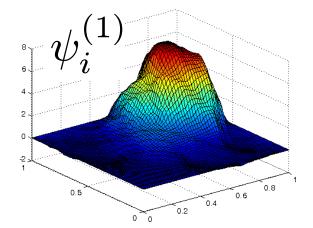


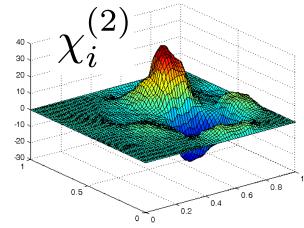


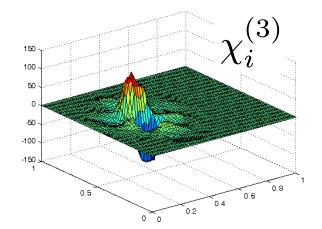


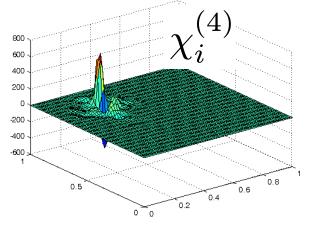


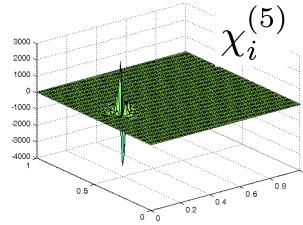
$$\chi_{i}^{(k)} = \psi_{i}^{(k)} - \psi_{i^{-}}^{(k)}$$

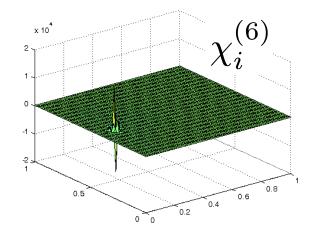












#### **Multiresolution decomposition of the solution space**

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

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

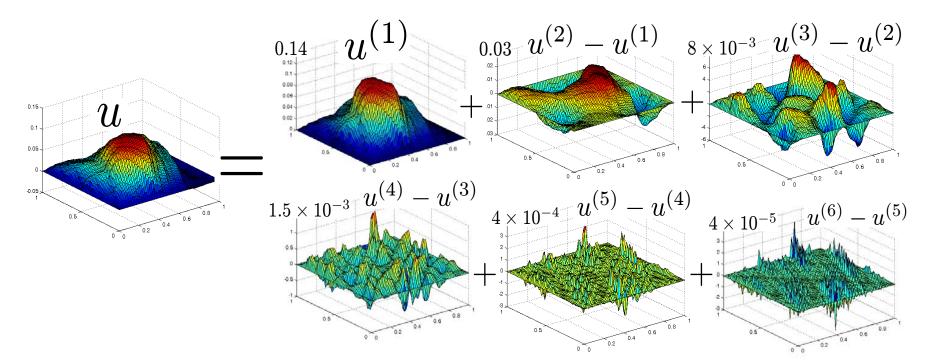
#### **Theorem**

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

#### **Multiresolution decomposition of the solution**

**Theorem** 

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

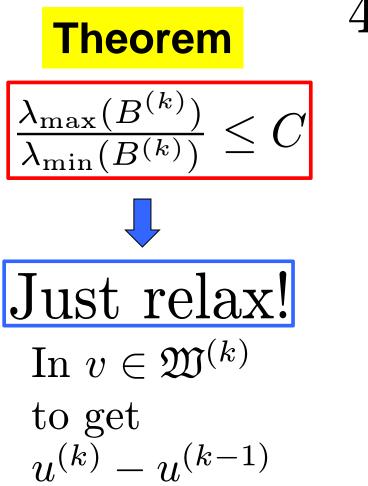


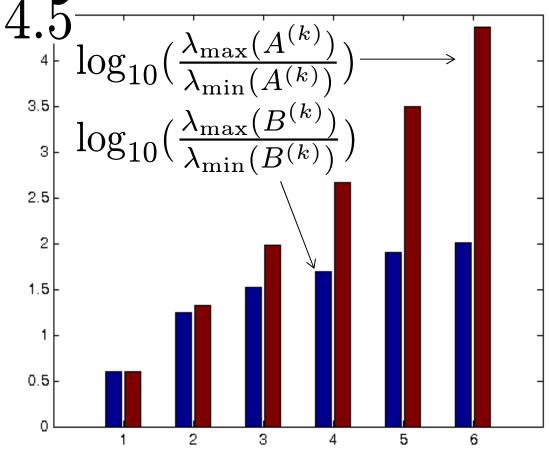
Subband solutions  $u^{(k+1)} - u^{(k)}$ can be computed independently

