Numerical Solution of PDEs: Bounds for Functional Outputs and Certificates

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ASC Workshop, 22-23 August 2005, Stanford University

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Acknowledgments

Singapore-MIT Alliance

Sandia National Laboratories

DARPA/AFOSR

Sleipner Platform Failure

- Sank in August 1991, causing an event registering 3.0 on the Richter scale and leaving nothing but a pile of debris at a depth of 220m

- Sinking traced to a failure of a concrete tricell
- FEM performed with NASTRAN under-estimated shear stresses by 47%
- More precise simulation of under-designed component predicted failure at 62m
- Actually sank at 65m

Basic Question

How do we know if the answer computed with a FE code is correct[1]?

given that:

- the solution may not be "well behaved"
- we may not have similar solutions to compare
- we may not have access to the source code
- the code may no longer exist !!

1 i.e. consistent with the mathematical model

Basic Question

How do we know if the answer computed with a FE code is correct ?

$\Rightarrow$ Provide a **Certificate**

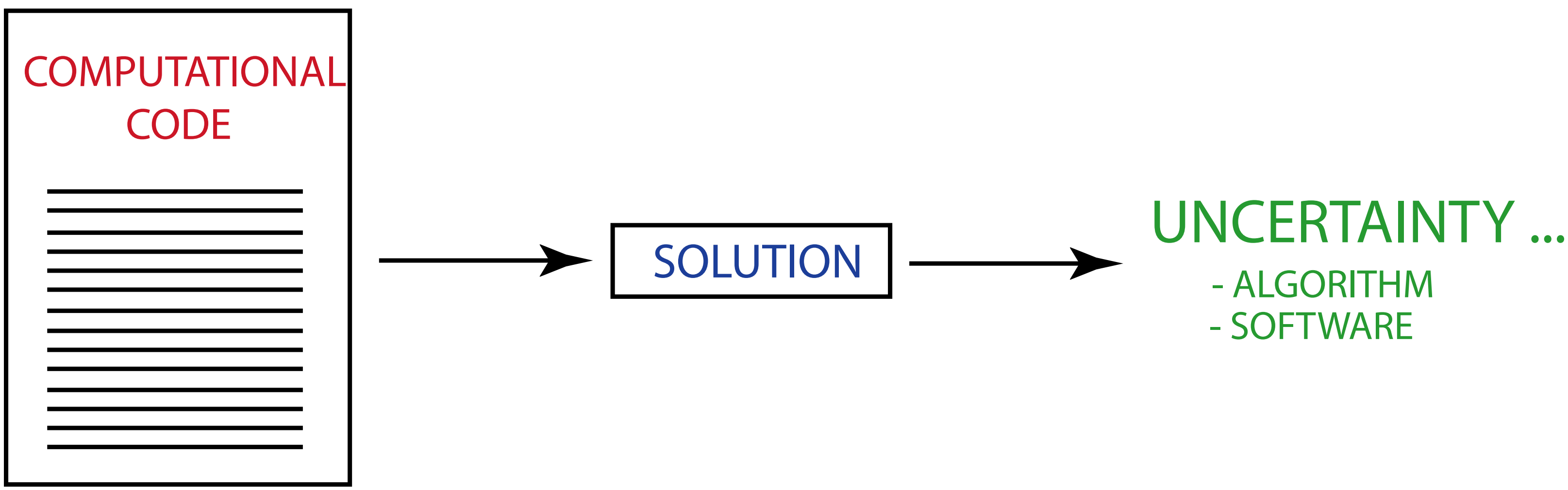
What is a Certificate?

A data set that documents a given claim

- Can be used to **rigorously** proof correctness
- **Simple** to exercise
- **Stand alone** - access to the code used to compute it not required
- The stronger the claim the “longer” the certificate (usually)

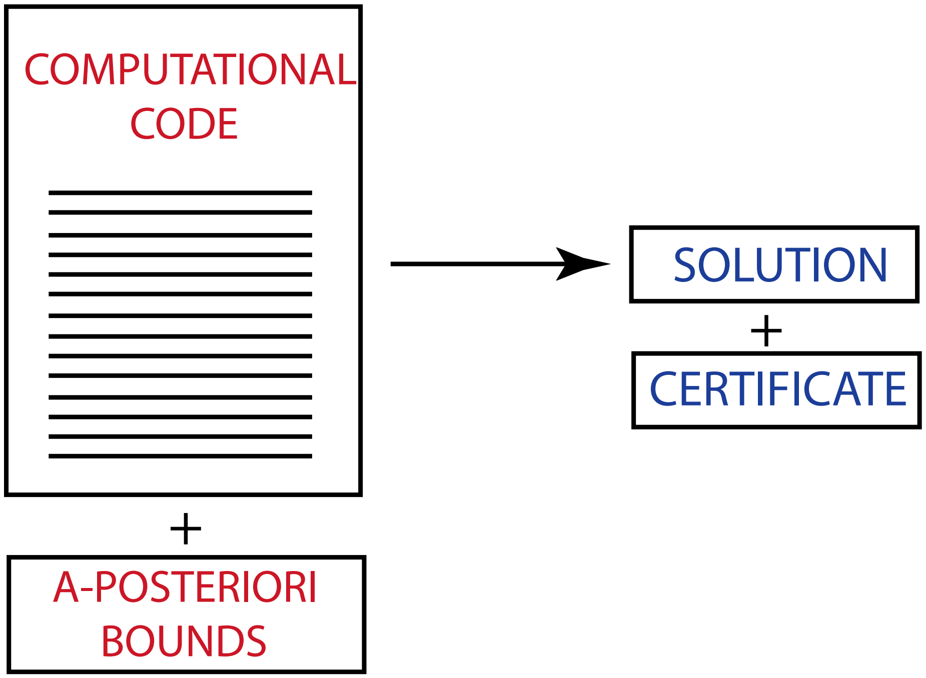
Certificates

Current Paradigm



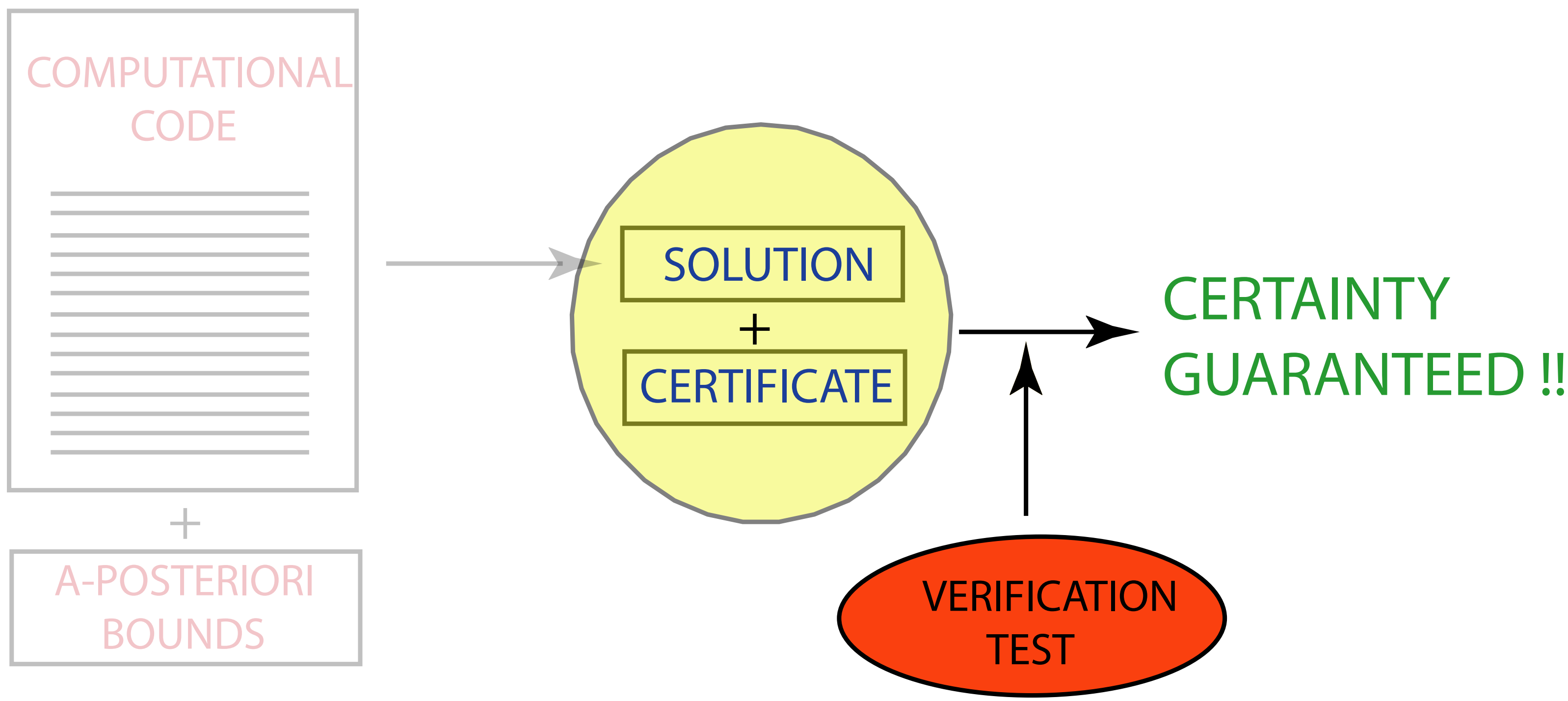
Certificates

Proposed Paradigm



Certificates

Proposed Paradigm



Certificates

Disclaimer

Physical Phenomenon

Modelling Uncertainty $\longrightarrow \Downarrow$

Continuous Mathematical Model

Discretization Uncertainty $\longrightarrow \Downarrow$

Discrete Mathematical Model

Software Uncertainty $\longrightarrow \Downarrow$

Prediction

Certificates

Disclaimer

Physical Phenomenon

Modelling Uncertainty $\longrightarrow \Downarrow$

Continuous Mathematical Model

$$\Downarrow$$

Prediction with certified error bounds

Certificates

Examples

Polynomial Bounds

Given a polynomial $F(x), \quad x \in \mathbb{R}^n$

Claim : $F(x) \geq \gamma, \quad \forall x$

Certificate : Polynomials $f_1(x), \ldots, f_m(x)$ s.t.

$$F(x) - \gamma = \sum_{i=1}^{m} f_i^2(x) \qquad \text{(SOS)}$$

or

$$\left(\sum_{i=1}^{n} f_i^2(x)\right) (F(x) - \gamma) = \sum_{i=n+1}^{m} f_i^2(x)$$

Certificates

Examples

Bounds for solutions of IVP...

