Introduction to Netgen-NGSolve with Python Getting started with C++ coding

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Schedule for today



- Introduction into C++ coding with NGSolve
- Run time evaluation vs. Code generation
- Shared memory parallelization
- Distributed memory parallelization



• Guest Lectures

Overview C++ Introduction



- How to build NGSolve extensions
- My Little NGSolve: create your own...
 - Finite Elements
 - DifferentialOperators
 - Finite Element Spaces
 - Integrators
- Some useful concepts: AutoDiff, IterateElements,...
- Create utility functions for performance critical operations
- Use NGSolve in a C++ only environment

How to build a NGSolve extension



- CMake: Easy, platform independent
- Export your classes and functions to Python



CMake makes setting up a new project with NGSolve easy: You need to provide a file CMakeLists.txt with:

This works for Linux, Windows and Mac!

If you want your package to be installable we recommend additionally:

```
# check if CMAKE_INSTALL_PREFIX is set by user, if not install in NGSolve python dir
if(CMAKE_INSTALL_PREFIX_INITIALIZED_TO_DEFAULT)
set(CMAKE_INSTALL_PREFIX ${NGSOLVE_INSTALL_DIR}/${NGSOLVE_INSTALL_DIR_PYTHON} CACHE
PATH "Install dir" FORCE)
endif(CMAKE_INSTALL_PREFIX_INITIALIZED_TO_DEFAULT)
install(TARGETS myngspy DESTINATION .)
```

Exporting to Python



There must be one .cpp file with the macro PYBIND11_PLUGIN. In this macro we define all our exported classes/functions

```
namespace py=pybind11;
PYBIND11_PLUGIN(myngspy) {
   py::module m("myngspy", "myngspy documentation string");
   ...
   return m.ptr();
}
```

Exporting Functions



If the arguments and the return value can be directly converted:

```
m.def("SomeFunction", &SomeCppFunction, "documentation");
```

Else:

Methods of classes are defined the same way.

Overload functions just by defining multiple versions.



Short constructor, arguments can be parsed into the c++ constructor:

No trivial constructor:

CAVE: Some NGSolve classes have creator functions and do not need to (but still can) export a constructor (i.e. FESpace)

MyLittleNGSolve



- Tutorial project for C++ programming with NGSolve
- 3 Sections:
 - Basic: How to create your own elements, spaces,... compiles into a python module, installs to CMAKE_INSTALL_PREFIX (default NGSolve python dir)
 - Advanced: Some further examples. Compile into local python module (cmake . && make)
 - Legacy: Old MyLittleNGS code, not maintained



Standard

Array, Table, Autodiff,...

Basic Linear Algebra

matrix, vector,...

Linear Algebra

direct solvers, iterative solvers, ...

Local: finite element, integrators (ngfem)

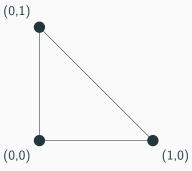
Global: spaces, (bi)linearforms (ngcomp)

Python Interface

Linear 'Hat' Finite Elements



Reference element:



Hat functions on reference element:

$$\varphi_1 = x$$

$$\varphi_2 = y$$

$$\varphi_3 = 1 - x - y$$



These functions calculate point evaluation of the shape functions and their derivatives on the reference domain.

