



Elmer

Software Development Practices APIs for Solver and UDF

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ElmerTeam

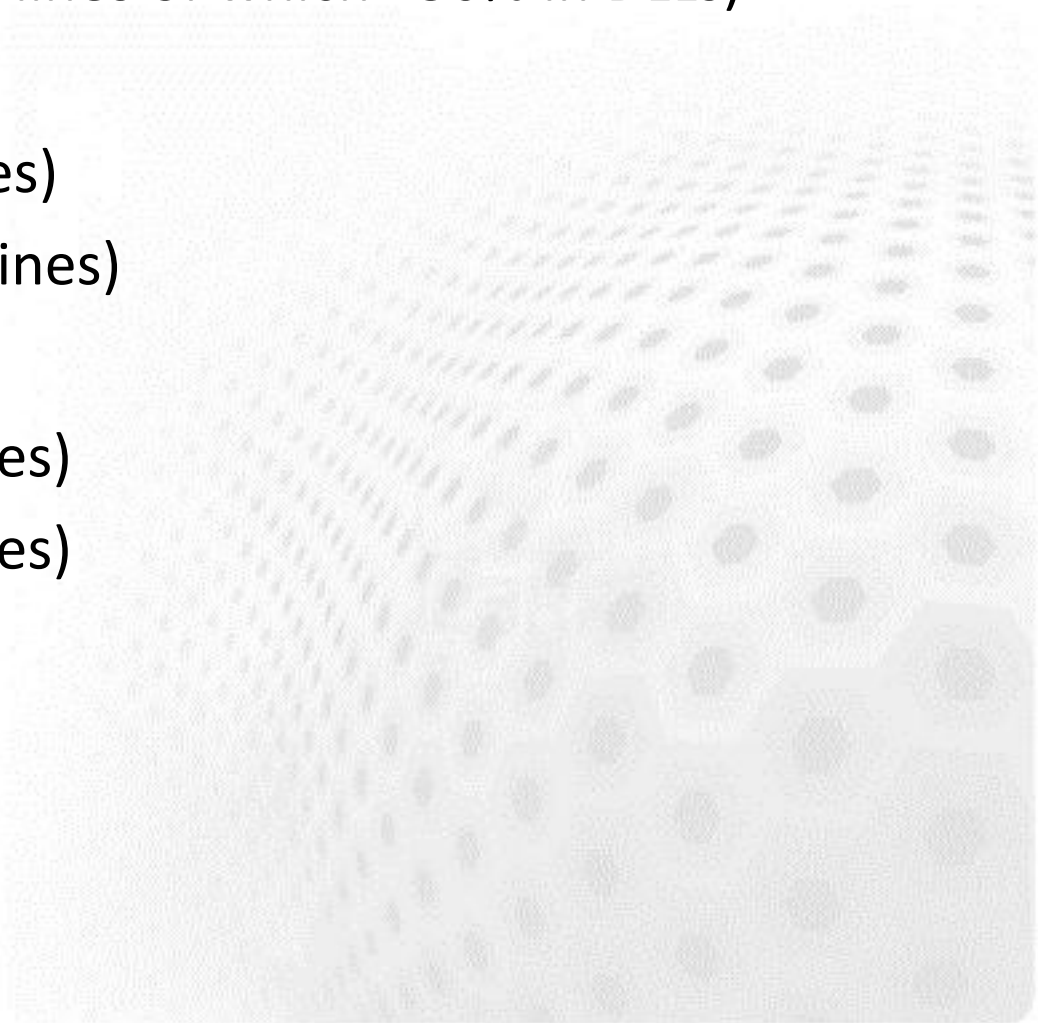
CSC – IT Center for Science

Warsaw, 21-22.10.2014

Elmer programming languages



- Fortran90 (and newer)
 - ElmerSolver (~240,000 lines of which ~50% in DLLs)
- C++
 - ElmerGUI (~18,000 lines)
 - ElmerSolver (~10,000 lines)
- C
 - ElmerPost (~45,000 lines)
 - ElmerGrid (~30,000 lines)
 - MATC (~11,000 lines)



Elmer libraries



➤ ElmerSolver

- Required: Matc, Hutilter, Lapack, Blas, Umfpack (GPL)
- Optional: Arpack, Mumps, Hypre, Pardiso, Trilinos, SuperLU, Cholmod, NetCDF, HDF5, ...

