Computational Mechanics: Linear Functional Outputs and Certificates

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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

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- More precise simulation of under-designed component predicted failure at 62m

Sleipner Platform Failure

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- 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]?

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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

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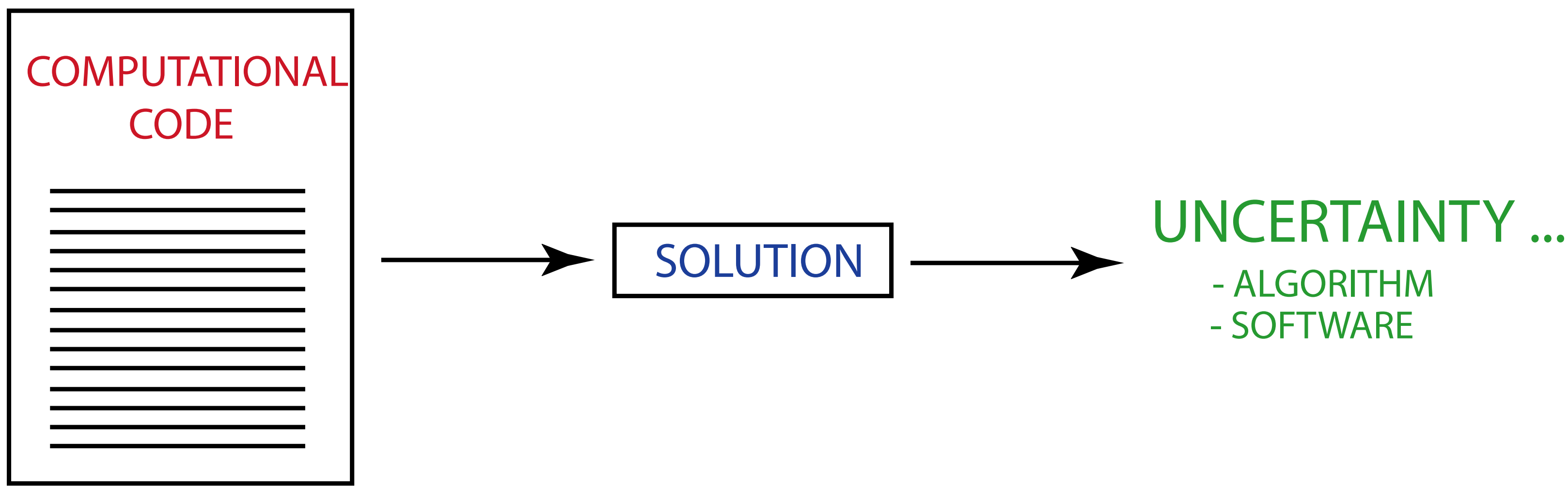
What is a Certificate?

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)

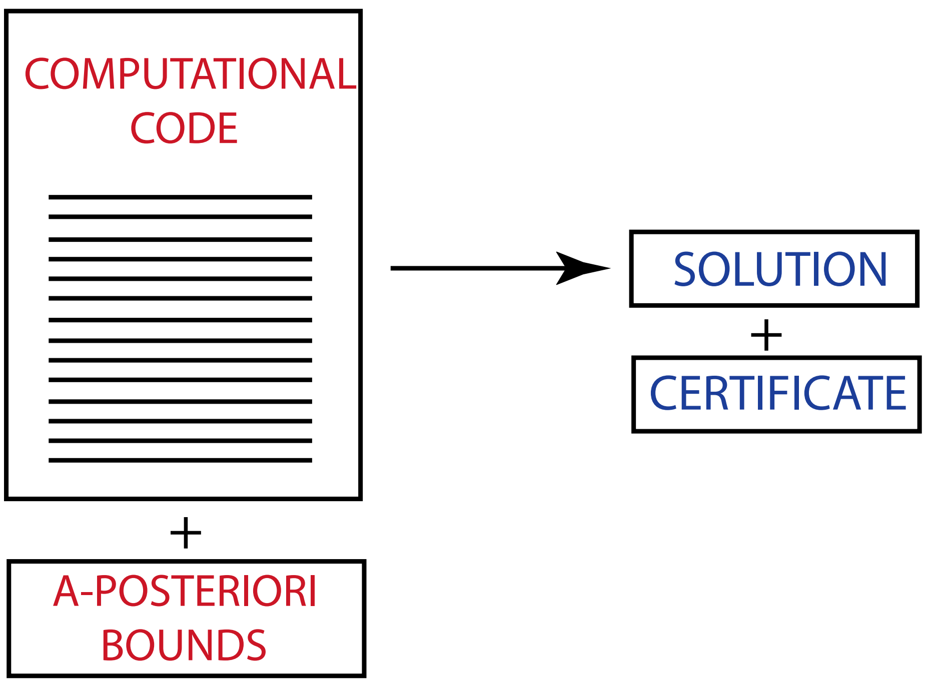
Certificates

Current Paradigm



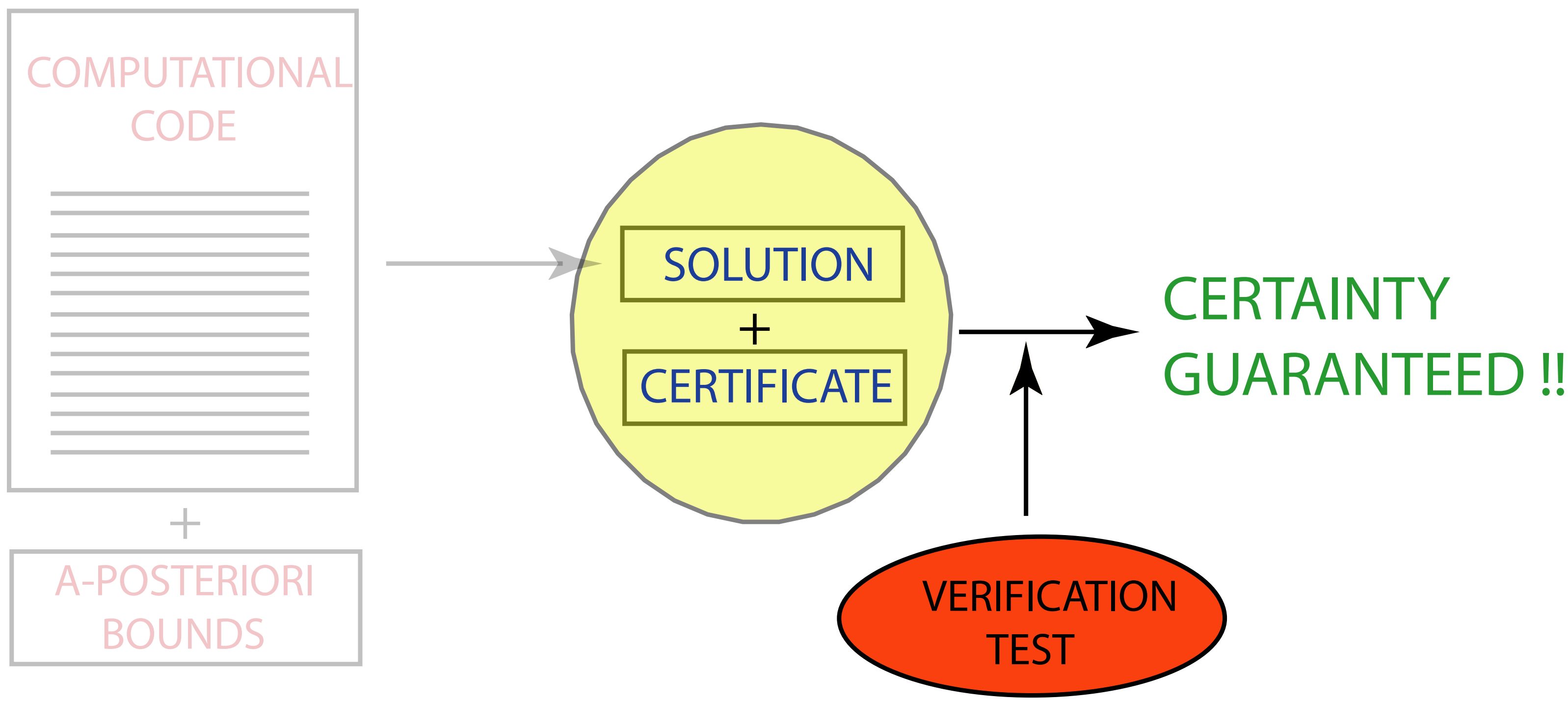
Certificates

Proposed Paradigm



Certificates

Proposed Paradigm



Certificates

Examples

Polynomial Bounds

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

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

Certificates

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

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

Certificates

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

Certificates

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

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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.

