Guaranteed Bounds for Solution of Parameter Dependent System of Equations

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22th Joint UTEP/NMSU Workshop on Mathematics, Computer Science, and Computational Sciences
Solution of PDE

Parameter dependent Boundary Value Problem

\[ A(p)u = f(p), u \in V(p), p \in P \]

Exact solution

\[ u = \inf_{p \in P} u(p), \overline{u} = \sup_{p \in P} u(p) \]

\[ u(x, p) \in [u(x), \overline{u}(x)] \]

Approximate solution

\[ u_h = \inf_{p \in P} u_h(p), \overline{u}_h = \sup_{p \in P} u_h(p) \]

\[ u_h(x, p) \in [u_h(x), \overline{u}_h(x)] \]
Linear and nonlinear equations.
Multiphysics (solid mechanics, fluid mechanics etc.)
Ordinary and partial differential equations, variational equations, variational inequalities, numerical methods, programming, visualizations, parallel computing etc.
Two point boundary value problem

Sample problem

\[
\begin{cases}
-(g(x, p)u'(x))' = f(x, p) \\
u(0) = 0, u(1) = 0
\end{cases}
\]

and \( u_h(x) \) is finite element approximation given by a weak formulation

\[
\int_0^1 g(x, p)u'_h(x)v'(x)dx = \int_0^1 f(x, p)v(x)dx, \forall v \in V_h^{(0)}
\]

or

\[ a(u_h, v) = l(v), \forall v \in V_h^{(0)} \subset H_0^1 \]

where \( u_h(x) = \sum_{i=1}^{n} u_i \varphi_i(x) \) and \( \varphi_i(x_j) = \delta_{ij} \).
The Finite Element Method

Approximate solution

$$\int_0^1 g(x, p) u'_h(x) v'(x) dx = \int_0^1 f(x, p) v(x) dx$$

$$\sum_{j=1}^n \left( \sum_{i=1}^n \int_0^1 g(x, p) \varphi_i(x) \varphi_j(x) dx u_i - \int_0^1 f(x, p) \varphi_j(x) dx \right) v_j = 0$$

Final system of equations (for one element) \( Ku = q \) where

$$K_{i,j} = \int_0^1 g(x, p) \varphi_i(x) \varphi_j(x) dx, q_i = \int_0^1 f(x, p) \varphi_i(x) dx$$
Global Stiffness Matrix

Global stiffness matrix

\[
\sum_{p=1}^{n} \left( \sum_{q=1}^{n} \sum_{e=1}^{n_e} \sum_{i=1}^{n_u} \sum_{j=1}^{n_u} U_{j,p}^e \int_{\Omega_e} g(x,p) \frac{\partial \varphi_i^e(x)}{\partial x} \frac{\partial \varphi_j^e(x)}{\partial x} dx\right) u_{i,q}^e -
\]

\[
\sum_{q=1}^{n} \sum_{e=1}^{n_e} \sum_{i=1}^{n_u} \sum_{j=1}^{n_u} U_{j,p}^e \int_{\Omega_e} f(x,p) \varphi_i^e(x) \varphi_j^e(x) dx \right) v_p = 0
\]

Final system of equations

\[ K(p)u = q(p) \Rightarrow F(u, p) = 0 \]
Nonlinear equation $F(u, p) = 0$ for $p \in P$.

$$F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$$

Implicit function $u = u(p) \iff F(u, p) = 0$

$$u(P) = \{ u : F(u, p) = 0, p \in P \}$$

Interval solution

$$\underline{u}_i = \min \{ u : F(u, p) = 0, p \in P \}$$

$$\overline{u}_i = \max \{ u : F(u, p) = 0, p \in P \}$$
Interval Methods


Interval solution

\[ u_i = \min \{ u(p) : p \in P \} = \min \{ u : F(u, p) = 0, p \in P \} \]

\[ \bar{u}_i = \max \{ u(p) : p \in P \} = \max \{ u : F(u, p) = 0, p \in P \} \]

\[ u_i = \begin{cases} 
\min u_i \\
F(u, p) = 0 \\
p \in P 
\end{cases}, \quad \bar{u}_i = \begin{cases} 
\max u_i \\
F(u, p) = 0 \\
p \in P 
\end{cases} \]
KKT Conditions

