```
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//
     in the file "license.txt" in the top-level Albany directory //
#ifndef HMCPROBLEM_HPP
#define HMCPROBLEM_HPP
#include "Teuchos_RCP.hpp"
#include "Teuchos_ParameterList.hpp"
#include "Albany_AbstractProblem.hpp"
#include "Phalanx.hpp"
#include "PHAL_Workset.hpp"
#include "PHAL_Dimension.hpp"
#include "PHAL_AlbanyTraits.hpp"
This source has been annotated with latex comments. Use the eqcc script to compile into a summary pdf. The source is best viewed using folding in
vim (i.e.,
 :g/\\begin{text}/foldc
namespace Albany {
 /*!
  * \brief Abstract interface for representing a 2-D finite element
  * problem.
  */
                                                      1
```

```
class HMCProblem : public Albany::AbstractProblem {
public:
  //! Default constructor
  HMCProblem(
    const Teuchos::RCP<Teuchos::ParameterList>& params_,
    const Teuchos::RCP<ParamLib>& paramLib_,
    const int numDim_);
  //! Destructor
  virtual ~HMCProblem();
  //! Return number of spatial dimensions
  virtual int spatialDimension() const { return numDim; }
  //! Build the PDE instantiations, boundary conditions, and initial solution
  virtual void buildProblem(
    Teuchos::ArrayRCP<Teuchos::RCP<Albany::MeshSpecsStruct> > meshSpecs,
    StateManager& stateMgr);
  // Build evaluators
  virtual Teuchos::Array< Teuchos::RCP<const PHX::FieldTag> >
  buildEvaluators(
    PHX::FieldManager<PHAL::AlbanyTraits>& fm0,
    const Albany::MeshSpecsStruct& meshSpecs,
   Albany::StateManager& stateMgr,
    Albany::FieldManagerChoice fmchoice,
    const Teuchos::RCP<Teuchos::ParameterList>& responseList);
  //! Each problem must generate it's list of valid parameters
 Teuchos::RCP<const Teuchos::ParameterList> getValidProblemParameters() const;
  void getAllocatedStates(Teuchos::ArrayRCP<Teuchos::RCP<Intrepid::FieldContainer<RealType> > > oldState_,
  Teuchos::ArrayRCP<Teuchos::ArrayRCP<Teuchos::RCP<Intrepid::FieldContainer<RealType>>>> newState_
  ) const;
```

```
private:
  //! Private to prohibit copying
  HMCProblem(const HMCProblem&);
  //! Private to prohibit copying
  HMCProblem& operator=(const HMCProblem&);
public:
  //! Main problem setup routine. Not directly called, but indirectly by following functions
  template <typename EvalT>
  Teuchos::RCP<const PHX::FieldTag>
  constructEvaluators(
    PHX::FieldManager<PHAL::AlbanyTraits>& fm0,
    const Albany::MeshSpecsStruct& meshSpecs,
    Albany::StateManager& stateMgr,
    Albany::FieldManagerChoice fmchoice,
    const Teuchos::RCP<Teuchos::ParameterList>& responseList);
  void constructDirichletEvaluators(const Albany::MeshSpecsStruct& meshSpecs);
  void constructNeumannEvaluators(const Teuchos::RCP<Albany::MeshSpecsStruct>& meshSpecs);
protected:
  //! Boundary conditions on source term
  bool haveSource;
  int numDim;
  std::string matModel;
  Teuchos::RCP<Albany::Layouts> dl;
  Teuchos::ArrayRCP<Teuchos::ArrayRCP<Teuchos::RCP<Intrepid::FieldContainer<RealType>>> oldState;
  Teuchos::ArrayRCP<Teuchos::ArrayRCP<Teuchos::RCP<Intrepid::FieldContainer<RealType>>> newState;
};
```

```
}
#include "Albany_SolutionAverageResponseFunction.hpp"
#include "Albany_SolutionTwoNormResponseFunction.hpp"
#include "Albany_SolutionMaxValueResponseFunction.hpp"
#include "Albany_Utils.hpp"
#include "Albany_ProblemUtils.hpp"
#include "Albany_ResponseUtilities.hpp"
#include "Albany_EvaluatorUtils.hpp"
#include "ElasticModulus.hpp"
#include "PoissonsRatio.hpp"
#include "PHAL_Source.hpp"
#include "Strain.hpp"
#include "DefGrad.hpp"
#include "Stress.hpp"
#include "PHAL_SaveStateField.hpp"
#include "ElasticityResid.hpp"
#include "Time.hpp"
#include "CapExplicit.hpp"
#include "CapImplicit.hpp"
template <typename EvalT>
Teuchos::RCP<const PHX::FieldTag>
Albany::HMCProblem::constructEvaluators(
  PHX::FieldManager<PHAL::AlbanyTraits>& fm0,
  const Albany::MeshSpecsStruct& meshSpecs,
  Albany::StateManager& stateMgr,
  Albany::FieldManagerChoice fieldManagerChoice,
  const Teuchos::RCP<Teuchos::ParameterList>& responseList)
   using Teuchos::RCP;
   using Teuchos::rcp;
   using Teuchos::ParameterList;
```

