Using ESSI Elastic - Plastic Material Model (Drucker Prager) in the **MOOSE** Framework

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Chapter 1

Introduction

1.1 Introduction

This report addresses the work is performed to design, implementation and testing of a framework to use elastic - plastic material models of ESSI in the tensor mechanics module of MOOSE.

1.2 The Purpose of the Project

MOOSE is a very power full framework for the multiphysics simulations and ESSI includes the state of the art capabilities in the finite element simulation of the Seismic Soil Structure Interaction Systems. It contains a very extensive material library for elastic - plastic modelling of solids. This project includes the design and implementation of how to use ESSI's Drucker Prager material model the MOOSE framework.

1.3 Review of MOOSE and ESSI Solid Mechanics Capabilities

MOOSE is a finite element framework for the development of coupled multiphysics solvers. It uses PETSc as the non-linear solver and libMesh (A particular version of libMesh is provided by MOOSE developers) to finite element discretization. MOOSE uses Jacobian-free Newton-Krylov method and this method only requires the residual. So addition of new physics is more simple. Kernels which includes the modules are in charge of providing the residuals and must be provided for any new physics. MOOSE provides the necessary core functionality for calculation of the residuals. libMesh provides the utilities for the finite element calculations, Mesh, I/O and the finite element library. It also provides the interface to the solver package(s).

MOOSE is a framework designed to solve the computational engineering problems in a well-planned, managed and coordinated way. It designed to reduce the cost and time of the new application development. It uses very robust solution methods, easily extendible and maintainable, and is efficient on both small and large number of processors. ESSI includes its own finite element library and a state of the art library of material models to simulate the elastic - plastic behaviour of the solids. Except pressure dependent finite elements, beam and truss elements, libMesh includes all of the other finite elements in ESSI. MOOSE and ESSI use different data structures so ESSI routines are not usable by MOOSE. MOOSE has a very efficient, organized and easy usable data structure very usable to implement different constitutive models. ESSI and MOOSE modules can not directly talk to each other so it is required to implement a communicator to make the ESSI talk to MOOSE. MOOSE uses libMesh to handle the finite elements and it includes hexahedral Lagrangian 8 node element. this is pretty similar to the eight node brick element in ESSI.

1.3.1 Evaluation of the Solid Mechanics Capabilities in MOOSE

Tensor Mechanics and solid mechanics modules are two mechanics modules in MOOSE to deal with the solid mechanics problems. The main difference between these two modules are summarized as below:

1. Rank two tensors are treated as length 6 vectors in Solid Mechanics Module but they are treated as rank two tensors in Tensor Mechanics Module/
2. Elasticity Tensor is treated as 6×6 matrix in Solid Mechanics Module but it is treated as rank four tensor in Tensor Mechanics module.
3. Materials are treated to be isotropic in Solid Mechanics module, but they are treated as anisotropic ones in Tensor Mechanics Module
4. Solid Mechanics is used for macro-scale simulations and Tensor Mechanics module is used for both meso-scale and macro-scale simulations.

MOOSE tensor mechanics module provides a system to solve the solid mechanics problems using *syntax based on tensor forms*. Tensor equations are implemented directly in **MOOSE** framework which makes the development of the models simple. Tensor mechanics module provides all of the routines to implement full plasticity models.

TensorMechanicsMaterial is the base class for materials and derived classes are linear elasticity, crystal nonlinearity and large - deformation plasticity. Stresses, strains and other related materials are calculated in material classes.

Depending on the material, up to twenty one independent stiffness tensor inputs can be introduced to *TensorMechanicsMaterial*. It can handle fully anisotropic single crystal elastic constants.

1.3.2 Evaluation of Solid Mechanics Materials in ESSI

Same as MOOSE's tensor mechanics module, ESSI treats the tensors as tensor but unlike MOOSE material class provides the tangent stiffness for the finite element part of the framework. It is more efficient for the elastic - plastic problems and need less iterations, but it can not be employed for multiphysics problems.

Chapter 2

Linking ESSI Material Models to be Used in MOOSE

Since the tensor mechanics module of MOOSE is more compatible with ESSI's material model library, tensor mechanics module of MOOSE is chosen to to be used as the interface to connect the MOOSE to the ESSI material library. An interface utility is designed to connect the tensor mechanics routines with the ESSI material library. "ESSI Material" class handles the communication between MOOSE and ESSI and "ESSI to MOOSE Tensor Converter" is in charge of the conversion between the tensor data of MOOSE with the nDarray library which is used by ESSI.