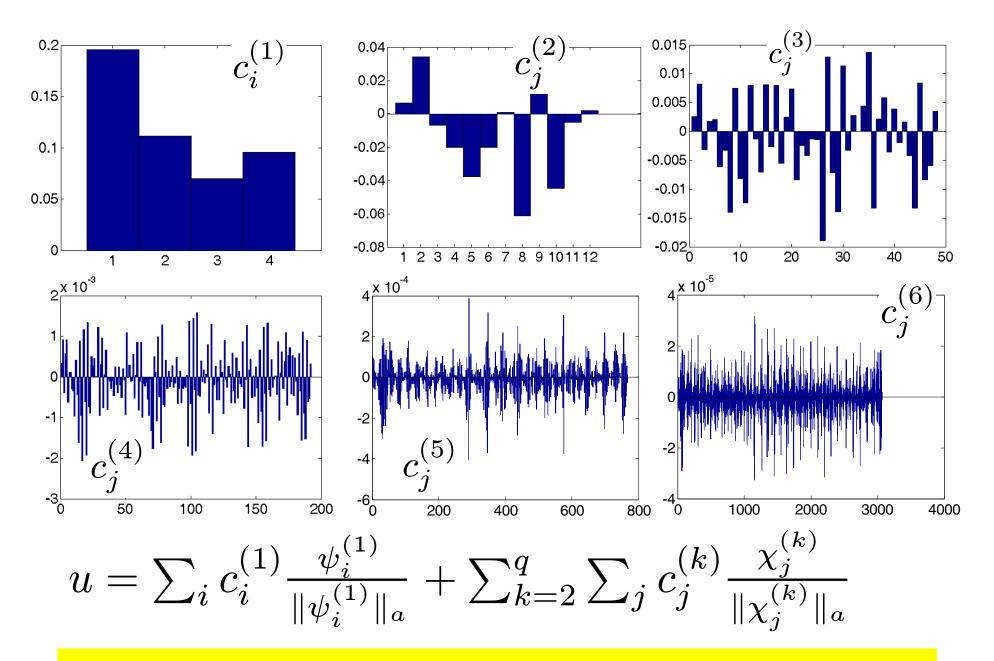
#### **Uniformly bounded condition numbers**