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```
using PHX::DataLayout;
using PHX::MDALayout;
using std::vector;
using PHAL::AlbanyTraits;
// get the name of the current element block
std::string elementBlockName = meshSpecs.ebName;
RCP<shards::CellTopology> cellType = rcp(new shards::CellTopology (&meshSpecs.ctd));
RCP<Intrepid::Basis<RealType, Intrepid::FieldContainer<RealType>>>
  intrepidBasis = Albany::getIntrepidBasis(meshSpecs.ctd);
const int numNodes = intrepidBasis->getCardinality();
const int worksetSize = meshSpecs.worksetSize;
Intrepid::DefaultCubatureFactory<RealType> cubFactory;
RCP <Intrepid::Cubature<RealType> > cubature = cubFactory.create(*cellType, meshSpecs.cubatureDegree);
const int numDim = cubature->getDimension();
const int numQPts = cubature->getNumPoints();
const int numVertices = cellType->getNodeCount();
*out << "Field Dimensions: Workset=" << worksetSize
     << ", Vertices= " << numVertices
     << ", Nodes= " << numNodes
     << ", QuadPts= " << numQPts
     << ", Dim= " << numDim << std::endl;
// Construct standard FEM evaluators with standard field names
dl = rcp(new Albany::Layouts(worksetSize,numVertices,numNodes,numQPts,numDim));
TEUCHOS_TEST_FOR_EXCEPTION(dl->vectorAndGradientLayoutsAreEquivalent==false, std::logic_error,
                            "Data Layout Usage in Mechanics problems assume vecDim = numDim");
Albany::EvaluatorUtils<EvalT, PHAL::AlbanyTraits> evalUtils(dl);
bool supportsTransient=true;
```

// 1.2 Gather Coordinates

```
// Define Field Names
   Teuchos::ArrayRCP<std::string> dof_names(1);
     dof_names[0] = "Displacement";
   Teuchos::ArrayRCP<std::string> dof_names_dotdot(1);
   if (supportsTransient)
     dof_names_dotdot[0] = dof_names[0]+"_dotdot";
   Teuchos::ArrayRCP<std::string> resid_names(1);
     resid_names[0] = dof_names[0]+" Residual";
// 1.1 Gather Solution
New evaluator: Gather solution data from solver data structures to grid based structures. Note that accelerations are added as an evaluated field if
appropriate.
Dependent Fields:
None.
Evaluated Fields:
     Nodal displacements ("Variable Name", "Displacement")
                                                                 dims(cell,nNodes,vecDim)
                         ("Variable Name", "Displacement_dotdot") dims(cell,nNodes,vecDim)
     Nodal accelerations
For implementation see:
problems/Albany_EvaluatorUtils_Def.hpp
evaluators/PHAL_GatherSolution_Def.hpp
   if (supportsTransient) fm0.template registerEvaluator<EvalT>
       (evalUtils.constructGatherSolutionEvaluator_withAcceleration(true, dof_names, Teuchos::null, dof_names_dotdot));
   else fm0.template registerEvaluator<EvalT>
       (evalUtils.constructGatherSolutionEvaluator_noTransient(true, dof_names));
```

New evaluator: Gather coordinate data from solver data structures to grid based structures. **Dependent Fields:** None.