2.1 ESSI to MOOSE Tensor Converter Utility

Since MOOSE and ESSI use different data structure to store and perform tensor operations, a class is designed implemented to convert these two formats of the tensors. This class is responsible to convert the nDarray data structure of ESSI with MOOSE's tensor data structure. This class is implemented and tested in several cases. Some of the tests of this utility are presented in Appendix **??** .

2.2 ESSI-Material

ESSI-Material class is in charge of getting the required information from MOOSE tensor mechanics module and passing them to the corresponding material in ESSI to perform the calculations. After performing the calculations by the ESSI's corresponding material, "ESSI- Material" gets the data from the material in ESSI and passes it to the tensor modulus of the MOOSE. Currently ESSI-Material implemented for the "Accelerated Drucker Prager Elastic - Perfectly Plastic", "Accelerated Drucker Prager Isotropic Hardening", and "NewTemplate3Dep Drucker Prager isotropic hardening" Materials from ESSI. "ESSI-Material" is designed and implemented generally and easily can be used to make the other ESSI material models work with the tensor mechanics module of MOOSE.

This class provides the features to make the communication between the MOOSE tensor mechanics module and the ESSI material models. It calls the appropriate methods and functions in ESSI's elastic - plastic material model and pass the required information to the MOOSE. Even ESSI is based on tangent stiffness but MOOSE uses the initial elastic stiffness as the initial stiffness and solves the system by doing several iterations in each step, the ESSI-Material is designed to provide the state of stress which is required by the tensor mechanics modulus.

2.3 ESSI-Material-Directory-Structure

Assuming "`tensor_mechanics`" folder as the root, source codes and header files are placed in "`./src`" and "`./include`" folders respectively:

1. **"ESSI Material"** related files are in "`./ESSI_Material`".

2. **"Moose-ESSI-Tensor-converter"** related files are in "`./utils/Moose_ESSI_Tensor_converter`".

3. **"nDarray"** related files are places in "`./utils/nDarray`".

Chapter 3

Test Example

All of the test problem includes a single eight node brick example loaded uniformly on top. Figure **??** shows the geometry, fixed boundary condition and the direction of the applied deformation pattern.

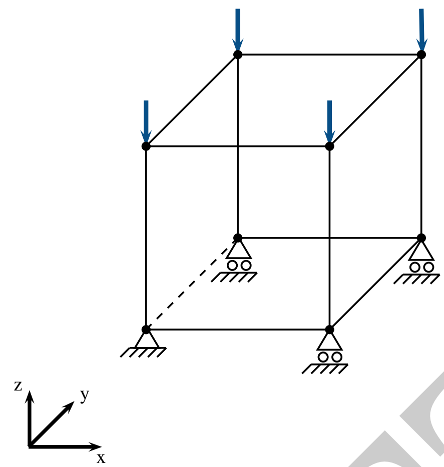

Figure 3.1: General view of the simulation geometry

3.1 Response of a Single Element for the Drucker Prager Material Model of NewTemplate3D

In this chapter, the response of a single eight node cube element loaded uniformly with the boundary conditions shown in figure **??**. Displacement versus force is shown in this section. Detailed material parameters including stress, strain, yield function and internal parameters are presented in Appendices.

3.1.1 Linear Branch Response

Displacement vs. force for the linear branch of the response of the test example (Figure **??**) is shown in the figure **??**

3.1.2 Elastic - Plastic with Isotropic Hardening

Displacement vs. force for the linear branch of the response of the test example (Figure **??**) is shown in the figure **??**