Given $\dot{x} = f(x,t), \;\; x(0) = x_0, \quad (f(x,t)$ polynomial)

Claim : $x(T) \leq \gamma$

Certificate : Polynomial function $B(x,t)$ s.t.

$$B_t(x,t) + B_x(x,t) f(x,t) \leq 0 \, , \qquad \forall x, t$$

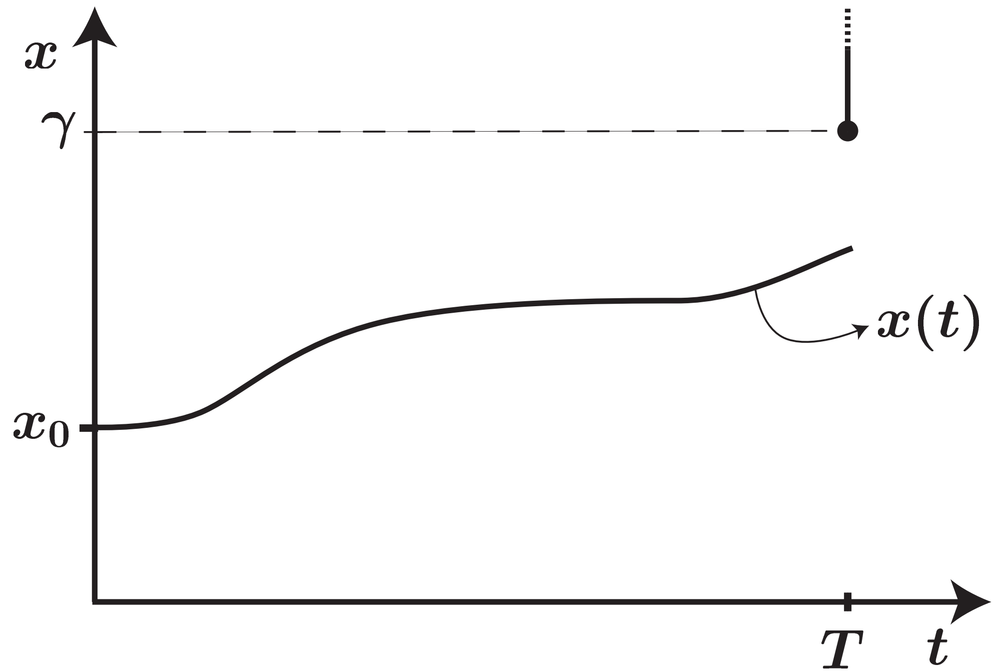
$$B(x_T, T) > B(x_0, 0) \, , \qquad \forall x_T \geq \gamma$$

Parrilo, Doyle, . . .

Certificates

Examples

...Bounds for solutions of IVP...



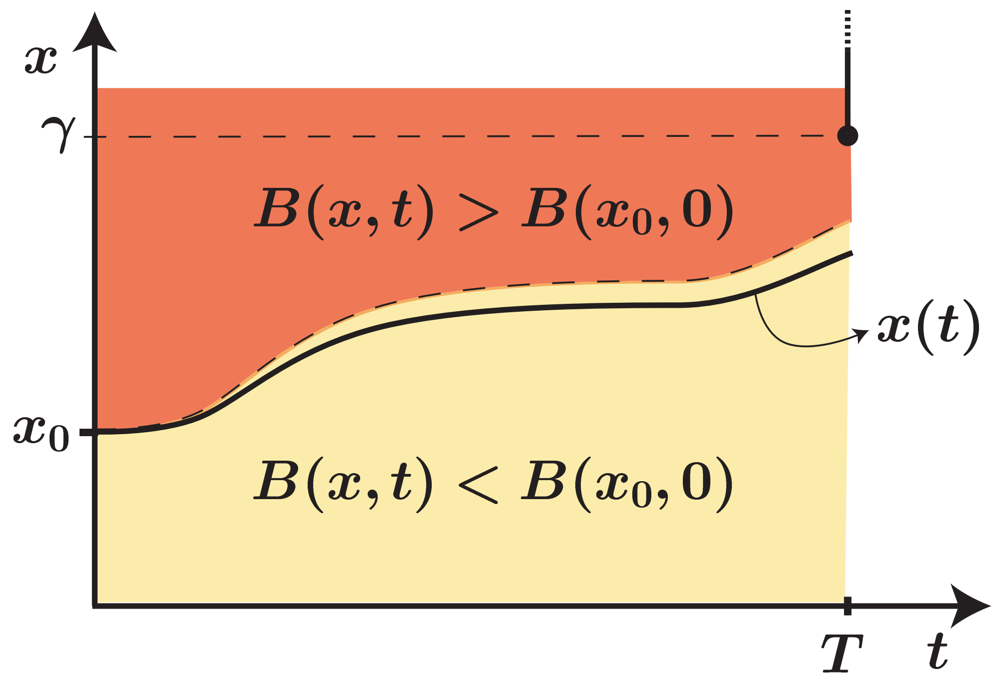
$$B_t(x,t) + B_x(x,t) f(x,t) \leq 0 \,, \qquad \forall x, t$$

$$B(x_T, T) > B(x_0, 0) \,, \qquad \forall x_T \geq \gamma$$

Certificates

Examples

...Bounds for solutions of IVP...



$$B_t(x,t) + B_x(x,t)f(x,t) \leq 0\ , \qquad \forall x, t$$

$$B(x_T,T) > B(x_0,0)\ , \qquad \forall x_T \geq \gamma$$

Certificates

Examples

...Bounds for solutions of IVP

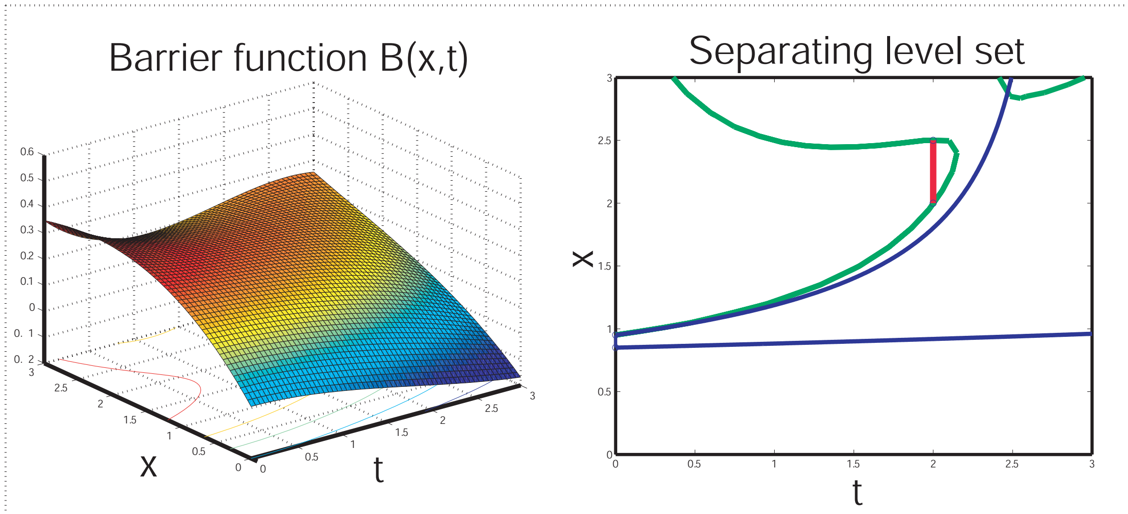
Given:

$$\dot{x} = px^3$$

$$x(0) \in [0.85, 0.95]$$

$$p \in [0.05, 0.2]$$

$$x(2) \overset{?}{\in} [2.0, 2.5]$$



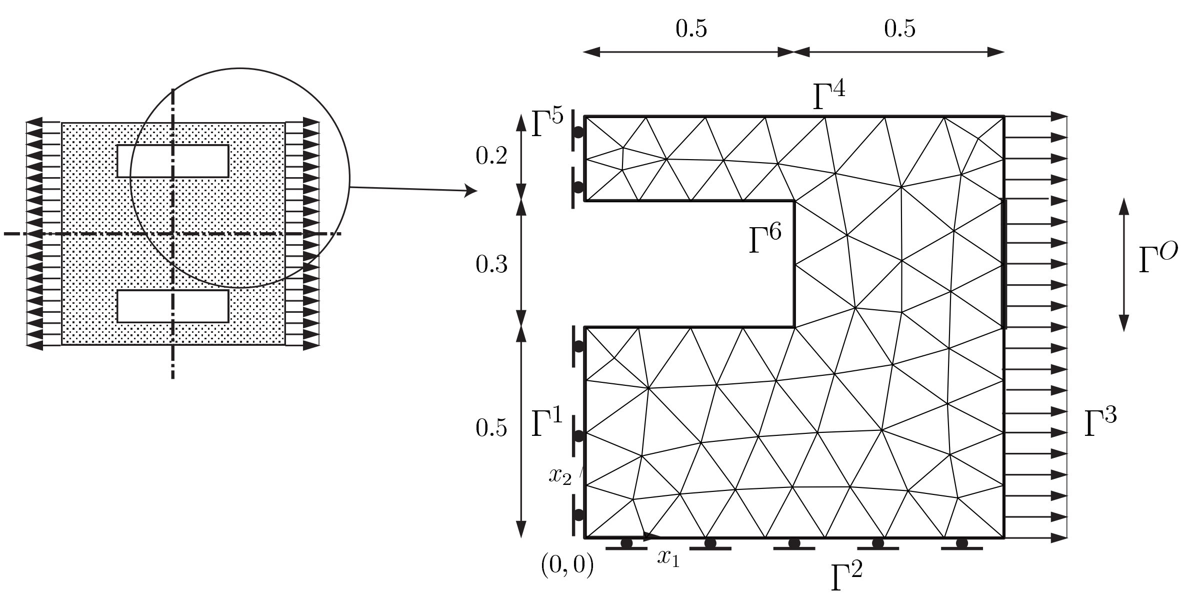
$$\Rightarrow \quad x(2) \notin [2.0, 2.5]$$

Objective

Compute Certificates for Bounds of Outputs of PDE's

- Work with **quantities** of interest
- Work with **equations** of interest
- Guarantee **certainty** even for low cost
- **Cost** effective

Non-regular solution (Plane Stress)



OUTPUTS

$$\ell(u) = \int_{\Gamma^O} u \, ds$$

$$\ell(u) = \int_{\Gamma^5} t_x \, ds$$

What can we do Today?

Linear Functional Outputs for:

- Convection-Diffusion-Reaction Equation (high Pe)
- Linear Elasticity Equations
- Stokes Equations (DG)

Collapse Loads in Limit Analysis (SOCP)

Energy Release Rates in Linear Elasticity

Outline

- Problem Description
- Function Minimization/Duality in $\mathbb{R}^n$
- Method Overview (for CG)

1.- Bounds for Energy

2.- Bounds for “Arbitrary” Outputs

3.- Bounds for “Arbitrary” Equations

4.- Domain Decomposition (Hybridization)

- Method Summary and Examples
- Extension to a non-linear Convex Problem: Limit Analysis

Problem Description

Let $u(x) \in X$, $x \in \Omega \subset \mathbb{R}^d$, be the solution of a PDE

$$\boxed{\mathcal{A} u = f\ .}$$

e.g. $\mathcal{A} \equiv -\nabla^2, -\nabla^2 + \mathrm{U} \cdot \nabla$, etc.

We are typically interested in *outputs* of the form

$$s = \ell(u) \in \mathbb{R} \qquad ,$$

$$e.g. \qquad \ell(v) \equiv v(x_0), \qquad \ell(v) = \int_{\Omega'} v_x \, dx, \qquad \ldots$$

Problem Description

- $u(x)$ is **not computable** ($\infty-$ dimensional)
- In practice, we compute approximation $\bar{u}(x)$, such that $||u - \bar{u}|| = C(\rightarrow 0)$ (as cost increases $\rightarrow \infty$).
  - For a given $\bar{u}$, C is **unknown**, and, any output approximation $\bar{s} = \ell(\bar{u})$, is uncertain.
- Existing error estimates are either,
  - **certain** but **uncomputable**, or,
  - **computable** but **uncertain**.