```
Evaluated Fields:
```

```
x<sub>iI</sub> Nodal coordinates ("Coordinate Vector Name", "Coord Vec") dims(cell,nNodes,vecDim)
```

For implementation see:

 $problems/Albany_EvaluatorUtils_Def.hpp$

evaluators/PHAL_GatherCoordinateVector_Def.hpp

```
fm0.template registerEvaluator<EvalT>
  (evalUtils.constructGatherCoordinateVectorEvaluator());
```

// 2.1 Compute gradient matrix and weighted basis function values in current coordinates

Register new evaluator.

Dependent Fields:

 x_{iI} Nodal coordinates ("Cordinate Vector Name", "Coord Vec") dims(cell,nNodes,vecDim)

Evaluated Fields:

For implementation see:

 $problems/Albany_EvaluatorUtils_Def.hpp$

evaluators/PHAL_ComputeBasisFunctions_Def.hpp

```
fm0.template registerEvaluator<EvalT>
   (evalUtils.constructComputeBasisFunctionsEvaluator(cellType, intrepidBasis, cubature));
```

// 3.1 Project displacements to Gauss points

$$u_i(\xi_p) = N_I(\xi_p)u_{iI}$$

 $(c, p, i) = (c, I, p) * (c, I, i)$

Dependent Fields:

 u_{iI} Nodal Displacements ("Variable Name", "Displacements") dims(cell,nNodes,vecDim) $N_I(\xi_p)$ Basis Functions ("BF Name", "BF") dims(cell,nNodes,nQPs)

Evaluated Fields:

 $u_i(\xi_p)$ Displacements at quadrature points ("Variable Name", "Displacements") dims(cell,nQPs,vecDim)

For implementation see: problems/Albany_EvaluatorUtils_Def.hpp evaluators/PHAL_DOFVecInterpolation_Def.hpp

fm0.template registerEvaluator<EvalT>
 (evalUtils.constructDOFVecInterpolationEvaluator(dof_names[0]));

// 3.2 Project accelerations to Gauss points

$$a_i(\xi_p) = N_I(\xi_p)a_{iI}$$

 $(c, p, i) = (c, I, p) * (c, I, i)$

Dependent Fields:

$$a_{iI}$$
 Nodal Acceleration ("Variable Name", "Displacement_dotdot") dims(cell,nNodes,vecDim) $N_I(\xi_p)$ Basis Functions ("BF Name", "BF") dims(cell,nNodes,nQPs)

Evaluated Fields:

 $a_i(\xi_p)$ Acceleration at quadrature points ("Variable Name", "Dsplacement_dotdot") dims(cell,nQPs,vecDim)

For implementation see: problems/Albany_EvaluatorUtils_Def.hpp evaluators/PHAL_DOFVecInterpolation_Def.hpp

if(supportsTransient) fm0.template registerEvaluator<EvalT>
 (evalUtils.constructDOFVecInterpolationEvaluator(dof_names_dotdot[0]));

// 3.3 Project nodal coordinates to Gauss points

New evaluator: Compute Gauss point locations from nodal locations.

$$x_{pi} = N_I(\xi_p)x_{iI}$$
$$(c, p, i) = (c, I, p) * (c, I, i)$$

Dependent Fields:

 x_{iI} Nodal coordinates ("Coordinate Vector Name", "Coord Vec") dims(cell,nNodes,vecDim)

Evaluated Fields:

 x_{pi} Gauss point coordinates ("Coordinate Vector Name", "Coord Vec") dims(cell,nQPs,vecDim)

For implementation see: problems/Albany_EvaluatorUtils_Def.hpp evaluators/PHAL_MapToPhysicalFrame_Def.hpp