➤ ElmerGUI

- Required: Qt, ElmerGrid, Netgen
- Optional: Tetgen, OpenCASCADE, VTK, QVT

Elmer licenses



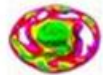
- ElmerSolver library is published under LGPL
 - Enables linking with all license types
 - It is possible to make a new solver even under propriety license
 - Note: some optional libraries may constrain this freedom
- Rest of Elmer is published under GPL
 - Derived work must also be under same license (“copyleft”)

Elmer at sourceforge.net



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Summary Files Reviews Support Develop Tracker Code



Elmer finite element software

apursula, juhar, juhavierinen, mlsf, mmalinen, raback, sjsillan, tzwinger

54 Recommendations

305 Downloads (This Week)

Tweet 0

+1 0

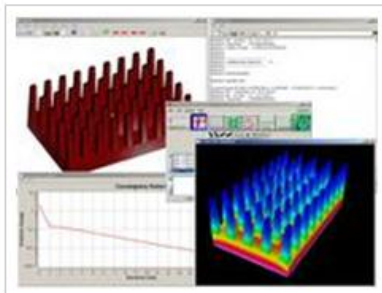
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Elmer-svn5475-2011-12-16.exe

Browse All Files



Description

Elmer is a finite element software for numerical solution of partial differential equations and multiphysical problems. It includes models of structural mechanics, fluid dynamics, heat transfer, electromagnetics etc. Elmer home is www.csc.fi/elmer

[Elmer finite element software Web Site >](http://www.csc.fi/elmer)

//

QUATTRO TITANIUM

10 000
näytepakkausta jaossa
KLIKKAA TÄSTÄ!

TreeGrid Web Gantt Chart

Fully customizable, fully interactive, auto and manual scheduling, 1000s tasks
Tasks, milestones, flags, dependencies (ss,fs,ff,lg; floats), constraints
Percent completion, price calculation, critical path, holidays, smooth zoom
Resources assigning, resource charts, any custom columns, custom bars
Sorting, filtering, grouping, tree, printing / PDF, paging, AJAX, localization



Obtaining the source code



- Note: elmerfem repository at sf.net was migrated into a new svn server in Jan 2013
- To check-out the code anonymously:
**svn checkout
svn://svn.code.sf.net/p/elmerfem/code/trunk
elmerfem-code**
- To check-out the code with a sf.net username:
**svn checkout --username=raback
svn+ssh://raback@svn.code.sf.net/p/elmerfem/code/trunk
elmerfem-code**
- We don't utilize branches and consider the trunk version to be stable and always backward compatible
 - The things under development may be little bit volatile

Code organization



Directory listing of elmerfem/trunk:

Name	Date modified	Type	
buildtools	25.11.2010 14:33	File folder	
eio	25.11.2010 14:37	File folder	Library for reading the mesh
elmergrid	18.4.2011 23:13	File folder	ElmerGrid
ElmerGUI	25.11.2010 14:37	File folder	ElmerGUI
ElmerGUIlogger	18.4.2011 23:13	File folder	
ElmerGUItester	25.11.2010 14:35	File folder	
elmerparam	25.11.2010 14:34	File folder	ElmerParam
fem	16.9.2011 9:42	File folder	ElmerSolver
front	25.11.2010 14:35	File folder	ElmerFront (obsolete)
hutiter	25.11.2010 14:33	File folder	
matc	25.11.2010 14:33	File folder	MATC library
mathlibs	18.4.2011 23:13	File folder	Basic math libraries
meshgen2d	25.11.2010 14:37	File folder	Mesh2D (almost obsolete)
misc	16.8.2011 13:26	File folder	Miscellaneous features
post	25.11.2010 14:34	File folder	ElmerPost
umfpack	25.11.2010 14:34	File folder	Umfpack
utils	25.11.2010 14:35	File folder	Various utilities
LICENSES	25.11.2010 14:37	File	Information on LICENCES

Cmake transition



- We are moving from gnu autotools to cmake
- Motivation
 - Cross compilation difficult with gnu autotools (configure & make)
 - Our installation script was quite hackish
 - Package creation difficult – our Windows installer creation was broken
 - Something had to be done
- Cmake is the solution?
 - Enables cross compilation (e.g. Intel MICs)
 - Installation scripts easier to maintain
 - Easy creation of installers using cpack etc.