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

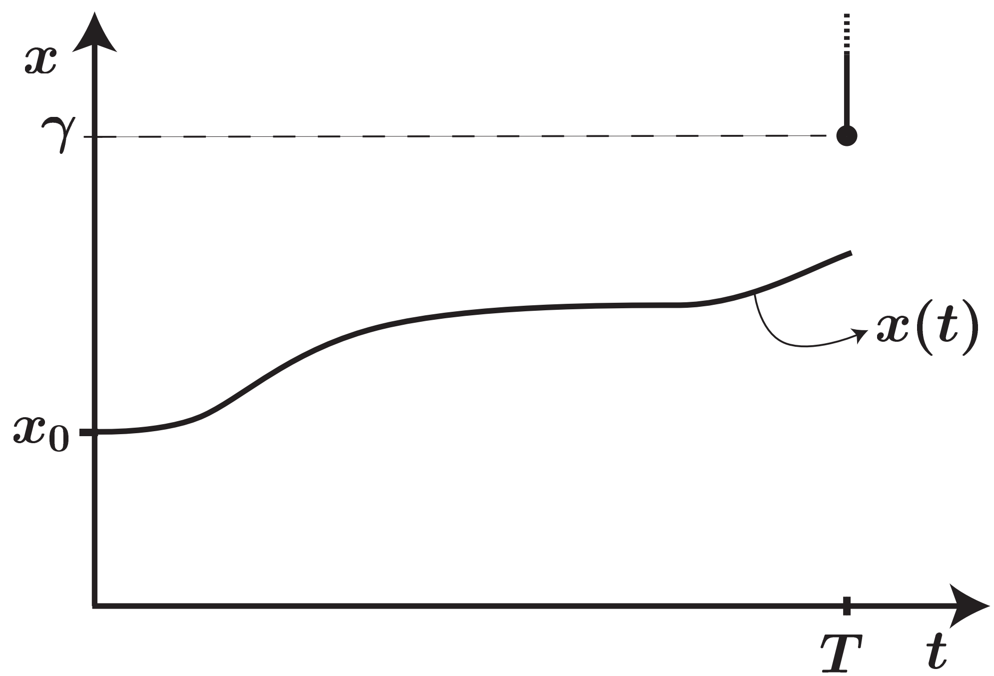
$$B(x_T, T) > B(x_0, 0) \,, \qquad \forall x_T \geq \gamma$$

Parrilo, Doyle, . . .

Certificates

Examples

...Bounds for solutions of IVP...



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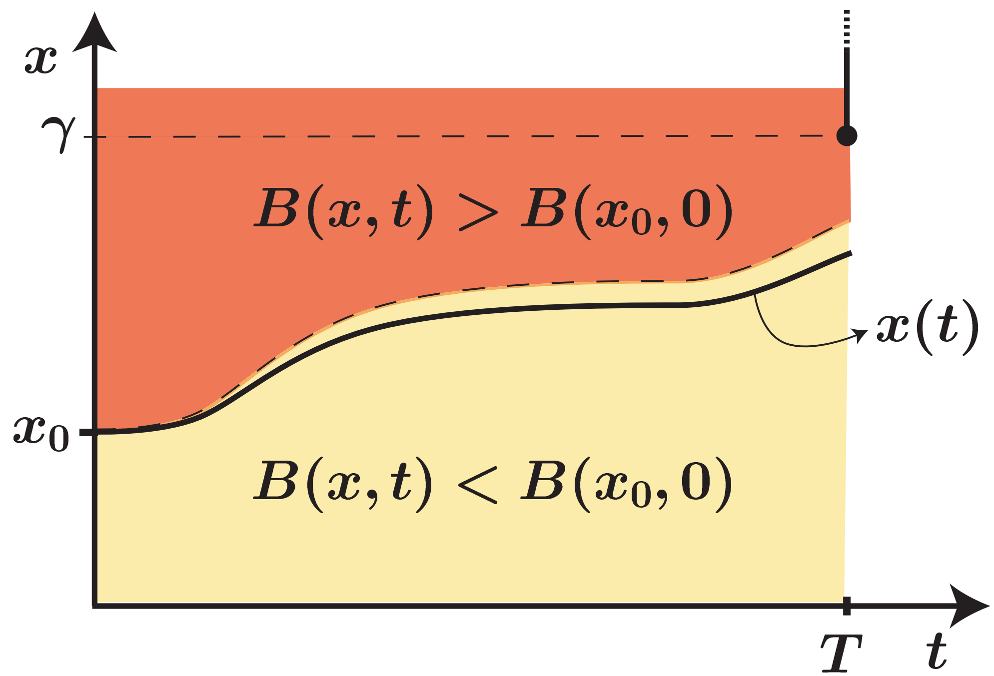

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...Bounds for solutions of IVP

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

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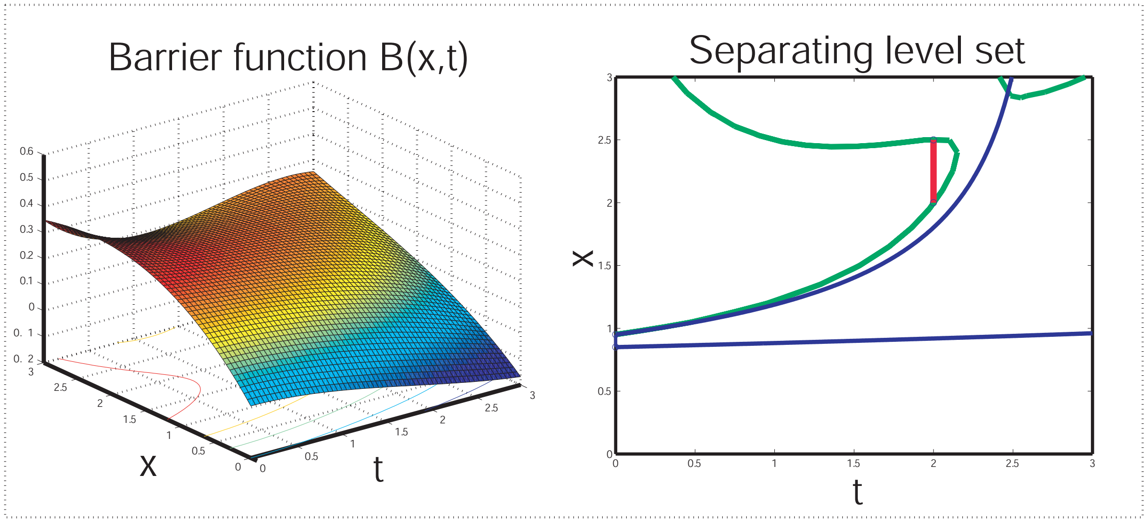

$$\Rightarrow \quad x(2) \notin [2.0, 2.5]$$

Objective

Compute Certificates for Bounds of Outputs of PDE's

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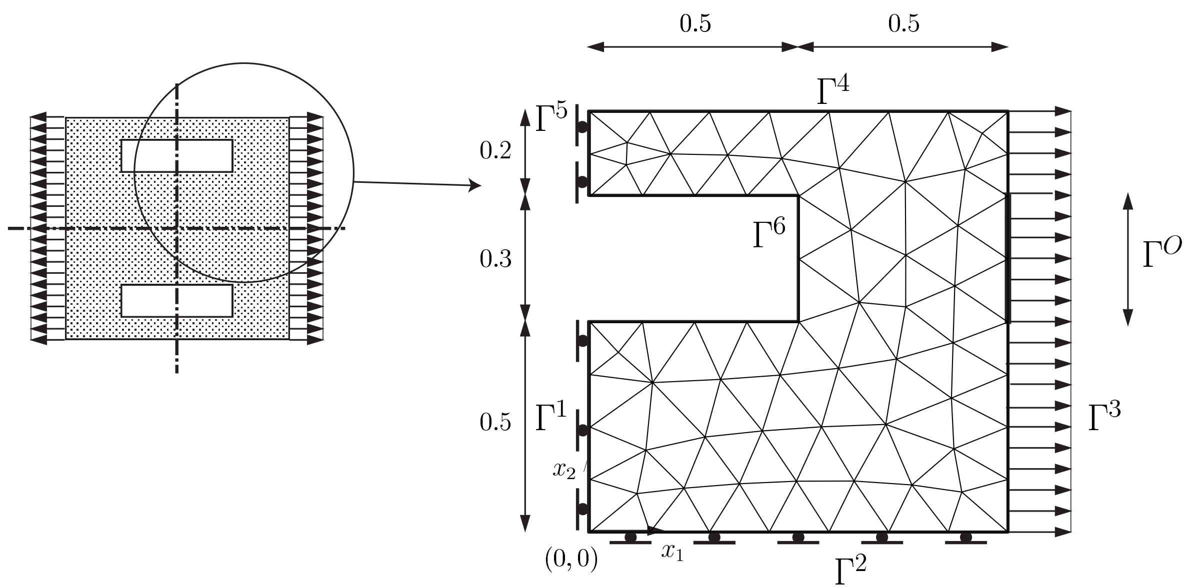
Compute Certificates for Bounds of Outputs of PDE's

- 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:

- Linear Convection-Diffusion-Reaction Equation

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Collapse Loads in Limit Analysis

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Collapse Loads in Limit Analysis

Energy Release Rates in Linear Elasticity

Outline

- Problem Description
- Method Overview

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

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

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

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- $u(x)$ is **not computable** ($\infty-$ dimensional)

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- 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.