```
fm0.template registerEvaluator<EvalT>
          (evalUtils.constructMapToPhysicalFrameEvaluator(cellType, cubature));
// 3.4 Compute displacement gradient
```

$$\begin{split} \frac{\partial u_i}{\partial x_j}\bigg|_{\xi_p} &= \partial_j N_I(\xi_p) u_{iI} \\ (c, p, i, j) &= (c, I, p, j) * (c, I, i) \end{split}$$

Dependent Fields:

 u_{iI} Nodal Displacement ("Variable Name", "Displacement") dims(cell,nNodes,vecDim) $B_I(\xi_p)$ Gradient of Basis Functions ("Gradient BF Name", "Grad BF") dims(cell,nNodes,nQPs,vecDim)

Evaluated Fields:

 $\left. \frac{\partial u_i}{\partial x_j} \right|_{\xi_p}$ Gradient of node vector ("Gradient Variable Name", "Displacement Gradient") dims(cell,nQPs,vecDim,spcDim)

For implementation see: problems/Albany_EvaluatorUtils_Def.hpp evaluators/PHAL_DOFVecGradInterpolation_Def.hpp

fm0.template registerEvaluator<EvalT>
 (evalUtils.constructDOFVecGradInterpolationEvaluator(dof_names[0]));

// 4.1 Compute strain

New evaluator:

$$\epsilon_{ij}^{p} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} \Big|_{\xi_p} + \frac{\partial u_j}{\partial x_i} \Big|_{\xi_p} \right)$$
$$(c, p, i, j) = ((c, p, i, j) + (c, p, j, i)/2.0)$$

Dependent Fields:

```
\frac{\partial u_i}{\partial x_j}\Big|_{\xi_p} Gradient of node vector ("Gradient Variable Name", "Displacement Gradient") dims(cell,nQPs,vecDim,spcDim)
```

Evaluated Fields:

```
\epsilon^p_{ij} Infinitesimal strain ("Strain Name", "Strain") dims(cell,nQPs,vecDim,spcDim)
```

For implementation see: problems/Albany_EvaluatorUtils_Def.hpp evaluators/PHAL_DOFVecGradInterpolation_Def.hpp

```
{ // Strain
  RCP<ParameterList> p = rcp(new ParameterList("Strain"));

//Input
p->set<std::string>("Gradient QP Variable Name", "Displacement Gradient");

//Output
p->set<std::string>("Strain Name", "Strain");

ev = rcp(new LCM::Strain<EvalT, AlbanyTraits>(*p,dl));
fm0.template registerEvaluator<EvalT>(ev);

if(matModel == "CapExplicit" || matModel == "GursonSD" || matModel == "CapImplicit"){
  p = stateMgr.registerStateVariable("Strain", dl->qp_tensor, dl->dummy, elementBlockName, "scalar", 0.0, true);
  ev = rcp(new PHAL::SaveStateField<EvalT, AlbanyTraits>(*p));
  fm0.template registerEvaluator<EvalT>(ev);
}

// 5.1 Compute stress
```

$$\sigma_{ij}^{p} = \lambda \epsilon_{kk}^{p} \delta_{ij} + 2\mu \epsilon_{ij}^{p}$$
$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$$
$$\mu = \frac{E}{2(1+\nu)}$$

Dependent Fields:

```
\begin{array}{lll} \epsilon_{ij}^{p} & \text{Infinitesimal strain} & (\text{"Strain Name", "Strain"}) & \text{dims(cell,nQPs,vecDim,spcDim)} \\ E & \text{Elastic modulus} & (\text{"Elastic Modulus Name", "Elastic Modulus"}) & \text{dims(cell,nQPs)} \\ \nu & \text{Poisson's ratio} & (\text{"Poissons Ratio Name", "Poissons Ratio"}) & \text{dims(cell,nQPs)} \\ \end{array}
```

Evaluated Fields:

```
\sigma_{ij}^p Stress ("Stress Name", "Stress") dims(cell,nQPs,vecDim,spcDim)
```

For implementation see:

LCM/evaluators/Stress_Def.hpp

```
{ // Linear elasticity stress
   RCP<ParameterList> p = rcp(new ParameterList("Stress"));

//Input
p->set<std::string>("Strain Name", "Strain");
p->set< RCP<DataLayout> >("QP Tensor Data Layout", dl->qp_tensor);

p->set<std::string>("Elastic Modulus Name", "Elastic Modulus");
p->set< RCP<DataLayout> >("QP Scalar Data Layout", dl->qp_scalar);

p->set<std::string>("Poissons Ratio Name", "Poissons Ratio"); // dl->qp_scalar also
//Output
p->set<std::string>("Stress Name", "Stress"); //dl->qp_tensor also
ev = rcp(new LCM::Stress<EvalT,AlbanyTraits>(*p));
```

