MATH 676

–

Finite element methods in scientific computing

Wolfgang Bangerth, Texas A&M University

Lecture 31.55:

Nonlinear problems

Part 2: Newton's method for PDEs

The minimal surface equation

Goal: Solve

$$-\nabla \cdot \left(A \frac{\nabla u}{\sqrt{1+|\nabla u|^2}} \right) = f \qquad \Leftrightarrow \qquad \underbrace{f + \nabla \cdot \left(A \frac{\nabla u}{\sqrt{1+|\nabla u|^2}} \right)}_{=: R(u)} = 0$$

Newton's method: Iterate

$$[R'(u_k)]\,\delta u_k = -R(u_k), \qquad u_{k+1} = u_k + \delta u_k$$

Questions:

- What is the variational formulation of this?
- What is $R'(u)$ anyway?

Derivatives for operators

Question: What is *R'(u)*?

Answer, part 1: Start with *R(u)*:

$$R(u) := f + \nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)$$

This is an operator that maps

$$R:\ u\in H_0^1 \rightarrow H^{-1}$$

Derivatives for operators

Question: What is *R'(u)*?

Answer, part 2: Start with *R(u)*:

$$R(u) \; := \; f + \nabla \cdot \left(A \frac{\nabla u}{\sqrt{1+|\nabla u|^2}} \right)$$

Then use the definition of a directional derivative:

$$R'(u)(\delta u) \; := \; \lim_{\epsilon \to 0} \frac{R(u+\epsilon \delta u) - R(u)}{\epsilon}$$

Derivatives for operators

Question: What is *R'(u)*?

Answer, part 3: Now we need to do some scary calculus:

$$R'(u)(\delta u) := \lim_{\epsilon \to 0} \frac{R(u+\epsilon\delta u)-R(u)}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{1}{\epsilon}\left[\left(f+\nabla\cdot\left(A\frac{\nabla(u+\epsilon\delta u)}{\sqrt{1+|\nabla(u+\epsilon\delta u)|^2}}\right)\right)-\left(f+\nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)\right)\right]$$

$$= \lim_{\epsilon \to 0} \frac{1}{\epsilon}\left[\nabla\cdot A\left(\frac{\nabla(u+\epsilon\delta u)}{\sqrt{1+|\nabla(u+\epsilon\delta u)|^2}}-\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)\right]$$

Derivatives for operators

Question: What is *R'(u)*?

Answer, part 3: Now we need to do some scary calculus:

$$R'(u)(\delta u) := \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left[\nabla\cdot A\left(\frac{\nabla(u+\epsilon\delta u)}{\sqrt{1+|\nabla(u+\epsilon\delta u)|^2}} - \frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)\right]$$

We need to do a Taylor expansion on a term of the form

$$f(\epsilon)=\frac{x+\epsilon y}{\sqrt{1+(x+\epsilon y)^2}} = \frac{x}{\sqrt{1+x^2}}+\left(\frac{y}{\sqrt{1+x^2}}-\frac{x^2 y}{(1+x^2)^{3/2}}\right)\epsilon+O(\epsilon^2)$$

This yields:

$$R'(u)(\delta u) := \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left[\nabla\cdot A\left(\frac{\nabla\epsilon\delta u}{\sqrt{1+|\nabla u|^2}} - \frac{(\nabla u\cdot\nabla\epsilon\delta u)\nabla u}{(1+|\nabla u|^2)^{3/2}}\right)+O(\epsilon^2)\right]$$

Derivatives for operators

Question: What is *R'(u)*?

Answer, part 3: After this step...

$$R'(u)(\delta u) \;:=\; \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\nabla\cdot A\left(\frac{\nabla\epsilon\delta u}{\sqrt{1+|\nabla u|^2}}-\frac{(\nabla u\cdot\nabla\epsilon\delta u)\nabla u}{\left(1+|\nabla u|^2\right)^{3/2}}\right)+O(\epsilon^2)\right]$$

... all we need to do is take the limit:

$$R'(u)(\delta u) \;:=\; \nabla\cdot\left(A\frac{\nabla\delta u}{\sqrt{1+|\nabla u|^2}}-A\frac{(\nabla u\cdot\nabla\delta u)\nabla u}{\left(1+|\nabla u|^2\right)^{3/2}}\right)$$

This operator is linear in the direction *δu* in which we take the derivative!

Derivatives for operators

Question: What is *R'(u)*?

Short answer: Really, taking derivatives of things like

$$R(u) \;:=\; f + \nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)$$

... works *almost* like taking normal derivatives. You just always have to provide the direction δu !

Derivatives for operators

Examples:

- $F(u) = au \quad \Rightarrow \quad F'(u)(\delta u) = a\,\delta u$
- $F(u) = u^2 \quad \Rightarrow \quad F'(u)(\delta u) = 2\,u\,\delta u$
- $F(u) = (\nabla u)^2 \quad \Rightarrow \quad F'(u)(\delta u) = 2\,(\nabla u)\cdot(\nabla \delta u)$
- $F(u) = \frac{1}{1+(\nabla u)^2} \quad \Rightarrow \quad F'(u)(\delta u) = -\frac{1}{\left(1+(\nabla u)^2\right)^2}\left(2\nabla u\cdot\nabla\delta u\right)$

Derivatives for operators

Question: What is *R'(u)*?