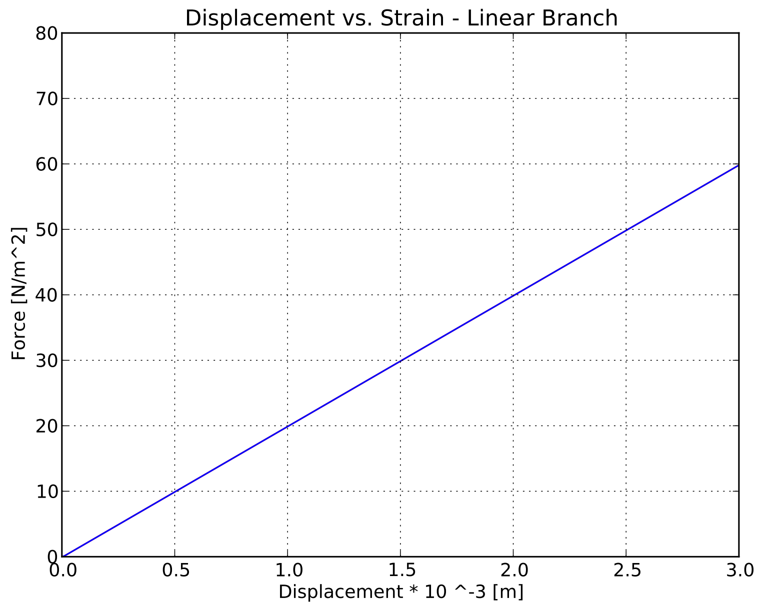

Figure 3.2: Linear Branch Response for the Drucker Prager Material (NewTemplate3Dep)

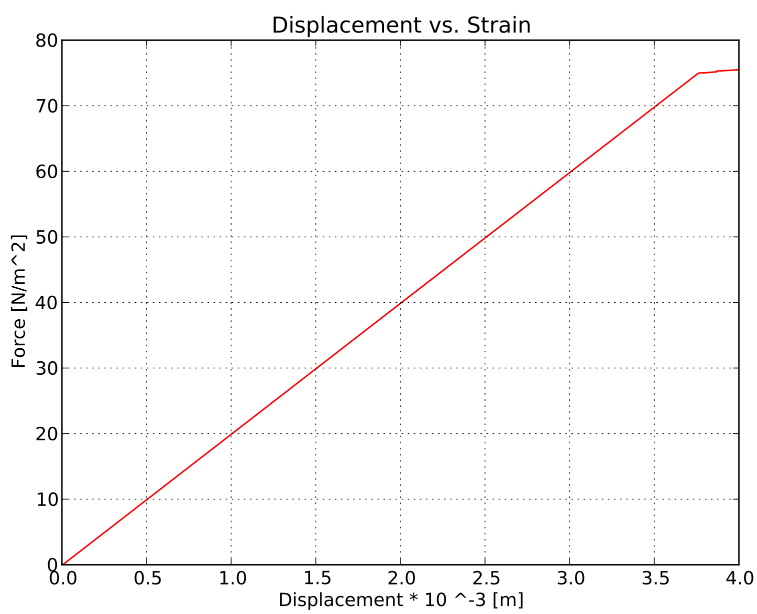

Figure 3.3: esponse for the Drucker Prager Material (NewTemplate3Dep)

Chapter 4

Summary and the Future Work

ESSI is a powerful tool which provides state of the art efficient elastic - plastic material models. At this moment, tensor mechanics module of MOOSE is chosen to be used but in next step a new module called ESSI module can be added to the MOOSE to take the full capabilities and deficiency of the ESSI to be used in seismic analysis. Since moose and ESSI use different data structure to work with the tensors, translating between these two makes the program not efficient. ESSI is a very extensive solid mechanics code which includes very useful capabilities to be used in seismic soil structure interaction systems. There are some capabilities in ESSI which can not be employed using the tensor module of the MOOSE. Development of a new module in MOOSE which devoted to use the capabilities of ESSI is the suggestion for the next step of the project. The summary of the performed project and also the suggestions for the future summarized as:

1. Implemented ESSI Material currently uses Drucker Prager material with isotropic hardening but it is easily extendible to use other material models from ESSI in MOOSE.

2. Performance of the implemented framework to make the tensor mechanics module work with ESSI material library is low due to lot of data conversion. Some of the features in the ESSI can not be employed because of the limitations in the tensor mechanics module.

3. In the current framework some of the calculations are performed by ESSI material library which are not required and used by the tensor mechanics module of MOOSE.

4. ESSI module is proposed to be implemented to communicate without going through the tensor mechanics module. It will be not only much more efficient than the current "ESSI Material" but also makes it possible to use the more features of the ESSI in MOOSE.

