

```

//*****//
//   Albany 2.0:  Copyright 2012 Sandia Corporation           //
//   This Software is released under the BSD license detailed  //
//   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"

// To do:
// -- Add multiblock support (See mechanics example problem)
// -- Add density as input.  Currently hardwired to implicit value of 1.0.
// -- Add Currant limit.  Newmark integrator only seems to work for beta=0.25.
// -- Add artificial viscosity.
// -- Add hourglass stabilization for single point integration.

```

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.
   */
  class HMCPProblem : public Albany::AbstractProblem {
  public:

    ///! Default constructor
    HMCPProblem(
      const Teuchos::RCP<Teuchos::ParameterList>& params_,
      const Teuchos::RCP<ParamLib>& paramLib_,
      const int numDim_,
      const Teuchos::RCP<const Epetra_Comm>& comm);

    ///! Destructor
    virtual ~HMCPProblem();

    ///! 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::ArrayRCP<Teuchos::RCP<Intrepid::FieldContainer<RealType> > > > oldState_,
        Teuchos::ArrayRCP<Teuchos::ArrayRCP<Teuchos::RCP<Intrepid::FieldContainer<RealType> > > > newState_
    ) const;

private:

    /// Private to prohibit copying
    HMCPProblem(const HMCPProblem&);

    /// Private to prohibit copying
    HMCPProblem& operator=(const HMCPProblem&);

    void parseMaterialModel(Teuchos::RCP<Teuchos::ParameterList>& p,
        const Teuchos::RCP<Teuchos::ParameterList>& params) const;

    Teuchos::RCP<QCAD::MaterialDatabase> material_db_;

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;
    int numMicroScales;
```

```
    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 "HMC_StrainDifference.hpp"
#include "HMC_TotalStress.hpp"
#include "FieldNameMap.hpp"
```

```
#include "Strain.hpp"
#include "DefGrad.hpp"
#include "HMC_Stresses.hpp"
#include "PHAL_SaveStateField.hpp"
#include "ElasticityResid.hpp"
```

```

#include "HMC_MicroResidual.hpp"

#include "Time.hpp"
#include "ConstitutiveModelParameters.hpp"
#include "ConstitutiveModelInterface.hpp"

#include <sstream>

template <typename EvalT>
Teuchos::RCP<const PHX::FieldTag>
Albany::HMCPProblem::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;
    using PHX::DataLayout;
    using PHX::MDALayout;
    using std::vector;
    using PHAL::AlbanyTraits;

    // get the name of the current element block
    std::string eb_name = meshSpecs.ebName;

    // get the name of the material model to be used (and make sure there is one)
    std::string material_model_name =
        material_db_->
            getElementBlockSublist(eb_name, "Material Model").get<std::string>(
                "Model Name");
    TEUCHOS_TEST_FOR_EXCEPTION(material_model_name.length() == 0, std::logic_error,
        "A material model must be defined for block: "

```

```

        + eb_name);

#ifdef ALBANY_VERBOSE
    *out << "In MechanicsProblem::constructEvaluators" << std::endl;
    *out << "element block name: " << eb_name << std::endl;
    *out << "material model name: " << material_model_name << std::endl;
#endif

    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);

```

```

const int numMacroScales = 1;

// Define Field Names
Teuchos::ArrayRCP<std::string> macro_dof_names(numMacroScales);
macro_dof_names[0] = "Displacement";
Teuchos::ArrayRCP<std::string> macro_resid_names(numMacroScales);
macro_resid_names[0] = macro_dof_names[0] + " Residual";

Teuchos::ArrayRCP< Teuchos::ArrayRCP<std::string> > micro_dof_names(numMicroScales);
Teuchos::ArrayRCP< Teuchos::ArrayRCP<std::string> > micro_resid_names(numMicroScales);
Teuchos::ArrayRCP< Teuchos::ArrayRCP<std::string> > micro_scatter_names(numMicroScales);
for(int i=0;i<numMicroScales;i++){
    micro_dof_names[i].resize(1);
    micro_resid_names[i].resize(1);
    micro_scatter_names[i].resize(1);
    std::stringstream dofname;
    dofname << "Microstrain_" << i;
    micro_dof_names[i][0] = dofname.str();
    micro_resid_names[i][0] = dofname.str() + " Residual";
    micro_scatter_names[i][0] = dofname.str() + " Scatter";
}