Nonlinear optimization problem for $f(x) = x_i$

$$\begin{align*}
\min_{x} f(x) \\
h(x) &= 0 \\
g(x) &\geq 0
\end{align*}$$

Lagrange function $L(x, \lambda, \mu) = f(x) + \lambda^T h(x) - \mu^T g(x)$

Optimality conditions can be solved by the Newton method.

$$\begin{align*}
\nabla_x L &= 0 \\
\nabla_\lambda L &= 0 \\
\mu_i &\geq 0 \\
\mu_i g_i(x) &= 0 \\
h(x) &= 0 \\
g(x) &\geq 0
\end{align*}$$
KKT Conditions - Newton Step

\[ F'(X) \Delta X = -F(X) \]

\[ F'(X) = \begin{bmatrix}
\left( \nabla_x^2 f(x) + \nabla_x^2 h(x)y \right)_{n \times n} & \nabla_x h(x)_{n \times m} & -I_{n \times n} \\
\nabla_x h(x)_{m \times n}^T & 0_{n \times m} & 0_{m \times n} \\
Z_{n \times n} & 0_{n \times m} & X_{m \times n}
\end{bmatrix} \]

\[ \Delta X = \begin{bmatrix}
\Delta x \\
\Delta y \\
\Delta z
\end{bmatrix}, \quad X = \begin{bmatrix}
x \\
y \\
z
\end{bmatrix} \]

\[ F(X) = -\begin{bmatrix}
\nabla_x f(x) + \nabla_x h^T(x)y - z \\
h(x) \\
XYe - \mu_k e
\end{bmatrix} \]
In order to find maximum/minimum of the function $u$ it is possible to apply the steepest descent algorithm.

1. Given $x_0$, set $k = 0$.
2. $d^k = -\nabla f(x_k)$. If $d^k = 0$ then stop.
3. Solve $\min_{\alpha} f(x_k + \alpha d^k)$ for the step size $\alpha_k$. If we know second derivative $H$ then $\alpha_k = \frac{d^T_k d_k}{d^T_k H(x_k) d_k}$.
4. Set $x_{k+1} = x_k + \alpha_k d_k$, update $k = k + 1$. Go to step 1.

New Approach for Finding Guaranteed Bounds

\[ g_1(P) \subset V_1, g_2(P) \subset V_2 \]
\[ \partial V_1 = \partial G_1^{\text{int}}, \partial V_2 \subset \partial G_2^{\text{int}} \]
Let's assume that $g : P \rightarrow \mathbb{R}$ is a continuous function, $P$ is a path-connected, compact subset of $\mathbb{R}$, then

$g(P) = \{ g(p) : p \in P \} = [g(p_{min}), g(p_{max})] = [x_{min}, x_{max}]$ is a closed interval and $p_{min}, p_{max} \in P$,

$x_{min} = \inf \{ g(x) : p \in P \}$, $x_{max} = \sup \{ g(x) : p \in P \}$. 
Theorem

Let’s assume that $g : P \to \mathbb{R}$ is a continuous function, $P$ is a path-connected, compact subset of $\mathbb{R}^m$, we know at least one value $x_0 = g(p_0)$ such that $p_0 \in P$, and exists some $\varepsilon > 0$ such that $x_0 + \Delta x \not\in g(P)$ for all $\Delta x \in (0, \varepsilon]$, then $x_0 = g(p_{\text{max}}) = g_{\text{max}}$ is a guaranteed upper bound of the set $g(P)$. 
New Approach for Finding Guaranteed Bounds

Theorem

Let’s assume that \( g : P \rightarrow \mathbb{R}^n \) is a continuous function that is defined as a unique solution of the equation \( f(x, p) = 0 \), \( P \) is a path-connected, compact subset of \( \mathbb{R}^m \), we know at least one value \( x_0 = g(p_0) \) such that \( p_0 \in P \), and exists some \( \varepsilon > 0 \) such that \( x_{0,i} + \Delta x_i \notin g_i(P) \) for all \( \Delta x_i \in (0, \varepsilon] \), then \( x_{0,i} = g_i(p_{\text{max}}) = g_{i,\text{max}} \) is a guaranteed upper bound of the set \( g_i(P) = [g_i,\text{min}(P), g_i,\text{max}(P)] \).