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  - 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

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

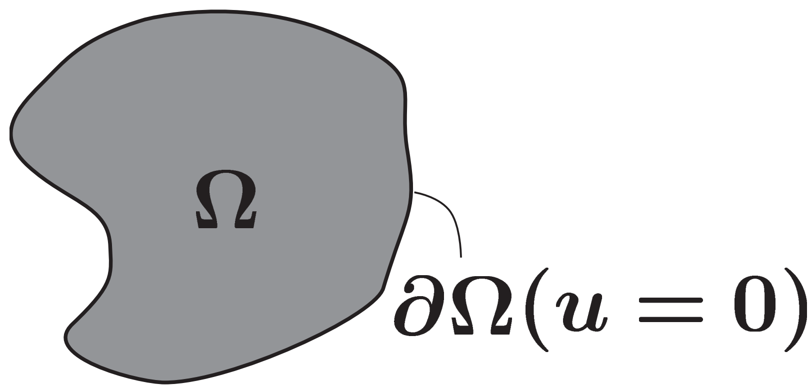
. . . and give **Certificates**

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

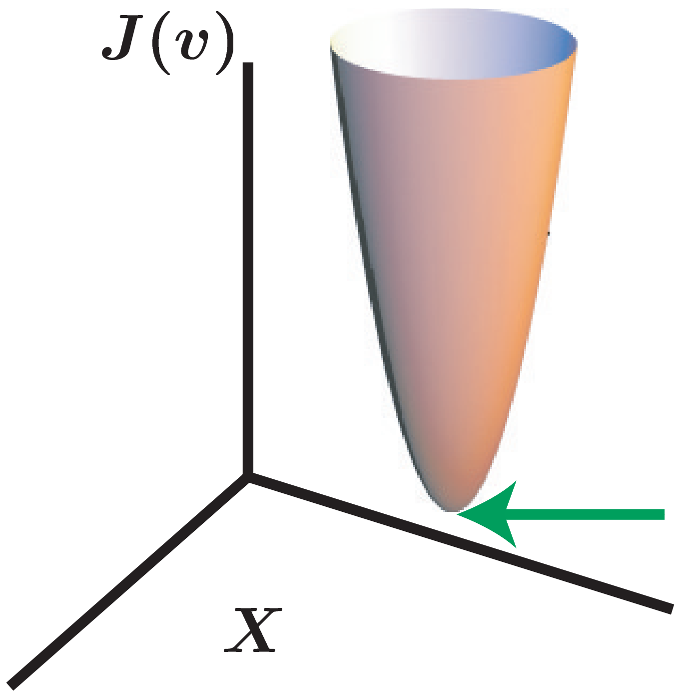
Minimization formulation

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

Method Overview

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

Minimization



$$J(u) = \min_{v \in X} J(v)$$

$$s = J(u) = -\int_\Omega u f \, dx$$

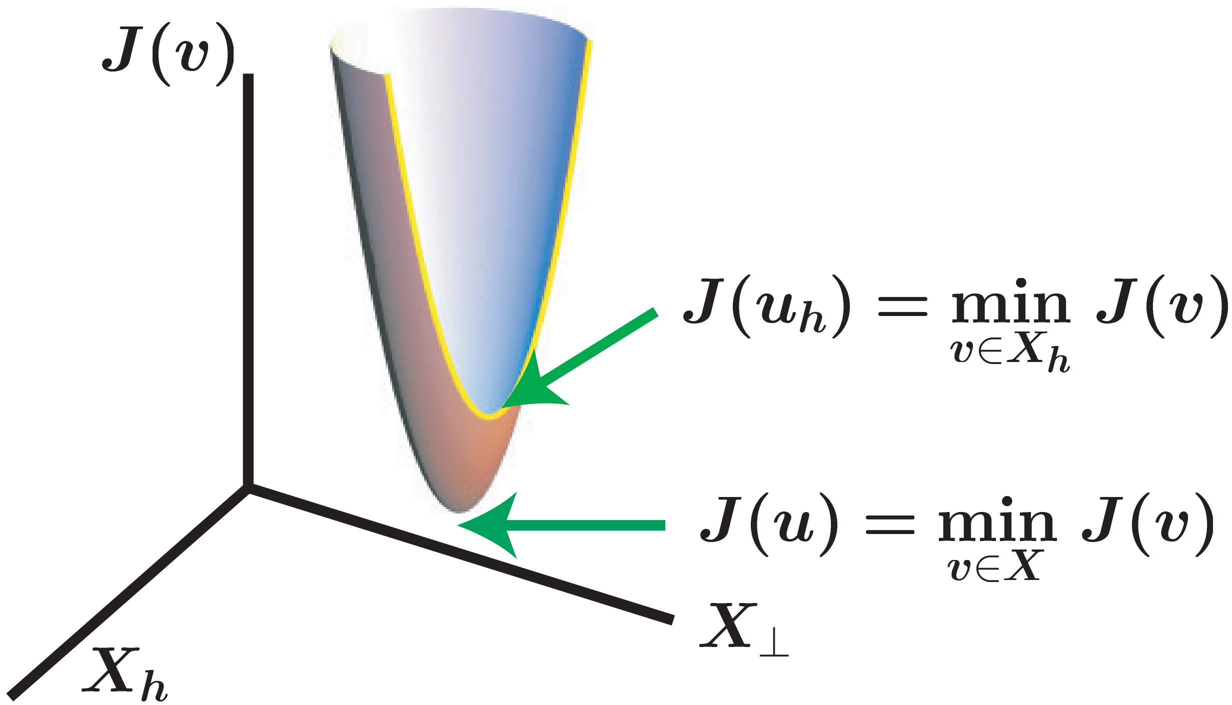
Method Overview

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

Upper Bound

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

(trivial)



Method Overview

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

Lower Bound...

Lower bound s^- (harder)

Construct **dual** problem

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

Method Overview

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

...Lower Bound...

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

Method Overview

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

...Lower Bound...

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

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

Method Overview

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

...Lower Bound...

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

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

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

Method Overview

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

...Lower Bound...

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

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

Method Overview

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

...Lower Bound...

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

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

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

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

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

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

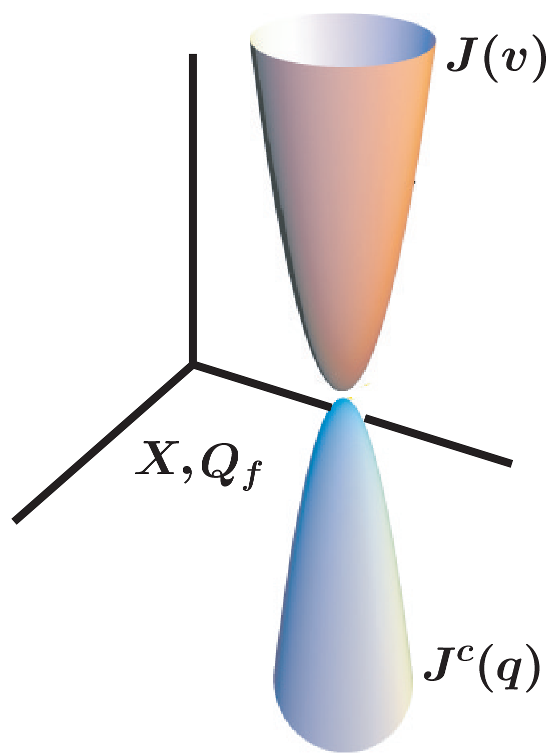
$$\boxed{J(v) \geq J^c(q), \qquad \forall v \in X, q \in Q_f}$$

Method Overview

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

...Lower Bound...

Duality

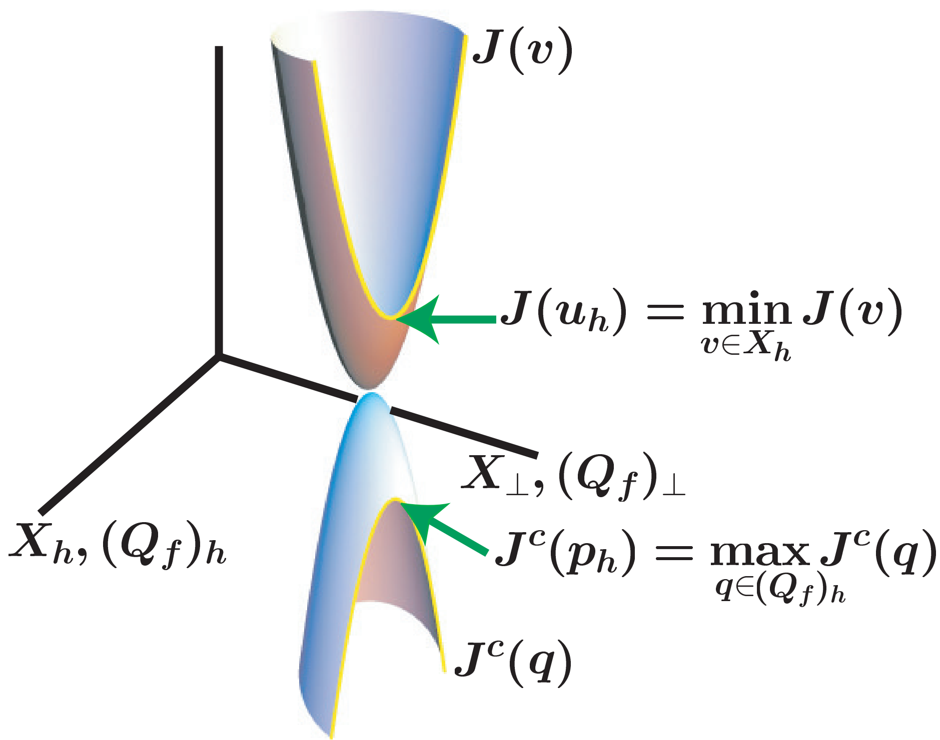


Method Overview

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

Method Overview

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

Lower Bound - Summary

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

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

Method Overview

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

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. $s^- \equiv J^c(p_h)$

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

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

Method Overview

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

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

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

or,

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

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or,

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

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

$$\mathcal{E}(v) \equiv \int_\Omega \nabla v \cdot \nabla v \, dx - \int_\Omega f v \, dx$$

Method Overview

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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

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

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

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

Method Overview

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

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

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

Method Overview

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

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

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

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

Method Overview

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

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...