Problem Description

Approach

Compute **Strict** upper and lower bounds for functional outputs of the **Exact** solutions of PDE's

. . . and give **Certificates**

Function Minimization

Unconstrained

$f : Y \mapsto \mathbb{R}$ e.g. $Y \equiv \mathbb{R}^n$

$$s = \min_{v \in Y} f(v) \equiv f(v^*)$$

Function Minimization

Unconstrained

Upper Bound

$$s = \min_{v \in Y} f(v) \equiv f(v^*)$$

$$\leq \underbrace{f(\bar{v})}_{\text{upper bound}} \equiv s^+, \quad \forall \bar{v} \in Y$$

EASY !

. . . we expect a reasonable bound if $\bar{v} \approx v^*$

Upper Bound: Example...

Linear-Quadratic Problem

$$f(v) = \frac{1}{2} v^T A v - v^T b, \; A \in \mathbb{R}^n \times \mathbb{R}^n \text{ SPD}, \; b, v \in \mathbb{R}^n$$

Stationarity condition

$$A v^* = b$$

$$s = \min_{v \in Y} f(v) = f(v^*) = -\frac{1}{2} v^{*T} A v^*$$

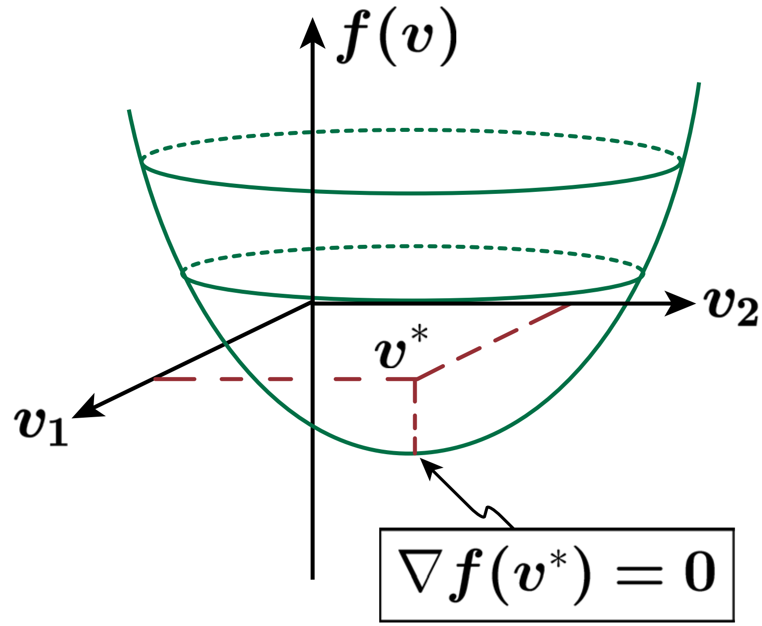
Function Minimization

Unconstrained

...Upper Bound: Example

Let $\bar{v} = v^* + \epsilon$

$$s^+ = f(\bar{v}) = f(v^*) + \frac{1}{2}\epsilon^T A \epsilon$$



"Error" is $\mathcal{O}(\epsilon^2)$

Function Minimization

Unconstrained

Lower Bound

$$s = \min_{v \in Y} f(v) \equiv f(v^*)$$

It appears that we need to know v^* explicitly

Not generally available ??

Function Minimization

Equality Constrained

$$f : Y \mapsto \mathbb{R}, \quad \text{objective}$$

$$g : Y \mapsto \Lambda \quad \text{constraints}$$

e.g. $Y \equiv \mathbb{R}^n, \ \Lambda \equiv \mathbb{R}^m$

$$s = \min_{\substack{v \in Y \\ g(v) = 0}} f(v)$$

Function Minimization

Equality Constrained

Lagrangian

$$L(v, \lambda) : Y \times \Lambda \to \mathbb{R}$$

$$L(v, \lambda) = f(v) + \lambda^T g(v)$$

λ : Lagrange multipliers

It follows that

$$s = \min_{v \in Y} \max_{\lambda \in \Lambda} \mathcal{L}(v, \lambda)$$

$$\min_{v\in Y}\ \max_{\lambda\in\Lambda}\ \mathcal{L}(v,\lambda) \geq \max_{\lambda\in\Lambda}\ \min_{v\in Y}\ \mathcal{L}(v,\lambda)$$

Proof: Let

$$L(v,\lambda^*(v)) \equiv \max_{\lambda\in\Lambda}\ L(v,\lambda)$$

$$L(v^*(\lambda),\lambda) \equiv \min_{v\in Y}\ L(v,\lambda)$$

Then,

$$L(v,\lambda^*(v)) \geq L(v,\lambda) \geq L(v^*(\lambda),\lambda), \quad \forall v,\lambda.$$

Function Minimization

Equality Constrained

Lower Bound

Since by duality,

$$s = \min_{v \in Y} \max_{\lambda \in \Lambda} L(v, \lambda) \geq \max_{\lambda \in \Lambda} \underbrace{\min_{v \in Y} L(v, \lambda)}_{L(v^*(\lambda), \lambda) \equiv G(\lambda)}$$

"Dual Function"

Then,

$$s \geq \max_{\lambda \in \Lambda} G(\lambda) \geq \underbrace{G(\bar{\lambda})}_{\text{lower bound}} \equiv s^-, \quad \forall \bar{\lambda} \in \Lambda$$

. . . reasonable bounds to be expected when $\bar{\lambda} \approx \lambda^*$

Function Minimization

Unconstrained

Lower Bound...

$$s = \min_{v \in Y} f(v)$$

Assume $f(v) \equiv F(v, g(v))$ and consider

$$s = \min_{\substack{v \in Y, w \in \Lambda \\ g(v) - w = 0}} F(v, w)$$

Function Minimization

Unconstrained

...Lower Bound

Lagrangian $L(v, w, \lambda) = F(v, w) + \lambda^T (g(v) - w)$

"Dual function"

$$G(\lambda) = \min_{v \in Y, w \in \Lambda} L(v, w, \lambda) = L(v^*(\lambda), w^*(\lambda), \lambda)$$

$$s = \min_{v \in Y} f(v) \geq \max_{\lambda \in \Lambda} G(\lambda) \geq G(\bar{\lambda}) \equiv s^-, \quad \forall \lambda$$

Linear-Quadratic Problem

$$f(v) = v^T K^T K v + v^T b, \qquad K \in \mathbb{R}^n \times \mathbb{R}^n\,,\; b, v \in \mathbb{R}^n$$

$$\begin{aligned} f(v) &\equiv F(v, g(v)) \\ &= g^T g + v^T b, \qquad\qquad g(v) = K v \in \mathbb{R}^n \end{aligned}$$

$$\Rightarrow \; L(v, w, \lambda) = w^T w + b^T v + \lambda^T (K v - w)$$

...Lower Bound: Example

"Dual Function"

$$G(\boldsymbol{\lambda}) = \min_{v \in Y, w \in \Lambda} L(v, w, \boldsymbol{\lambda}) = \begin{cases} -\frac{1}{2}\boldsymbol{\lambda}^T\boldsymbol{\lambda} & \text{if } K^T\boldsymbol{\lambda} = b \\ -\infty & \text{otherwise} \end{cases}$$

$$s = \min_{v \in Y} f(v) \geq \max_{\lambda \in \Lambda} G(\boldsymbol{\lambda})$$

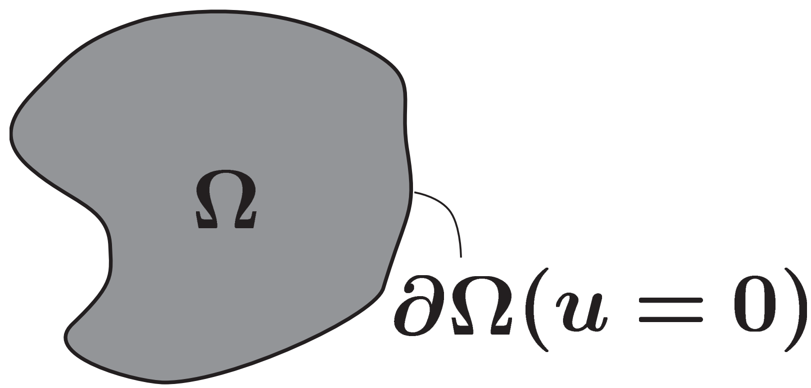
$$\geq -\frac{1}{2}\bar{\boldsymbol{\lambda}}^T\bar{\boldsymbol{\lambda}} \equiv s^-, \quad \forall \bar{\boldsymbol{\lambda}} \text{ s.t. } K\boldsymbol{\lambda} = b$$