If the equation \( f(x, p) = 0 \) has multiple solutions \( x = g_i(p) \) \( (i = 1, \ldots, s) \), then

\[
g(P) = g_1(P) \cup g_2(P) \cup \ldots \cup g_s(P)
\]
Let's consider the equation nonlinear equation with uncertain parameter

\[ x^2 - 4p^2 = 0 \quad \text{for} \quad p \in [1, 2]. \]

Presented equation has two solutions \( x = g_1(p) = 2p \) and \( x = g_2(p) = -2p \).

Non-guaranteed solutions are
\[ [x_1, x_1] = g_1([1, 2]) = [2, 4] \]  and 
\[ [x_2, x_2] = g_2([1, 2]) = [-4, -2]. \]
Example 1

Let’s check if the number $x_1 = 4 + \Delta x$ is a solution for $\Delta x > 0$.

$$0 \in f(4 + \Delta x, [1, 2])$$
$$0 \in (4 + \Delta x)^2 - 4[1, 2]^2$$
$$0 \in 16 + 8\Delta x + \Delta x^2 - 4[1, 4]$$
$$0 \in 16 + 8\Delta x + \Delta x^2 - [4, 16]$$
$$0 \in [8\Delta x + \Delta x^2, 12 + 8\Delta x + \Delta x^2]$$

Last condition is not satisfied then $x_1 = 4 + \Delta x$ is not a solution for any $\Delta x > 0$ then $\bar{x} = 4$. 
Example 1

Let’s check if the number \( x_1 = 2 - \Delta x \) is a solution for \( \Delta x > 0 \).

\[
0 \in f(2 - \Delta x, [1, 2])
\]
\[
0 \in (2 - \Delta x)^2 - 4[1, 2]^2
\]
\[
0 \in 4 - 4\Delta x + \Delta x^2 - 4[1, 2]
\]
\[
0 \in 4 - 4\Delta x + \Delta x^2 + [-8, -4]
\]
\[
0 \in [-4 - 4\Delta x + \Delta x^2, -4\Delta x + \Delta x^2]
\]

For small \( \Delta x \) it is possible to neglect the quadratic term and \(-4\Delta x + \Delta x^2 < 0\). Last condition is not satisfied then \( x_1 = 2 - \Delta x \) is not a solution for small \( \Delta x > 0 \) then \( x = 2 \). The interval solution \([x_1, \bar{x}_1] = [2, 4]\) is guaranteed.
Example 2

Let’s consider the following system of linear interval equations

\[
\begin{aligned}
[-4, -3] x_1 + [-2, 2] x_2 &= [-8, 8] \\
[-2, 2] x_1 + [-4, -3] x_2 &= [-8, 8]
\end{aligned}
\] (1)

Let’s assume that the non-guaranteed solution is \(x_1 \in [-8, 8], x_2 \in [-8, 8]\).
Example 2

Let $x_1 = 8 + \Delta x_1$ and $\Delta x_1 > 0$.

\[
\begin{cases}
  a_{11}(8 + \Delta x_1) + a_{12}x_2 = b_1 \\
  a_{21}(8 + \Delta x_1) + a_{22}x_2 = b_2
\end{cases}
\]

\[
\begin{aligned}
  &a_{11}(8 + \Delta x_1) + a_{12} \left( \frac{b_2 - a_{21}(8+\Delta x_1)}{a_{22}} \right) = b_1 \\
  &x_2 = \frac{b_2 - a_{21}(8+\Delta x_1)}{a_{22}}
\end{aligned}
\]

\[
\begin{aligned}
  &a_{11}(8 + \Delta x_1) + \frac{a_{12}b_2}{a_{22}} - \frac{a_{12}a_{21}(8 + \Delta x_1)}{a_{22}} = b_1 \\
  &(8 + \Delta x_1) \left( a_{11} - \frac{a_{12}a_{21}}{a_{22}} \right) + \frac{a_{12}b_2}{a_{22}} - b_1 = 0
\end{aligned}
\]
Example 2

\[(8 + \Delta x_1) \left( a_{11} - \frac{a_{12} a_{21}}{a_{22}} \right) + \frac{a_{12} b_2}{a_{22}} - b_1 = 0 \]

\[0 \in (8 + \Delta x_1) \left( a_{11} - \frac{a_{12} a_{21}}{a_{22}} \right) + \frac{a_{12} b_2}{a_{22}} - b_1 \]

\[0 \in (8 + \Delta x_1) \left[ -\frac{16}{3}, -\frac{5}{3} \right] + \left[ -\frac{16}{3}, \frac{16}{3} \right] - [-8, 8] \]

\[0 \in \left[ -\frac{128}{3} - \frac{16}{3} \Delta x_1, -\frac{40}{3} - \frac{5}{3} \Delta x_1 \right] + \left[ -\frac{40}{3}, \frac{40}{3} \right] \]

\[0 \in \left[ -56 - \frac{16}{3} \Delta x_1, -\frac{5}{3} \Delta x_1 \right] \]

