HiperLife Tutorial: PoissonSurfaceNeumann

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₁ 1 Introduction

2 1.1 Problem Definition

- The Poisson equation is the canonical elliptic PDE. For a domain $\Omega \subset \mathbb{R}^n$ with boundary $\partial\Omega$, the Poisson
- 4 equation is like:

$$-\Delta U = f \quad \text{in } \Omega$$

$$\nabla U \cdot n = g \quad \text{on } \partial \Omega$$
(1)

- Here, f and g are input data which in this case we assume that f = 1 and $g = x_2 \cos(3\pi x_1)$, and n denotes the
- 6 normal vector of boundary.

7 1.2 Boundary Condition

We have used Neumann Condition along the lines $x_2 = 0$, and $x_2 = 1$, as depicted in Figure 1.

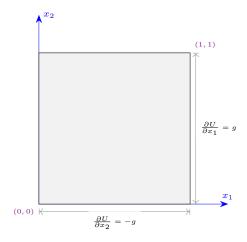


Figure 1: Illustration of Geometry in $\Omega = [0,1] \times [0,1]$ and Boundary conditions on $\partial\Omega$.

⁹ 2 Formulation

10 2.1 Weak Form

To establish the weak form of Eq. (1), it is multiplied with a weight-function, $w(x_1, x_2)$ to obtain

$$-w\nabla^2 U = wf \quad \text{in } \Omega$$

$$w\nabla U \cdot n = wg \quad \text{on } \partial\Omega$$
 (2)

By integrating this expression over Ω , we have

$$-\int_{\Omega} w \nabla^2 U = \int_{\Omega} w f \tag{3}$$

We know from calculus that $\nabla(w\nabla U) = \nabla w \cdot \nabla U + w\nabla^2 U$. So we can write

$$-\int_{\Omega} w \nabla^2 U = \int_{\Omega} \nabla w \cdot \nabla U - \int_{\Omega} \nabla (w \nabla U) \tag{4}$$

14 according to Gauss's theorem

$$\int_{\Omega} \nabla(w\nabla U)dA = \int_{\delta\Omega} w\nabla U \cdot ndS \tag{5}$$

by applying Eq. (5) to Eq. (4)

$$-\int_{\Omega} w \nabla^2 U = \int_{\Omega} \nabla w \cdot \nabla U - \int_{\delta\Omega} w \nabla U \cdot n dS \tag{6}$$

the right-hand side of the Eq. (5) is the second part of Eq. (2), So now we can rewrite the Eq. (4) like this

$$\int_{\Omega} \nabla w \cdot \nabla U dA = \int_{\Omega} w f dA + \int_{\partial \Omega} w g dS \tag{7}$$

17 2.2 Basis Function

We need to define basis functions for our 2D-domain and by it we can give an approximation of U.

$$U(x,y) = \sum_{i=1}^{n} u_i \phi_i(x_1, x_2)$$
 (8)

by applying Galerkin method the weight function is the same as basis function.

$$w_i = \phi_i \tag{9}$$

in isoparametric concept even geometry is interpolated by same function. so

$$X(x_1, x_2) = \sum_{i=1}^{n} x_i \phi_i(x_1, x_2)$$
(10)

21 2.3 Element

22 Triangular Element is used for discretization of bulk in this example, as shown in Fig. 2a,

The quadratic element consists of 9 nodes would have interpolation functions for geometry and field variables like this. Let $\phi_I = N_I$ at element T.

$$N_{1}(\xi, \eta) = \xi(2\xi - 1) \qquad N_{2}(\xi, \eta) = 4\xi(1 - \xi - \eta)$$

$$N_{3}(\xi, \eta) = (1 - \xi - \eta)(1 - 2\xi - 2\eta) \qquad N_{4}(\xi, \eta) = 4\xi\eta$$

$$N_{5}(\xi, \eta) = 4\eta(1 - \xi - \eta) \qquad N_{6}(\xi, \eta) = \eta(2\eta - 1)$$
(11)

For the purpose of discretization of the boder in this example, 3-node line element is used, as shown in Fig. 2b. which its interpolation functions would be like this.

$$N_1(\xi,\eta) = \frac{1}{2}\xi(\xi-1) \quad N_2(\xi,\eta) = 4\xi(1-\xi^2) \quad N_3(\xi,\eta) = \frac{1}{2}\xi(\xi+1)$$
 (12)