5. Current implementation is limited to use of the libMesh finite element features. This platform is originally aimed to use by the aerospace engineering purposes . Completion of the element library of the libMesh to include structural elements such as beam, truss and shells will help the use of MOOSE framework in the simulation of the seismic soil structure interaction problems taking the advantage of unique multiphysics capabilities of MOOSE considering several physics involved in the simulation of the response of the complex systems such as nuclear poser plants.

6. Multiphysics nature of MOOSE needs to solve all the system of equations together so the tangent stiffness can not be used for the solid mechanics applications. It needs lot of iterations to be done to make the solution converged. Using appropriate preconditioning matrices can improve the performance of the method for the elastic - plastic problems. It should be considered in the implementation of the ESSI module for MOOSE.

Appendix A

How to install MOOSE in UBUNTU 14.04

If you already installed OpenMPI, following the **MOOSE** installation procedure might damage your current installation of OpenMPI.

A.1 Installing the Dependencies

First following ubuntu packages need to be installed:

```
sudo -E apt-get install build-essential \
tcl8.5 \
libx11-dev \
python-pyside \
python-matplotlib \
python-yaml \
gfortran \
git \
m4
```

A.2 Downloading and Installing the Pre-Compiled Installable Packages

Pre-compiled installable packages should be downloaded and installed with the following command:

```
sudo dpkg -i moose-environment_ubuntu_14.04_1.1-3.x86_64.deb
```

```
mkdir ~/projects
cd ~/projects
git clone https://github.com/idaholab/moose.git
cd ~/projects/moose
git checkout master
```

After installing, following lines should be added to the .bashrc file:

```
# Source MOOSE Environment
if [ -f /opt/moose/environments/moose_profile ]; then
  . /opt/moose/environments/moose_profile
fi
```

Afterwards, all the terminals should be closed. Open a new terminal window and enter the following command:

```
module list
```

You should see themodules with prefix 'moose'.

MOOSE can be uninstalled by the following command:

```
sudo -E dpkg -r moose-environment
```

A.3 Cloning the MOOSE from the Repository, Installing and Testing

Next step is cloning the MOOSE by following commands in terminal:

```
mkdir ~/projects
cd ~/projects
git clone https://github.com/idaholab/moose.git
cd ~/projects/moose
git checkout master
```

LIBMESH should be installed with the following command:

```
cd ~/projects/moose
scripts/update_and_rebuild_libmesh.sh
```

Test it with the following commands:

```
cd ~/projects/moose/test
make -j8
./run_tests -j8
```

Appendix B

Material Parameters Evolution in the Course of the Simulation for the Test Problem

In this part, stress, strain, internal variables, yield function value for the Test Problems in chapter **??** are presented. They compared with the theoretical values from the closed form solutions.

B.1 Response of a Single Element for the Drucker Prager Material Model of NewTemplate3D