Then \( x_1 = 8 + \Delta x_1 \) is not a solution for \( \Delta x_1 > 0 \) and \( x_1 = 8 \).
Sample boundary value problem

\[ \frac{d}{dx} \left( EA \frac{du}{dx} \right) = 0, \; u(0) = 0, \; EA \frac{du(L)}{dx} = P \]

After discretization

\[
\begin{bmatrix}
  k_1 + k_2 & -k_2 & 0 & \ldots & 0 & 0 \\
  -k_2 & k_2 + k_3 & -k_3 & \ldots & 0 & 0 \\
  \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
  0 & 0 & 0 & \ldots & k_{n-1} + k_n & -k_n \\
  0 & 0 & 0 & \ldots & -k_n & k_n \\
\end{bmatrix}
\begin{bmatrix}
  u_1 \\
  u_2 \\
  \ldots \\
  u_{n-1} \\
  u_n \\
\end{bmatrix} = \begin{bmatrix}
  0 \\
  0 \\
  \ldots \\
  0 \\
  P \\
\end{bmatrix}
\]

Let \( n = 2 \) and \( k_1, k_2 \in \left[ \frac{1}{3}, \frac{1}{2} \right] \) and \( P = 1 \) then the non-guaranteed solution is \( u_1 \in [2, 3], \; u_2 \in [4, 6] \).
Example 3

Let’s assume that \( u_1 = 3 + \Delta u_1, \Delta u_1 > 0 \) then

\[
\begin{aligned}
(k_1 + k_2)(3 + \Delta u_1) - k_2 u_2 &= 0 \\
-k_2(3 + \Delta u_1) + k_2 u_2 &= P
\end{aligned}
\]

\[
\begin{aligned}
(k_1 + k_2)(3 + \Delta u_1) - k_2 u_2 &= 0 \\
u_2 &= \frac{P + k_2(3 + \Delta u_1)}{k_2}
\end{aligned}
\]

\[
\begin{aligned}
(k_1 + k_2)(3 + \Delta u_1) - k_2 \frac{P + k_2(3 + \Delta u_1)}{k_2} &= 0 \\
(k_1 + k_2)(3 + \Delta u_1) - P - k_2(3 + \Delta u_1) &= 0 \\
k_1(3 + \Delta u_1) - P &= 0
\end{aligned}
\]
Example 3

By assumption $k_1 \in \left[ \frac{1}{3}, \frac{1}{2} \right]$, $P = 1$ then

$$0 \in \left[ \frac{1}{3}, \frac{1}{2} \right] (3 + \Delta u_1) - P,$$

$$0 \in \left[ \frac{1}{3}(3 + \Delta u_1), \frac{1}{2}(3 + \Delta u_1) \right] - 1,$$

$$0 \in \left[ \frac{1}{3} \Delta u_1, \frac{1}{2} + \frac{1}{2} \Delta u_1 \right].$$

The last condition cannot be satisfied because $\Delta u_1 > 0$ consequently $u_1 = 3 + \Delta u_1$ cannot be a solution of the system for any $\Delta u_1 > 0$ and $3 = \bar{u}_1$ is guaranteed upper-bound of the solution $u_1$. 
Methodology presented in this paper can be applied for wide range of parameter dependent system of equations and eigenvalue problems. The method can be applied not only for the solution of the equations with set-valued parameters but also for finding values of the functions that depends of such solutions which is very important in the practical applications. By using theory from the presentation, in some cases, in order to use guaranteed bounds of the solution it is possible existing, well established computational methods and at the end prove that the solution is guaranteed. Methodology presented in this presentation can be applied to selected solutions or to all solutions of the systems of nonlinear equations.