```
fm0.template registerEvaluator<EvalT>(ev);
    p = stateMgr.registerStateVariable("Stress",dl->qp_tensor, dl->dummy, elementBlockName, "scalar", 0.0);
    ev = rcp(new PHAL::SaveStateField<EvalT,AlbanyTraits>(*p));
    fm0.template registerEvaluator<EvalT>(ev);
}
// X.X Scatter nodal forces
```

New evaluator: Scatter the nodal forces (i.e., "Displacement Residual") from the grid based structures to the solver data structures. **Dependent Fields:** u_{iI} Displacement residual ("Residual Name", "Displacement Residual") dims(cell,nNodes,vecDim)

Evaluated Fields:

None.

For implementation see: problems/Albany_EvaluatorUtils_Def.hpp evaluators/PHAL_ScatterResidual_Def.hpp

```
fm0.template registerEvaluator<EvalT>
    (evalUtils.constructScatterResidualEvaluator(true, resid_names));

// Temporary variable used numerous times below
Teuchos::RCP<PHX::Evaluator<AlbanyTraits> > ev;

{    // Time
    RCP<ParameterList> p = rcp(new ParameterList);

p->set<std::string>("Time Name", "Time");
p->set<std::string>("Delta Time Name", "Delta Time");
p->set< RCP<DataLayout> >("Workset Scalar Data Layout", dl->workset_scalar);
p->set<RCP<ParamLib> >("Parameter Library", paramLib);
p->set<bool>("Disable Transient", true);

ev = rcp(new LCM::Time<EvalT,AlbanyTraits>(*p));
```

```
fm0.template registerEvaluator<EvalT>(ev);
  p = stateMgr.registerStateVariable("Time",dl->workset_scalar, dl->dummy, elementBlockName, "scalar", 0.0, true);
  ev = rcp(new PHAL::SaveStateField<EvalT, AlbanyTraits>(*p));
  fm0.template registerEvaluator<EvalT>(ev);
}
{ // Elastic Modulus
  RCP<ParameterList> p = rcp(new ParameterList);
  p->set<std::string>("QP Variable Name", "Elastic Modulus");
  p->set<std::string>("QP Coordinate Vector Name", "Coord Vec");
  p->set< RCP<DataLayout> >("Node Data Layout", dl->node_scalar);
  p->set< RCP<DataLayout> >("QP Scalar Data Layout", dl->qp_scalar);
  p->set< RCP<DataLayout> >("QP Vector Data Layout", dl->qp_vector);
  p->set<RCP<ParamLib> >("Parameter Library", paramLib);
  Teuchos::ParameterList& paramList = params->sublist("Elastic Modulus");
  p->set<Teuchos::ParameterList*>("Parameter List", &paramList);
  ev = rcp(new LCM::ElasticModulus<EvalT,AlbanyTraits>(*p));
  fm0.template registerEvaluator<EvalT>(ev);
}
{ // Poissons Ratio
  RCP<ParameterList> p = rcp(new ParameterList);
  p->set<std::string>("QP Variable Name", "Poissons Ratio");
  p->set<std::string>("QP Coordinate Vector Name", "Coord Vec");
  p->set< RCP<DataLayout> >("Node Data Layout", dl->node_scalar);
  p->set< RCP<DataLayout> >("QP Scalar Data Layout", dl->qp_scalar);
  p->set< RCP<DataLayout> >("QP Vector Data Layout", dl->qp_vector);
  p->set<RCP<ParamLib> >("Parameter Library", paramLib);
  Teuchos::ParameterList& paramList = params->sublist("Poissons Ratio");
  p->set<Teuchos::ParameterList*>("Parameter List", &paramList);
```