Teuchos::ArrayRCP<std::string> macro_dof_names_dotdot(numMacroScales);
Teuchos::ArrayRCP<std::string> macro_resid_names_dotdot(numMacroScales);
Teuchos::ArrayRCP< Teuchos::ArrayRCP<std::string> > micro_dof_names_dotdot(numMicroScales);
Teuchos::ArrayRCP< Teuchos::ArrayRCP<std::string> > micro_resid_names_dotdot(numMicroScales);
Teuchos::ArrayRCP< Teuchos::ArrayRCP<std::string> > micro_scatter_names_dotdot(numMicroScales);
macro_dof_names_dotdot[0] = macro_dof_names[0]+"_dotdot";
macro_resid_names_dotdot[0] = macro_resid_names[0]+" Residual";
for(int i=0;i<numMicroScales;i++){
    micro_dof_names_dotdot[i].resize(1);
    micro_resid_names_dotdot[i].resize(1);
    micro_scatter_names_dotdot[i].resize(1);
    micro_dof_names_dotdot[i][0] = micro_dof_names[i][0]+"_dotdot";
    micro_resid_names_dotdot[i][0] = micro_resid_names_dotdot[i][0]+" Residual";
    micro_scatter_names_dotdot[i][0] = micro_scatter_names_dotdot[i][0]+" Scatter";
}

```

```
}

```

```
// Gather Solution (displacement and acceleration)

```

Gather solution data from solver data structures to grid based structures.

DEPENDENT FIELDS:

None.

EVALUATED FIELDS:

u_{Ii}	Nodal displacements	"Displacement"	<code>dims(cell,I=nNodes,i=vecDim)</code>
a_{Ii}	Nodal accelerations	"Displacement_dotdot"	<code>dims(cell,I=nNodes,i=vecDim)</code>

```
int vectorRank = 1;
fm0.template registerEvaluator<EvalT>
    (evalUtils.constructGatherSolutionEvaluator_withAcceleration(vectorRank, macro_dof_names, Teuchos::null, macro_dof_names_dotdot));

```

```
// Gather Solution (microstrains and micro accelerations)

```

Gather solution data from solver data structures to grid based structures.

DEPENDENT FIELDS:

None.

EVALUATED FIELDS:

ϵ_{Iij}^n	Nodal microstrains at scale 'n'	"Microstrain_n"	<code>dims(cell,I=nNodes,i=vecDim,j=vecDim)</code>
$\ddot{\epsilon}_{Iij}^n$	Nodal micro accelerations at scale 'n'	"Microstrain_n_dotdot"	<code>dims(cell,I=nNodes,i=vecDim,j=vecDim)</code>

```
int dof_offset = numDim; // dof layout is {x, y, ..., xx, xy, xz, yx, ...}
int dof_stride = numDim*numDim;
int tensorRank = 2;
for(int i=0;i<numMicroScales;i++){
    fm0.template registerEvaluator<EvalT>
        (evalUtils.constructGatherSolutionEvaluator_withAcceleration(
            tensorRank, micro_dof_names[i], Teuchos::null, micro_dof_names_dotdot[i], dof_offset+i*dof_stride) );
}

```



