NGsolve::Give me your element

And let your eyes delight in my ways

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Download code (works only on version 6.0) for these notes from here.

"Give me your heart / And let your eyes delight in my ways." –The Bible

Contents

Automatic differentiation

Goal: Create variables that know how to (exactly) differentiate themselves.

Idea:

- Differentiation obeys some rules (product rule, quotient rule etc) that we can implement by overloading operators, e.g., overload * to implement
$$\partial_i(f * g) = f(\partial_i g) + g(\partial_i f).$$
- Suppose an object representing x_i (the ith coordinate) knows its value **and** the value of its derivatives, at any given point. Then, we can compute both the value and the value of derivatives of $x_i * x_j$ by overloading * as above.

A minimalist class for differentiation

```
template<int D> class MyDiffVar{// My differentiable variables
                                // File: differentiables.hpp
  double Value;
  double Derivatives[D];

public:

  MyDiffVar () {};

  MyDiffVar (double xi, int i) { // i-th coordinate xi has
    Value = xi;                  // grad = i-th unit vector
    for (auto & d : Derivatives) d = 0.0;
    Derivatives[i] = 1.0;
  }

  double  GetValue() const  {return Value;}
  double& SetValue()        {return Value;}
  double  GetDerivative(int i) const {return Derivatives[i];}
  double& SetDerivative(int i)       {return Derivatives[i];}
};
```

Overload * for the differentiables

Template implementation of implement $\partial_i(f * g) = f(\partial_i g) + g(\partial_i f)$:

```
// implement product rule

template<int D> MyDiffVar<D>
operator* (const MyDiffVar<D> & f, const MyDiffVar<D> & g) {

  MyDiffVar<D> fg;

  fg.SetValue() = f.GetValue() * g.GetValue();

  for (int i=0; i<D; i++)
    fg.SetDerivative(i) = f.GetValue() * g.GetDerivative(i)
                        + g.GetValue() * f.GetDerivative(i) ;
  return fg;
}
```

Quiz: Open the file and provide operators $+, -$, and $/$.

Using your class

```
#include "differentiables.hpp"          // File d0.cpp
using namespace std;

int main() {

  MyDiffVar<2> x(0.5, 0), y(2.0, 1);

  cout << "x:" << x << endl
       << "y:" << y << endl
       << "x*y:" << x*y << endl
       << "x*y*y+y:" << x*y*y+y << endl;
}
```

Using your simple class, you can now differentiate polynomial expressions built using x and y coordinates (or x_i, $i = 1, \ldots, N$, in N-dimensions).

Exercise!

How would you modify `differentiables.hpp` so that you can also differentiate expressions like $\sin(xy)$?

Make sure your modified file compiles and runs correctly with this driver:

```
#include "differentiables.hpp"          // File d0x.cpp
using namespace std;

int main() {

  MyDiffVar<2> x(0.5, 0), y(2.0, 1);

  cout << "x:" << x << endl
       << "y:" << y << endl
       << "sin(x*y)/y:"<< sin(x*y)/y << endl;
}
```

Netgen's `AutoDiff` class

An implementation of these ideas is available in
`$NGSRC/netgen/libsrc/general/autodiff.hpp`.
Here is an example showing how to use it:

```
#include <fem.hpp>                              // File d1.cpp
using namespace std;

int main() {

  AutoDiff<2>  x(0.5, 0), y(2.0, 1);    // x and y coords
  AutoDiff<2>  b[3] = { x, y, 1-x-y }; // barycentric coords

  cout << "x:" << x << endl
       << "y:" << y << endl
       << "x*y:" << x*y << endl
       << "x*y*y+y:" << x*y*y+y << endl
       << "(b0*b1*b2-1)/y:" << (b[0]*b[1]*b[2] - 1)/y << endl;
}
```

We will use `AutoDiff` and the following classes to program finite elements.