B.1.1 Linear Response

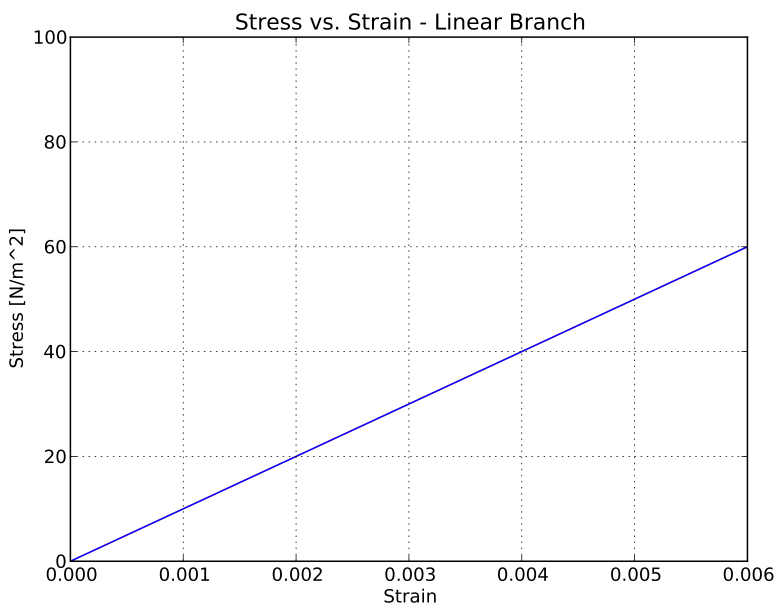

Figure B.1: General view of the simulation geometry

B.1.2 Elastic - Plastic with Isotropic Hardening

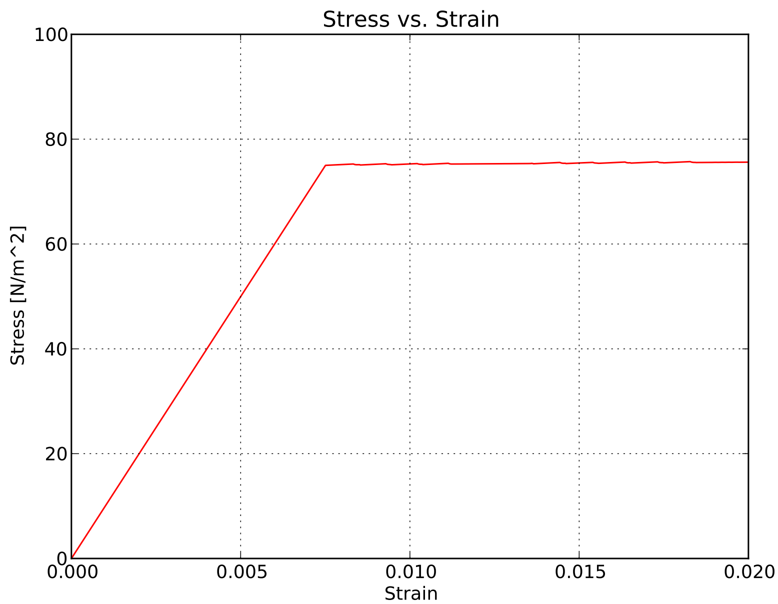

Figure B.2: General view of the simulation geometry

Appendix C

ESSI to MOOSE Tensor Converter Utility Test

ESSI to MOOSE Tensor Converter is developed to exchange the data between the MOOSE and ESSI data structures between MOOSe and ESSI. Several tests performed to make sure the developed utility works correctly. A Sample of performed test for each of the conversions are presented in this section.

C.1 Rank Two Tensors

Test results for the exchange of rank two tensors between the MOOSE and ESSI are presented in tables **??** and **??**.

i	j	ESSI	MOOSE	i	j	ESSI	MOOSE	i	j	ESSI	MOOSE
1	1	7.01	7.01	1	1	1184.69	1184.69	1	1	91.13	91.13
1	2	2.43	2.43	1	2	21.87	21.87	1	2	7.29	7.29
1	3	2.34	2.34	1	3	37.44	37.44	1	3	9.36	9.36
2	1	5.45	5.45	2	1	136.25	136.25	2	1	27.25	27.25
2	2	6.87	6.87	2	2	247.32	247.32	2	2	41.22	41.22
2	3	6.09	6.09	2	3	298.41	298.41	2	3	42.63	42.63
3	1	3.78	3.78	3	1	3.78	3.78	3	1	3.78	3.78
3	2	19.02	19.02	3	2	10061.58	10061.58	3	2	437.46	437.46
3	3	2.14	2.14	3	3	34.24	34.24	3	3	8.56	8.56

Table C.1: Sample of ESSI to MOOSE Tensor Converter Utility Test - Rank Two Tensor (Conversion from ESSI to MOOSE

i	j	ESSI	MOOSE	i	j	ESSI	MOOSE	i	j	ESSI	MOOSE
1	1	56.09	56.09	1	1	9479.21	9479.21	1	1	729.17	729.17
1	2	8.6	8.6	1	2	77.4	77.4	1	2	25.8	25.8
1	3	5.02	5.02	1	3	80.32	80.32	1	3	20.08	20.08
2	1	3.5	3.5	2	1	87.5	87.5	2	1	17.5	17.5
2	2	6.56	6.56	2	2	236.16	236.16	2	2	39.36	39.36
2	3	4.56	4.56	2	3	223.44	223.44	2	3	31.92	31.92
3	1	0.09	0.09	3	1	0.09	0.09	3	1	0.09	0.09
3	2	1.23	1.23	3	2	650.67	650.67	3	2	28.29	28.29
3	3	3.45	3.45	3	3	55.2	55.2	3	3	13.8	13.8