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

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



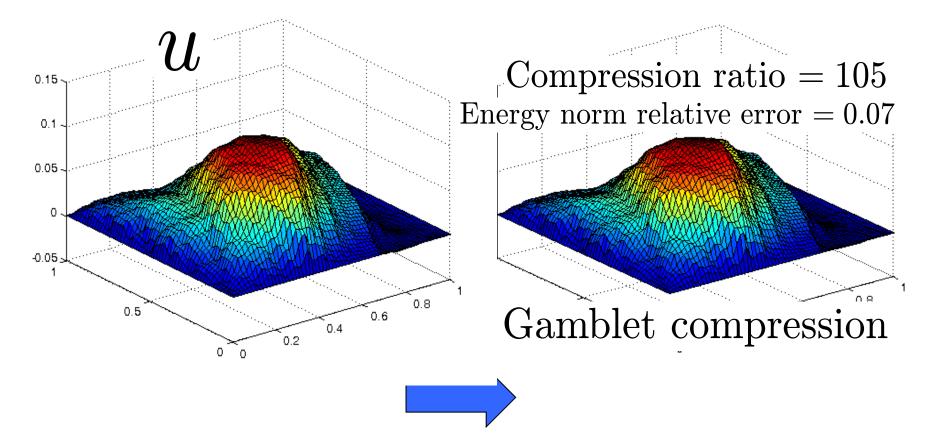




**Coefficients of the solution in the gamblet basis** 

# **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

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

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

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

**Localization** 

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

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

#### **Theorem**

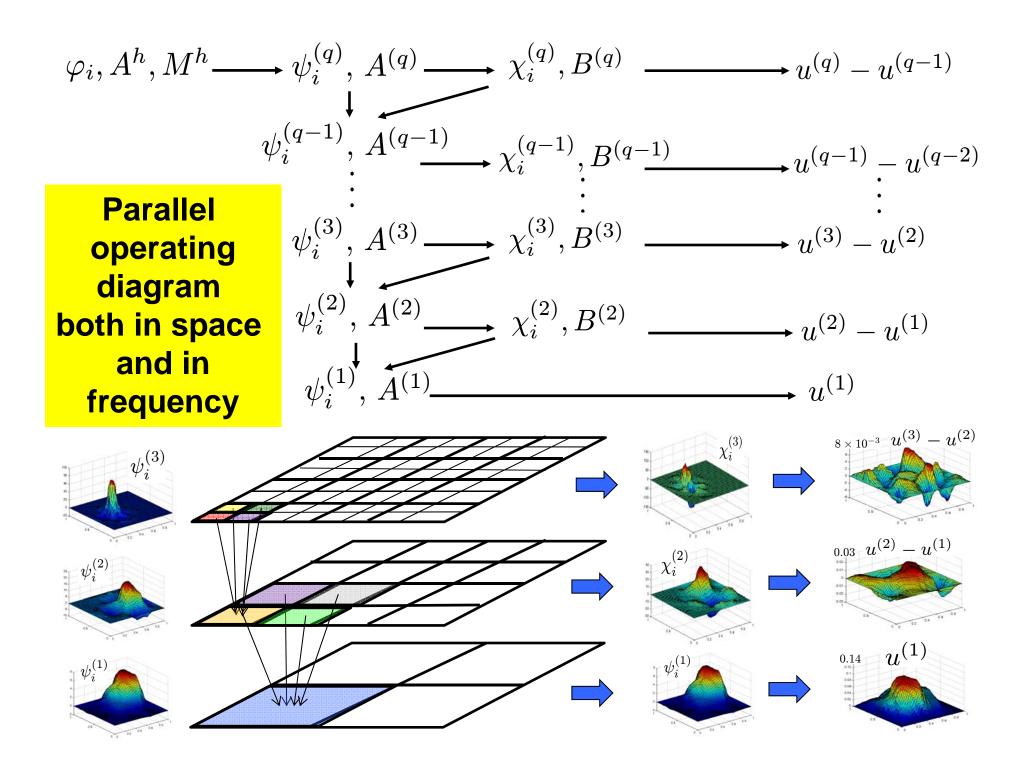
Localizing 
$$(\psi_i^{(k)})_{i \in \mathcal{I}_k}$$
 and  $(\chi_i^{(k)})_i$  to subdomains of size  
 $\geq CH_k \ln^2 \frac{1}{H_k} \Longrightarrow$  Cond. No  $(B^{(k), \text{loc}}) \leq C$   
 $\geq CH_k (\ln^2 \frac{1}{H_k} + \ln \frac{1}{\epsilon}) \Longrightarrow$   
 $\left\| u - u^{(1), \text{loc}} - \sum_{k=1}^{q-1} (u^{(k+1), \text{loc}} - u^{(k), \text{loc}}) \right\|_a \leq \epsilon$ 