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

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

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

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

For a given $\bar{\psi}$, $\boldsymbol{L(v,\bar{\psi})}$, contains quadratic and linear terms in $\boldsymbol{v}$

Method Overview

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

...Lower Bound...

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

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,

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

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Idea:

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

Summary

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

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

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Certificate :

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

3.- Non-symmetric equations

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

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or,

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

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

or,

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

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

$$\mathcal{E}(v) \equiv \int_\Omega \nabla v \cdot \nabla v \, dx - \int_\Omega f v \, dx$$

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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...

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

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

Lagrangian...

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

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Method Overview

3.- Non-symmetric equations

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

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

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

Lagrangian...

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

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

...

Idea :

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

Summary

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

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

Summary

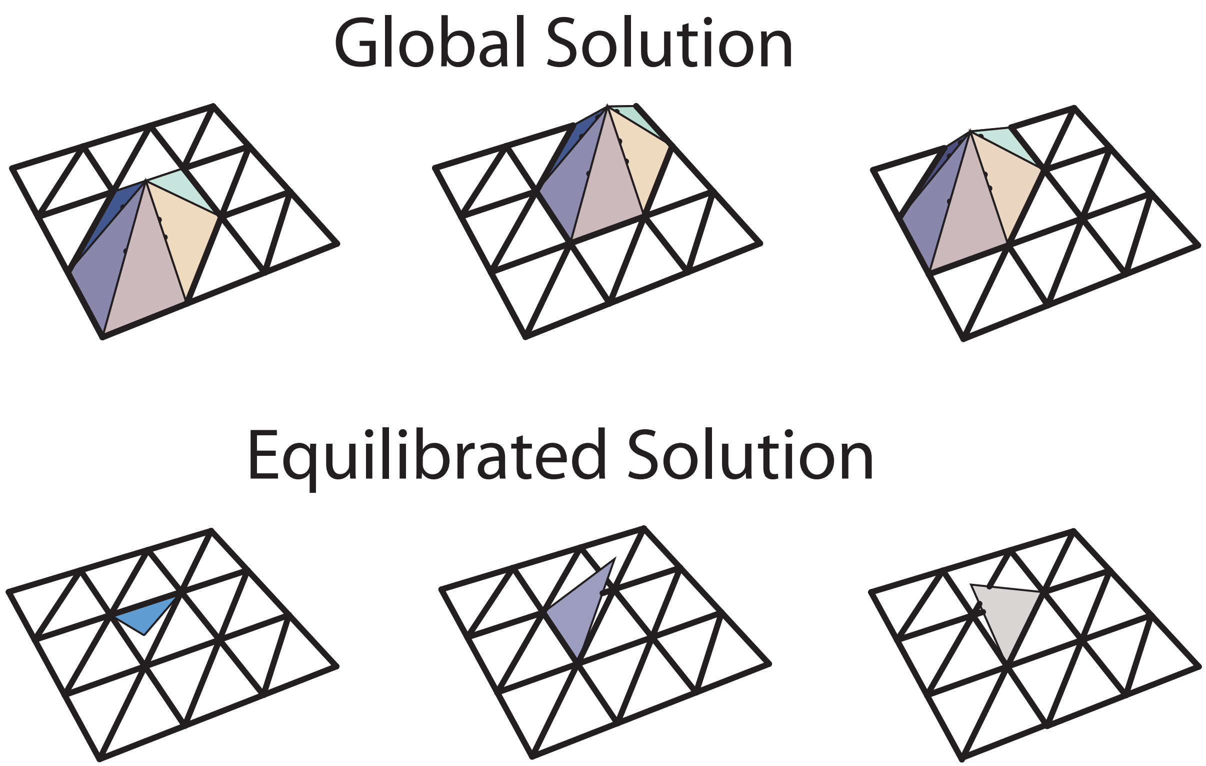
1. Primal problem: $u_h \in X_h$

$$\mathcal{A} u_h = f$$

2. Dual problem: $\bar{\psi} \in X_h$

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

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



4. Obtain lower bounds for local minimization problems

$$\longrightarrow \quad \boldsymbol{s}^{+} \;\; \boldsymbol{s}^{-}$$

. . . and **piecewise polynomial certificates**

4. Obtain lower bounds for local minimization problems

$$\longrightarrow \quad \boldsymbol{s}^+ \quad \boldsymbol{s}^-$$

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

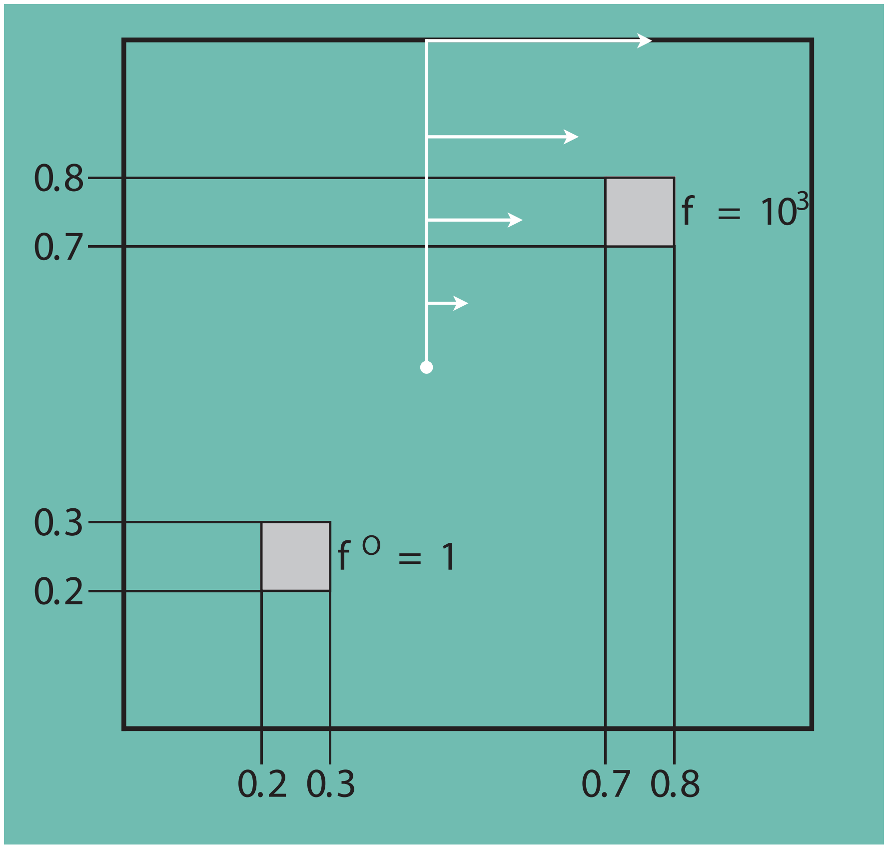
$$\boldsymbol{s}^+ - \boldsymbol{s}^- = \sum_{T_e \in \mathcal{T}_H} \boldsymbol{\Delta}_e$$

with $\boldsymbol{\Delta}_e \geq 0$

... $\Rightarrow$ **Adaptivity**

Examples

Convection-Diffusion

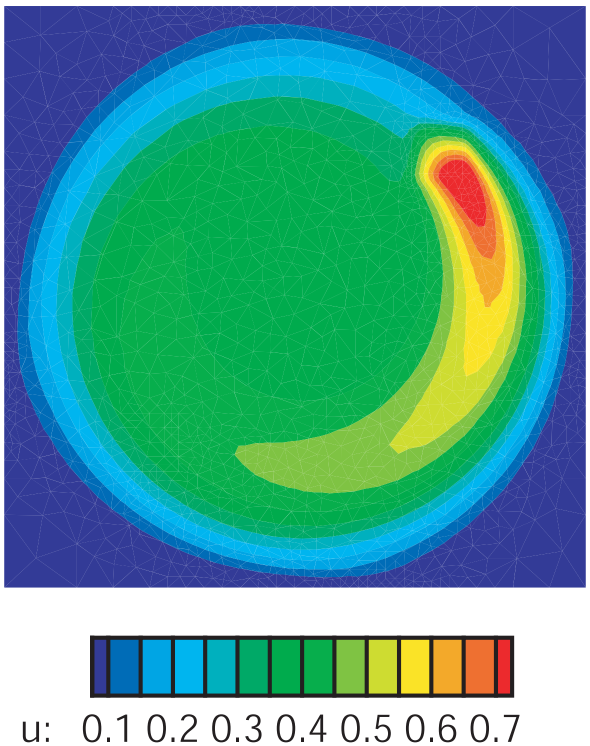


$$-\nu\nabla^2 u + U\cdot\nabla u = f$$

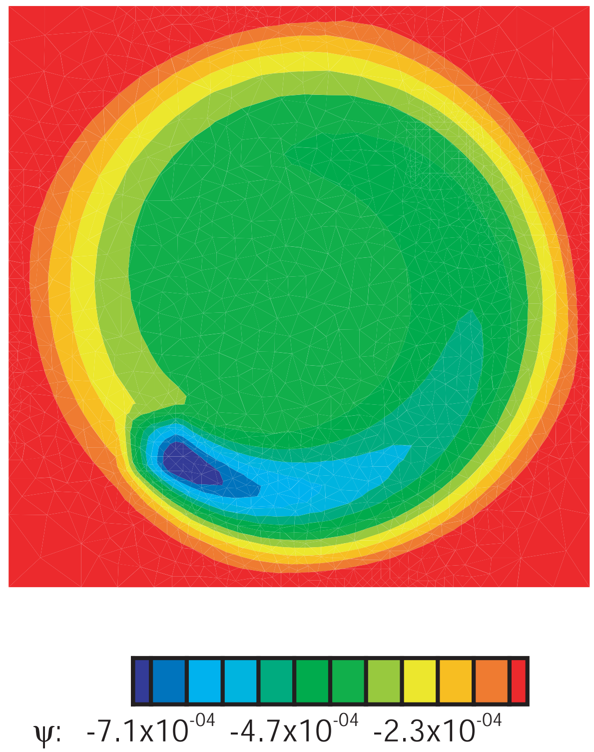
$$s = \ell(u) = \int_\Omega f^{\mathcal{O}} u\,dx$$