Table C.2: Sample of ESSI to MOOSE Tensor Converter Utility Test - Rank Two Tensor (Conversion from MOOSE to ESSI

C.2 Rank Four Tensors

Test results for the exchange of rank two tensors between the MOOSE and ESSI are presented in tables **??** and **??**.

i	j	k	l	ESSI	MOOSE	i	j	k	l	ESSI	MOOSE	i	j	k	l	ESSI	MOOSE
1	1	1	1	2.5	2.5	2	1	1	1	422.5	422.5	3	1	1	1	32.5	32.5
1	1	1	2	5.2	5.2	2	1	1	2	46.8	46.8	3	1	1	2	15.6	15.6
1	1	1	3	45.32	45.32	2	1	1	3	725.12	725.12	3	1	1	3	181.28	181.28
1	1	2	1	77.23	77.23	2	1	2	1	1930.75	1930.75	3	1	2	1	386.15	386.15
1	1	2	2	9.12	9.12	2	1	2	2	328.32	328.32	3	1	2	2	54.72	54.72
1	1	2	3	8.17	8.17	2	1	2	3	400.33	400.33	3	1	2	3	57.19	57.19
1	1	3	1	7.13	7.13	2	1	3	1	7.13	7.13	3	1	3	1	7.13	7.13
1	1	3	2	2.14	2.14	2	1	3	2	1132.06	1132.06	3	1	3	2	49.22	49.22
1	1	3	3	2.98	2.98	2	1	3	3	47.68	47.68	3	1	3	3	11.92	11.92
1	2	1	1	7.23	7.23	2	2	1	1	41760.48	41760.48	3	2	1	1	549.48	549.48
1	2	1	2	5.19	5.19	2	2	1	2	15134.04	15134.04	3	2	1	2	280.26	280.26
1	2	1	3	4.18	4.18	2	2	1	3	4280.32	4280.32	3	2	1	3	133.76	133.76
1	2	2	1	4.23	4.23	2	2	2	1	8565.75	8565.75	3	2	2	1	190.35	190.35
1	2	2	2	0.01	0.01	2	2	2	2	5.29	5.29	3	2	2	2	0.23	0.23
1	2	2	3	9.13	9.13	2	2	2	3	18488.25	18488.25	3	2	2	3	410.85	410.85
1	2	3	1	32.24	32.24	2	2	3	1	144725.36	144725.36	3	2	3	1	2160.08	2160.08
1	2	3	2	76.98	76.98	2	2	3	2	609758.58	609758.58	3	2	3	2	6851.22	6851.22
1	2	3	3	34.23	34.23	2	2	3	3	2772.63	2772.63	3	2	3	3	308.07	308.07
1	3	1	1	56.34	56.34	2	3	1	1	8112.96	8112.96	3	3	1	1	676.08	676.08
1	3	1	2	21.32	21.32	2	3	1	2	24645.92	24645.92	3	3	1	2	724.88	724.88
1	3	1	3	49.02	49.02	2	3	1	3	142942.32	142942.32	3	3	1	3	2647.08	2647.08
1	3	2	1	5.23	5.23	2	3	2	1	20757.87	20757.87	3	3	2	1	329.49	329.49
1	3	2	2	6.23	6.23	2	3	2	2	3295.67	3295.67	3	3	2	2	143.29	143.29
1	3	2	3	3.12	3.12	2	3	2	3	5768.88	5768.88	3	3	2	3	134.16	134.16
1	3	3	1	8.21	8.21	2	3	3	1	25746.56	25746.56	3	3	3	1	459.76	459.76
1	3	3	2	1.19	1.19	2	3	3	2	7239.96	7239.96	3	3	3	2	92.82	92.82
1	3	3	3	2.34	2.34	2	3	3	3	18954	18954	3	3	3	3	210.6	210.6