Method Overview

1.- Energy $s = J(u)$

Poisson's Equation: Find $u \in X(\Omega)$

$$-\nabla^2 u = f(x), \quad x \in \Omega, \qquad (+ \text{ b.c.'s})$$



"Energy" functional: $J(v) : X \rightarrow \mathbb{R}$

$$J(v) = \int_\Omega \nabla v \cdot \nabla v \, dx - 2 \int_\Omega f v \, dx$$

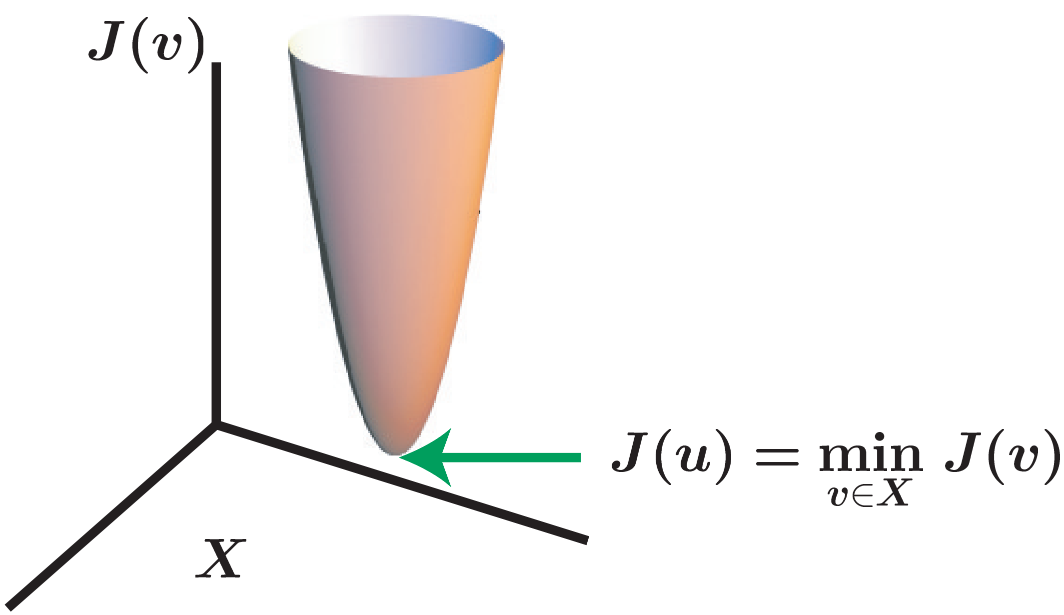
Method Overview

1.- Energy $s = J(u)$

Minimization

Minimization formulation

$$\min_{v \in X} J(v) = J(u) \qquad = -\int_\Omega u f \, dx$$



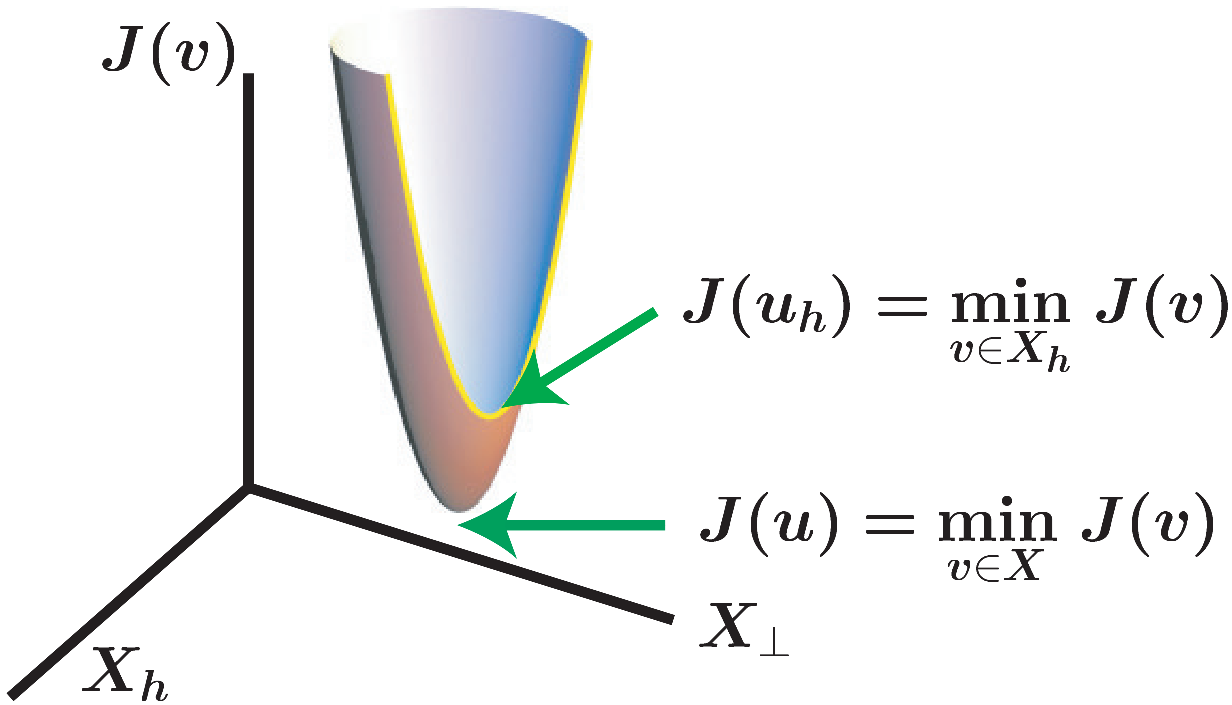
Method Overview

1.- Energy $s = J(u)$

Upper Bound

Upper bound $s^+ \equiv J(u_h), \qquad \forall u_h \in X_h \subset X$

(trivial)



Lower bound s^- (harder)

Construct **dual** problem

$$(J(u) =)\ \ J^c(p) = \max_{q \in Q_f} J^c(q)\ ,$$

Method Overview

1.- Energy $s = J(u)$

...Lower Bound...

$$s = \min_{v \in X} \int_\Omega (\nabla v \cdot \nabla v - 2 v f)\, dx \qquad (q = \nabla v)$$

$$= \min_{v \in X} \max_{q \in Q} \int_\Omega (-q \cdot q + 2 q \cdot \nabla v - 2 v f)\, dx$$

$$\geq \max_{q \in Q} \min_{v \in X} \int_\Omega (-q \cdot q + 2 q \cdot \nabla v - 2 v f)\, dx$$

$$= \max_{q \in Q_f} \int_\Omega -q \cdot q \, dx$$

$$Q_f = \{ q \in Q \mid \underbrace{\int_\Omega q \cdot \nabla v \, dx = \int_\Omega f v \, dx, \quad \forall v \in X}_{-\nabla \cdot q = f} \}$$

Method Overview

1.- Energy $s = J(u)$

...Lower Bound...

$$
\begin{aligned}
s &= \min_{v \in X} \quad J(v) \\
&= \min_{v \in X} \max_{q \in Q} \int_\Omega (-q \cdot q + 2q \cdot \nabla v - 2vf)\, dx \\
&\geq \max_{q \in Q} \min_{v \in X} \int_\Omega (-q \cdot q + 2q \cdot \nabla v - 2vf)\, dx \\
&= \max_{q \in Q_f} \quad J^c(q)
\end{aligned}
$$

$$
Q_f = \{ q \in Q \mid \underbrace{\int_\Omega q \cdot \nabla v \, dx = \int_\Omega f v \, dx, \quad \forall v \in X}_{-\nabla \cdot q = f} \}
$$

Method Overview

1.- Energy $s = J(u)$

...Lower Bound...

or, in a different way ... $\int_\Omega (q - \nabla v)^2 \, dx \geq 0 \,, \; \forall v \in X, q \in Q$

$$\int_\Omega q \cdot q \, dx - 2 \int_\Omega q \cdot \nabla v \, dx + \int_\Omega \nabla v \cdot \nabla v \, dx \geq 0, \; \forall v \in X, q \in Q$$

$$\underbrace{\int_\Omega q \cdot q \, dx}_{-J^c(q)} \underbrace{- 2 \int_\Omega f v \, dx + \int_\Omega \nabla v \cdot \nabla v \, dx}_{+ \quad J(v)} \geq 0, \; \forall v \in X, q \in Q_f$$

$$-J^c(q) \quad + \quad J(v) \geq 0, \; \forall v \in X, q \in Q_f$$

$$Q_f = \{ q \in Q \mid \int_\Omega q \cdot \nabla v \, dx = \int_\Omega f v \, dx, \quad \forall v \in X \} \qquad (-\nabla \cdot q = f)$$

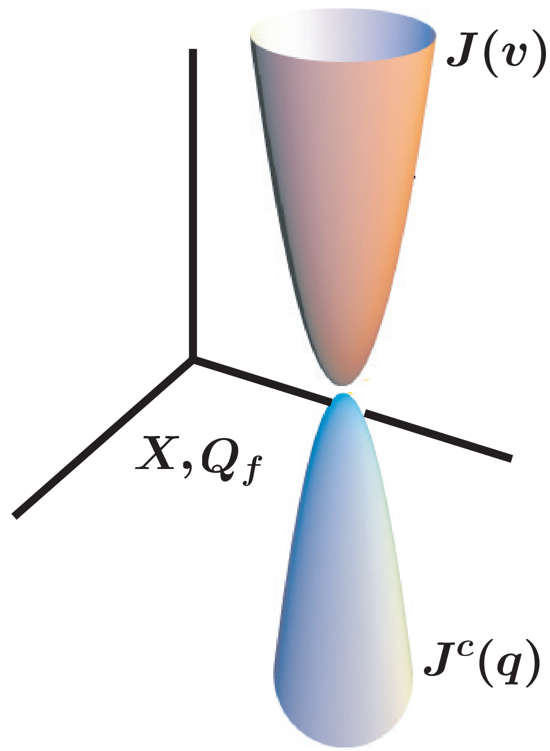
$$\boxed{J(v) \geq J^c(q), \qquad \forall v \in X, q \in Q_f}$$

Method Overview

1.- Energy $s = J(u)$

...Lower Bound...

Duality

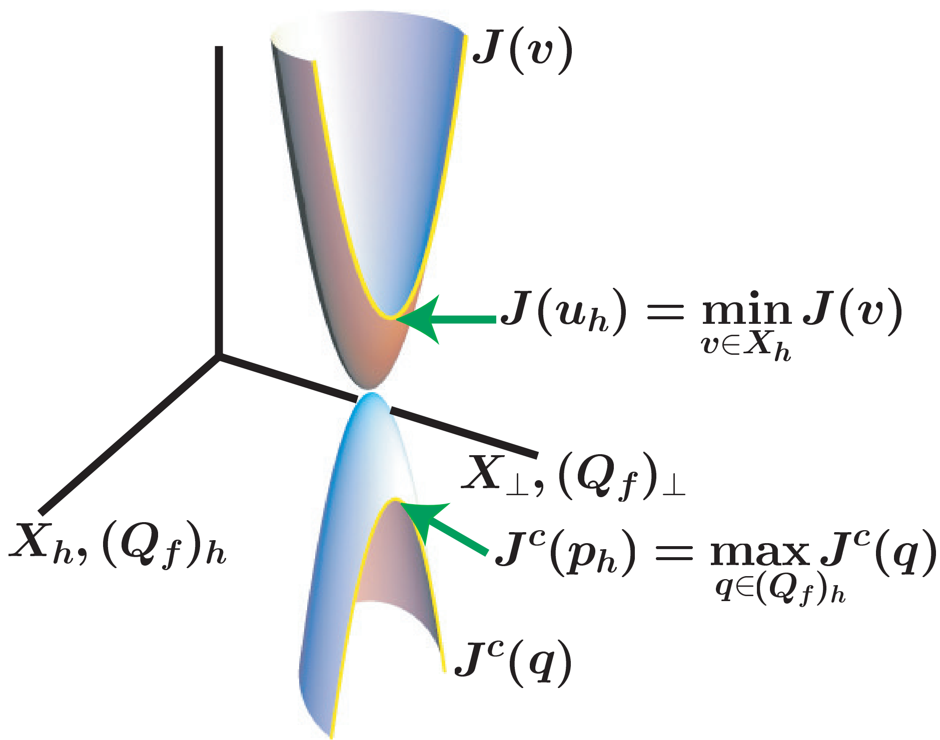


Method Overview

1.- Energy $s = J(u)$

...Lower Bound...

Then, $s^- \equiv J^c(p_h), \; \forall p_h \in (Q_f)_h \subset Q_f$.



Method Overview

1.- Energy $s = J(u)$

...Lower Bound

Idea :

We can exchange an **infinite** dimensional **minimization** problem by a **finite** dimensional **feasibility** problem while retaining the bounding property

Lower Bound - Summary

Given $-\nabla^2 u = f(x)$

Claim : $s = J(u) = -\int_\Omega u f \, dx \geq s^-$

Certificate : Any $p_h \in (Q_f)_h \subset Q_f$ s.t. $s^- \equiv J^c(p_h)$

Recall:

$$Q_f = \{ q \in Q \mid \int_\Omega q \cdot \nabla v \, dx = \int_\Omega f v \, dx, \quad \forall v \in X \} \qquad (-\nabla \cdot q = f)$$

Method Overview

2.- General Outputs $s = \ell(u)$

Find $s = \ell(u)$, where $u \in X(\Omega)$ $\quad$ ($\ell(v) = \int_\Omega f^{\mathcal{O}} v \, dx$)

$$-\nabla^2 u = f(x), \quad x \in \Omega, \qquad (+ \text{ b.c.'s})$$

or,

$$\int_\Omega (\nabla u \cdot \nabla v - f v) \, dx = 0, \quad \forall v \in X$$

Modified Energy : $\mathcal{E}(v) : X \longrightarrow \mathbb{R}$

$$\mathcal{E}(v) \equiv \int_\Omega \nabla v \cdot \nabla v \, dx - \int_\Omega f v \, dx \qquad \Rightarrow \mathcal{E}(u) = 0$$

Method Overview

2.- General Outputs $s = \ell(u)$

Lagrangian

$$s = \ell(u) = \min_{\substack{v \in X \\ \int_\Omega (\nabla v \cdot \nabla \psi - f\psi)\,dx = 0,\ \forall \psi \in X}} \ell(v) \ + \mathcal{E}(v)$$

Lagrangian : $L(v, \psi) : X \times X \longrightarrow \mathbb{R}$

$$L(v, \psi) = \mathcal{E}(v) + \ell(v) + \int_\Omega (\nabla v \cdot \nabla \psi - f\psi)\,dx$$

$$s = \ell(u) = \min_v \max_\psi L(v, \psi)$$

Lower Bound...