CalcShape & CalcDShape



```
void MyLinearTrig :: CalcShape
  (const IntegrationPoint & ip,
    BareSliceVector<> shape) const
{
    double x = ip(0);
    double y = ip(1);
    shape(0) = x;
    shape(1) = y;
    shape(2) = 1-x-y;
}
```

```
void MyLinearTrig :: CalcDShape
  (const IntegrationPoint & ip,
    SliceMatrix <> dshape)
    const
{
    dshape(0,0) = 1;
    dshape(0,1) = 0;
    dshape(1,0) = 0;
    dshape(1,1) = 1;
    dshape(2,0) = -1;
    dshape(2,1) = -1;
}
```



```
class MyFESpace : public FESpace
 int ndof. nvert:
public:
  MyFESpace (shared ptr < MeshAccess > ama, const Flags & flags);
 // calculate number of dofs
 virtual void Update(LocalHeap & lh);
  virtual size t GetNDof () const { return ndof; }
 // return dofs of element ei in dnums arrav
  virtual void GetDofNrs (ElementId ei, Array OofId > & dnums) const;
 // return finite element ei allocated on alloc
  virtual FiniteElement & GetFE (ElementId ei.
                                 Allocator & alloc) const;
 // some new functionality our space should have in Python
 int GetNVert() { return nvert: }
};
```



```
MyFESpace :: MyFESpace (const MeshAccess & ama,
 const Flags & flags) : FESpace (ama, flags)
 evaluator[VOL] =
      make_shared < T_DifferentialOperator < DiffOpId <2>>>();
 flux evaluator[VOL] =
      make shared < T DifferentialOperator < DiffOpGradient < 2>>>():
  evaluator[BND] =
      make shared < T DifferentialOperator < DiffOpIdBoundary < 2>>>();
 // (still) needed to draw solution. SetValues
 integrator[VOL] =
      GetIntegrators().CreateBFI("mass", ma->GetDimension(),
        make shared < Constant Coefficient Function > (1));
void MyFESpace :: Update(LocalHeap & lh)
 ndof = ma.GetNV(); // number of vertices
 nvert = ndof:
```



```
FiniteElement & MyFESpace :: GetFE (ElementId ei,
                    Allocator & alloc) const
 if (ei.IsVolume())
   return * new (alloc) MyLinearTrig;
 else
   return * new (alloc) FE_Segm1;
void MyFESpace :: GetDofNrs (ElementId ei,
                Array < DofId > & dnums) const
 // returns dofs of element ei
 // may be a volume triangle or boundary segment
 dnums.SetSize(0):
 // first dofs are vertex numbers:
 for (auto v : ma->GetElVertices(ei))
   dnums.Append (v);
```



- Allocator Base class calls new to allocate object
- LocalHeap Optimized memory handler:
 - Calls new for a memory block with predefined size
 - Overloaded new operator with efficient allocation on block
 - HeapReset to reset pointer to stored position ⇒ free memory





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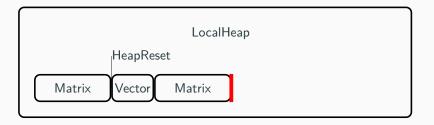


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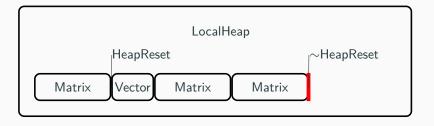


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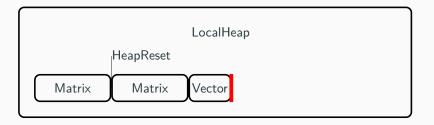


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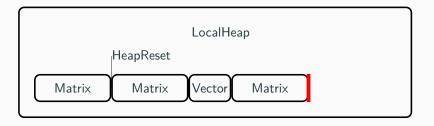


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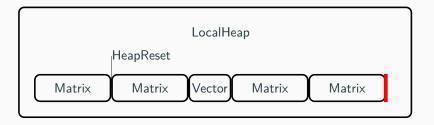


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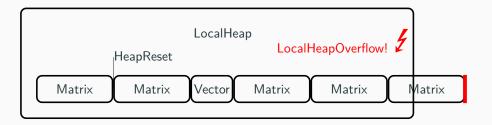


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FESpace constructor converts kwargs to Flags

 \Rightarrow use FESpace constructor and don't write your own Python __init__

For this we need to register the FESpace in NGSolve

```
static RegisterFESpace<MyFESpace> initifes ("myfespace");
```

If we want additional functionality: export without constructor

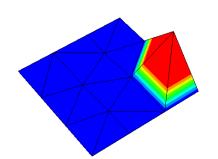
```
py::class_<MyFESpace, shared_ptr<MyFESpace>, FESpace>
(m, "MyFESpace", "FESpace with first order trigs on 2d mesh")
// export some additional function
.def("GetNVert", &MyFESpace::GetNVert)
;
```

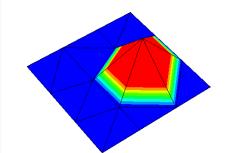
Shapetester



```
mesh = Mesh(unit_square.GenerateMesh(maxh=0.2))
fes = FESpace("myfespace", mesh)
u = GridFunction(fes,"shapes")
Draw(u)

# we can use the additionally exported function here
for i in range(fes.GetNVert()):
    print("Draw basis function ", i)
    u.vec[:] = 0
    u.vec[i] = 1
    Redraw()
    input("press key to draw next shape function")
```







 ${\sf Differential Operator}$

 $T_Differential Operator$

DiffOp

Your Diff Op



 ${\sf Differential Operator}$

 $T_DifferentialOperator$

?