```
}
```

```
// Gather Coordinates
```

Gather coordinate data from solver data structures to grid based structures.

DEPENDENT FIELDS:

None.

EVALUATED FIELDS:

x_{Ii} Nodal coordinates "Coord Vec" dims(cell,I=nNodes,i=vecDim)

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

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

Register new evaluator.

DEPENDENT FIELDS:

x_{Ii} Nodal coordinates "Coord Vec" dims(cell,I=nNodes,i=vecDim)

EVALUATED FIELDS:

$\det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted measure	"Weights"	dims(cell,p=nQPs)
$\det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right)$	Jacobian determinant	Jacobian Det"	dims(cell,p=nQPs)
$N_I(\mathbf{x}_p)$	Basis function values	"BF"	dims(cell,I=nNodes,p=nQPs)
$N_I(\mathbf{x}_p) \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted basis function values	"wBF"	dims(cell,I=nNode,p=nQPs)
$\frac{\partial N_I(\mathbf{x}_p)}{\partial \xi_k} J_{kj}^{-1}$	Gradient matrix wrt physical frame	"Grad BF"	dims(cell,I=nNodes,p=nQPs,j=spcDim)
$\frac{\partial N_I(\mathbf{x}_p)}{\partial \xi_k} J_{kj}^{-1} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted gradient matrix wrt current config	"wGrad BF"	dims(cell,I=nNodes,p=nQPs,j=spcDim)

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

```
// Project displacements to Gauss points
```

Register new evaluator:

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

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

DEPENDENT FIELDS:

u_{Ii}	Nodal Displacements	"Displacements"	dims(cell,I=nNodes,i=vecDim)
$N_I(\xi_p)$	Basis Functions	"BF"	dims(cell,I=nNodes,p=nQPs)

EVALUATED FIELDS:

$u_i(\xi_p)$	Displacements at quadrature points	"Displacements"	dims(cell,p=nQPs,i=vecDim)
--------------	------------------------------------	-----------------	----------------------------

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

```
// Project microstrains to Gauss points
```

Register new evaluator:

$$\epsilon_{ij}^n(\xi_p) = N_I(\xi_p)\epsilon_{ijI}^n$$

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

DEPENDENT FIELDS:

ϵ_{ij}^n	Nodal microstrains at scale 'n'	"Microstrain_n"	dims(cell,I=nNodes,i=vecDim,j=vecDim)
$N_I(\xi_p)$	Basis Functions	"BF"	dims(cell,I=nNodes,p=nQPs)

EVALUATED FIELDS:

$\epsilon_{ij}^n(\xi_p)$	Microstrains at scale 'n' at quadrature points	"Microstrain_n"	dims(cell,p=nQPs,i=vecDim,j=spcDim)
--------------------------	--	-----------------	-------------------------------------

```
for(int i=0;i<numMicroScales;i++)
  fm0.template registerEvaluator<EvalT>
```

```
(evalUtils.constructDOFTensorInterpolationEvaluator(micro_dof_names[i][0],
dof_offset+i*dof_stride));
```

```
// Project accelerations to Gauss points
```

Register new evaluator:

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

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

DEPENDENT FIELDS:

a_{Ii}	Nodal Acceleration	"Displacement_dotdot"	dims(cell,I=nNodes,i=vecDim)
$N_I(\xi_p)$	Basis Functions	"BF"	dims(cell,I=nNodes,p=nQPs)

EVALUATED FIELDS:

$a_i(\xi_p)$	Acceleration at quadrature points	"Displacement_dotdot"	dims(cell,p=nQPs,i=vecDim)
--------------	-----------------------------------	-----------------------	----------------------------

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

```
// Project micro accelerations to Gauss points
```

Register new evaluator:

$$\tilde{\epsilon}_{ij}^n(\xi_p) = N_I(\xi_p) \epsilon_{Iij}^n$$

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

DEPENDENT FIELDS:

$\tilde{\epsilon}_{Iij}^n$	Nodal micro acceleration at scale 'n'	"Microstrain_n_dotdot"	dims(cell,I=nNodes,i=vecDim,j=vecDim)
$N_I(\xi_p)$	Basis Functions	"BF"	dims(cell,I=nNodes,p=nQPs)

EVALUATED FIELDS:

$\tilde{\epsilon}_{ij}^n(\xi_p)$	Micro acceleration at scale 'n' at quadrature points	"Microstrain_n_dotdot"	dims(cell,p=nQPs,i=vecDim,j=vecDim)
----------------------------------	--	------------------------	-------------------------------------