Weak duality + Relaxation

$$\begin{aligned} s = \ell(u) &= \min_{v} \max_{\psi} L(v, \psi) \\ &\geq \max_{\psi} \min_{v} L(v, \psi) \\ &\geq \min_{v} L(v, \bar{\psi}), \ \forall \bar{\psi} \in X \end{aligned}$$

Method Overview

2.- General Outputs $s = \ell(u)$

...Lower Bound...

$$\boldsymbol{L(v,\bar{\psi}) = \int_\Omega \nabla v \cdot \nabla v \, dx - \int_\Omega f v \, dx}$$

$$\boldsymbol{+ \ell(v) + \int_\Omega (\nabla v \cdot \nabla \bar{\psi} - f \bar{\psi}) \, dx}$$

For a given $\bar{\psi}$, $\boldsymbol{L(v,\bar{\psi})}$, contains quadratic and linear terms in $\boldsymbol{v} \Rightarrow$ identical to $\boldsymbol{J(v)}$ (for an appropriate $\boldsymbol{f_{\bar{\psi}}}$).

$$\boldsymbol{L(v,\bar{\psi}) = \int_\Omega \nabla v \cdot \nabla v \, dx - 2 \int_\Omega f_{\bar{\psi}} v \, dx - \int_\Omega f \bar{\psi} \, dx}$$

...Lower Bound

Idea :

Write output as a **constrained** minimization problem. **Relax** constraint to obtain an **energy-like** minimization problem. Obtain **lower bound** by finding a **feasible** solution of the dual problem.

Method Overview

2.- General Outputs $s = \ell(u)$

Upper Bound

Define $\ell_*(v) = -\ell(v)$ and compute,

$$s_*^- \le \ell_*(u)$$

$$s^+ \equiv -s_*^- \ge -\ell_*(u) = \ell(u)$$

Idea:

Upper Bound for $\ell(v) \equiv -$ **Lower Bound** for $-\ell(v)$

Summary

Given $-\nabla^2 u = f(x)$

Claim : $s^{+} \geq s = \ell(u) \geq s^{-}$

Certificate :

$$\bar{\psi} \in X_h \subset X,$$
$$p_h^{+} \in (Q_{f^+})_h \subset Q_{f^+},$$
$$p_h^{-} \in (Q_{f^-})_h \subset Q_{f^-}$$

Method Overview

3.- Non-symmetric equations

$$-\nabla^2 u + \boldsymbol{U} \cdot \nabla u = f(x), \quad x \in \Omega, \qquad (+ \text{ b.c.'s})$$

or,

$$\int_\Omega (\nabla u \cdot \nabla v + (\boldsymbol{U} \cdot \nabla u) v - f v)\, dx = 0, \quad \forall v \in X$$

Modified Energy : $\mathcal{E}(v) : X \longrightarrow \mathbb{R}$

$$\mathcal{E}(v) \equiv \int_\Omega \nabla v \cdot \nabla v \, dx - \int_\Omega f v \, dx \qquad \Rightarrow \mathcal{E}(u) = 0$$

Method Overview

3.- Non-symmetric equations

Lagrangian...

$$s = \ell(u) = \min_{v \in X} \ell(v) + \mathcal{E}(v)$$

$$\int_\Omega (\nabla v \cdot \nabla \psi + (U \cdot \nabla v)\psi - f\psi)\, dx = 0, \forall \psi \in X$$

Lagrangian : $L(v, \psi) : X \times X \longrightarrow \mathbb{R}$

$$L(v,\psi) = \mathcal{E}(v) + \ell(v) + \int_\Omega (\nabla v \cdot \nabla \psi + (U \cdot \nabla v)\psi - f\psi)\, dx$$

$$s = \ell(u) = \min_v \max_\psi L(v, \psi)$$

. . .

Method Overview

3.- Non-symmetric equations

...Lagrangian

Idea :

Non-symmetric terms do not contribute to the **"energy"** and only enter in the Lagrangian linearly. After relaxation, minimization problem retains **convex** structure.

4.- Domain Decomposition

Recall that a lower bound for $s = J(u)$, is given by
$s^- = J^c(q), \forall q \in Q_f$

$$Q_f = \{q \in Q \mid \int_\Omega q \cdot \nabla v \, dx = \int_\Omega f v \, dx, \quad \forall v \in X\}$$

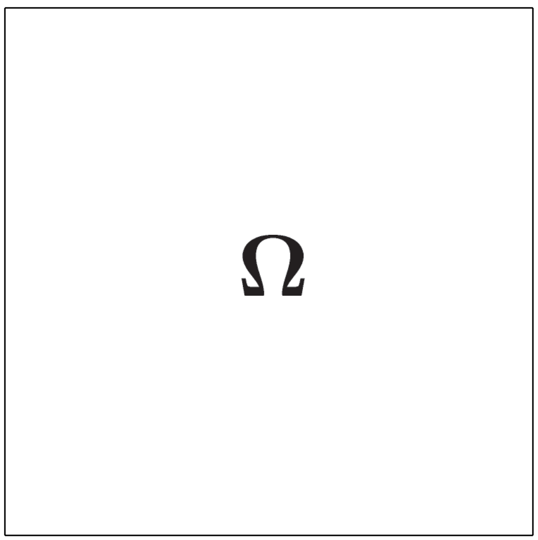
i.e. find $q \in Q$ s.t.

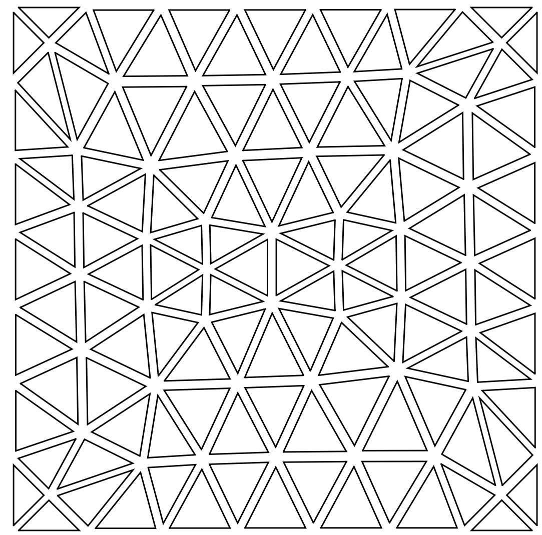
$$\nabla \cdot q = f, \qquad \text{in} \quad \Omega$$

. . . **not trivial**

$v \in X(\Omega)$ continuous

$\hat{v} \in \hat{X}(\Omega)$ discontinuous

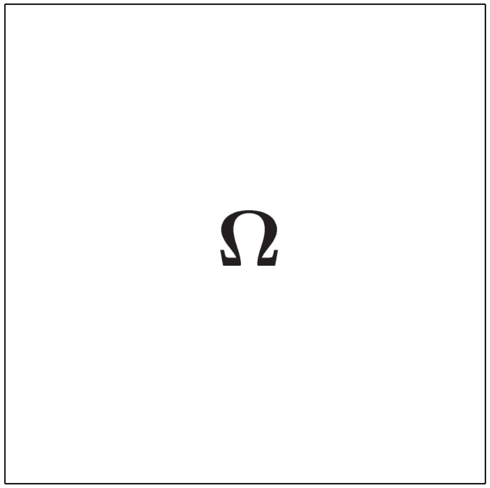


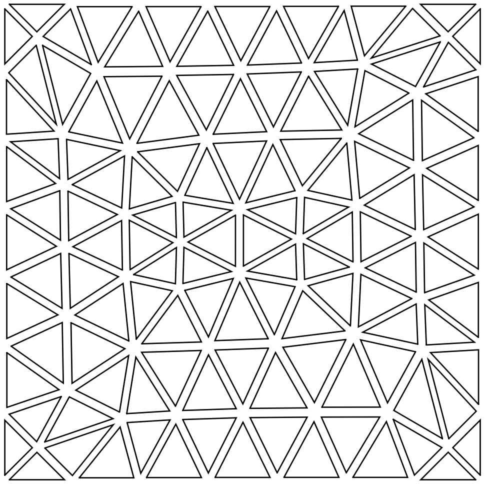


$$X \subset \hat{X}$$

4.- Domain Decomposition

$v \in X(\Omega)$ continuous $\qquad \hat{v} \in \hat{X}(\Omega)$ discontinuous





Idea : solve **local** minimization problems

$\Rightarrow$ use **piecewise polynomial certificates**

Continuity Form

"Jump" bilinear form $b : \hat{X}(\Omega) \times \Lambda(\Gamma) \longrightarrow \mathbb{R}$

$$\boldsymbol{b}(\hat{\boldsymbol{v}}, \boldsymbol{\lambda}) = \sum_{\gamma} \int_{\gamma} [\hat{\boldsymbol{v}}]_{\gamma} \cdot \boldsymbol{\lambda}|_{\gamma} \, \boldsymbol{ds},$$

$$\boldsymbol{X} \equiv \{\hat{\boldsymbol{v}} \in \hat{\boldsymbol{X}} \mid \boldsymbol{b}(\hat{\boldsymbol{v}}, \boldsymbol{\lambda}) = \boldsymbol{0}, \forall \boldsymbol{\lambda} \in \boldsymbol{\Lambda}\}$$

Relaxation...

$$J(u) = \min_{v \in X} J(v) = \min_{\substack{\hat{v} \in \hat{X} \\ b(\hat{v}, \boldsymbol{\lambda}) = 0, \forall \boldsymbol{\lambda} \in \boldsymbol{\Lambda}}} J(\hat{v})$$

$$= \min_{\hat{v} \in \hat{X}} \max_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} J(\hat{v}) + b(\hat{v}, \boldsymbol{\lambda})$$

$$\geq \min_{\hat{v} \in \hat{X}} \underbrace{J(\hat{v}) + b(\hat{v}, \bar{\boldsymbol{\lambda}})}_{J_{\bar{\lambda}}(\hat{v})}, \quad \forall \bar{\boldsymbol{\lambda}} \in \boldsymbol{\Lambda} \text{ (equil.)}$$

$\Rightarrow$ Solve local minimization problems

Feasibility problem over each triangle

$$\nabla \cdot q = f, \qquad \text{in} \quad T_e$$

$$q \cdot n = \bar{\lambda}, \qquad \text{on} \quad \partial T_e$$

has an explicit solution provided f and $\bar{\lambda}$ are **polynomial**

Ladeveze . . .