DiffOp

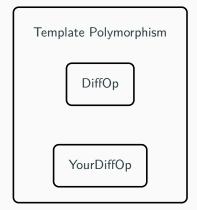
Your Diff Op



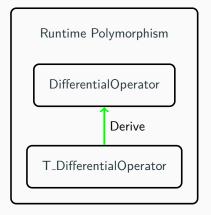
Runtime Polymorphism

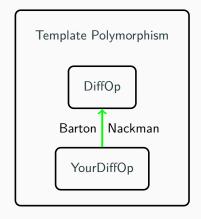
 ${\sf Differential Operator}$

 $T_DifferentialOperator$

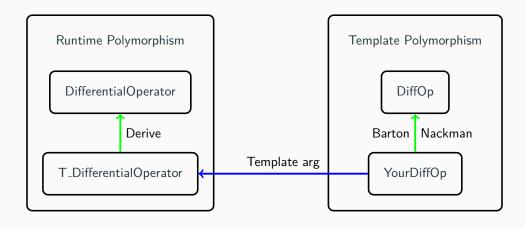




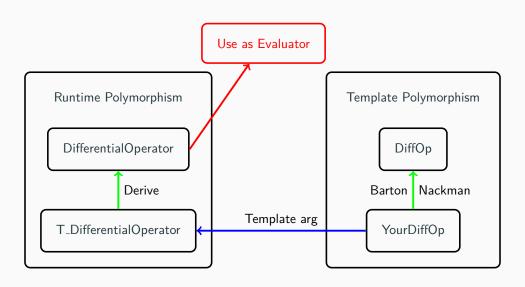














```
class MyIdentity : public DiffOp < MyIdentity >
public:
  enum { DIM = 1 };
  enum { DIM SPACE = 2 }:
  enum { DIM_ELEMENT = 2 };
  enum { DIM DMAT = 1 }:
  enum { DIFFORDER = 0 };
  template <typename FEL, typename MIP, typename MAT>
  static void GenerateMatrix (const FEL & fel, const MIP & mip,
                  MAT && mat, LocalHeap & lh)
    HeapReset hr(1h):
    mat.Row(0) = static_cast < const ScalarFiniteElement < 2 > & > (fel).GetShape(mip.IP(), lh);
};
```



Add GetAdditionalEvaluators to MyFESpace

```
virtual SymbolTable<shared_ptr<DifferentialOperator>> GetAdditionalEvaluators () const
    override
{
    SymbolTable<shared_ptr<DifferentialOperator>> additional;
    additional.Set ("myId", make_shared<T_DifferentialOperator<MyIdentity>>());
    return additional;
}
```

From Python we can call it on ProxyFunctions and GridFunctions

```
u,v = fes.TrialFunction(), fes.TestFunction()
a += SymbolicBFI(u.Operator("myId")*v.Operator("myId"))
gfu = GridFunction(fes)
Draw(gfu.Operator("myId"),mesh,"myId")
```



$$\int_{\Omega} \lambda \nabla u \nabla v \, dx$$

```
class MyLaplaceIntegrator : public BilinearFormIntegrator
  shared_ptr<CoefficientFunction> coef_lambda;
public:
  MyLaplaceIntegrator(shared ptr < CoefficientFunction > coeffs)
  : coef lambda(coef) { : }
  virtual bool IsSymmetric () const { return true; }
  virtual VorB VB() const { return VOL; }
  virtual void
  CalcElementMatrix (const FiniteElement & fel.
              const ElementTransformation & eltrans.
              FlatMatrix < double > elmat,
              LocalHeap & 1h) const;
};
```



```
void MyLaplaceIntegrator ::
CalcElementMatrix (const FiniteElement & base fel,
            const ElementTransformation & eltrans.
            FlatMatrix < double > elmat.
            LocalHeap & lh) const
 const ScalarFiniteElement<2> & fel =
   dynamic_cast < const ScalarFiniteElement < 2 > & > (base_fel);
 int ndof = fel.GetNDof():
 elmat = 0:
 Matrix <> dshape ref(ndof, 2);
 Matrix <> dshape(ndof, 2);
 IntegrationRule ir(fel.ElementType(), 2*fel.Order());
 for (int i = 0 ; i < ir.GetNIP(); i++)</pre>
      MappedIntegrationPoint < 2,2 > mip(ir[i], eltrans);
      double lam = coef lambda -> Evaluate (mip):
      fel.CalcDShape (ir[i], dshape_ref);
      dshape = dshape ref * mip.GetJacobianInverse();
      double fac = mip.IP().Weight() * mip.GetMeasure();
      elmat += (fac*lam) * dshape * Trans(dshape);
```