```
ev = rcp(new LCM::PoissonsRatio<EvalT,AlbanyTraits>(*p));
    fm0.template registerEvaluator<EvalT>(ev);
  }
// ?
  if (haveSource) { // Source
    TEUCHOS_TEST_FOR_EXCEPTION(true, Teuchos::Exceptions::InvalidParameter,
                       "Error! Sources not implemented in HMC yet!");
    RCP<ParameterList> p = rcp(new ParameterList);
    p->set<std::string>("Source Name", "Source");
    p->set<std::string>("Variable Name", "Displacement");
    p->set< RCP<DataLayout> >("QP Scalar Data Layout", dl->qp_scalar);
    p->set<RCP<ParamLib> >("Parameter Library", paramLib);
    Teuchos::ParameterList& paramList = params->sublist("Source Functions");
    p->set<Teuchos::ParameterList*>("Parameter List", &paramList);
    ev = rcp(new PHAL::Source<EvalT,AlbanyTraits>(*p));
    fm0.template registerEvaluator<EvalT>(ev);
  }
// 6.1 Compute residual (stress divegence + inertia term)
```

$$f_{iI} = \sum_{p} \frac{\partial N_{I}(\mathbf{x}_{p})}{\partial \xi_{k}} J_{kj}^{-1} det \left(\frac{\partial x_{ip}}{\partial \xi_{j}}\right) \omega_{p} \sigma_{ij}^{p} + \sum_{p} N_{I}(\mathbf{x}_{p}) det \left(\frac{\partial x_{ip}}{\partial \xi_{j}}\right) \omega_{p} a_{i}(\xi_{p})$$

Dependent Fields:

Dependent Fields			
$\sigma^{ar{p}}_{ij}$	Stress	("Stress Name", "Stress")	${\rm dims}({\rm cell,nQPs,vecDim,spcDim})$
$\frac{\partial \tilde{N}_I(\mathbf{x}_p)}{\partial \xi_k} J_{kj}^{-1} det \left(\frac{\partial x_{ip}}{\partial \xi_i} \right) \omega_p$	Weighted GradBF	("Weighted Gradient BF Name", "Weighted Gradient BF")	dims(cell,nNodes,nQPs,spcDim)
$a_i(\xi_p)$	Acceleration at quadrature points	("Variable Name", "Dsplacement_dotdot")	dims(cell,nQPs,vecDim)
$N_I(\mathbf{x}_p) \ det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted BF	("Weighted BF Name", "wBF")	${\rm dims}({\rm cell,nNode,nQPs})$

Evaluated Fields:

```
f_{iI}(x_iI) \quad \text{Residual ("Residual Name", "Residual")} \quad \text{dims(cell,nNodes,spcDim)} For implementation see:  \frac{\text{LCM/evaluators/ElasticityResid\_Def.hpp}}{\text{LCM/evaluators/ElasticityResid\_Def.hpp}}
```

```
{ // Displacement Resid
  RCP<ParameterList> p = rcp(new ParameterList("Displacement Resid"));
  //Input
  p->set<std::string>("Stress Name", "Stress");
  p->set< RCP<DataLayout> >("QP Tensor Data Layout", dl->qp_tensor);
  // \todo Is the required?
  p->set<std::string>("DefGrad Name", "Deformation Gradient"); //dl->qp_tensor also
  p->set<std::string>("Weighted Gradient BF Name", "wGrad BF");
  p->set< RCP<DataLayout> >("Node QP Vector Data Layout", dl->node_qp_vector);
  // extra input for time dependent term
  p->set<std::string>("Weighted BF Name", "wBF");
  p->set< RCP<DataLayout> >("Node QP Scalar Data Layout", dl->node_qp_scalar);
  p->set<std::string>("Time Dependent Variable Name", "Displacement_dotdot");
  p->set< RCP<DataLayout> >("QP Vector Data Layout", dl->qp_vector);
  //Output
  p->set<std::string>("Residual Name", "Displacement Residual");
  p->set< RCP<DataLayout> >("Node Vector Data Layout", dl->node_vector);
  ev = rcp(new LCM::ElasticityResid<EvalT,AlbanyTraits>(*p));
  fm0.template registerEvaluator<EvalT>(ev);
}
```

```
if (fieldManagerChoice == Albany::BUILD_RESID_FM) {
    PHX::Tag<typename EvalT::ScalarT> res_tag("Scatter", dl->dummy);
    fm0.requireField<EvalT>(res_tag);
    return res_tag.clone();
}
else if (fieldManagerChoice == Albany::BUILD_RESPONSE_FM) {
    Albany::ResponseUtilities<EvalT, PHAL::AlbanyTraits> respUtils(dl);
    return respUtils.constructResponses(fm0, *responseList, stateMgr);
}
return Teuchos::null;
}
#endif // ALBANY_ELASTICITYPROBLEM_HPP
```