GitHub transition



- ➊ Elmer has been hosted at sourceforge.net since 2007 using subversion (svn)
 - It is rather cumbersome to use branches in svn
 - As an end-results we are working in one development tree only
- ➋ Git was developed by Linus Torvalds in host Linux kernel development
 - Distributed version control system
 - It is much easier to maintain several development branches
 - There are much more options and hence also the learning curve is a bit steeper
- ➌ GitHub is a portal providing Git and some additional services

Status of the Cmake & GitHub transition



- The cmake related changes into the code are disruptive
 - Choices required for cmake breaks the Gnu autotools scripts
- Cmake related development is already being carried out at GitHub
- Other development is still being carried out at SVN
 - Modifications are merged with the GitHub version
- When the cmake version is fully functional we will move all development to GitHub
 - Short transition period

Compilation of Elmer with cmake



The new version of Elmer that can be compiled with cmake is hosted at GitHub.
The development work is carried out in the "devel" branch.

```
# clone the git repository.
```

```
$ git clone https://www.github.com/ElmerCSC/elmerfem
```

```
# Switch to devel branch
```

```
$ cd elmerfem      $ cmake -DWITH_ELMERGUI:BOOL=FALSE -
```

```
$ git checkout devel WITH_MPI:BOOL=FALSE -
```

```
$ cd ..           DCMAKE_INSTALL_PREFIX=../install  
                  ../elmerfem
```

```
# create build directory
```

```
$ mkdir build
```

```
$ cd build
```

```
$ cmake <flags>
```

```
# You can tune the compilation parameters graphically with $ ccmake or $cmake-gui .
```

```
$ make install
```

```
# or alternatively compile in parallel (4 procs) $ make -j4 install
```

Installers



- Still partly under developed
- Fresh Windows installers
 - Currently only 64 bit version
 - Also a parallel version with msmpi
 - <http://www.nic.funet.fi/pub/sci/physics/elmer/bin/windows/>
- Elmer for Debian & Ubuntu etc. at launchpad
 - Nightly builds from Git repository
 - To install
 - \$ sudo apt-add-repository ppa:juhmat/elmer-test
 - \$ sudo apt-get update
 - \$ sudo apt-get install elmerfem-csc

Consistency tests



- Simple shell script to run through the cases + piece of C-code to compare the norm of solutions
- There are about 290 consistency tests (April 2014)
 - Located under fem/tests
- Each time a significant commit is made the tests are run with the fresh version
 - Aim: trunk version is a stable version
 - New tests for each major new feature
- The consistency tests provide a good starting point for taking some Solver into use
 - cut-paste from sif file
- Note: the consistency tests have often poor time and space resolution for rapid execution

Consistency tests - example



```
raback@hippu2:/fs/proj1/elmer/raback/elmerfem/fem/tests> ./runtests
$ELMER_HOME undefined, setting it to ../src
test 1 :                1dtests                [PASSED], CPU time=0.1
test 2 :                1sttime                [PASSED], CPU time=0.58
test 3 :                2ndtime                [PASSED], CPU time=1.09
test 4 :                AdvReactDG            [PASSED], CPU time=1.53
test 5 :                BlockLinElast1        [PASSED], CPU time=2.06
test 6 :                BlockLinElast2        [PASSED], CPU time=2.32
test 7 :                BlockLinElast3        [PASSED], CPU time=6.32
test 8 :                BlockPoisson1         [PASSED], CPU time=6.46
test 9 :                BlockPoisson2         [PASSED], CPU time=6.7
test 10 :               BlockPoisson3         [PASSED], CPU time=7.37
test 11 :               CapacitanceMatrix     [PASSED], CPU time=7.66
test 12 :               CavityLid            [PASSED], CPU time=8.46
test 13 :               CavityLid2           [PASSED], CPU time=14.21
test 14 :               ConditionalFlow look at [ConditionalFlow/test.log] for c
test 15 :               CoordinateScaling     [PASSED], CPU time=14.34
...
test 189 :              vortex3d              [PASSED], CPU time=809.12
Tests completed, passed: 188 out of total 189 tests
Cumulative CPU time used in test: 809.12 s
```