FlatVector, SliceVector, etc.

```
#include <bla.hpp>                        // File: flatvec.cpp
using namespace std; using namespace ngbla;

int main() {

  double mem[] = {1,2,3,4,5,6,7,8,9,10};

  FlatVector<double> f1(2,mem);   // A vector class that steals
  FlatVector<double> f2(2,mem+3);// memory from elsewhere.
  cout << "f1:\n" << f1 << endl; // This prints 1, 2.
  cout << "f2:\n" << f2 << endl; // This prints 5, 6.

  SliceVector<> s1(4,2,mem);      // Also steals memory.
  cout << "s1:\n" << s1 << endl; // This prints 1, 3, 5, 7.
  SliceVector<> s2(5,1,mem+4);   // What is this?
  // :
```

- `SliceVector` class does not allocate or delete memory.
- Their constructors just create/copy pointers.

class ScalarFiniteElement

```
template <int D>
class ScalarFiniteElement : public FiniteElement {

  virtual void CalcShape(const IntegrationPoint & ip,
                         SliceVector<> shape) const = 0;

  virtual void CalcDShape(const IntegrationPoint & ip,
                          SliceMatrix<> dshape) const = 0;
  // ...
};
```

- `shape` and `dshape` are cheap to pass by value as function arguments even when they contain many elements.
- Any derived finite element class must provide shape functions and their derivatives.

Visualizing finite element “shape functions”

```
#                                              FILE: shapes.pde
geometry = square.in2d
mesh = squareTrg.vol

fespace v -type=h1ho -order=2
gridfunction u -fespace=v

numproc shapetester nptest -gridfunction=u
```

- The `numproc shapetester` is an NGsolve tool to visualize global basis functions (called **global shape functions**) of an `FESpace`.
- Load this PDE file. Click `Solve` button before doing anything else.
- Look for a tiny window called `Shape Tester` that pops up.
- The number (0,1,. . .) that you input in `Shape Tester` window determines which basis function will be set in `gridfunction u`.
- Got to `Visual` menu and pick `gridfunction u` to visualize.

Visualizing finite element “shape functions”

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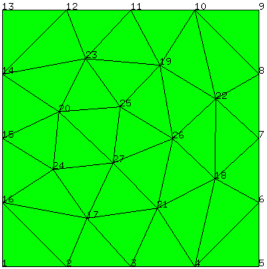
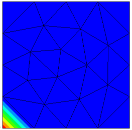
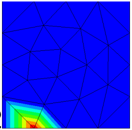
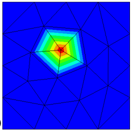


1 , 2 , . . . 25  . . . etc.

Global shape functions

Prepare to write your own finite element

Study these files in the folder `my_little_ngsolve`:

- `myElement.hpp`, `myElement.cpp`, `myHOElement.hpp`, `myHOElement.cpp`

  All elements in a mesh are mapped from a fixed “reference element”. Pay particular attention to `CalcShape(..)` and `CalcDshape(..)`. They give the values and derivatives of all **local shape functions** on the reference element.

- `myFESpace.hpp`, `myFESpace.cpp`, `myHOFESpace.hpp`, `myHOFESpace.cpp`

  Each global degree of freedom (“dof”) gives a global basis function and is associated to a geometrical object of the mesh (like a vertex, edge, or element). Pay particular attention to `GetDofNrs(...)`, which return global dof-numbers connected to an element.

Homework

Your assignment is to code the bicubic finite **element** Q_3 in `bicubicelem.cpp`. On the reference element, the unit square, this element consists of the space of functions

$$Q_3 = \mathrm{span}\{x^i y^j : \ 0 \le i \le 3, \ 0 \le j \le 3\}.$$

Also code a bicubic finite element **space** (derived from `FESpace`), for any mesh of quadrilateral elements, in file `bicubicspace.cpp`

Then, use your space to approximate the operator $-\Delta + I$ and solve a Neumann boundary value problem. Tabulate errors.

The ensuing slides give you hints to complete this homework and suggest separating the work into smaller separate tasks.

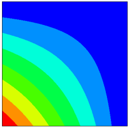
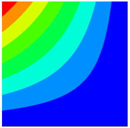
Bicubic shape functions on unit square

Task 1: In `bicubicelem.cpp`, provide shape functions.