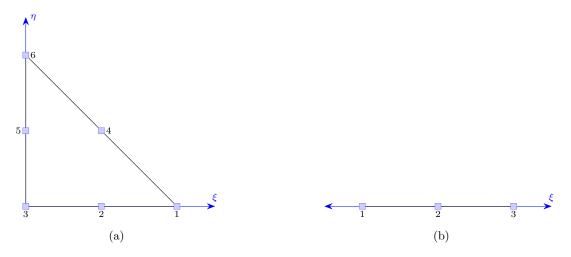


Figure 2: Schematic of the (a) bulk element (b) border element

27 2.4 Elemental Integral

We want to compute the integral at Eq. (7) over the element T

$$\int_{\Omega_T} \left(\frac{\partial N}{\partial x_1} \frac{\partial N}{\partial x_1} + \frac{\partial N}{\partial x_2} \frac{\partial N}{\partial x_2} \right) U dA = \int_{\Omega_T} N f dA + \int_{\partial \Omega} N g dS \tag{13}$$

by the linear mapping between (ξ, η) and (x_1, x_2) , we can define $\frac{\partial N}{\partial x_1}$ and $\frac{\partial N}{\partial x_2}$

$$\frac{\partial N}{\partial \xi} = \frac{\partial N}{\partial x_1} \frac{\partial x_1}{\partial \xi} + \frac{\partial N}{\partial x_2} \frac{\partial x_2}{\partial \eta}
\frac{\partial N}{\partial \eta} = \frac{\partial N}{\partial x_1} \frac{\partial x_1}{\partial \xi} + \frac{\partial N}{\partial x_2} \frac{\partial x_2}{\partial \eta}$$
(14)

Since $x = x(\xi, \eta)$, we get

$$\begin{bmatrix} dx_1 \\ dx_2 \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial \xi} & \frac{\partial x_2}{\partial \xi} \\ \frac{\partial x_1}{\partial \eta} & \frac{\partial x_2}{\partial \eta} \end{bmatrix} \begin{bmatrix} d\xi \\ d\eta \end{bmatrix}$$
(15)

31 by defining Jacobian as

$$J = \begin{bmatrix} \frac{\partial x_1}{\partial \xi} & \frac{\partial x_2}{\partial \xi} \\ \frac{\partial x_1}{\partial x} & \frac{\partial x_2}{\partial x} \end{bmatrix}$$
 (16)

so we can rewrite the Eq. (13)

$$\begin{bmatrix} \frac{\partial N}{\partial x_1} \\ \frac{\partial N}{\partial x_2} \end{bmatrix} = J^{-1} \begin{bmatrix} \frac{\partial N}{\partial \xi} \\ \frac{\partial N}{\partial x} \end{bmatrix} \tag{17}$$

by obtaining the terms Eq. (12) now we can calculate the integral. So the elements of tangent matrix K could

34 be defined as

$$K(i,j) = \int_{\Omega_T} \left(\frac{\partial N_i}{\partial x_1} \frac{\partial N_j}{\partial x_1} + \frac{\partial N_i}{\partial x_2} \frac{\partial N_j}{\partial x_2}\right) dA \tag{18}$$

35 and for right-hand side

$$F(i) = \int_{\Omega_T} N_i^{bulk} f dA + \int_{\partial \Omega} N_i^{border} g dS$$
 (19)

Note that as it discussed earlier, different types of elements is used for bulk and border. At last we define j as j = det(J) because $dA = dx_1 \times dx_2 = jd\xi d\eta$.

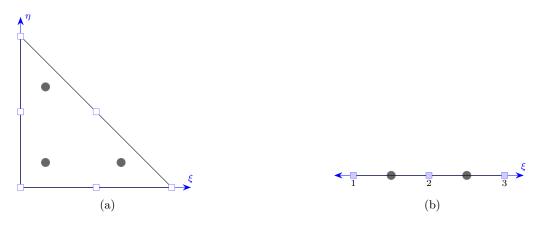


Figure 3: (a) 2-D integration on Triangle element (b) 1-D integration on line element

38 2.5 Integration method

Let $f(\xi_i, \eta_i) = j(\frac{\partial N_i}{\partial x_1} \frac{\partial N_j}{\partial x_1} + \frac{\partial N_i}{\partial x_2} \frac{\partial N_j}{\partial x_2})$, then by Gauss–Legendre quadrature we have

$$\int_{-1}^{1} \int_{-1}^{1} f(\xi_i, \eta_i) d\xi d\eta = \sum_{k=1}^{n} \sum_{l=1}^{m} \omega_k \omega_l f(\hat{\xi}_i, \hat{\eta}_i)$$
 (20)

where n and m are the number of integration points used in each direction, ω is quadrature weights, $\hat{\xi_i}$ and $\hat{\eta_i}$ are the roots of the nth Legendre polynomial. In this example we use 3 points integration as it shown in Fig. 3a. $[W_p = \{\frac{1}{6}, \frac{1}{6}, \frac{1}{6}\}, (\xi_p, \eta_p) = \{(\frac{1}{6}, \frac{1}{6}), (\frac{1}{6}, \frac{2}{3}), (\frac{2}{3}, \frac{1}{6})\}]$. At the border we use 2 points integration as it shown in Fig. 3b. $[W_p = 1, \xi_p = \mp \frac{1}{\sqrt{3}}]$

44 3 Implementation

In this section, we present implementation of our solution in the Hiperlife.