Doxygen – WWW documentation



The screenshot shows a Mozilla Firefox browser window with the address bar displaying `http://www.elmerfem.org/doxygen/modules.html`. The page title is "Elmer finite element software" and the subtitle is "preliminary version open for comments". The navigation menu includes "Main Page", "Related Pages", "Modules" (selected), "Data Types List", and "Files". A search box is located in the top right of the navigation area. The left sidebar contains a tree view with "Modules" expanded, showing sub-items like "Elmer library", "Utility programs", "Class List", "Data Types", "Data Fields", "File List", and "File Members". The main content area is titled "Modules" and contains the text "Here is a list of all modules:" followed by a bulleted list of modules and their sub-modules. The footer indicates the page was generated on "Fri Sep 16 2011 09:28:55" for Elmer finite element software by Doxygen 1.7.5.1.

Elmer finite element software: Modules - Mozilla Firefox

File Edit View History Bookmarks Tools Help

`http://www.elmerfem.org/doxygen/modules.html`

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Elmer finite element software

preliminary version open for comments

Main Page Related Pages **Modules** Data Types List Files Search

▼ Elmer finite element software

- ▶ Related Pages
- ▼ **Modules**
 - ▶ Elmer library
 - Dynamically linked solvers
 - Dynamically linked functions
 - ▶ Utility programs
 - ▶ Class List
 - Data Types
 - Data Fields
 - ▶ File List
 - File Members

Modules

Here is a list of all modules:

- **Elmer library**
 - Default API
- **Dynamically linked solvers**
- **Dynamically linked functions**
- **Utility programs**
 - Program ResultToPost
 - Program ResultToResult
 - Program ViewFactors

Generated on Fri Sep 16 2011 09:28:55 for Elmer finite element software by **doxygen** 1.7.5.1

Done

Doxygen – Example in code



Special comment indicators: !> and <!

```
!-----  
!> Subroutine for computing fluxes and gradients of scalar fields.  
!> For example, one may compute the the heat flux as the negative grad.  
!> field multiplied by the heat conductivity.  
!> \ingroup Solvers  
!-----  
SUBROUTINE FluxSolver( Model, Solver, dt, Transient )  
!-----  
USE CoordinateSystems  
USE DefUtils  
IMPLICIT NONE  
!-----  
TYPE(Solver_t) :: Solver    !< Linear & nonlinear equation solver options  
TYPE(Model_t)  :: Model    !< All model information (mesh, materials, BC  
REAL(KIND=dp) :: dt       !< Timestep size for time dependent simulation  
LOGICAL :: Transient     !< Steady state or transient simulation  
!-----  
!     Local variables  
!-----  
TYPE(ValueList_t), POINTER :: SolverParams
```


Doxygen – Example in WWWW



```
subroutine FluxSolver ( TYPE(Model_t) Model,  
                      TYPE(Solver_t) Solver,  
                      REAL(KIND=dp) dt,  
                      LOGICAL Transient  
                      )
```

Subroutine for computing fluxes and gradients of scalar fields. For example, one may compute the the heat flux as the negative gradient of temperature field multiplied by the heat conductivity.

Parameters:

Solver Linear & nonlinear equation solver options
Model All model information (mesh, materials, BCs, etc...)
dt Timestep size for time dependent simulations
Transient Steady state or transient simulation

References [BulkAssembly\(\)](#).