$$\int_{\Omega} f v \, dx$$



```
void MySourceIntegrator ::
CalcElementVector (const FiniteElement & base fel.
            const ElementTransformation & eltrans.
            FlatVector < double > elvec.
            LocalHeap & lh) const
 const ScalarFiniteElement<2> & fel =
   dynamic_cast < const ScalarFiniteElement < 2 > & > (base_fel);
 int ndof = fel.GetNDof();
 elvec = 0;
 Vector <> shape(ndof);
 IntegrationRule ir(fel.ElementType(), 2*fel.Order());
 for (int i = 0 ; i < ir.GetNIP(); i++)</pre>
      MappedIntegrationPoint <2,2> mip(ir[i], eltrans);
      double f = coef f -> Evaluate (mip):
      fel.CalcShape (ir[i], shape);
      double fac = mip.IP().Weight() * mip.GetMeasure();
      elvec += (fac*f) * shape;
```

Exporting Integrators





```
from netgen.geom2d import unit_square
from ngsolve import *
from myngspy import *
mesh = Mesh(unit_square.GenerateMesh(maxh=0.2))
fes = FESpace("myfespace", mesh, dirichlet="top|bottom|right|left")
u.v = fes.TrialFunction(), fes.TestFunction()
a = BilinearForm(fes)
a += MyLaplace(CoefficientFunction(1))
f = LinearForm(fes)
f += MySource(x*y)
a. Assemble()
f.Assemble()
u = GridFunction(fes)
u.vec.data = a.mat.Inverse(fes.FreeDofs()) * f.vec
Draw(u)
```



```
mesh = Mesh(unit square.GenerateMesh(maxh=0.1))
for i in range(6):
   mesh.Refine()
fes = H1(mesh, order=1)
print("ndof = ", fes.ndof)
timing={}
integrators = {"MyLaplace" : MyLaplace(CoefficientFunction(1)),
          "Symbolic": SymbolicBFI(grad(fes.TrialFunction())*grad(fes.TestFunction()))}
for name, integrator in integrators.items():
    start = time()
   with TaskManager():
        a = BilinearForm(fes)
        a += integrator
        a. Assemble()
    timing[name] = time()-start
for name, value in timing.items():
    print(name, " needed ", value, " seconds for assembling")
```



```
class MyHighOrderTrig : public ScalarFiniteElement <2>,
                        public VertexOrientedFE < ET_TRIG >
public:
 // ScalarFE with (order+1)*(order+2)/2 ndofs and order 'order'
  MvHighOrderTrig (int order)
  : ScalarFiniteElement <2> ((order+1)*(order+2)/2, order) { : }
  virtual ELEMENT_TYPE ElementType() const { return ET_TRIG; }
  virtual void CalcShape (const IntegrationPoint & ip,
              BareSliceVector<> shape) const;
  virtual void CalcDShape (const IntegrationPoint & ip,
                SliceMatrix <> dshape) const;
private:
  template <class T>
  void T_CalcShape (const T & x, const T & y,
                    BareSliceVector <T> shape) const;
};
```

T_CalcShape



```
template <class T>
void MyHighOrderTrig :: T_CalcShape (const T & x, const T & y,
                              BareSliceVector <T> shape) const {
 T lami[3] = { x, y, 1-x-y };
 for (int i = 0; i < 3; i++) shape[i] = lami[i];</pre>
 int ii = 3:
 ArrayMem < T. 20 > polx(order+1), poly(order+1);
 for (int i = 0; i < 3; i++)
   if (order >= 2) {
   auto edge = GetVertexOrientedEdge(i);
    ScaledIntegratedLegendrePolynomial (order,
               lami[edge[1]]-lami[edge[0]],
               lami[edge[0]]+lami[edge[1]], polx);
   for (int j = 2; j <= order; j++)</pre>
      shape[ii++] = polx[i]:
 if (order >= 3) {
      T bub = x * y * (1-x-y);
      ScaledLegendrePolynomial(order-2, lami[1]-lami[0],
                   lami[1]+lami[0], polx);
      LegendrePolynomial (order-1, 2*lami[2]-1, poly);
      for (int i = 0; i <= order-3; i++)</pre>
   for (int j = 0; j \le order - 3 - i; j + +)
      shape[ii++] = bub * polx[i] * poly[j];
```