Summary

1. Primal problem: $\boldsymbol{u}_h \in \boldsymbol{X}_h$

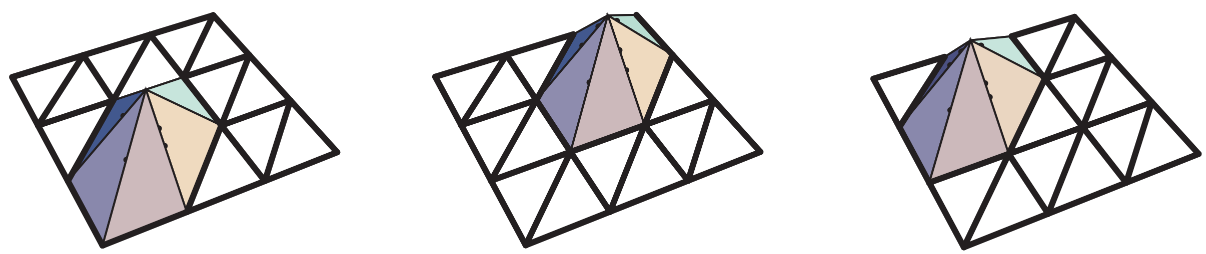
$$\boldsymbol{\mathcal{A}} \boldsymbol{u}_h = \boldsymbol{f}$$

2. Dual problem: $\bar{\psi} \in \boldsymbol{X}_h$

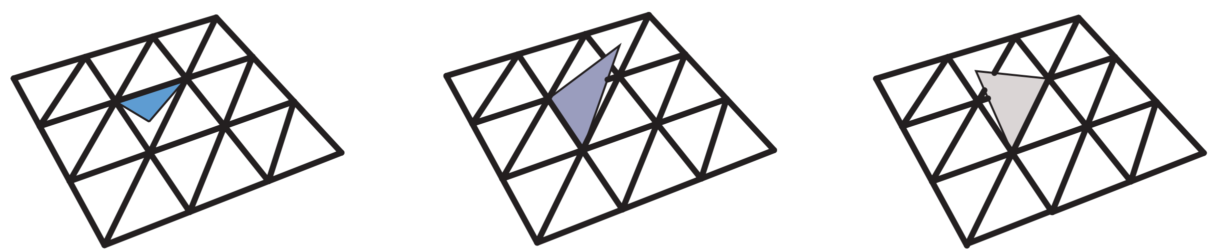
$$\boldsymbol{\mathcal{A}}^* \bar{\psi} = \boldsymbol{f}^{\mathcal{O}}, \quad \left(\ell(v) = \int_\Omega f^{\mathcal{O}} v \, dx \right)$$

3. Domain decomposition (Equilibration) $\longrightarrow \bar{\lambda}$

Global Solution



Equilibrated Solution



Summary

4. Obtain lower bounds for local minimization problems

$$\longrightarrow \quad s^+ \;\; s^-$$

... and **piecewise polynomial certificates**

5. It can be shown that the bound gap can be written as

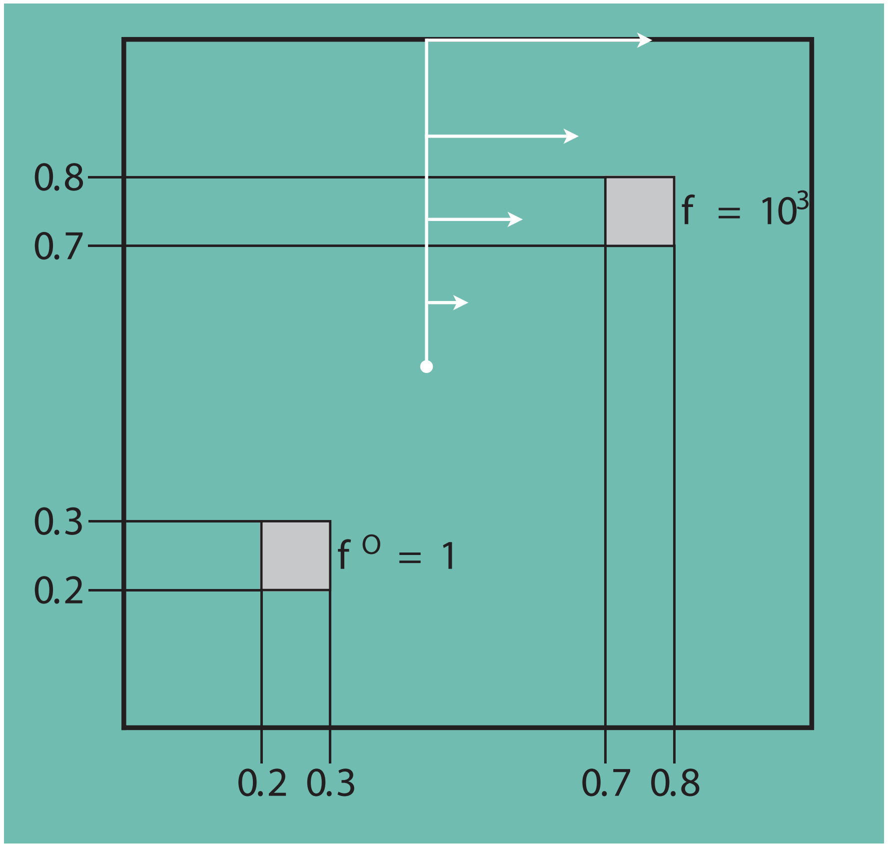
$$s^+ - s^- = \sum_{T_e \in \mathcal{T}_H} \Delta_e$$