Here is the call graph for this function:



Compilation of the whole code



- To compile the whole code see example scripts under www.csc.fi/elmer and www.elmerfem.org

```
#!/bin/sh -f
# Compile Elmer modules and install it
# replace these with your compilers:
export CC=gcc
export CXX=g++
export FC=gfortran
export F77=gfortran

modules="matc umfpack mathlibs elmergrid meshgen2d eio hutiter fem"
for m in $modules; do
  cd $m
  make clean
  ./configure --prefix=/fs/proj1/elmer/raback/elmerbin
  make
  make install
  cd ..
done
```

Compilation of a DLL module



- Applies both to Solvers and User Defined Functions (UDF)
- Assumes that there is a working compile environment that provides "**elmerf90**" script
 - Comes with the Windows installer, and Linux packages
 - Generated automatically when ElmerSolver is compiled

```
elmerf90 MySolver.f90 -o MySolver.so
```

Elmer – High level abstractions



- The quite good success of Elmer as a multiphysics code may be addressed to certain design choices
 - Solver is an abstract dynamically loaded object
 - Parameter value is an abstract property fetched from a list
- The abstractions mean that new solvers may be implemented without much need to touch the main library
 - Minimizes need of central planning
 - Several applications fields may live their life quite independently (electromagnetics vs. glaciology)
- MATC – a poor man's Matlab adds to flexibility as algebraic expressions may be evaluated on-the-fly

Solver as an abstract object



- Solver is an dynamically loaded object (.dll or .so)
 - May be developed and compiled seperately
- Solver utilizes heavily common library utilities
 - Most common ones have interfaces in DefUtils
- Any solver has a handle to all of the data
- Typically a solver solves a weak form of a differential equation
- Currently ~50 different Solvers,
roughly half presenting physical phenomena
 - No upper limit to the number of Solvers
- Solvers may be active in different domains,
and even meshes
- The menu structure of each solver in ElmerGUI may be
defined by an `.xml` file

Property as an abstract object



- Properties are saved in a list structure by their name
- Namespace of properties is not fixed, they may be introduced in the command file
 - E.g. `"MyProperty = Real 1.23"` adds a property "MyProperty" to a list structure related to the solver block
- In code parameters are fetched from the list
 - E.g. `"val = GetReal(Material, 'MyProperty', Found)"` retrieves the above value 1.23 from the list
- A "Real" property may be any of the following
 - Constant value
 - Linear or cubic dependence via table of values
 - Expression given by MATC (MatLab-type command language)
 - User defined functions with arbitrary dependencies
 - Real vector or tensor
- As a result solvers may be weakly coupled without any *a priori* defined manner
- There is a price to pay for the generic approach but usually it is less than 10%
- `SOLVER.KEYWORDS` file may be used to give the types for the keywords in the command file

- DefUtils module includes wrappers to the basic tasks common to standard solvers
 - E.g. "**DefaultDirichlet()**" sets Dirichlet boundary conditions to the given variable of the Solver
 - E.g. "**DefaultSolve()**" solves linear systems with all available direct, iterative and multilevel solvers, both in serial and parallel
- Programming new Solvers and UDFs may usually be done without knowledge of other modules

DefUtils – some functions



Public Member Functions

TYPE(Solver_t) function, pointer	GetSolver ()
TYPE(Matrix_t) function, pointer	GetMatrix (USolver)
TYPE(Mesh_t) function, pointer	GetMesh (USolver)
TYPE(Element_t) function, pointer	GetCurrentElement (Element)
INTEGER function	GetElementIndex (Element)
INTEGER function	GetNOFActive (USolver)
REAL(KIND=dp) function	GetTime ()
INTEGER function	GetTimeStep ()
INTEGER function	GetTimeStepInterval ()
REAL(KIND=dp) function	GetTimestepSize ()
REAL(KIND=dp) function	GetAngularFrequency (ValueList, Found)
INTEGER function	GetCoupledIter ()
INTEGER function	GetNonlinIter ()
INTEGER function	GetNOFBoundaryElements (UMesh)
subroutine	GetScalarLocalSolution (x, name, UElement, USolver, tStep)
subroutine	GetVectorLocalSolution (x, name, UElement, USolver, tStep)
INTEGER function	GetNofEigenModes (name, USolver)
subroutine	GetScalarLocalEigenmode (x, name, UElement, USolver, NoEigen, ComplexPart)
subroutine	GetVectorLocalEigenmode (x, name, UElement, USolver, NoEigen, ComplexPart)
CHARACTER(LEN=MAX_NAME_LEN) function	GetString (List, Name, Found)
INTEGER function	GetInteger (List, Name, Found)
LOGICAL function	GetLogical (List, Name, Found)
recursive REAL(KIND=dp) function	GetConstReal (List, Name, Found, x, y, z)
recursive REAL(KIND=dp) function	GetCReal (List, Name, Found)
recursive REAL(KIND=dp) function, dimension(:), pointer	GetReal (List, Name, Found, UElement)