- Class supporting automatic differentiation
- instance knows it's value and derivative
- \bullet Algebraic operations are overloaded using product-rule, \dots

```
// AutoDiff with 2 dim derivative, value is 3,
// derivative is 0-th unit vector
AutoDiff<2> x (3.0, 0);
```



```
void MyHighOrderTrig :: CalcShape (const IntegrationPoint & ip,
                    BareSliceVector<> shape) const
 double x = ip(0);
 double y = ip(1);
 T_CalcShape (x, y, shape);
void MyHighOrderTrig :: CalcDShape (const IntegrationPoint & ip,
                    SliceMatrix <> dshape) const
 AutoDiff <2> adx (ip(0), 0);
 AutoDiff <2> adv (ip(1), 1);
 Vector < AutoDiff < 2> > shapearray(ndof);
 T CalcShape < AutoDiff < 2>> (adx, ady, shapearray);
 for (int i = 0: i < ndof: i++)</pre>
      dshape(i, 0) = shapearray[i].DValue(0);
      dshape(i, 1) = shapearray[i].DValue(1);
```



```
class MyHighOrderFESpace : public FESpace
 int order;
 int ndof;
  Array<int> first_edge_dof;
  Array<int> first_cell_dof;
public:
  MyHighOrderFESpace (shared_ptr < MeshAccess > ama,
                      const Flags & flags);
  virtual void Update(LocalHeap & lh);
  virtual size t GetNDof () const { return ndof; }
  virtual void GetDofNrs (ElementId ei, Array < DofId > & dnums) const;
  virtual FiniteElement & GetFE (ElementId ei,
                                  Allocator & alloc) const;
};
```



```
void MyHighOrderFESpace :: Update(LocalHeap & lh)
  int n_vert = ma->GetNV();
 int n_edge = ma->GetNEdges();
 int n cell = ma->GetNE();
 first_edge_dof.SetSize (n_edge+1);
 int ii = n vert;
 for (int i = 0; i < n_edge; i++, ii+=order-1)</pre>
   first_edge_dof[i] = ii;
 first_edge_dof[n_edge] = ii;
 first cell dof.SetSize (n cell+1);
 for (int i = 0; i < n cell; i++, ii+=(order-1)*(order-2)/2)
   first cell dof[i] = ii:
 first_cell_dof[n_cell] = ii;
 ndof = ii;
```



```
void MyHighOrderFESpace :: GetDofNrs (ElementId ei,
                  Array < DofId > & dnums) const
 dnums.SetSize(0):
 Ngs_Element ngel = ma->GetElement (ei);
 // vertex dofs
 for (auto v : ngel.Vertices())
   dnums.Append(v);
 // edge dofs
 for (auto e : ngel.Edges())
     int first = first_edge_dof[e];
     int next = first edge dof[e+1];
     for (int j = first; j < next; j++)
       dnums.Append (j);
 // cell dofs
 if (ei.IsVolume())
     int first = first_cell_dof[ei.Nr()];
      int next = first_cell_dof[ei.Nr()+1];
     for (int j = first; j < next; j++)
       dnums.Append (j);
```



```
FiniteElement & MyHighOrderFESpace :: GetFE (ElementId ei,
                               Allocator & alloc) const
 Ngs Element ngel = ma->GetElement (ei);
  switch (ngel.GetType())
   case ET TRIG:
   MyHighOrderTrig * trig = new (alloc) MyHighOrderTrig(order);
   trig->SetVertexNumbers (ngel.vertices);
   return *trig;
    case ET_SEGM:
   MyHighOrderSegm * segm = new (alloc) MyHighOrderSegm(order);
   segm -> SetVertexNumbers (ngel.vertices);
   return *segm;
   default:
      throw Exception (string("Element type ")+
              ToString(ngel.GetType())+" not supported");
```



```
from netgen.geom2d import unit_square
from ngsolve import *
from myngspy import *
mesh = Mesh(unit_square.GenerateMesh(maxh=0.2))
fes = FESpace("myhofespace", mesh, dirichlet="top|bottom|right|left", order = 5)
u.v = fes.TrialFunction(), fes.TestFunction()
a = BilinearForm(fes)
a += MyLaplace(CoefficientFunction(1))