Examples

Convection-Diffusion



Solution



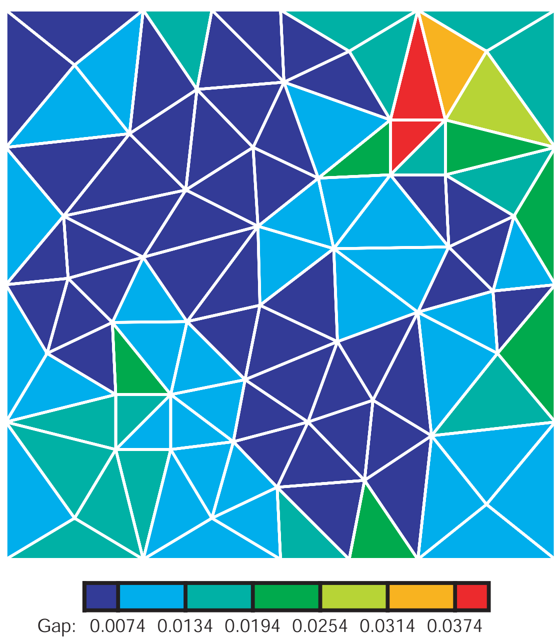
Adjoint

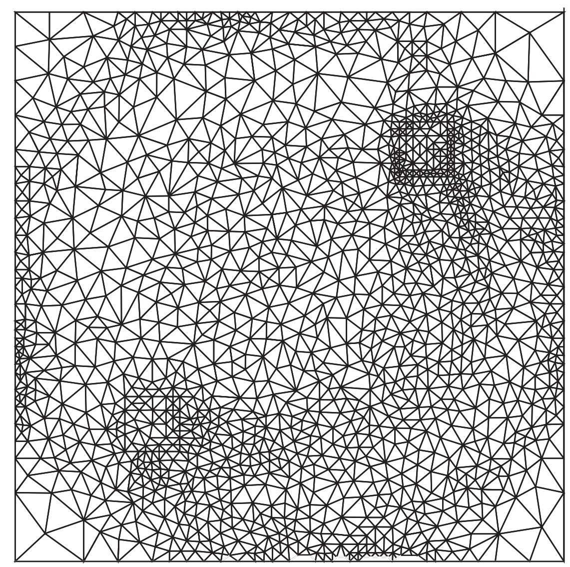
Examples

Convection-Diffusion

Adaptive Solution

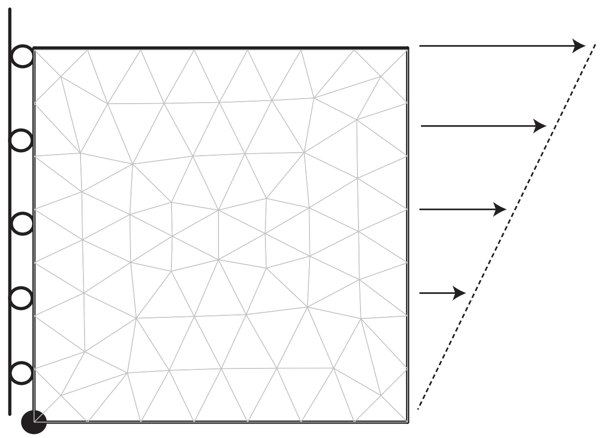
$$\Delta_{gap} = 0.0005 \qquad s = 0.00370 \pm 0.00049$$





2917 Elements

Uniform refinement would require 6356 elements



Find $u \in X$ such that

$$\nabla \cdot \sigma(u) = 0$$

$$\sigma(u) \cdot n = y \quad x = L$$

Exact Solution:

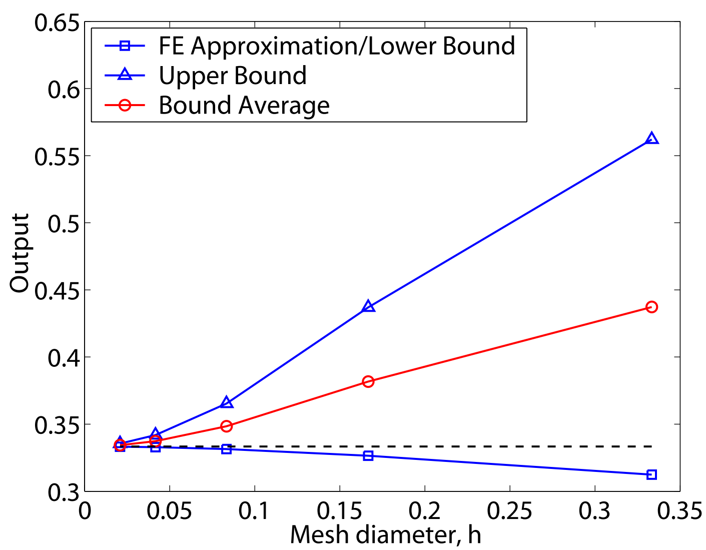
$$u = (2xy, -\nu(y^2 - x^2)/(2\lambda), \quad (x, y) \in [0, L]^2$$

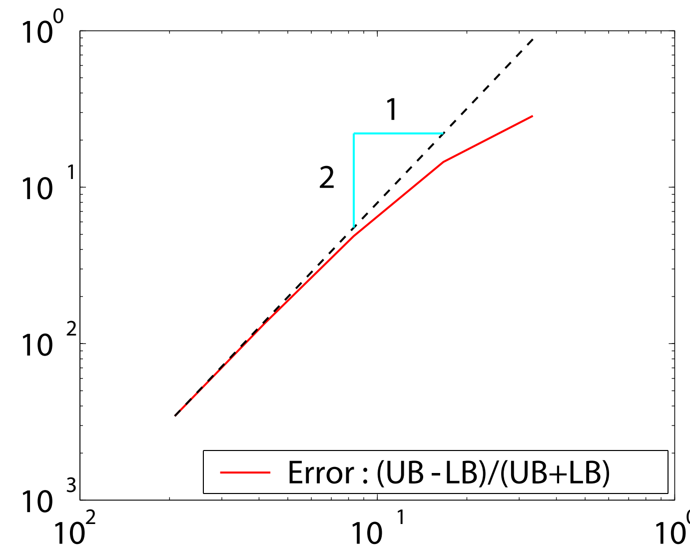
Examples

Elasticity

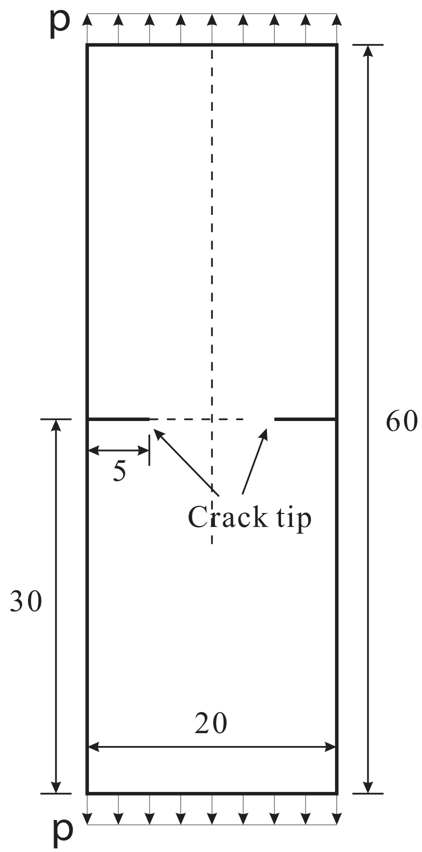
Linear Functionals

$$\ell(u) = \int_{x=L} y u_1 \, ds \quad (= L^4/3\lambda)$$





Examples



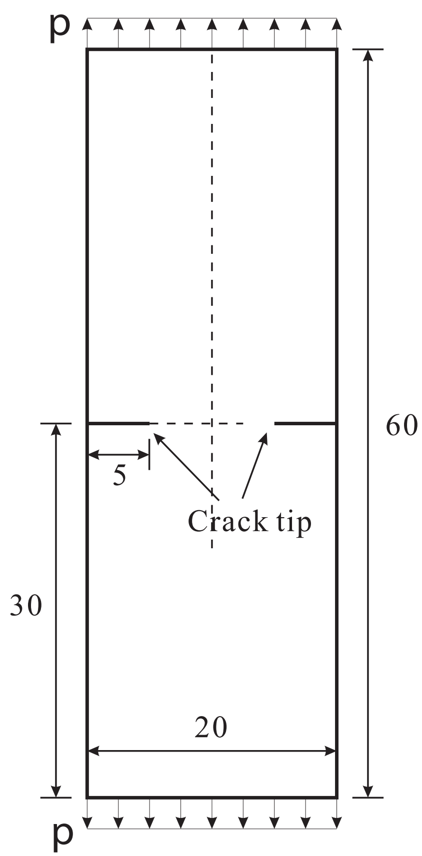
Total Potential Energy

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

Displacement solution u minimizes $\Pi(v)$

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

Examples



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

Energy Release Rate $J(u)$

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

$\ldots\ell$ crack length

Examples

Elasticity

...Energy Release Rates...