Solver API



```
!-----  
!> Standard API for Solver  
!-----  
SUBROUTINE MySolver( Model, Solver, dt, Transient )  
!-----  
    USE DefUtils  
    IMPLICIT NONE  
!-----  
    TYPE(Solver_t) :: Solver    !< Current solver  
    TYPE(Model_t)  :: Model     !< Handle to all data  
    REAL(KIND=dp) :: dt        !< Timestep size  
    LOGICAL :: Transient       !< Time-dependent or not  
!-----  
    Actual code ...
```

Solver API



```
Solver 1
```

```
Equation = "MySolver"
```

```
Procedure = "MyModule" "MySolver"
```

```
...
```

```
End
```

- Solver is typically a FEM implementation of a physical equation
- But it could also be an auxiliary solver that does something completely different
- Solver is usually called once for each coupled system iteration

User defined function API



```
!-----  
!> Standard API for UDF  
!-----  
FUNCTION MyProperty( Model, n, t ) RESULT(f)  
!-----  
    USE DefUtils  
    IMPLICIT NONE  
!-----  
    TYPE(Model_t) :: Model    !< Handle to all data  
    INTEGER :: n              !< Current node  
    REAL(KIND=dp) :: t        !< Parameter(s)  
    REAL(KIND=dp) :: f        !< Parameter value at node  
!-----  
    Actual code ...
```


Function API



```
MyProperty = Variable time  
"MyModule" "MyProperty"
```

- User defined function (UDF) typically returns a real valued property at a given point
- It can be located in any section that is used to fetch these values from a list
 - Boundary Condition, Initial Condition, Material,...

Example: Poisson equation

$$-\nabla^2 \phi = \rho$$


- Implemented as an dynamically linked solver
 - Available under tests/1dtests
- Compilation by:
Elmerf90 Poisson.f90 -o Poisson.so
- Execution by:
ElmerSolver case.sif
- The example is ready to go massively parallel and with all a plethora of elementtypes in 1D, 2D and 3D

Poisson equation: code Poisson.f90



```
!-----  
!> Solve the Poisson equation  $-\nabla \cdot \nabla \phi = \rho$   
!-----  
SUBROUTINE PoissonSolver( Model,Solver,dt,TransientSimulation )  
!-----  
USE DefUtils  
IMPLICIT NONE  
...  
  
!Initialize the system and do the assembly:  
!-----  
CALL DefaultInitialize()  
  
active = GetNOFActive()  
DO t=1,active  
  Element => GetActiveElement(t)  
  n = GetElementNOFNodes()  
  
  LOAD = 0.0d0  
  BodyForce => GetBodyForce()  
  IF ( ASSOCIATED(BodyForce) ) &  
    Load(1:n) = GetReal( BodyForce, 'Source', Found )  
  
  ! Get element local matrix and rhs vector:  
  !-----  
  CALL LocalMatrix( STIFF, FORCE, LOAD, Element, n )  
  
  ! Update global matrix and rhs vector from local contribs  
  !-----  
  CALL DefaultUpdateEquations( STIFF, FORCE )  
END DO  
  
CALL DefaultFinishAssembly()  
CALL DefaultDirichletBCs()  
Norm = DefaultSolve()
```