with $\Delta_e \geq 0$

$\ldots \Rightarrow$ **Adaptivity**

Examples

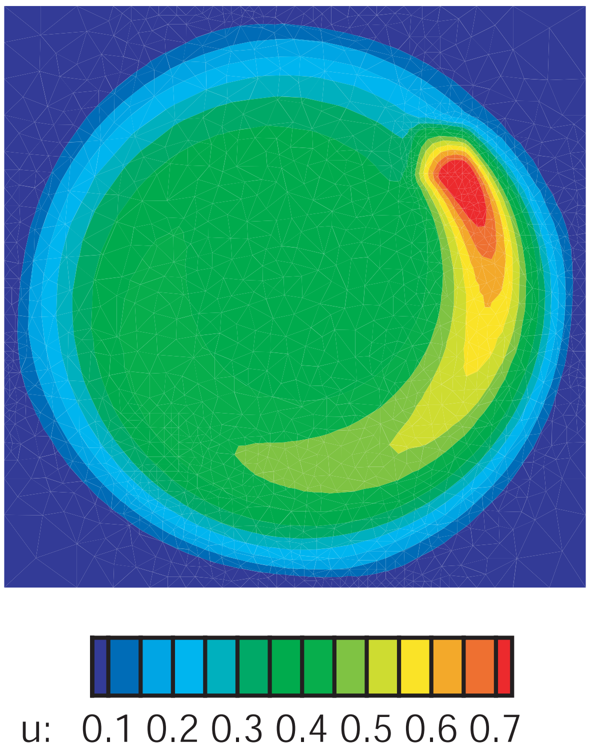
Convection-Diffusion

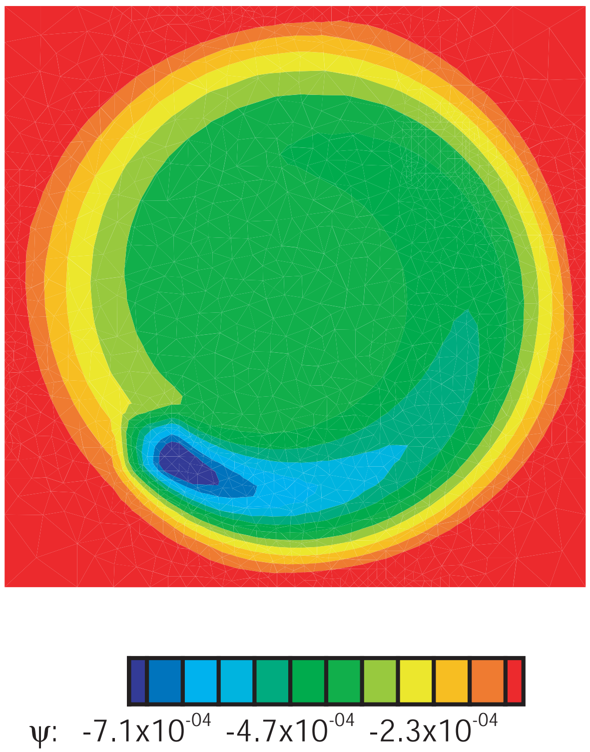


$$-\nu \nabla^2 u + U \cdot \nabla u = f$$

$$s = \ell(u) = \int_\Omega f^{\mathcal{O}} u \, dx$$

Convection-Diffusion





Solution

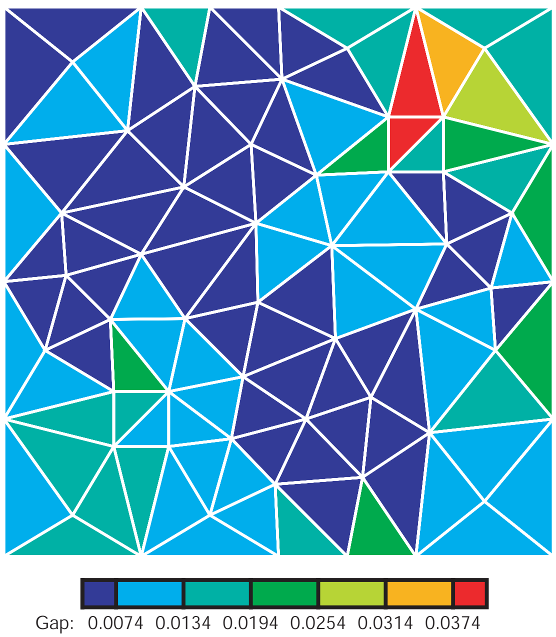
Adjoint

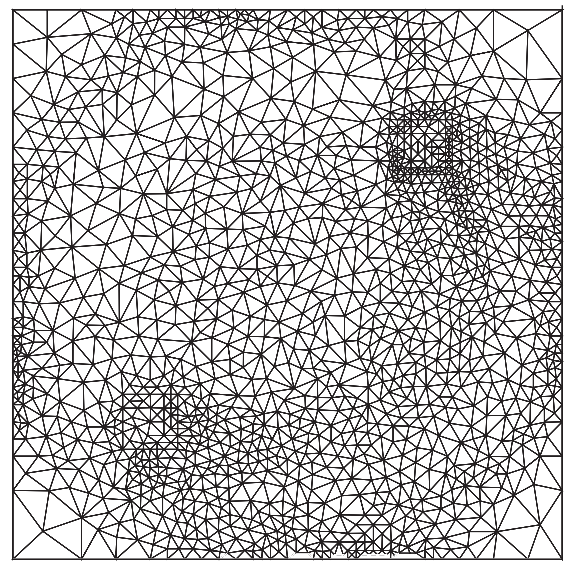
Examples

Convection-Diffusion

Adaptive Solution

$$\Delta_{gap} = 0.0005 \qquad s = 0.00370 \pm 0.00049$$

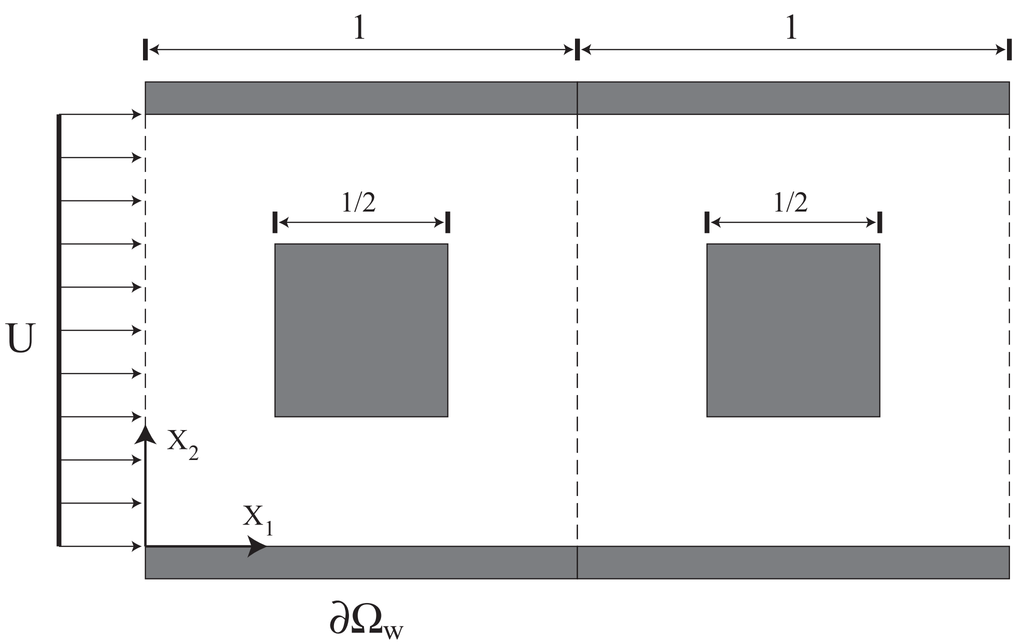




2917 Elements

Uniform refinement would require 6356 elements

Examples



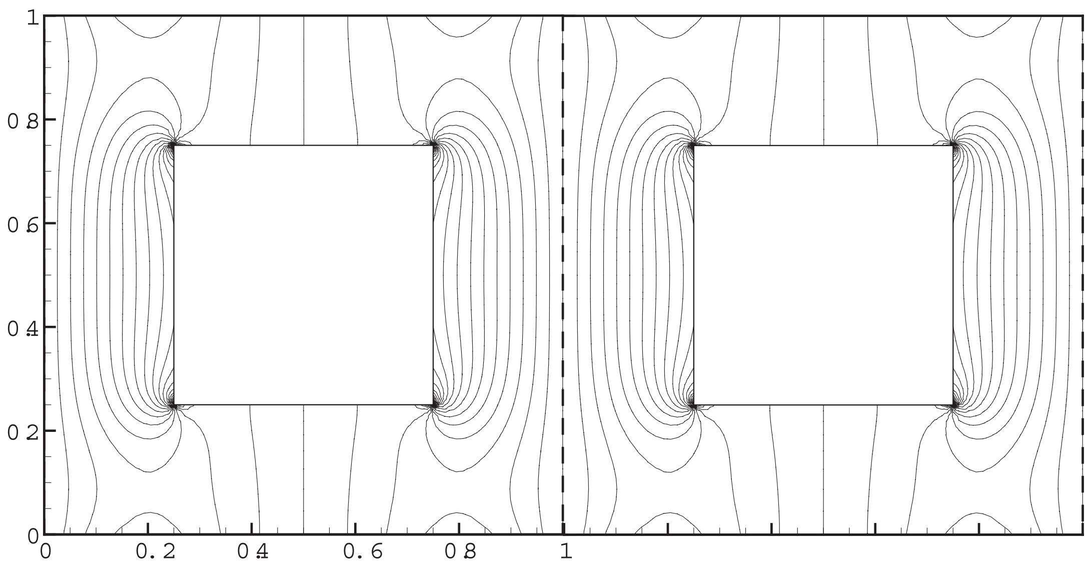
$$-\nabla \cdot \sigma + \nabla(p + \bar{p}) = f$$

$$\nabla \cdot u = 0$$

$$\frac{\partial \bar{p}}{\partial x_1} = -1$$

$$\ell(u) = \int_{\text{cylinder}} t_x \, ds$$

Pressure



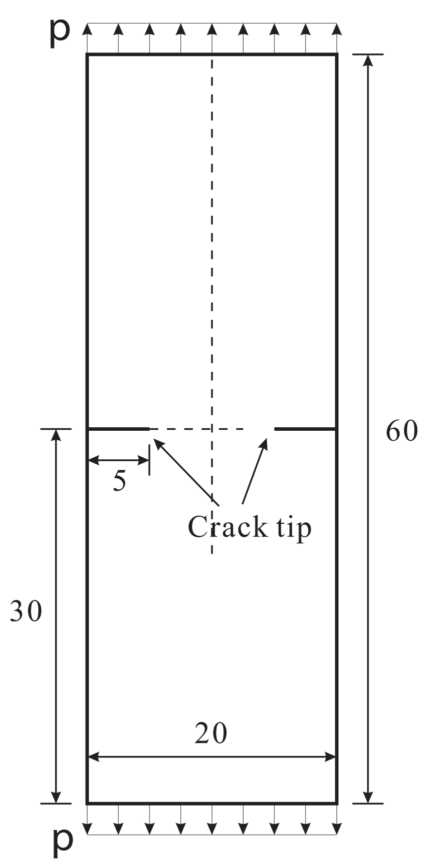
h	S^-	S^+
$1/8$	-0.487292	-0.483790
$1/16$	-0.485439	-0.484383
$1/32$	-0.484883	-0.484553

Special attention paid to incompressibility constraint !!

Examples

Linear Elasticity

Energy Release Rates...



Total Potential Energy

$$\Pi(v) = \frac{1}{2}a(v,v) - (f,v) - \langle g, v\rangle$$

Displacement solution u minimizes $\Pi(v)$

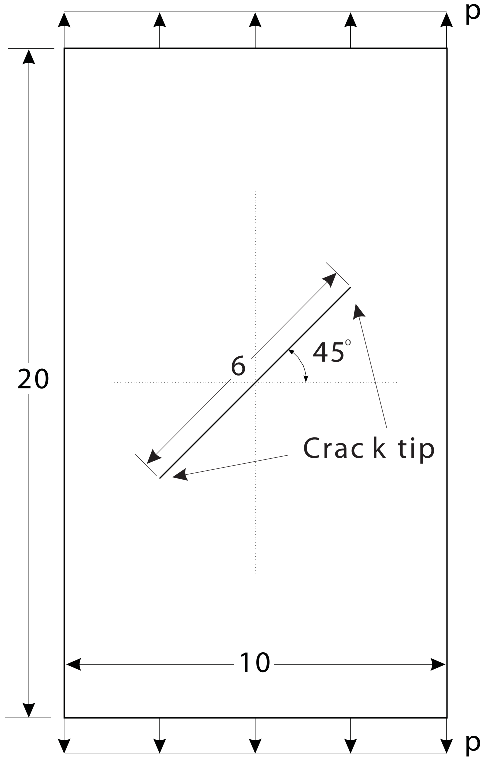
$$\Pi(u) = -\frac{1}{2}a(u,u) = -\frac{1}{2}|||u|||$$

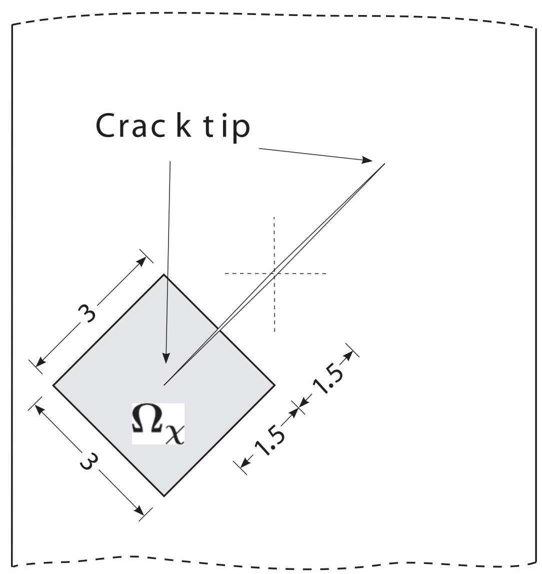
Energy Release Rate $J(u)$

$$\delta\Pi(u) = -\mathcal{J}(u)\,\delta\ell$$

$\ldots\ell$ crack length

Mixed mode crack problem (Plane Strain, $\nu = 0.3$)

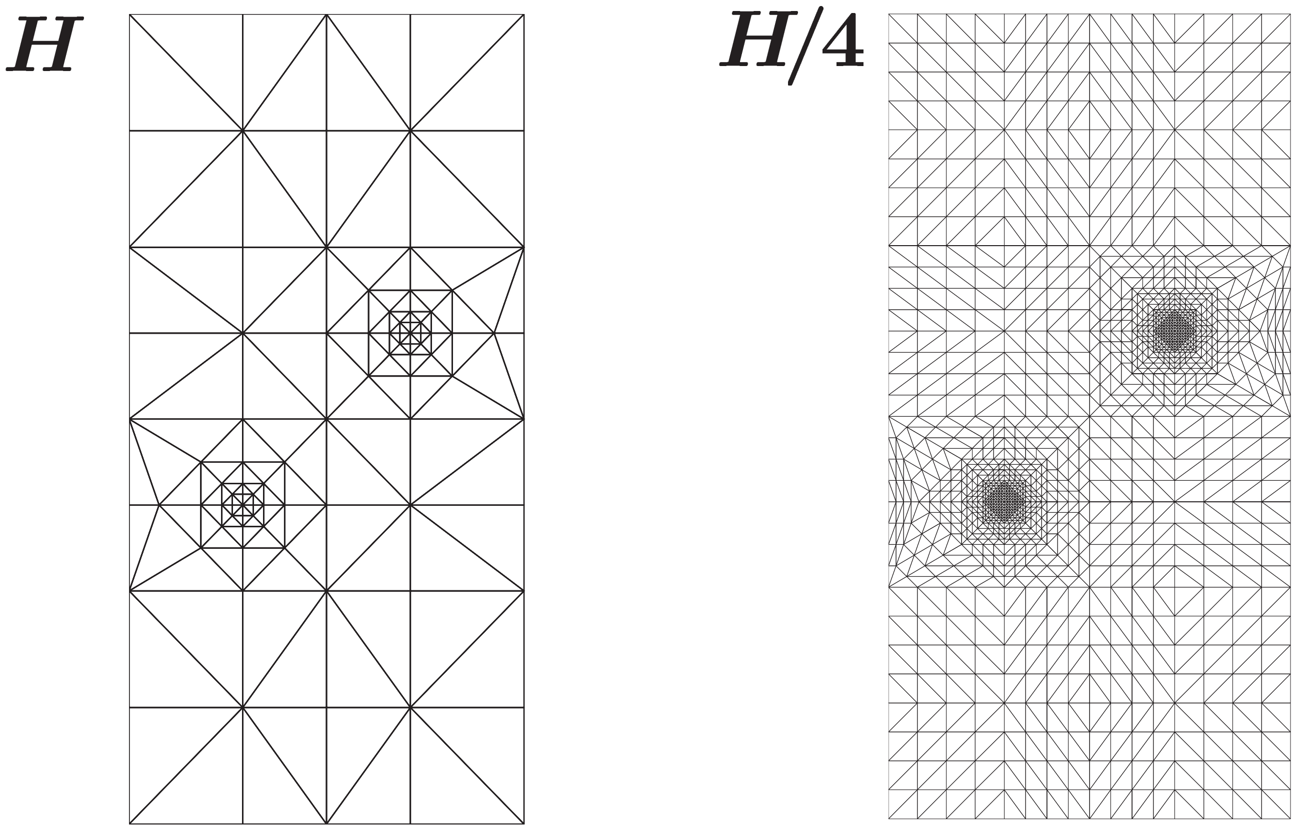




Examples

Linear Elasticity

...Energy Release Rates...