Table C.3: Sample of ESSI to MOOSE Tensor Converter Utility Test - Rank Four Tensor (Conversion from ESSI to MOOSE

i	j	k	l	MOOSE	ESSI	i	j	k	l	MOOSE	ESSI	i	j	k	l	MOOSE	ESSI
1	1	1	1	5.67	5.67	2	1	1	1	958.23	958.23	3	1	1	1	73.71	73.71
1	1	1	2	8.76	8.76	2	1	1	2	78.84	78.84	3	1	1	2	26.28	26.28
1	1	1	3	2.32	2.32	2	1	1	3	37.12	37.12	3	1	1	3	9.28	9.28
1	1	2	1	4.09	4.09	2	1	2	1	102.25	102.25	3	1	2	1	20.45	20.45
1	1	2	2	8.09	8.09	2	1	2	2	291.24	291.24	3	1	2	2	48.54	48.54
1	1	2	3	2.65	2.65	2	1	2	3	129.85	129.85	3	1	2	3	18.55	18.55
1	1	3	1	4.34	4.34	2	1	3	1	4.34	4.34	3	1	3	1	4.34	4.34
1	1	3	2	2.34	2.34	2	1	3	2	1237.86	1237.86	3	1	3	2	53.82	53.82
1	1	3	3	5.78	5.78	2	1	3	3	92.48	92.48	3	1	3	3	23.12	23.12
1	2	1	1	6.89	6.89	2	2	1	1	39796.64	39796.64	3	2	1	1	523.64	523.64
1	2	1	2	2.31	2.31	2	2	1	2	6735.96	6735.96	3	2	1	2	124.74	124.74
1	2	1	3	4.21	4.21	2	2	1	3	4311.04	4311.04	3	2	1	3	134.72	134.72
1	2	2	1	3.42	3.42	2	2	2	1	6925.5	6925.5	3	2	2	1	153.9	153.9
1	2	2	2	3.56	3.56	2	2	2	2	1883.24	1883.24	3	2	2	2	81.88	81.88
1	2	2	3	7.59	7.59	2	2	2	3	15369.75	15369.75	3	2	2	3	341.55	341.55
1	2	3	1	4.53	4.53	2	2	3	1	20335.17	20335.17	3	2	3	1	303.51	303.51
1	2	3	2	2.59	2.59	2	2	3	2	20515.39	20515.39	3	2	3	2	230.51	230.51
1	2	3	3	6.34	6.34	2	2	3	3	513.54	513.54	3	2	3	3	57.06	57.06
1	3	1	1	199.01	199.01	2	3	1	1	28657.44	28657.44	3	3	1	1	2388.12	2388.12
1	3	1	2	21.23	21.23	2	3	1	2	24541.88	24541.88	3	3	1	2	721.82	721.82
1	3	1	3	2.45	2.45	2	3	1	3	7144.2	7144.2	3	3	1	3	132.3	132.3
1	3	2	1	6.23	6.23	2	3	2	1	24726.87	24726.87	3	3	2	1	392.49	392.49
1	3	2	2	7.23	7.23	2	3	2	2	3824.67	3824.67	3	3	2	2	166.29	166.29
1	3	2	3	9.12	9.12	2	3	2	3	16862.88	16862.88	3	3	2	3	392.16	392.16
1	3	3	1	2.13	2.13	2	3	3	1	6679.68	6679.68	3	3	3	1	119.28	119.28
1	3	3	2	7.23	7.23	2	3	3	2	43987.32	43987.32	3	3	3	2	563.94	563.94
1	3	3	3	4.56	4.56	2	3	3	3	36936	36936	3	3	3	3	410.4	410.4

Table C.4: ESSI to MOOSE Tensor Converter Utility Test - Rank Four Tensor (Conversion from MOOSE to ESSI

Appendix D

Source Codes and Examples

A GIT repository has been set up on GitHub for the project related source code, examples and the documentation. The repository address is "`https://github.com/babakkamrani/MOOSE_ESSI.git`". Source and header files are in "`./src`" and "`./include`" folders respectively. They are organization structure and the place which they should be copied in the tensor mechanics module of MOOSE are:

1. "`./ESSI_Material`" includes the **"ESSI Material"** related and corresponding ESSI material library files. This folder should be copied to the "`./tensor_mechanics/src/materials/`"
2. "`./Moose_ESSI_Tensor_converter`" includes the **"Moose-ESSI-Tensor-converter"** related files. They should be copied to the "`./tensor_mechanics/src/utils/`".
3. "`./utils/nDarray`" folder includes the **"nDarray"** related files and this folder should be placed in "`./tensor_mechanics/src/utils/`".
4. "`./Examples`" includes the example files".
5. "`ESSI_Material.h`" should be included in "`TensorMechanicsApp.C`" to make the MOOSE work with the ESSI Material.