Given (an approximate) solution u_H, $e = u - u_H$

$$\mathcal{J}(u) = \mathcal{J}(u_H) + \delta\mathcal{J}_u(u_H; e) + \mathcal{J}(e)$$

Examples

Elasticity

...Energy Release Rates...

Given (an approximate) solution u_H, $\quad e = u - u_H$

$$\mathcal{J}(u) = \mathcal{J}(u_H) + \delta\mathcal{J}_u(u_H; e) + \mathcal{J}(e)$$

- $\delta\mathcal{J}_u(u_H; e)$ linear $\longrightarrow \quad L^- \le \delta\mathcal{J}_u(u_H; e) \le L^+$
- $\mathcal{J}(e)$ quadratic $\longrightarrow \quad |\mathcal{J}(e)| \le \eta_\chi |||e|||^2 \equiv Q$

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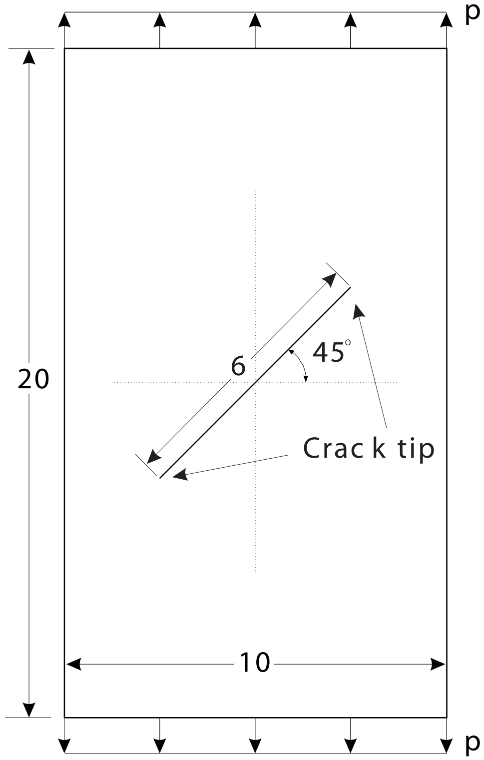
$$\boxed{\mathcal{J}^- \equiv \mathcal{J}(u_H) - Q + L^- \le \mathcal{J}(u) \le \mathcal{J}(u_H) + Q + L^+ \equiv \mathcal{J}^+}$$

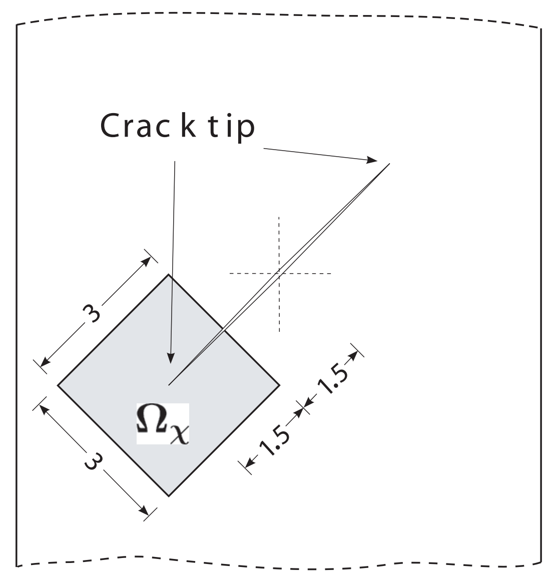
Examples

Elasticity

...Energy Release Rates...

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



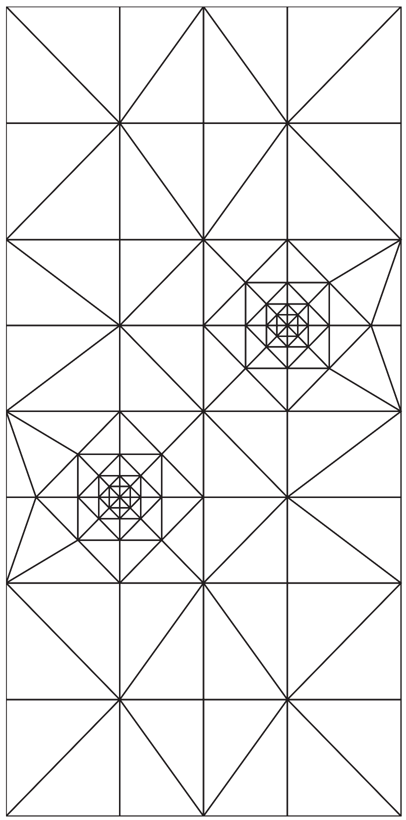


Examples

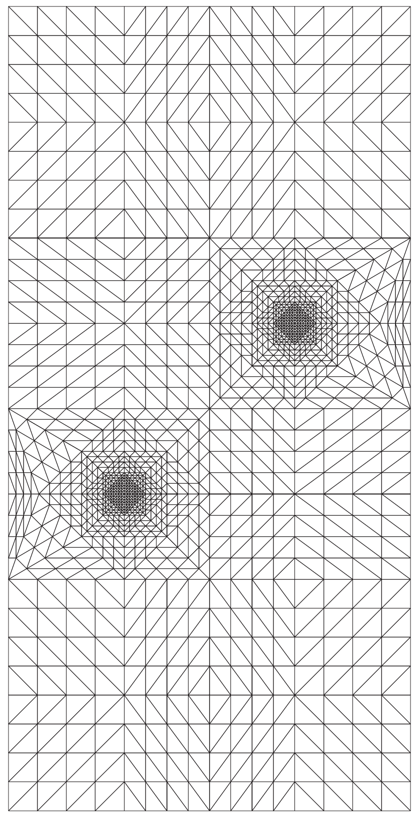
Elasticity

...Energy Release Rates...

H



$H/4$



Examples

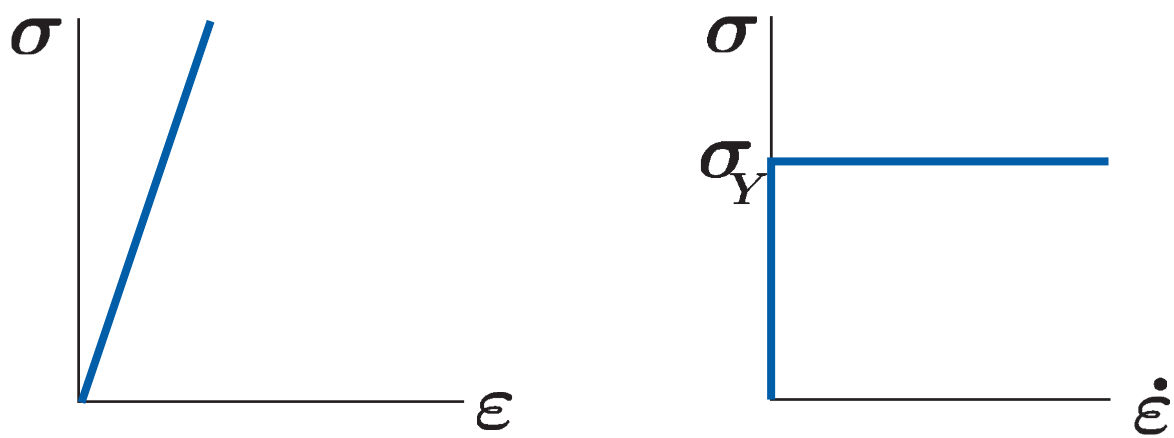
Elasticity

...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**



Nonlinear Extension

Limit Analysis

Formulation

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

$$\boldsymbol{F}(\boldsymbol{v}) = \int_\Omega \boldsymbol{f}\boldsymbol{v}\, d\boldsymbol{x} + \int_{\partial\Omega} \boldsymbol{g}\boldsymbol{v}\, d\boldsymbol{s}$$

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

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

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

$$\begin{aligned} \varphi^* &= \max_{\substack{\exists \boldsymbol{\sigma} \in \Sigma \\ a(\boldsymbol{\sigma}, v) = \varphi F(v), \forall v \in X}} \varphi \\ &= \min_{\boldsymbol{v} \in \boldsymbol{X_F}} \max_{\boldsymbol{\sigma} \in \boldsymbol{\Sigma}} \boldsymbol{a}(\boldsymbol{\sigma}, \boldsymbol{v}) \\ &= \max_{\boldsymbol{\sigma} \in \boldsymbol{\Sigma}} \min_{\boldsymbol{v} \in \boldsymbol{X_F}} \boldsymbol{a}(\boldsymbol{\sigma}, \boldsymbol{v}) \end{aligned}$$

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

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

- By choosing appropriate piecewise polynomial interpolations for v and $\boldsymbol{\sigma}$ we can obtain **strict upper and lower bounds** on φ