Examples

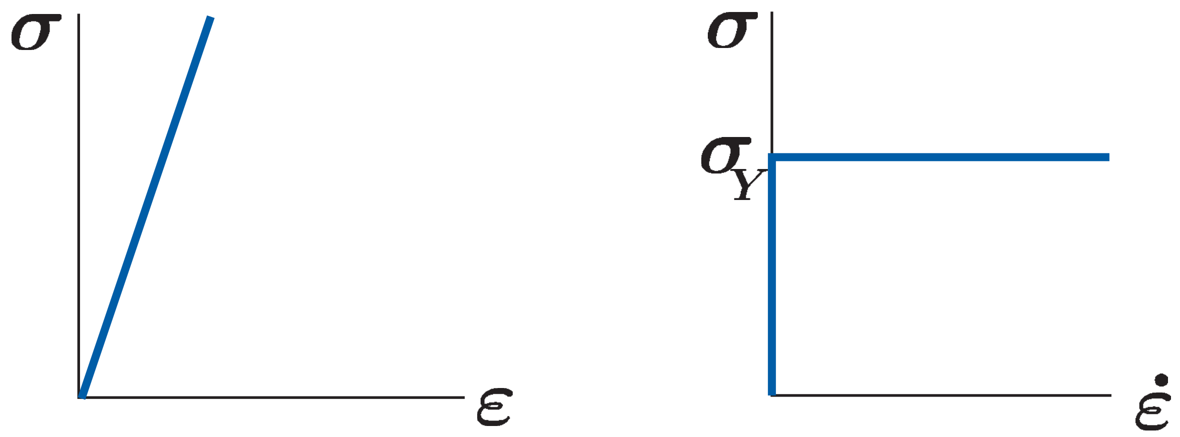
Linear Elasticity

...Energy Release Rates

Mesh size	H	$H/2$	$H/4$	$H/8$	$H/16$
$\mathcal{J}(u_H)$	4.1722	5.3889	5.9313	6.1325	6.2034
$\eta_\chi \vert\vert\vert e \vert\vert\vert^2$	10.7902	3.4107	0.8012	0.1829	0.0411
$\mathcal{J}^-$	-16.8051	-3.3567	3.3228	5.4447	6.0829
$\mathcal{J}^+$	34.6587	17.1489	9.3096	7.0083	6.4621

Compute **Bounds** on the **Collapse Load** under the assumption of **rigid-plastic** material behavior

Linear vs. **Rigid-Plastic**



Limit Analysis vs Non-linear Analysis

CONS

- Limited Physics

PROS

- Existence of solution
- Uniqueness of solution
- Computable
- Certifiable
- . . .

Nonlinear Extension

Limit Analysis

Formulation

$$a(\boldsymbol{\sigma}, v) = \int_\Omega \boldsymbol{\sigma} : \dot{\varepsilon}(v)\, dx$$

$$F(v) = \int_\Omega f v\, dx + \int_{\partial\Omega} g v\, ds$$

$$X_F = \{v \in X \mid F(v) = 1\}$$

$$\Sigma = \{\boldsymbol{\sigma} \mid f(\boldsymbol{\sigma}) \leq \sigma_Y\}$$

$$\dot{\varepsilon}(v) = \begin{cases} 0 & \text{if } f(\boldsymbol{\sigma}) < \sigma_Y \\ \kappa \frac{\partial f}{\partial \sigma} & \text{if } f(\boldsymbol{\sigma}) = \sigma_Y \end{cases}$$

$$\varphi^* = \max_{\substack{\exists \sigma \in \Sigma \\ a(\sigma, v) = \varphi F(v), \forall v \in X}} \varphi$$

$$= \min_{v \in X_F} \max_{\sigma \in \Sigma} a(\boldsymbol{\sigma}, v)$$

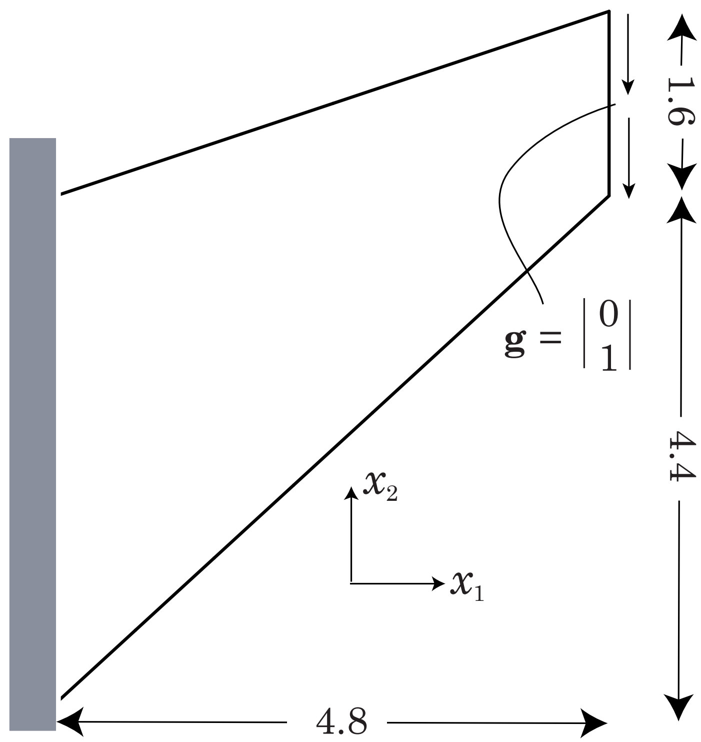
$$= \max_{\sigma \in \Sigma} \min_{v \in X_F} a(\boldsymbol{\sigma}, v)$$

$\max_{\sigma \in \Sigma} a(\boldsymbol{\sigma}, \bar{v}) \longrightarrow$ Upper Bound

$\min_{v \in X_F} a(\bar{\boldsymbol{\sigma}}, v) \longrightarrow$ Lower Bound

- By choosing appropriate piecewise polynomial interpolations for $\boldsymbol{v}$ and $\boldsymbol{\sigma}$ we can obtain **strict upper and lower bounds** on φ
- Discrete minimization/maximization problems are convex (SOCP) and solved (globally) with an IPM
- $\varphi^+ - \varphi^-$ can be decomposed into elemental contributions $\longrightarrow$ Adaptivity

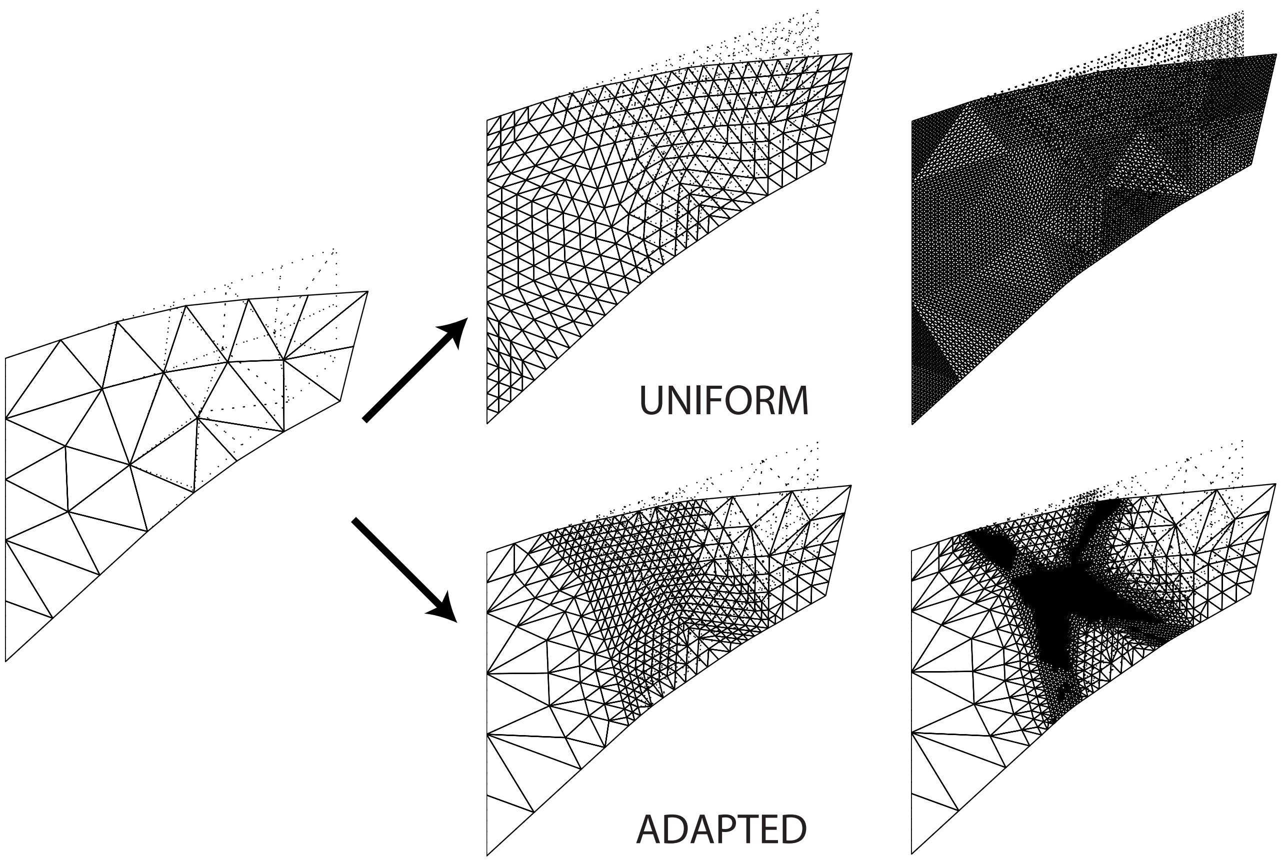
- Cantilever Beam in Plane Stress



Nonlinear Extension

Limit Analysis

...Examples...



Nonlinear Extension

Limit Analysis

...Examples...

Uniform Mesh						
Number of refin.	Number of elem.	Low. Bound λ_h^{*LB}	Upp. Bound λ_h^{*UB}	Bound Gap Δ_h	Low. Bound Error (%)	Upp. Bound Error (%)
0	34	0.52186	0.75759	0.23573	23.821	10.591
1	136	0.65432	0.71936	0.06503	4.484	5.010
2	544	0.68079	0.69704	0.01624	0.620	1.752
3	2176	0.68349	0.68983	0.00634	0.226	0.699
4	8704	0.68440	0.68662	0.00223	0.093	0.231

Adaptive Mesh						
Number of refin.	Number of elem.	Low. Bound λ_h^{*LB}	Upp. Bound λ_h^{*UB}	Bound Gap Δ_h	Low. Bound Error (%)	Upp. Bound Error (%)
0	34	0.52186	0.75759	0.23573	23.821	10.591
1	90	0.65782	0.71951	0.06169	3.973	5.032
2	300	0.68079	0.69704	0.01625	0.620	1.752
3	882	0.68349	0.68989	0.00640	0.226	0.708
4	2450	0.68440	0.68667	0.00227	0.093	0.238

Conclusions

- **Uniform** bounds on
- **Relevant** engineering outputs (linear functionals) of
- **Exact** weak solutions of linear PDEs, with a
- Stand-alone **certificate** of precision, including
- **Non-symmetric** operators, using
- Standard FE solutions and purely **local** subproblems.

Conclusions

Certificates allow to

- **Standardize** the use of more accurate and safer mathematical models (e.g. construction codes)
- Eliminate **costlier-than-necessary** computations
- Allow for true **black boxes** that can be used by non-experts in numerical analysis
- **Document** computations
- Address **software error** issues
- . . .

Current Work

- Exploit Discontinuous Galerkin Discretizations
- Time dependent parabolic problems
- $\mu-$PDE's
- Non-coercive operators with positivity constraints on the solution
- Deformation theory of plasticity

Recent papers can be found at:

`http://raphael.mit.edu`