Finite volume method: further aspects

Julia packages supporting PDE solution

Up to now we used the Triangulate.jl in order to access mesh generation, for all other functionality, standard Julia packages were used.

There are a number of PDE solution packages in Julia, in particular for the finite element method. During this course, we will use a number of recently developed packages supporting basic functionality for the solution of PDEs. They emerged from the WIAS pdelib project and from scientific computing courses from previous years. These are:

- ExtendableGrids.jl: unstructured grid management library
- · GridVisualize.jl: grid and function visualization related to ExtendableGrids.jl
- · SimplexGridFactory.jl: unified high level mesh generator interface
- · ExtendableSparse.jl: convenient and efficient sparse matrix assembly

We will use all of them in this lecture.

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Dirichlet boundary conditions

 $\begin{array}{ll} -\nabla \delta \cdot \nabla u = f & \quad \text{in } \Omega \\ u = g & \quad \text{on } \partial \Omega \end{array}$

Three main possibilities to implement Dirichlet boundary conditions:

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- Eliminate Dirichlet BC algebraically after building of the matrix, i.e. fix ``known unknowns" at the Dirichlet boundary \Rightarrow highly technical
- Modifiy matrix such that equations at boundary exactly result in Dirichlet values \Rightarrow loss of symmetry of the matrix
- Penalty method: replace the Dirichlet boundary condition by a Robin boundary condition with high transfer coefficient

We discuss these possibilities for a 1D problem in $\Omega=(0,1)$ with tridiagonal matrix:

$$-\Delta u = f$$
 in Ω
 $u(0) = g_0$
 $u(1) = g_1$

Algebraic manipulation

• Matrix A of homogeneous Neumann problem - no regard to boundary values.

$$AU = \begin{pmatrix} \frac{1}{h} & -\frac{1}{h} & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}$$

- A is diagonally dominant, but neither idd, nor sdd.
- Fix the value of u_1 and eliminate the corresponding equation:

• A' is idd and stays symmetric

This operation is quite technical to implement, even more so for triangular meshes or for systems with multiple PDEs.

Modification of boundary equations

· Modify equation at boundary to exactly represent Dirichlet values

$$A'U = \begin{pmatrix} \frac{1}{h} & 0 & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \frac{1}{h}g \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}$$

- A' is idd ?
- + Loss of symmetry \Rightarrow problem e.g. with CG method

Penalty method: the "lazy" way

This corresponds to replacing the Dirichlet boundary condition u = g with a Robin boundary condition

$$\delta \partial_n u + \frac{1}{\varepsilon} u = \frac{1}{\varepsilon} g$$

In practice we perform this operation on a discrete level:

$$A'U = \begin{pmatrix} \frac{1}{\varepsilon} + \frac{1}{h} & -\frac{1}{h} & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_1 + \frac{1}{\varepsilon}g \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}$$



- A' is idd, symmetric, and the realization is technically easy.
- + If arepsilon is small enough, $u_1=g$ will be satisfied exactly within

floating point accuracy.

- · Drawback: this creates a large condition number
- Iterative methods should be initialized with Dirichlet values, so we start in a subspace where this is not relevant
- · Works also nonlinear problems, finite volume methods

Matrix assembly

trifactors! (generic function with 1 method)

bfacefactors! (generic function with 1 method)