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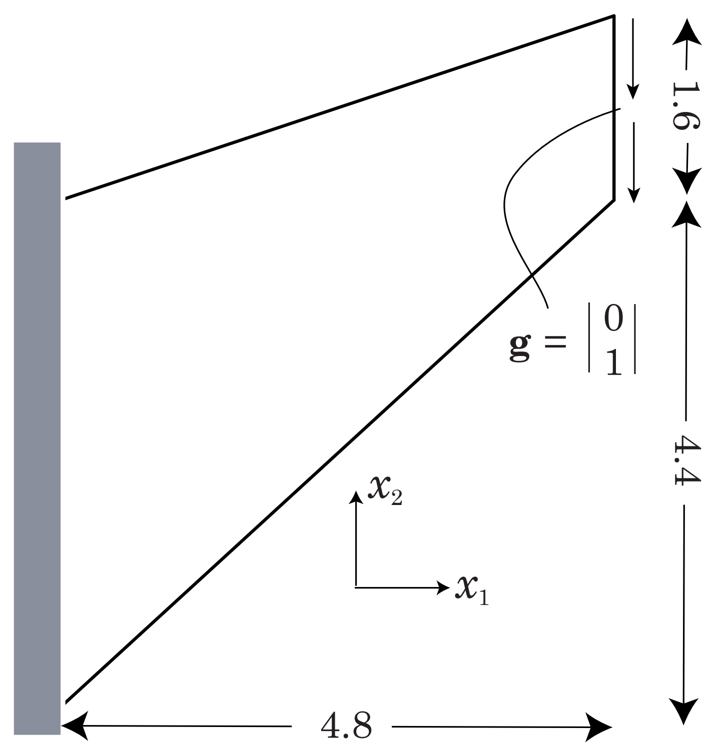
- By choosing appropriate piecewise polynomial interpolations for $\boldsymbol{v}$ and $\boldsymbol{\sigma}$ we can obtain **strict upper and lower bounds** on φ
- Discrete minimization/maximization problems are convex (SOCP) and solved (globally) with an IPM
- $\varphi^+ - \varphi^-$ can be decomposed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

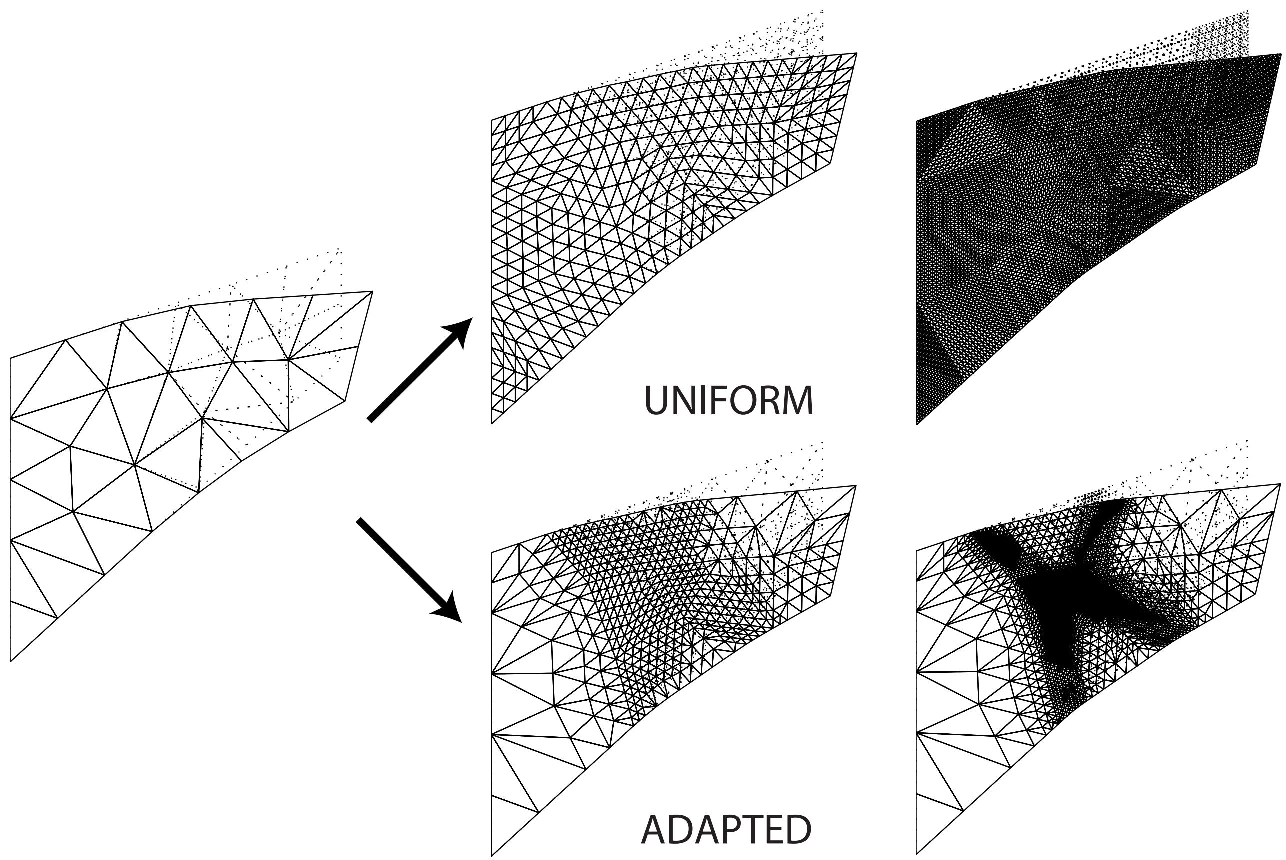
- Cantilever Beam in Plane Stress



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

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- **Non-symmetric** operators, using
- Standard FE solutions and purely **local** subproblems.

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- Address **software error** issues
- . . .

Current Work

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- Deformation theory of plasticity

Recent papers can be found at:

`http://raphael.mit.edu`

Current Work

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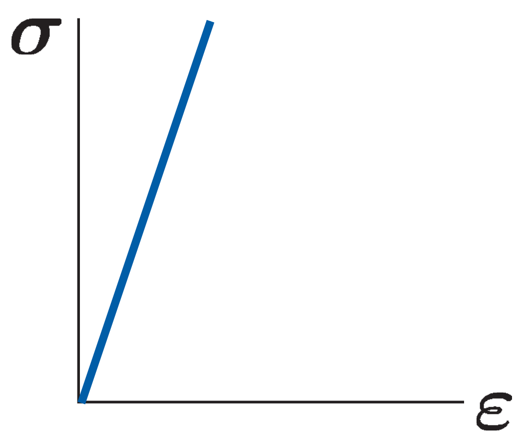
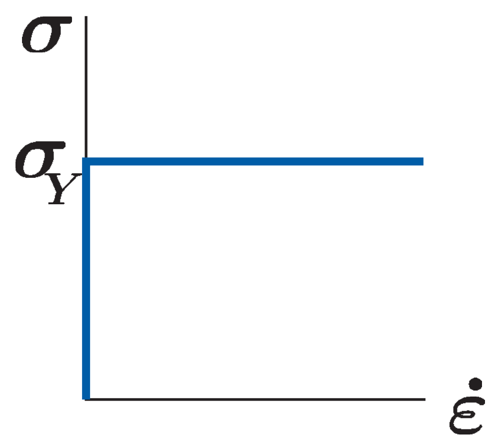
Linear vs. **Rigid-Plastic**





Current Work

Limit Analysis

Continuous Formulation

Current Work

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Continuous Formulation

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

$$F(\mathrm{u}) = \int_\Omega f \mathrm{u}\, dx + \int_{\partial\Omega^N} g \mathrm{u}\, ds$$

$$C = \{\mathrm{u} \in Y \,|\, F(\mathrm{u}) = 1\}$$

$$B = \{\boldsymbol{\sigma} \in X \,|\, f(\boldsymbol{\sigma}) \leq \boldsymbol{\sigma}_Y\}$$

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

$$\begin{aligned} \boldsymbol{\lambda}^* &= \sup \boldsymbol{\lambda} \\ & \quad s.t. \begin{cases} \exists \boldsymbol{\sigma} \in B \\ a(\boldsymbol{\sigma}, \mathrm{u}) = \boldsymbol{\lambda} F(\mathrm{u}), \forall \mathrm{u} \in Y \end{cases} \\ &= \sup_{\boldsymbol{\sigma} \in B} \inf_{\mathrm{u} \in C} a(\boldsymbol{\sigma}, \mathrm{u}) \\ &= \inf_{\mathrm{u} \in C} \sup_{\boldsymbol{\sigma} \in B} a(\boldsymbol{\sigma}, \mathrm{u}) \\ &= \inf_{\mathrm{u} \in C} D(\mathrm{u}). \end{aligned}$$

$\sup_{\boldsymbol{\sigma} \in B} a(\boldsymbol{\sigma}, u^*) \longrightarrow$ Lower Bound

$\inf_{u \in C} a(\boldsymbol{\sigma}^*, u) \longrightarrow$ Upper Bound

Current Work

Limit Analysis

Discrete Formulation

Mesh the domain Ω and choose interpolation spaces $\boldsymbol{X}_h$ for $\boldsymbol{\sigma}$ and $\boldsymbol{Y}_h$ for $\mathbf{u}$.

$$\lambda_h^* = \max_{s.t.\begin{cases} \exists \boldsymbol{\sigma}_h \in \boldsymbol{B}_h \\ \boldsymbol{a}(\boldsymbol{\sigma}_h, \mathbf{u}_h) = \boldsymbol{\lambda} \boldsymbol{F}(\mathbf{u}_h), \forall \mathbf{u}_h \in \boldsymbol{Y}_h \end{cases}} \boldsymbol{\lambda}$$

$$= \max_{\boldsymbol{\sigma}_h \in \boldsymbol{B}_h} \min_{\mathbf{u}_h \in \boldsymbol{C}_h} \boldsymbol{a}(\boldsymbol{\sigma}_h, \mathbf{u}_h)$$

$$= \min_{\mathbf{u}_h \in \boldsymbol{C}_h} \max_{\boldsymbol{\sigma}_h \in \boldsymbol{B}_h} \boldsymbol{a}(\boldsymbol{\sigma}_h, \mathbf{u}_h)$$

$$= \min_{\mathbf{u}_h \in \boldsymbol{C}_h} \boldsymbol{D}_h(\mathbf{u}_h).$$

Current Work

Discrete Formulation...