Short answer: Really, taking derivatives of things like

$$R(u) := f + \nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)$$

… works *almost* like taking normal derivatives:

$$R'(u)(\delta u) := \nabla\cdot\left(A\frac{\nabla \delta u}{\sqrt{1+|\nabla u|^2}} - A\frac{(\nabla u\cdot\nabla\delta u)\nabla u}{\left(1+|\nabla u|^2\right)^{3/2}}\right)$$

Derivatives for operators

Question: What is $R'(u)$?

Some more theory:

- We call $R'(u)(\delta u)$ the *Gateaux differential* of R at u in direction δu .
- If $R'(u)(\delta u)$ exists for all δu then we say that R is *Gateaux differentiable* at u.
- Under certain conditions (linearity, continuity, ...) we can define a linear operator $R'(u)$ and then we can write

$$R'(u)(\delta u) = R'(u)\, \delta u$$

The minimal surface equation

Goal: Solve

$$-\nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)=f \qquad \Leftrightarrow \qquad \underbrace{f+\nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)}_{=:R(u)}=0$$

Newton's method: Iterate

$$[R'(u_k)]\,\delta u_k=-R(u_k), \qquad u_{k+1}=u_k+\delta u_k$$

Questions:

- What is the variational formulation of this?
- What is $R'(u)$ anyway?

Newton's method for PDEs

Question: What is the variational formulation of

$$[R'(u_k)]\,\delta u_k = -R(u_k), \qquad u_{k+1} = u_k + \delta u_k$$

Answer: With...

$$R(u) := f + \nabla\cdot\left(A\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)$$

...we get:

$$R'(u)(\delta u) := \nabla\cdot\left(A\frac{\nabla \delta u}{\sqrt{1+|\nabla u|^2}} - A\frac{(\nabla u\cdot\nabla\delta u)\nabla u}{\left(1+|\nabla u|^2\right)^{3/2}}\right)$$

Newton's method for PDEs

Question: What is the variational formulation of

$$[R'(u_k)]\,\delta u_k = -R(u_k), \qquad u_{k+1} = u_k + \delta u_k$$

Answer: With...

$$(\phi, R'(u_k)(\delta u_k)) := \left(\nabla\phi, \frac{A}{\sqrt{1+|\nabla u_k|^2}}\nabla\delta u_k\right) - \left(\nabla\phi, \frac{A(\nabla u_k\cdot\nabla\delta u_k)}{\left(1+|\nabla u_k|^2\right)^{3/2}}\nabla u_k\right)$$

$$(\phi, R(u_k)) := (\phi, f) + \left(\nabla\phi, \frac{A}{\sqrt{1+|\nabla u_k|^2}}\nabla u_k\right)$$

...we arrive at this in each Newton step:

$$\left(\nabla\phi, \frac{A}{\sqrt{1+|\nabla u_k|^2}}\nabla\delta u_k\right) - \left(\nabla\phi, \frac{A(\nabla u_k\cdot\nabla\delta u_k)}{\left(1+|\nabla u_k|^2\right)^{3/2}}\nabla u_k\right)$$

$$= -(\phi, f) - \left(\nabla\phi, \frac{A}{\sqrt{1+|\nabla u_k|^2}}\nabla u_k\right) \qquad \forall\phi\in H_0^1$$

Practical considerations

Question: What if $R(u)$ is already really complicated?

Answer 1: Then your $R'(u)$ will be even more complicated. You will probably make mistakes calculating it, or implementing it.

Practical considerations

Question: What if *R(u)* is already really complicated?

Answer 2: You could use a symbolic math package to compute the derivative (e.g., Maple, Mathematics, …)

Practical considerations

Question: What if *R(u)* is already really complicated?

Answer 3: Or you could use automatic differentiation from within the code:
- in the code you only implement *R(u)*
- which you need anyway
- and get *R'(u)* for free (and correct!) if you do it right

Step-33 shows an example of how to do this.

Practical considerations

Question: How accurate do we have to be?

Observation: In the first few Newton steps, we are still far away from the solution!

– We could compute Newton updates δu_k on a coarse mesh
– We could solve the linear system inaccurately

In practice, this is exactly what is done.

Practical considerations

Question: But Newton's method does not always converge?

Answer: Yes. In many cases on needs a “globalization” strategy such as
– line search
– a trust region method

Newton's method for PDEs

Summary: For Newton's method on PDEs, we need to think about what the *derivative* of the residual *R(u)* should mean.

In practice: The derivative can be computed *almost* as normal.

We can then define each Newton iteration in weak form as

$$\left(\phi, [R'(u_k)]\,\delta u_k\right) = -\left(\phi, R(u_k)\right), \qquad u_{k+1} = u_k + \delta u_k$$

We then solve for the Newton updates δu_k on finer and finer meshes with more and more accuracy.

MATH 676

–

Finite element methods in scientific computing

Wolfgang Bangerth, Texas A&M University