46 3.1 Headers

```
#include <iostream>
#include <fstream>
#include "hl_Core.h"

#include "hl_ParamStructure.h"

#include "hl_Parser.h"

#include "hl_TypeDefs.h"

#include "hl_MeshLoader.h"

#include "hl_StructMeshGenerator.h"

#include "hl_DistributedMesh.h"

#include "hl-FillStructure.h"

#include "hl-FillStructure.h"

#include "hl-FillStructure.h"

#include "hl-FillStructure.h"

#include "hl-DoFsHandler.h"

#include "hl-JoofsHandler.h"

#include "hl-JoofsHandler.h"
```

1 3.2 Parameters

```
68
69
               enum StringParameters
70
71
                           filemesh
                };
72
73
               HL_PARAMETER_LIST Default Values {
74
                           {"filemesh", ""},
{"strength", 1.0},
75
76
                };
77
    };
78
```

3.3 Initializing

```
void LS(hiperlife::FillStructure& fillStr);
void RHS_Border(hiperlife::FillStructure& fillStr);

int main(int argc, char** argv)
{
    using namespace std;
    using namespace hiperlife;
```

3.4 Defining parameters of the model

SmartPtr<ParamStructure> paramStr = ReadParamsFromCommandLine<PoissonParams>();

89 3.5 Mesh Generation

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```
SmartPtr<StructMeshGenerator> mesh = Create<StructMeshGenerator>();
mesh->setElemType(ElemType::Triang);
mesh->setBasisFuncType(BasisFuncType::Lagrangian);
mesh->setBasisFuncOrder(2);
mesh->genSquare(4,1.0);
```

5 3.6 Mesh Distribution

```
SmartPtr<DistributedMesh> disMesh = Create<DistributedMesh>();
disMesh->setMesh(mesh);
disMesh->setBalanceMesh(true);
disMesh->Update();
```

3.7 DOFs Handler

```
SmartPtr<DOFsHandler> dofHand = Create<DOFsHandler>(disMesh);
dofHand->setNameTag("dofHand");
dofHand->setNumDOFs(1);
dofHand->setNumElemAuxF(1);
dofHand->Update();
```

3.8 Boundary conditions and Constraints

3.9 HiperProblem

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152

```
SmartPtr<HiPerProblem> hiperProbl = Create<HiPerProblem>();
123
124
            hiperProbl->setParameterStructure(paramStr);
125
            hiperProbl->setDOFsHandlers({dofHand});
126
127
            hiperProbl->setIntegration("Integ", {"dofHand"});
128
            hiperProbl->setCubatureGauss("Integ",3);
129
            hiperProbl->setElementFillings("Integ", LS);
130
131
            hiperProbl->setIntegration("BorderInteg", {"dofHand"});
132
            hiperProbl->setCubatureBorderGauss("BorderInteg", 2, {MAxis::Xmax, MAxis::Ymin});
133
            hiperProbl->setElementFillings("BorderInteg", nullptr, nullptr, RHS_Border);
134
135
            hiperProbl->setGlobalIntegrals({"BorderLength"});
136
137
            hiperProbl->Update();
138
```

3.10 Solver Settings

```
SmartPtr<AztecOOIterativeLinearSolver> solver=Create<AztecOOIterativeLinearSolver>();
140
             solver->setHiPerProblem(hiperProbl);
141
             solver->setTolerance(1.E-8);
142
             solver -\!\!> \!set MaxNum Iterations \, (500) \, ;
143
             solver -> setSolver (AztecOOIterativeLinearSolver :: Solver :: Gmres);
144
145
             solver -> set Preconditioner (Aztec O O I terative Linear Solver :: Preconditioner :: Neumann);
             solver->setDefaultParameters();
146
             solver -> setVerbosity (AztecOOIterativeLinearSolver :: Verbosity :: High);
147
148
             solver->Update();
149
             solver->solve();
150
             solver -> UpdateSolution();
151
```

3.11 Finalization and Postprocessing