- In general, for a given choice of $\boldsymbol{X}_h \times \boldsymbol{Y}_h$, $\boldsymbol{\lambda}_h^*$ is only an approximation to $\boldsymbol{\lambda}^*$, but not a bound.

Current Work

Limit Analysis

Discrete Formulation...

- In general, for a given choice of $\boldsymbol{X}_h \times \boldsymbol{Y}_h$, $\boldsymbol{\lambda}_h^*$ is only an approximation to $\boldsymbol{\lambda}^*$, but not a bound.
- For appropriately-chosen combinations of the interpolation spaces $\boldsymbol{X}_h \times \boldsymbol{Y}_h$, then $\boldsymbol{\lambda}_h^*$ is either a lower bound ($\boldsymbol{\lambda}_h^{*LB} \leq \boldsymbol{\lambda}^*$) or an upper bound ($\boldsymbol{\lambda}^* \leq \boldsymbol{\lambda}_h^{*UB}$).

Current Work

Limit Analysis

Discrete Formulation...

- In general, for a given choice of $\boldsymbol{X}_h \times \boldsymbol{Y}_h$, $\boldsymbol{\lambda}_h^*$ is only an approximation to $\boldsymbol{\lambda}^*$, but not a bound.
- For appropriately-chosen combinations of the interpolation spaces $\boldsymbol{X}_h \times \boldsymbol{Y}_h$, then $\boldsymbol{\lambda}_h^*$ is either a lower bound ($\boldsymbol{\lambda}_h^{*LB} \leq \boldsymbol{\lambda}^*$) or an upper bound ($\boldsymbol{\lambda}^* \leq \boldsymbol{\lambda}_h^{*UB}$).
- Purely **static spaces** $\boldsymbol{X}_h^{LB} \times \boldsymbol{Y}_h^{LB}$ yield lower bounds. Purely **kinematic spaces** $\boldsymbol{X}_h^{UB} \times \boldsymbol{Y}_h^{UB}$ yield upper bounds.

Current Work

...Discrete Formulation...

- Purely **static spaces** $\boldsymbol{X}_h^{LB} \times \boldsymbol{Y}_h^{LB}$:
  - Plane stress/strain - $\boldsymbol{\sigma}_h$: elementally discontinuous linear interpolations, $\mathbf{u}_h$: constant spaces on the elements and additional linear interpolations in the inter-element edges.
- Purely **kinematic spaces** $\boldsymbol{X}_h^{UB} \times \boldsymbol{Y}_h^{UB}$:
  - Plane stress - $\boldsymbol{\sigma}_h$: constant spaces on the elements, $\mathbf{u}_h$: continuous piecewise linear interpolations.
  - Plane strain - $\boldsymbol{\sigma}_h$: constant spaces on the elements and additional linear tractions in the inter-element edges; $\mathbf{u}_h$: elementally discontinuous linear spaces.

Current Work

Limit Analysis

Conic Programming...

- Primal (P) and Dual (D) canonical forms of Conic Programs:
  $$(\boldsymbol{P})\ \ \min\ \left\{\boldsymbol{c}^T\boldsymbol{x} \mid \boldsymbol{A}\boldsymbol{x}=\boldsymbol{b},\ \boldsymbol{x}\in\mathcal{K}\right\},$$
  $$(\boldsymbol{D})\ \ \max\ \left\{\boldsymbol{b}^T\boldsymbol{y} \mid \boldsymbol{A}^T\boldsymbol{y}+\boldsymbol{s}=\boldsymbol{c},\ \boldsymbol{s}\in\mathcal{K}_*\right\}$$
  where $\mathcal{K}\subset\mathbb{R}^n$ is a closed, convex cone with a nonempty interior and $\mathcal{K}_*=\left\{\boldsymbol{s}\in\mathbb{R}^n \mid \boldsymbol{s}^T\boldsymbol{x}\geq 0,\ \forall\boldsymbol{x}\in\mathcal{K}\right\}$ is its dual.
- Canonical Self-Dual Cones $\mathcal{K}\equiv\mathcal{K}_*$: Positive orthant (LP)- $\mathbb{R}^n_+$;
  Lorentz cone (SOCP): $\mathcal{L}^n=\left\{\boldsymbol{x}\in\mathbb{R}^n \mid x_1\geq\sqrt{\sum_{i=2}^n x_i^2}\right\}$;
  Positive semidefinite cone (SDP): $\equiv \S^n_+$
- Mixed Conic Program:
  $$\mathcal{K}=\mathbb{R}^{n_1}\times\mathcal{L}^{n_2}\times\ldots\times\mathcal{L}^{n_r}\times\S_+^{n_{r+1}}\times\ldots\times\S_+^{n_q}\equiv\mathcal{K}_*$$

Current Work

Limit Analysis

Conic Programming...

Example: Lower Bound Problem as a SOCP

$$\lambda_h^{*LB} \equiv \max \lambda$$

$$s.t. \begin{cases} \begin{pmatrix} \underline{\underline{A}}^{eq1} & \vdots & \underline{F}_h^{eq1} & \vdots & \underline{\underline{0}} \\ \underline{\underline{A}}^{eq2} & \vdots & \underline{F}_h^{eq2} & \vdots & \underline{\underline{0}} \\ \underline{\underline{A}}_\delta^{soc} & \vdots & \underline{0} & \vdots & \underline{\underline{I}}_\delta \end{pmatrix} \begin{pmatrix} \underline{\sigma}_h \\ \lambda \\ \underline{x}_\delta^{soc} \end{pmatrix} = \begin{pmatrix} \underline{0} \\ \underline{0} \\ \underline{b}_\delta^{soc} \end{pmatrix} \\ \underline{\sigma}_h \text{ free}, \ \lambda \geq 0, \ \underline{x}_\delta^{soc} \in \mathcal{K} \end{cases}$$

where $\mathcal{K} = \overbrace{\mathcal{L}^n \times \cdots \times \mathcal{L}^n}^{3\times E}$, $\delta = 1$ refers to plane stress ($n = 5$) and $\delta = 2$, to plane strain ($n = 3$).

Solution of the Bound Problems

- Both the upper and the lower bound problems are SOCPs.
- This is important mainly for two reasons:

1. State of the art primal-dual interior point methods (IPMs), particularly developed for SOCP, can be used. They guarantee global convergence and efficiency in the solution process.
2. The bound problems can be solved using any generic conic programming optimization package.

Current Work

Limit Analysis

Certificates...

- Claim: $\boldsymbol{\lambda}_h^{*LB} \leq \boldsymbol{\lambda}_h^{*} \leq \boldsymbol{\lambda}_h^{*UB}$
- Certificate:
  - Information about the computational mesh $\mathcal{T}_h$
  - $(\boldsymbol{\lambda}_h^{*LB}, \underline{\boldsymbol{\sigma}}_h^{LB}) \Longrightarrow$ check that equilibrium and membership to the yield condition hold point by point.
  - $(\boldsymbol{\lambda}_h^{*UB}, \underline{\boldsymbol{u}}_h^{UB}) \Longrightarrow$ check that $\underline{\boldsymbol{u}}_h^{UB}$ is a kinematically admissible velocity field and that $\boldsymbol{\lambda}_h^{*UB} = \boldsymbol{D}(\underline{\boldsymbol{u}}_h^{UB})$.

Current Work

Limit Analysis

...Mesh Adaptivity

- Objective: refine the mesh $\mathcal{T}_h$ efficiently, by only dividing the elements that contribute more to the numerical error. Here, the error is measured by the **bound gap**, $\boldsymbol{\Delta}_h = \boldsymbol{\lambda}_h^{*UB} - \boldsymbol{\lambda}_h^{*LB}$.
- The **elemental bound gap**, Δ_h^e, gives the contribution of each element, e, in the mesh to the total bound gap:

$$\boldsymbol{\Delta}_h^e = \underbrace{\int_{\Omega^e} \boldsymbol{\sigma}_y \boldsymbol{\varepsilon}_{eq}(\mathbf{u}_{UB}^e)}_{D^e(\mathbf{u}_{UB}^e)} - \underbrace{\left(\int_{\Omega^e} (-\nabla \cdot \boldsymbol{\sigma}_{LB}^e) \cdot \mathbf{u}_{UB}^e \, dV + \int_{\partial\Omega^e} (\mathbf{n}^{\xi_e} \cdot \boldsymbol{\sigma}_{LB}^e) \cdot \mathbf{u}_{UB}^e \, dS \right)}_{F^e(\mathbf{u}_{UB}^e)},$$

- Properties of $\boldsymbol{\Delta}_h^e$: 1) $\boldsymbol{\Delta}_h^e \geq \mathbf{0}, \ \forall e \in \mathcal{T}_h$, 2) $\sum_{e \in \mathcal{T}_h} \boldsymbol{\Delta}_h^e = \boldsymbol{\Delta}_h$.
- Adaptive strategy: refine only the elements with higher $\boldsymbol{\Delta}_h^e$.