```

for(int i=0;i<numMicroScales;i++)
  fm0.template registerEvaluator<EvalT>
    (evalUtils.constructDOFTensorInterpolationEvaluator(micro_dof_names_dotdot[i][0],
      dof_offset+i*dof_stride));

```

```
// Project nodal coordinates to Gauss points
```

Register 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 "Coord Vec" dims(cell,I=nNodes,i=vecDim)

EVALUATED FIELDS:

x_{pi} Gauss point coordinates "Coord Vec" dims(cell,p=nQPs,i=vecDim)

```

fm0.template registerEvaluator<EvalT>
  (evalUtils.constructMapToPhysicalFrameEvaluator(cellType, cubature));

```

```
// Compute displacement gradient
```

New evaluator:

$$\left. \frac{\partial u_i}{\partial x_j} \right|_{\xi_p} = \partial_j N_I(\xi_p) u_{iI}$$

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

DEPENDENT FIELDS:

u_{Ii} Nodal Displacement "Displacement" dims(cell,I=nNodes,i=vecDim)

$B_I(\xi_p)$ Gradient of Basis Functions "Grad BF" dims(cell,I=nNodes,p=nQPs,i=vecDim)

EVALUATED FIELDS:

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

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

```
// Compute microstrain gradient
```

Register new evaluator:

$$\left. \frac{\partial \epsilon_{ij}^n}{\partial x_k} \right|_{\xi_p} = \partial_k N_I(\xi_p) \epsilon_{Iij}^n$$

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

DEPENDENT FIELDS:

ϵ_{Iij}^n	Nodal microstrain at scale 'n'	"Microstrain_n"	dims(cell,I=nNodes,i=vecDim,j=vecDim)
$B_I(\xi_p)$	Gradient of Basis Functions	"Grad BF"	dims(cell,I=nNodes,p=nQPs,i=vecDim)

EVALUATED FIELDS:

$\left. \frac{\partial \epsilon_{ij}^n}{\partial x_k} \right _{\xi_p}$	Microstrain gradient at scale 'n'	"Microstrain_n Gradient"	dims(cell,p=nQPs,i=vecDim,j=vecDim,k=spcDim)
--	-----------------------------------	--------------------------	--

```
for(int i=0;i<numMicroScales;i++)
  fm0.template registerEvaluator<EvalT>
    (evalUtils.constructDOFTensorGradInterpolationEvaluator(micro_dof_names[i][0],dof_offset+i*dof_stride));
```

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

```
// Compute strain
```

New evaluator:

$$\epsilon_{ij}^p = \frac{1}{2} \left(\left. \frac{\partial u_i}{\partial x_j} \right|_{\xi_p} + \left. \frac{\partial u_j}{\partial x_i} \right|_{\xi_p} \right)$$

$$(c, p, i, j) = ((c, p, i, j) + (c, p, j, i))/2.0$$

DEPENDENT FIELDS:

$\left. \frac{\partial u_i}{\partial x_j} \right|_{\xi_p}$ Gradient of displacement "Displacement Gradient" dims(cell, p=nQPs, i=vecDim, j=spcDim)

EVALUATED FIELDS:

ϵ_{ij}^p Infinitesimal strain "Strain" dims(cell, p=nQPs, i=vecDim, j=spcDim)

```
{
  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,d1));
  fm0.template registerEvaluator<EvalT>(ev);
}

// Compute microstrain difference
```

Register new evaluator:

$$\Delta \epsilon_{ij}^{np} = \epsilon_{ij}^p - \epsilon_{ij}^{np}$$

DEPENDENT FIELDS:

ϵ_{ij}^p Macro strain "Strain" dims(cell, p=nQPs, i=vecDim, j=spcDim)
 ϵ_{ijI}^n Nodal microstrains at scale 'n' "Microstrain_1" dims(cell, I=nNodes, i=vecDim, j=vecDim)

EVALUATED FIELDS:

$\Delta \epsilon_{ij}^{np}$ Strain Difference at scale 'n' "Strain Difference n" dims(cell, p=nQPs, i=vecDim, j=spcDim)