f = LinearForm(fes)
f += MySource(x*y)
a.Assemble()
f.Assemble()
u = GridFunction(fes)
u.vec.data = a.mat.Inverse(fes.FreeDofs()) * f.vec
Draw(u)
```



```
#include <solve.hpp>
using namespace ngsolve;
int main(int argc, char** argv)
  auto ma = make shared < MeshAccess > ("square.vol");
  Flags flags fes:
  flags fes.SetFlag ("order", 4):
  auto fes = make shared < H1HighOrderFESpace > (ma, flags fes);
  Flags flags gfu;
  auto gfu = make shared < T GridFunction < double >> (fes, "u",
                                                      flags gfu):
  Flags flags bfa:
  auto bfa = make shared < T BilinearFormSymmetric < double >> (fes,
                                                      "a", flags bfa);
  shared ptr <BilinearFormIntegrator > bfi =
      make_shared < LaplaceIntegrator < 2 >> (
           make_shared < ConstantCoefficientFunction > (1));
  bfa -> AddIntegrator (bfi);
  Array < double > penalty (ma -> Get NBoundaries ());
  penaltv = 0.0:
  penalty[0] = 1e10:
  bfi = make shared < Robin Integrator < 2>> (
          make_shared < Domain Constant Coefficient Function > (penalty));
  bfa -> AddIntegrator (bfi):
```



```
. . .
Flags flags lff:
auto lff = make_shared < T_LinearForm < double >> (fes, "f", flags_lff);
auto lfi = make shared < SourceIntegrator < 2>> (
                 make shared < ConstantCoefficientFunction > (5));
lff -> AddIntegrator (lfi):
LocalHeap lh(100000);
fes -> Update(lh);
fes -> FinalizeUpdate(lh);
gfu -> Update():
bfa -> Assemble(lh):
lff -> Assemble(lh);
const BaseMatrix & mata = bfa -> GetMatrix():
const BaseVector & vecf = lff -> GetVector():
BaseVector & vecu = gfu -> GetVector();
auto inverse = mata.InverseMatrix(fes->GetFreeDofs());
vecu = *inverse * vecf:
cout << "Solution vector = " << endl << vecu << endl;</pre>
return 0;
```



```
shared ptr < GridFunction > MyAssemble (shared ptr < FESpace > fes,
          shared_ptr <BilinearFormIntegrator > bfi,
          shared_ptr <LinearFormIntegrator > 1fi)
  auto ma = fes->GetMeshAccess();
  int ndof = fes->GetNDof():
  int ne = ma->GetNE():
  Array < int > dnums;
  Array < int > cnt(ne);
  for (auto ei : ma->Elements(VOL))
      fes->GetDofNrs (ei. dnums):
      cnt[ei.Nr()] = dnums.Size();
 Table < int > el2dof(cnt):
  for (auto ei : ma->Elements(VOL))
      fes->GetDofNrs (ei, dnums);
      el2dof[ei.Nr()] = dnums;
  auto mat = make_shared < SparseMatrixSymmetric < double >> (ndof,
                                                         el2dof):
  VVector < double > vecf (fes -> GetNDof());
  *mat = 0.0:
  vecf = 0.0:
  . . .
```



```
. . .
LocalHeap lh(100000);
IterateElements(*fes, VOL, lh, [&] (FESpace::Element el,
                                      LocalHeap &lh)
  const ElementTransformation& eltrans = ma->GetTrafo(el,1h);
  const FiniteElement& fel = fes->GetFE(el.lh):
  auto dofs = el.GetDofs():
  FlatMatrix <> elmat(dofs.Size().lh):
  bfi->CalcElementMatrix(fel,eltrans,elmat,lh);
  mat -> AddElementMatrix (dofs, elmat);
  FlatVector <> elvec(dofs.Size().lh):
  lfi->CalcElementVector(fel, eltrans, elvec, lh);
  vecf.AddIndirect(dofs,elvec);
  });
shared ptr <BaseMatrix > inv = mat -> InverseMatrix (fes -> GetFreeDofs()):
Flags gfuFlags;
auto gfu=make shared < T GridFunction < double >> (fes. "u". gfuFlags):
gfu->Update();
gfu -> GetVector() = (*inv) * vecf;
return gfu;
```

Thank you for your attention!