## **Theorem**

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

Complexity

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



Generalization to linear systems of equations

Identification of the optimal prior/mixed strategy in that setting

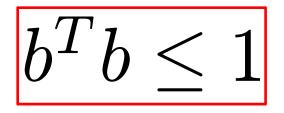
## Approximate solution x of

$$Ax = b$$

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

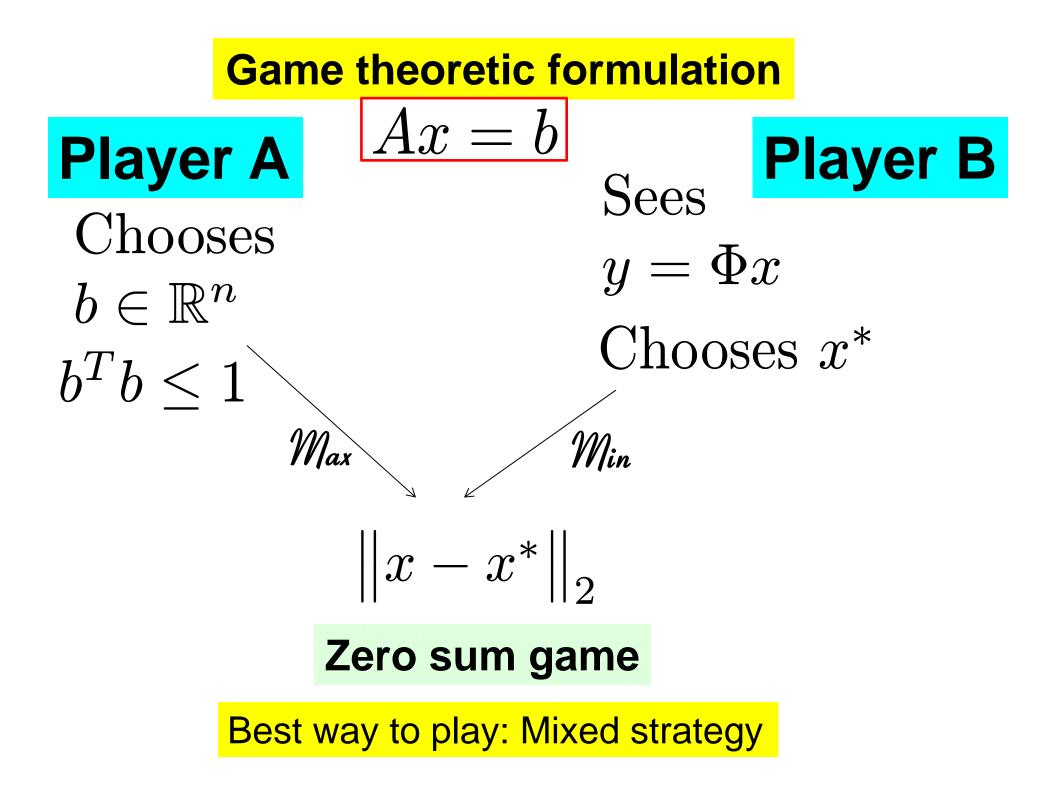
 $b{:}\ {\rm Unknown}\ {\rm element}\ {\rm of}\ \mathbb{R}^n$  Based on the information that

$$\Phi x = y$$



 $\Phi: \text{Known } m \times n$ rank m matrix (m < n)

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



# Player B's mixed strategyAx = b $\checkmark$ $AX = \xi$ $\xi \sim \mathcal{N}(0, Q)$

**Player's B bet** 

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

#### **Theorem**

**Accuracy of the recovery** 

$$\|x - x^*\|_{K^{-1}} = \min_{z \in \mathbb{R}^m} \|Q^{-\frac{1}{2}}b - Q^{-\frac{1}{2}}A^{\frac{1}{2}}K^{\frac{1}{2}}\Phi^T z\|$$

$$\|x\|_{K^{-1}}^2 := x^T K^{-1} x \qquad \qquad K = A^{-1} Q A^{-1}$$

## **Player B's optimal decision**

$$Q = A \implies K = A^{-1}$$

#### **Theorem**

$$\|x - x^*\|_A = \min_{z \in \mathbb{R}^m} \|A^{-\frac{1}{2}}b - A^{-\frac{1}{2}}\Phi^T z\|$$