```
for(int i=0;i<numMicroScales;i++){
```

```

RCP<ParameterList> p = rcp(new ParameterList("Strain Difference"));

//Input
p->set<std::string>("Micro Strain Name", micro_dof_names[i][0]);
p->set<std::string>("Macro Strain Name", "Strain");

//Output
std::stringstream sd;
sd << "Strain Difference " << i;
p->set<std::string>("Strain Difference Name", sd.str());

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

{ // Constitutive Model Parameters
RCP<ParameterList> p = rcp(
    new ParameterList("Constitutive Model Parameters"));
std::string matName = material_db_->getElementBlockParam<std::string>(
    eb_name, "material");
Teuchos::ParameterList& param_list =
    material_db_->getElementBlockSublist(eb_name, matName);

// pass through material properties
p->set<Teuchos::ParameterList*>("Material Parameters", &param_list);

RCP<LCM::ConstitutiveModelParameters<EvalT, AlbanyTraits> > cmpEv =
    rcp(new LCM::ConstitutiveModelParameters<EvalT, AlbanyTraits>(*p, dl));
fm0.template registerEvaluator<EvalT>(cmpEv);
}

// Compute stresses

```

Register new evaluator:

$$\{\sigma_{ij}^p, \bar{\beta}_{ij}^{np}, \bar{\beta}_{ijk}^{np}\} = f(\{\epsilon_{ij}^p, \Delta\epsilon_{ij}^{np}, \epsilon_{ij,k}^{np}\})$$

DEPENDENT FIELDS:

ϵ_{ij}^p	Macro strain	"Strain"	$\text{dims}(\text{cell}, p=\text{nQPs}, i=\text{vecDim}, j=\text{spcDim})$
$\Delta\epsilon_{ij}^{np}$	Strain Difference 'n'	"Strain Difference 1"	$\text{dims}(\text{cell}, p=\text{nQPs}, i=\text{vecDim}, j=\text{spcDim})$
$\epsilon_{ij,k}^{np}$	Microstrain gradient 'n'	"Microstrain_n Gradient"	$\text{dims}(\text{cell}, p=\text{nQPs}, i=\text{vecDim}, j=\text{vecDim}, k=\text{spcDim})$

EVALUATED FIELDS:

σ_{ij}^p	Macro Stress	"Stress"	$\text{dims}(\text{cell}, p=\text{nQPs}, i=\text{vecDim}, j=\text{spcDim})$
β_{ij}^{np}	Micro stress 'n'	"Micro Stress n"	$\text{dims}(\text{cell}, p=\text{nQPs}, i=\text{vecDim}, j=\text{spcDim})$
$\bar{\beta}_{ijk}^{np}$	Double stress 'n'	"Double Stress n"	$\text{dims}(\text{cell}, p=\text{nQPs}, i=\text{vecDim}, j=\text{spcDim}, k=\text{spcDim})$

```
{
  RCP<ParameterList> p = rcp(new ParameterList("Constitutive Model Interface"));
  std::string matName = material_db_->getElementBlockParam<std::string>(eb_name, "material");
  Teuchos::ParameterList& param_list = material_db_->getElementBlockSublist(eb_name, matName);

  // construct field name map
  // required
  LCM::FieldNameMap
  field_name_map(false);
  RCP<std::map<std::string, std::string> >
  fnm = field_name_map.getMap();
  param_list.set<RCP<std::map<std::string, std::string> > >("Name Map", fnm);
  p->set<Teuchos::ParameterList*>("Material Parameters", &param_list);
  // end required

  p->set<Teuchos::ParameterList*>("Material Parameters", &param_list);

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

  // register state variables
```



```

for (int sv(0); sv < cmiEv->getNumStateVars(); ++sv) {
    cmiEv->fillStateVariableStruct(sv);
    p = stateMgr.registerStateVariable(cmiEv->getName(),
        cmiEv->getLayout(),
        dl->dummy,
        eb_name,
        cmiEv->getInitType(),
        cmiEv->getInitValue(),
        cmiEv->getStateFlag(),
        cmiEv->getOutputFlag());
    ev = rcp(new PHAL::SaveStateField<EvalT, AlbanyTraits>(*p));
    fm0.template registerEvaluator<EvalT>(ev);
}
}

```