assemble! (generic function with 1 method)

```
    function assemble!(matrix, # System matrix
    rhs, # Right hand side vector
    δ, # heat conduction coefficient
    f::Function, # Source/Sink function function
    g::Function, # boundary condition function

                                 pointlist.
                                  trianglelist,
                                 segmentlist)
         penalty=1.0e30
num_nodes_per_cell=3;
         num_edges_per_cell=3;
         num_nodes_per_bface=2
         ntri=size(trianglelist,2)
         nbface=size(segmentlist,2)
        # Local edge-node connectivity
local_edgenodes=[ 2 3; 3 1; 1 2]'
         # Storage for form factors
         e=zeros(num_nodes_per_cell)
         w=zeros(num_edges_per_cell)
         v=zeros(num_nodes_per_bface)
         # Initialize right hand side to zero
         rhs.=0.0
         # Loop over all triangles
         for itri=1:ntri
                trifactors!(w,e,itri,pointlist,trianglelist)
         # Assemble nodal contributions to right hand side
                for k_local=1:num_nodes_per_cell
                      k_global=trianglelist[k_local,itri]
                      x=pointlist[1,k_global]
y=pointlist[2,k_global]
rhs[k_global]+=f(x,y)*w[k_local]
                end
                # Assemble edge contributions to matrix
               # Assemble edge contributions to matrix
for iedge=linum.edges_per_cell
k_global=trianglelist[local_edgenodes[1,iedge],itri]
u_global=trianglelist[local_edgenodes[2,iedge],itri]
matrix[k_global,k_global]==5*e[iedge]
matrix[k_global,k_global]==5*e[iedge]
matrix[k_global,L_global]==5*e[iedge]
                      matrix[l_global,l_global]+=&*e[iedge]
                end
         end
         # Assemble boundary conditions
         for ibface=1:nbface
         bfacefactors!(v,ibface, pointlist, segmentlist)
for k_local=1:num_nodes_per_bface
    k_global=segmentlist[k_local,ibface]
                      x=pointlist[1,k_global]
y=pointlist[2,k_global]
                      rhs[k_global]+=penalty*g(x,y)
               end
         end

    end
```

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Calculation example

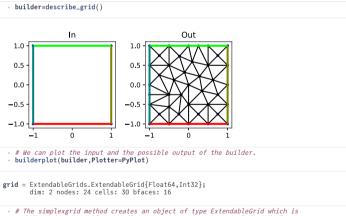
Now we are able to solve our intended problem.

Grid generation

describe_grid (generic function with 1 method) # We use the SimplexGridBuilder from SimplexGridFactory.jl function describe_grid() # Create a SimplexGridBuilder structure which can collect # geometry information builder=SimplexGridBuilder(Generator=Triangulate) # Add points, record their numbers
p1=point!(builder,-1,-1) p2=point!(builder,1,-1) p3=point!(builder,1,1) p4=point!(builder,-1,1) # Connect points by respective facets (segments) facetregion!(builder,1) facet!(builder,p1,p2) facetregion! (builder, 2) facet!(builder,p2,p3)
facetregion!(builder,3) facet!(builder,p3,p4) facetregion!(builder,4) facet!(builder,p4,p1) options!(builder,maxvolume=0.1) builder end

builder =

SimplexGridBuilder(Triangulate, 4, 1, 1.0, 1.0e-12, Int32[1, 2, 3, 4], Array{Int32,



- # defined in ExtendableGrids.jl. We can overwrite the maxvolume default
 # which we used in `describe_grid`.
- grid=simplexgrid(builder,maxvolume=4/desired_number_of_triangles)

Desired number of triangles

From the desired number of triangles, we can calculate a value fo the maximum area constraint passed to the mesh generator: Desired number of triangles: 20

Solving the problem

Problem data

```
f (generic function with 1 method)
 f(x,y)=sinpi(x)*sinpi(y)
```

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 $\delta = 1$

Data of the grid are accessed in a Dictionary like fashion. Coordinates, CellNodes and BFaceNodes are abstract types defined in ExtendableGrids.il. Behind this is a dictionary with types as keys allowing type-stable access of the contents like in a struct and easy extension by defining additional key types. See here for more information.

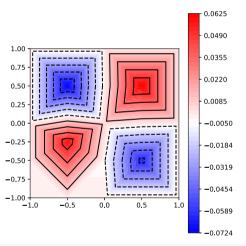
solve_example (generic function with 1 method)

```
function solve_example(grid)
     # Initialize sparse matrix and right hand side
     n=num_nodes(grid)
     matrix=spzeros(n,n)
     # call the assemble function.
assemble!(matrix,rhs,\delta,f,g,
             grid[Coordinates],
grid[CellNodes],
grid[BFaceNodes])
      # Solve
     sol=matrix\rhs
end
```

solution =

Float64[7.58983e-63, -1.58037e-62, 1.56301e-62, -1.8106e-62, 0.00546284, 1.23156e-32,

solution=solve_example(grid)



scalarplot from GridVisualize.jl allows easy handling of plotting
 # on unstructured grids with reasonable defaults.
 scalarplot(grid,solution,Plotter=PyPlot,resolution=

(300,300), isolines=11, colormap=:bwr)

Convergence test

How good is our implementation and the choice of the penalty method for Dirichlet boundary conditions ? - Perform a convergence test on ever finer grids!