E.g., here is a valid basis set of shape functions (you may use others) :

Vertex basis

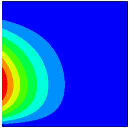
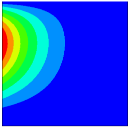
$$\phi_0 = (1-x)(1-y)$$
$$\phi_1 = (1-x)y$$
$$\phi_2 = x(1-y)$$
$$\phi_3 = xy$$

...

Edge basis

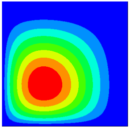
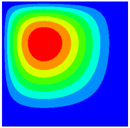
$$\phi_4 = (\phi_0\phi_1)\phi_0$$
$$\phi_5 = (\phi_0\phi_1)\phi_1$$
$$\phi_6 = (\phi_1\phi_3)\phi_3$$
$$\phi_7 = (\phi_1\phi_3)\phi_1$$
$$\vdots$$

...

Interior basis

$$\phi_4 = (1-x)(1-y)xy\phi_0$$
$$\phi_4 = (1-x)(1-y)xy\phi_1$$
$$\vdots$$

...

Bicubic shape functions on unit square

Task 1: In `bicubicelem.cpp`, provide shape functions.

- Your basis expressions should go into the `CalcShape` member function.
- For the `CalcDShape` member function, you can use `AutoDiff` variables and the same expressions you need in `CalcShape`.
- Consider simplifying your code so that you only type the basis expressions once.

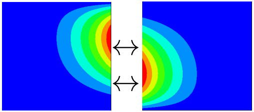
Orientation

Task 2: In `bicubicspace.cpp`, write your finite element space.

Remember to keep track of matching local and global orientation (go back and revise your `bicubicelem.cpp` if necessary).

```
/* What is the local orientation? Is the ordering of vertices
 * and edges within the reference element
 *
 *   v2     e1       v3         v3     e1       v2
 *      o----------o              o----------o
 *      |          |              |          |
 *   e2 |          | e3        e2 |          | e3
 *      |          |              |          |
 *      o----------o              o----------o          or something
 *   v0     e0       v1  ,      v0     e0       v1  ,   else?         */
```

What is the global orientation? NGsolve's mesh edges are directed/oriented. If edge shape functions from adjacent elements are not given in that orientation, then you may lose continuity!



Check your basis

Task 3: Compile the code you wrote and make a shared library

`make libmyquad.so`

and check your basis functions on the three given quadrilateral mesh files.

```
#                                    FILE : bicubicshapes.pde
geometry = square.in2d
#mesh = squareQuad1.vol.gz
#mesh = squareQuad2.vol.gz
mesh = squareQuad3.vol.gz

shared = libmyquad
define fespace v -type=myquadspace

define gridfunction u -fespace=v

numproc shapetester nptest -gridfunction=u
```

Solve a PDE

Task 4: Using your finite element space, solve this boundary value problem:

$$\begin{aligned} -\Delta u + u &= f \quad \text{on } \Omega \\ \partial u / \partial n &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

Hints:

- Do you know the variational formulation for this problem?
- You want to write a PDE file that mixes your finite element space with the NGSolve integrators.
- E.g., the NGSolve integrator `laplace`, can work with any finite element which provides `CalcDShape`, by dynamic polymorphism.

Solve a PDE

Task 4: Using your finite element space, solve this boundary value problem:

$$\begin{aligned} -\Delta u + u &= f \quad \text{on } \Omega \\ \partial u / \partial n &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

This task includes these steps:

1. Set f so that your exact solution is $u = \sin(\pi x)^2 \sin(\pi y)^2$.
2. Compute the $L^2(\Omega)$ error (code this either in your own C++ `numproc` – like we did before – or find facilities to directly do it in the `pde` file).
3. Solve on `mesh = squareQuad3.vol.gz` by loading your `pde` file and pressing the `Solve` button. Compute the $L^2(\Omega)$-error. Note it down.
4. Pressing the `Solve` button again to solve and compute the L^2-error on a uniformly refined mesh. Note the L^2-error. Repeat (until you can't).
5. What is the rate of convergence of L^2-error with meshsize?

Project

Student Team Project: Learn about the "DPG method" and download an implementation of it in GitHub. Your job is to extend it to quadrilateral elements. You will need to code a new finite element space that will serve as the "test" space for the DPG method. Details will be progressively made clear as you proceed with the project.