```
dofHand->printFileLegacyVtk("PoissonSurface");
153
154
155
             if (dofHand \rightarrow myRank() = 0)
             cout << std::scientific << std::setprecision(5) << "Border-Length == " << endl;
156
             cout<<hiperProbl->globalIntegral("BorderLength")<<endl;</pre>
157
158
             ofstream rhsFile;
159
             rhsFile.open(paramStr->getStringParameter(PoissonParams::filemesh)+
160
              to_string(dofHand->myRank())+".txt");
161
             hiperProbl->sol->Print(rhsFile);
162
             rhsFile.close();
163
164
              hiperlife :: Finalize ();
165
             return 0;
166
167
```

3.12 Filling left-hand side matrix

```
void LS(hiperlife::FillStructure& fillStr)
169
170
171
             using namespace std;
             using namespace hiperlife;
172
             using hiperlife::Tensor::tensor;
173
174
             double strength = fillStr.getRealParameter(PoissonParams::strength);
175
176
             SubFillStructure& subFill = fillStr["dofHand"];
177
             int DOF = subFill.numDOFs;
178
             int eNN = subFill.eNN;
179
             int nDim = subFill.nDim;
180
             int pDim = subFill.pDim;
181
             vector<double>& nborCoords = subFill.nborCoords;
182
183
             double* bf = subFill.nborBFs();
184
             double* dbf_l = subFill.nborBFsGrads();
185
             double x[3] = \{\};
186
             for (int i = 0; i < eNN; i++) // i from 0 to 5
187
188
                      for (int n = 0; n < nDim; n++) // n from 0 to 2
189
190
                               x[n] += nborCoords[i*nDim+n] * bf[i];
191
192
193
             }
194
             double g_cc[4] = \{\};
195
             double xu[3] = \{\};
196
             double xv[3] = \{\};
197
             SurfLagrParam:: MetricTensor(g_cc, xu, xv, eNN, nborCoords.data(), dbf_l);
198
199
             double g_CC[4] = \{\};
200
             Math::Invert2x2(g_CC, g_cc);
201
             double jac = sqrt (Math::DetMat2x2(g_cc));
203
204
             double source = strength * x[1]*cos(3.0*M_PI*x[0]);
205
206
             for (int i = 0; i < eNN; i++)
207
208
                      double* dbf_lI_c = &dbf_l[pDim*i];
210
                      double dbf_1I_C[2] = \{\};
211
                      Math:: MatProduct(dbf_II_C, 2, 2, 1, g_CC, dbf_II_c);
212
213
214
                      for (int j = 0; j < eNN; j++)
215
                               double* dbf_lJ_c = \&dbf_l[pDim*j];
216
217
                               fillStr.Ak(0,0)[i*DOF*eNN+j*DOF] += jac*Math::Dot2D(dbf_lI_C,dbf_lJ_c);
218
219
220
                      fillStr.Bk(0)[i*DOF] += jac * bf[i] * source;
221
222
             }
223
224
             return;
225
```

3.13 Filling right-hand side vector

```
using hiperlife::Tensor::tensor;
231
232
                SubFillStructure& subFill = fillStr["dofHand"];
233
234
               int DOF = subFill.numDOFs;
               int eNN = subFill.eNN;
235
               int nDim = subFill.nDim;
236
                {\tt vector}{<} \textbf{double}{>} \& \ {\tt nborCoords} \ = \ {\tt subFill.nborCoords} \ ;
237
               double *bf = subFill.nborBFs();
238
               double *dbf_l = subFill.nborBFsGrads();
240
                \mathbf{double} \ \mathrm{Ip}\left[4\right], \ \mathrm{xu}\left[3\right], \ \mathrm{xv}\left[3\right];
241
               SurfLagrParam:: MetricTensor(Ip\,,\ xu\,,\ xv\,,\ eNN,\ nborCoords.data()\,,\ dbf\_l\,);
242
243
               auto bTangentRef = subFill.tangentsBoundaryRef();
               double bTangent[3] = \{\};
245
                for (int n = 0; n < nDim; n++)
246
                bTangent[n] \ = \ bTangentRef[0] \ * \ xu[n] \ + \ bTangentRef[1]*xv[n];
247
               double jac = Math::Norm3D(bTangent);
248
249
                \quad \mathbf{for} \ (\mathbf{int} \ i \ = \ 0\,; \ i \ < \ \mathrm{eNN}\,; \ i + +)
250
                fillStr.Bk(0)[i*DOF] += jac*bf[i];
251
252
                fillStr.addToGlobalIntegral("BorderLength", jac);
253
254
```

55 4 Results