For this purpose we need to calculate error norms. Based on the L2-Norm

$$||u||_2^2 = \int_\Omega u^2 d\omega$$

we implement a discrete analogon for a discrete solution $u_h = (u_k)_{k \in \mathcal{N}}$

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 $||u_h||^2_{2,h} = \int_\Omega u_h^2 d\omega = \sum_{k\in\mathcal{N}} |\omega_k|u_k^2$

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Further, we implement the "h1"-norm wich measures the error in the gradient. We may discuss the details later.

fvnorms (generic function with 1 method)

```
    # ## Calculate norms of solution

  function fvnorms(u,pointlist,trianglelist)
        local_edgenodes=[ 2 3; 3 1; 1 2]
num_nodes_per_cell=3;
        num_edges_per_cell=3;
        e=zeros(num_nodes_per_cell)
ω=zeros(num_edges_per_cell)
         l2norm=0.0
        h1norm=0.0
        ntri=size(trianglelist,2)
         for itri=1:ntri
               trifactors!(w,e,itri,pointlist,trianglelist)
for k_local=1:num_nodes_per_cell
                     k=trianglelist[k_local.itri]
                     x=pointlist[1,k]
y=pointlist[2,k]
l2norm+=u[k]^2*w[k_local]
               end
               for iedge=1:num_edges_per_cell
    k=trianglelist[local_edgenodes[1,iedge],itri]
    l=trianglelist[local_edgenodes[2,iedge],itri]
    hinorm+=(u[k]-u[l])^2*e[iedge]
               end
        end
        return (sqrt(l2norm), sqrt(h1norm));

    end
```

Run convergence test for a number of grid refinement levels

convergence_test (generic function with 1 method)

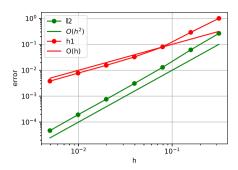
```
• function convergence_test(;nref0=0, nref1=1,k=1,l=1,extsparse=false)
     allh=[
      alll2=
     allh1=[]
     gbc(x,y)=0
      # We know the anayltical expression for the right hand side which
      # corresponds to this solution
      fexact(x,y)=sinpi(k*x)*sinpi(l*y);
      frhs(x,y)=(k^2+l^2)*pi^2*fexact(x,y);
      for iref=nref0:nref1
       # define the refinement level via the maximum area constraint
          area=0.1*2.0^(-2*iref)
          h=sgrt(area)
          grid=simplexgrid(builder,maxvolume=area)
          n=num_nodes(grid)
          rhs=zeros(n)
          # Optionally, use the sparse matrix from ExtendableGrids
          if extsparse
              matrix=ExtendableSparseMatrix(n.n)
          else
              matrix=spzeros(n,n)
          and
          rhs=zeros(n)
          assemble!(matrix,rhs,\delta,frhs,gbc,
grid[Coordinates],grid[CellNodes],grid[BFaceNodes])
sol=matrix\rhs
          uexact=map(fexact,grid)
          (l2norm,h1norm)=fvnorms(uexact-sol,grid[Coordinates],grid[CellNodes])
          push!(allh.h)
          push!(allh1,h1norm)
          push!(alll2,l2norm)
      end
     allh,alll2,allh1

    end
```

(Any[0.316228, 0.158114, 0.0790569, 0.0395285, 0.0197642, 0.00988212, 0.00494106], A

allh,alll2,allh1=convergence_test(nref0=0,nref1=6,extsparse=false)

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Conclusions

We see the second order convergence of the solution and first order convergence of the gradient. This is the typical behavior which we also would expect from the finite element method.

Concerning the complexity, the ExtendableSparseMatrix uses an intermediate data structure for collecting the matrix entries. If we directly insert data into a compressed column data structure, there is a considerable overhead for reorganization of the long arrays describing the matrix.