CONTAINS

```
!-----  
SUBROUTINE LocalMatrix( STIFF, FORCE, LOAD, Element, n )  
!-----  
...  
  
CALL GetElementNodes( Nodes )  
STIFF = 0.0d0  
FORCE = 0.0d0  
  
! Numerical integration:  
!-----  
IP = GaussPoints( Element )  
DO t=1,IP % n  
  ! Basis function values & derivatives at the integration point:  
  !-----  
  stat = ElementInfo( Element, Nodes, IP % U(t), IP % V(t), &  
    IP % W(t), detJ, Basis, dBasisdx )  
  
  ! The source term at the integration point:  
  !-----  
  LoadAtIP = SUM( Basis(1:n) * LOAD(1:n) )  
  
  ! Finally, the elemental matrix & vector:  
  !-----  
  STIFF(1:n,1:n) = STIFF(1:n,1:n) + IP % s(t) * DetJ * &  
    MATMUL( dBasisdx, TRANSPOSE( dBasisdx ) )  
  FORCE(1:n) = FORCE(1:n) + IP % s(t) * DetJ * LoadAtIP * Basis(1:n)  
END DO  
!-----  
END SUBROUTINE LocalMatrix  
!-----  
END SUBROUTINE PoissonSolver  
!-----
```

Poisson equation: command file case.sif



Check Keywords "Warn"

Header

Mesh DB "." "mesh"

End

Simulation

Coordinate System = "Cartesian"

Simulation Type = Steady State

Steady State Max Iterations = 50

End

Body 1

Equation = 1

Body Force = 1

End

Equation 1

Active Solvers(1) = 1

End

Solver 1

Equation = "Poisson"

Variable = "Potential"

Variable DOFs = 1

Procedure = "Poisson" "PoissonSolver"

Linear System Solver = "Direct"

Linear System Direct Method = umfpack

Steady State Convergence Tolerance = 1e-09

End

Body Force 1

Source = Variable Potential

Real Procedure "Source" "Source"