```
// Compute total stress
```

Register new evaluator:

$$\sigma_{ij}^{tp} = \sigma_{ij}^p + \sum_n \bar{\beta}_{ij}^{np}$$

DEPENDENT FIELDS:

σ_{ij}^{tp} Total stress "Total Stress" dims(cell, p=nQPs, i=vecDim, j=spcDim)

EVALUATED FIELDS:

σ_{ij}^p Macro Stress "Stress" dims(cell, p=nQPs, i=vecDim, j=spcDim)

β_{ij}^{np} Micro stress 'n' "Micro Stress n" dims(cell, p=nQPs, i=vecDim, j=spcDim)

```

{
    RCP<ParameterList> p = rcp(new ParameterList("Total Stress"));

    p->set<int>("Additional Scales", numMicroScales);

    //Input
    p->set<std::string>("Macro Stress Name", "Stress");
}

```

```

p->set< RCP<DataLayout> >("QP 2Tensor Data Layout", dl->qp_tensor);
for(int i=0;i<numMicroScales;i++){
    std::string ms = Albany::strint("Micro Stress",i);
    std::string msname(ms); msname += " Name";
    p->set<std::string>(msname, ms);
}
//Output
p->set<std::string>("Total Stress Name", "Total Stress");

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

```

// Compute macro residual

Register new evaluator:

$$f_{Ii} = \sum_p \frac{\partial N_I(\mathbf{x}_p)}{\partial \xi_k} J_{kj}^{-1} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p \sigma_{ij}^{tp} + \sum_p N_I(\mathbf{x}_p) \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p a_i^p$$

DEPENDENT FIELDS:

σ_{ij}^{tp}	Total stress	"Total Stress"	dims(cell, p=nQPs, i=vecDim, j=spcDim)
$\frac{\partial N_I(\mathbf{x}_p)}{\partial \xi_k} J_{kj}^{-1} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted Gradient matrix wrt current config	"wGrad BF"	dims(cell, I=nNodes, p=nQPs, i=spcDim)
a_i^p	Acceleration at quadrature points	"Displacement_dotdot"	dims(cell, p=nQPs, i=vecDim)
$N_I(\mathbf{x}_p) \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted BF	"wBF"	dims(cell, I=nNodes, p=nQPs)

EVALUATED FIELDS:

f_{Ii}	Macroscale Residual	"Displacement Residual"	dims(cell, I=nNodes, i=spcDim)
----------	---------------------	-------------------------	--------------------------------

```

{
    RCP<ParameterList> p = rcp(new ParameterList("Displacement Resid"));

    //Input

```

```

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

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", macro_dof_names_dotdot[0]);
p->set< RCP<DataLayout> >("QP Vector Data Layout", dl->qp_vector);

//Output
p->set<std::string>("Residual Name", macro_resid_names[0]);
p->set< RCP<DataLayout> >("Node Vector Data Layout", dl->node_vector);