Perspectives

#### How is this related to model uncertainty?

Motivations for developing this kind of framework

## Solving PDEs: Two centuries ago

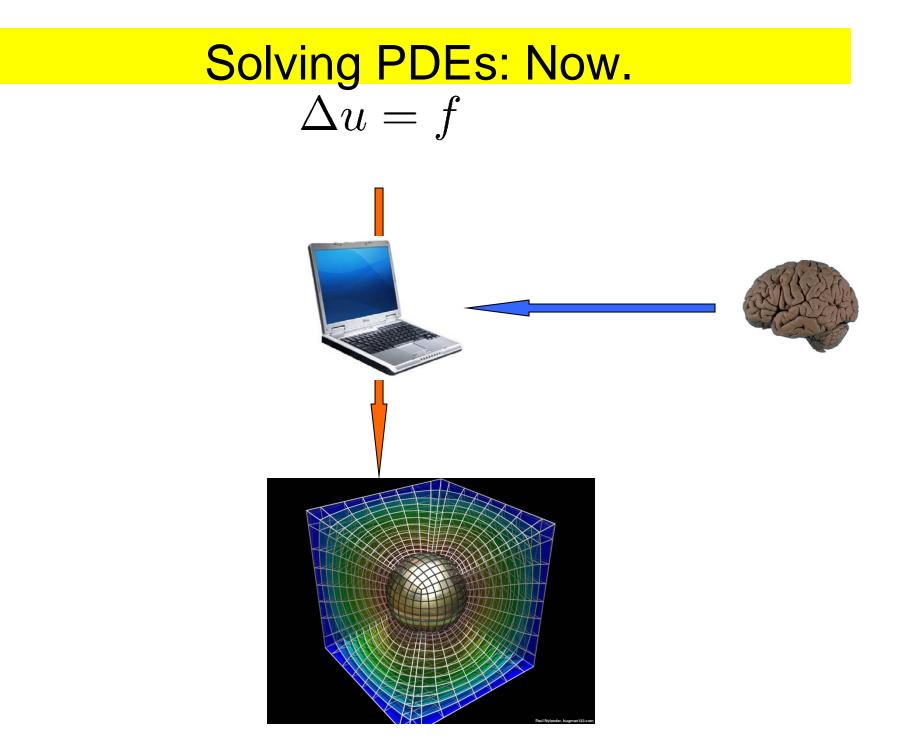
 $\Delta u = f$ 



A. L. Cauchy (1789-1857)

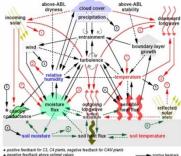
S. D. Poisson (1781-1840)

By the Hurglots integral binula,  $f_n(z) = \int_{0}^{2\pi} \frac{e^{i\theta} + z^i}{e^{i\theta} - z^i} \operatorname{Refn}(ae^{i\theta} + 5) \frac{d\theta}{2\pi}$ , 50  $\int \frac{1}{n(z)} - f_n(\omega) = \left(\int_{0}^{2\pi} \left(\frac{e^{i\theta} + z^i}{e^{i\theta} - z^i} - \frac{e^{i\theta} + iz^i}{e^{i\theta} - z^i}\right) \operatorname{Refn}(ae^{i\theta} + 5) \frac{d\theta}{2\pi}\right)$   $\leq \int_{0}^{2\pi} \frac{1}{(e^{i\theta} - z^i)} \frac{e^{i\theta} + z^i}{e^{i\theta} - z^i} - \frac{e^{i\theta} + iz^i}{e^{i\theta} - \omega^i} \operatorname{Refn}(ae^{i\theta} + 5) \frac{d\theta}{2\pi}$ Since k is compact.  $\exists M > 0$  such that  $|ae^{i\theta} + b| - (az^i + b)| = a|e^{i\theta} - z^i| \ge M$  $\forall z \in K$ . Since  $ZRefn \in K$  is converges unlinker on  $\partial_i$ , it is unlimber to under the estimates in  $\frac{1}{M^2} = \frac{2Ma}{M^2} |z - \omega|$ .



#### Find the best climate model now

and-surface - ABL - radiation interactio



8 10 12 14 16 18 20 22 24 26



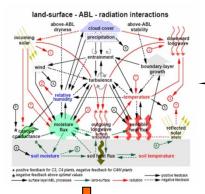


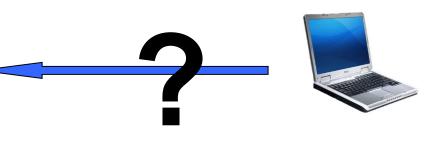
#### Find a 95% interval of confidence on average global temperatures in 50 years

## **Problem**

- Incomplete information on underlying processes
- Limited computation capability
- You don't know P
- You have limited data

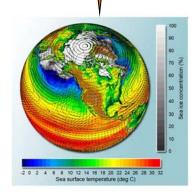
#### Can a machine compute the best climate model?





## **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**



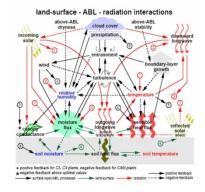
## **Chooses candidate**



# Sees data

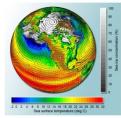


## **Chooses model**



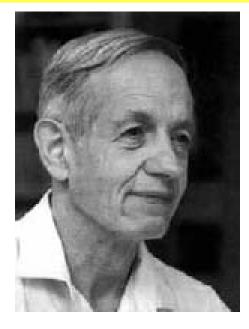
# $\mathcal{E}(\text{candidate}, \text{model}(\text{data}))$





## 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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