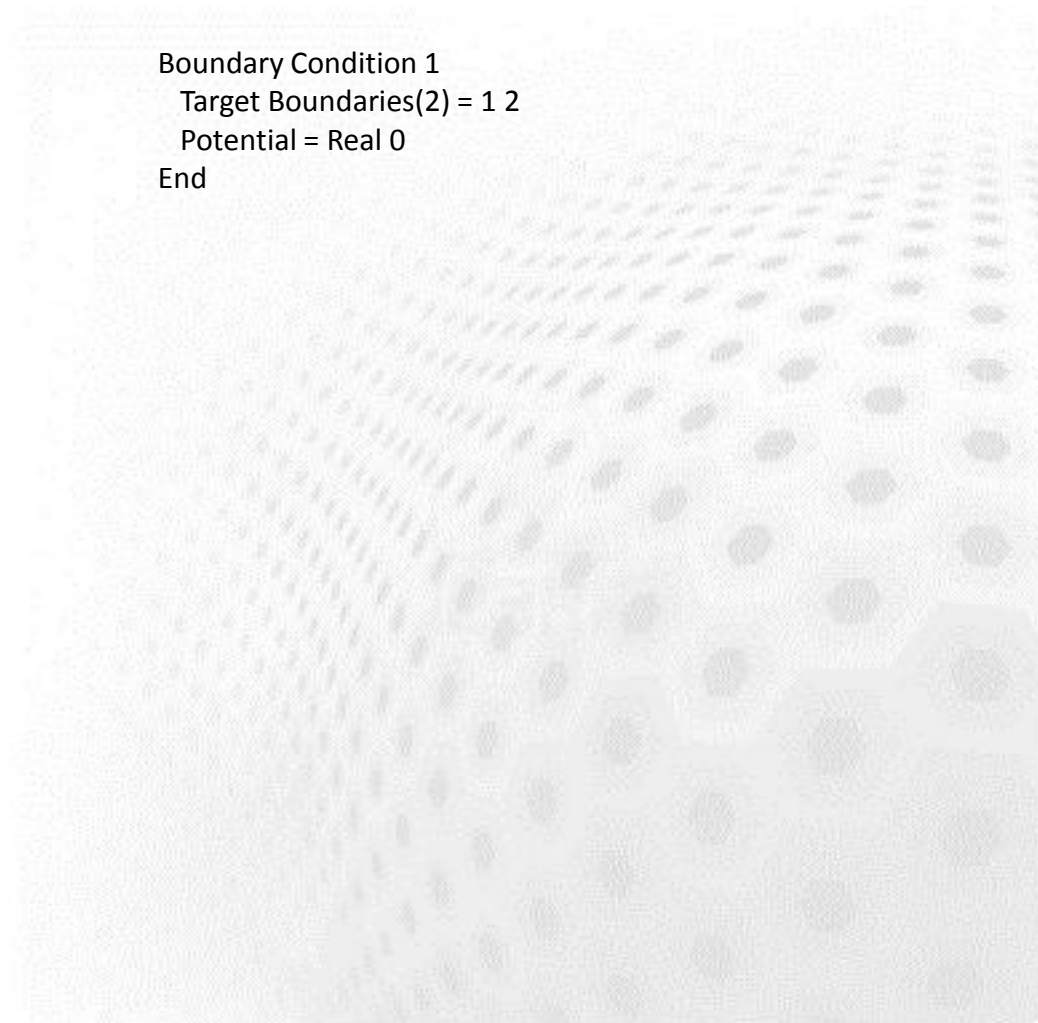
End

Boundary Condition 1

Target Boundaries(2) = 1 2

Potential = Real 0

End



Poisson equation: source term, examples



Constant source:

```
Source = 1.0
```

Source depending piecewise linear on x:

```
Source = Variable Coordinate 1
Real
  0.0 0.0
  1.0 3.0
  2.0 4.0
End
```

Source depending on x and y:

```
Source = Variable Coordinate
Real MATC "sin(2*pi*tx(0))*cos(2*pi(tx(1)))"
```

Source depending on anything

```
Source = Variable Coordinate 1
Procedure "Source" "MySource"
```


Poisson equation: ElmerGUI menus



```
<?xml version='1.0' encoding='UTF-8'?>
<!DOCTYPE edf>
<edf version="1.0" >
  <PDE Name="Poisson" >
    <Name>Poisson</Name>

    <BodyForce>
      <Parameter Widget="Label" > <Name> Properties </Name> </Parameter>
        <Parameter Widget="Edit" >
          <Name> Source </Name>
          <Type> String </Type>
          <Whatis> Give the source term. </Whatis>
        </Parameter>
      </BodyForce>

      <Solver>
        <Parameter Widget="Edit" >
          <Name> Procedure </Name>
          <DefaultValue> "Poisson" "PoissonSolver" </DefaultValue>
        </Parameter>
        <Parameter Widget="Edit">
          <Name> Variable </Name>
          <DefaultValue> Potential</DefaultValue>
        </Parameter>
      </Solver>

      <BoundaryCondition>
        <Parameter Widget="Label" > <Name> Dirichlet conditions </Name> </Parameter>
        <Parameter Widget="Edit">
          <Name> Potential </Name>
          <Whatis> Give potential value for this boundary. </Whatis>
        </Parameter>
      </BoundaryCondition>
    </PDE>
  </edf>
```

Development tools for ElmerSolver



➤ Basic use

- Editor (emacs, vi, notepad++, jEdit,...)
- elmerf90 script

➤ Advanced

- Editor
- svn client
- Compiler suite (gfortran, ifort, pathf90, pgf90,...)
- Documentation tools (Doxygen, LaTeX)
- Debugger (gdb)
- Profiling tools
- ...

Elmer – some best practices



- Use version control when possible
 - If the code is left to your own local disk, you might as well not write it at all
 - Never fork! (userbase of 1000's)
- Always make a consistency test for a new feature
 - Always be backward compatible
 - If not, implement a warning to the code
- Maximize the level of abstraction
 - Essential for multiphysics software
 - E.g. any number of physical equations, any number of computational meshes, any number of physical or numerical parameters – without the need for recompilation

Migration to cmake



- We're in the process in going from gnu autotools to cmake
- The change is hoped to help in development and packing on different platforms
 - Intel MICs
 - Windows distribution
- The change is disruptive for some interfaces
 - We will start to utilize iso-C bindings
- Development version under development in github
- Developments will become the main Elmer distribution hopefully during summer months
- Going on in: <https://github.com/ElmerCSC/elmerfem>