ev = rcp(new LCM::ElasticityResid<EvalT,AlbanyTraits>(*p));
fm0.template registerEvaluator<EvalT>(ev);
}
// Compute micro residuals

```

Register new evaluator:

$$f_{Iij}^n = \sum_p \frac{\partial N_I(\mathbf{x}_p)}{\partial \xi_i} J_{lk}^{-1} \bar{\beta}_{ijk}^{np} \} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p + \sum_p N_I(\mathbf{x}_p) \bar{\beta}_{ij}^{np} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p + \sum_p N_I(\mathbf{x}_p) \bar{\epsilon}_{ij}^{np} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$$

DEPENDENT FIELDS:

β_{ij}^{np}	Micro stress 'n'	"Micro Stress n"	dims(cell, p=nQPs, i=vecDim, j=spcDim)
$\bar{\beta}_{ijk}^{np}$	Double stress 'n'	"Double Stress n"	dims(cell, p=nQPs, i=vecDim, j=spcDim, k=spcDim)
$\bar{\epsilon}_{ij}^n$	micro accel at scale 'n'	"Microstrain_n_dotdot"	dims(cell, I=nNodes, i=vecDim, j=vecDim)
$\frac{\partial N_I(\mathbf{x}_p)}{\partial \xi_k} J_{kj}^{-1} \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted Gradient matrix wrt current config	"wGrad BF"	dims(cell, I=nNodes, p=nQPs, i=spcDim)
$N_I(\mathbf{x}_p) \det \left(\frac{\partial x_{ip}}{\partial \xi_j} \right) \omega_p$	Weighted BF	"wBF"	dims(cell, I=nNodes, p=nQPs)

EVALUATED FIELDS:

f_{Iij}^n	Residual at scale 'n'	"Microstrain_n Residual"	dims(cell, I=nNodes, i=vecDim, j=vecDim)
-------------	-----------------------	--------------------------	--

```
for(int i=0;i<numMicroScales;i++){
  RCP<ParameterList> p = rcp(new ParameterList("Microstrain Resid"));

  //Input: Micro stresses
  std::string ms = Albany::strint("Micro Stress",i);
  p->set<std::string>("Micro Stress Name", ms);
  p->set< RCP<DataLayout> >("QP Tensor Data Layout", dl->qp_tensor);

  std::string ds = Albany::strint("Double Stress",i);
  p->set<std::string>("Double Stress Name", ds);
  p->set< RCP<DataLayout> >("QP 3Tensor Data Layout", dl->qp_tensor3);

  p->set<std::string>("Weighted Gradient BF Name", "wGrad BF");
  p->set< RCP<DataLayout> >("Node QP Vector Data Layout", dl->node_qp_vector);

  p->set<std::string>("Weighted BF Name", "wBF");
  p->set< RCP<DataLayout> >("Node QP Scalar Data Layout", dl->node_qp_scalar);

  // extra input for time dependent term
  p->set<std::string>("Time Dependent Variable Name", micro_dof_names[i][0]+"_dotdot");
  p->set< RCP<DataLayout> >("QP Vector Data Layout", dl->qp_vector);

  //Output
  p->set<std::string>("Residual Name", micro_resid_names[i][0]);
  p->set< RCP<DataLayout> >("Node Tensor Data Layout", dl->node_tensor);

  ev = rcp(new HMC::MicroResidual<EvalT,AlbanyTraits>(*p));
  fm0.template registerEvaluator<EvalT>(ev);
}

// Scatter macroscale forces
```

Register new evaluator: Scatter the nodal forces from grid based structures to solver data structures.

DEPENDENT FIELDS:

f_{Ii} Macroscale Residual "Displacement Residual" dims(cell, I=nNodes, i=vecDim)

EVALUATED FIELDS:

None.

```
fm0.template registerEvaluator<EvalT>
    (evalUtils.constructScatterResidualEvaluator(vectorRank, macro_resid_names));
```

```
// Scatter microscale forces
```

Register new evaluator: Scatter the nodal forces from grid based structures to solver data structures.

DEPENDENT FIELDS:

f_{Iij}^n Microscale Residual "Microstrain_n Residual" dims(cell, I=nNodes, i=vecDim, j=vecDim)

EVALUATED FIELDS:

None.

```
int numTensorFields = numDim*numDim;
int dofOffset = numDim;
for(int i=0;i<numMicroScales;i++){ // Micro forces
    fm0.template registerEvaluator<EvalT>
        (evalUtils.constructScatterResidualEvaluator(tensorRank, micro_resid_names[i], dofOffset, micro_scatter_names[i][0]));
    dofOffset += numTensorFields;
}

{ // 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, eb_name, "scalar", 0.0, true);
    ev = rcp(new PHAL::SaveStateField<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);
    for(int i=0;i<numMicroScales;i++){ // Micro forces
        PHX::Tag<typename EvalT::ScalarT> res_tag(micro_scatter_names[i][0], 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

```