

Elmer

Software Development Practices APIs for Solver and UDF

ElmerTeam
CSC – IT Center for Science

Elmer programming languages



- Fortran90 (and newer)
 - ElmerSolver (~"280,000 lines of which ~50% in DLLs)
- - ElmerGUI (~18,000 lines)
 - ElmerSolver (~15,000 lines)
- C
 - ElmerPost (~45,000 lines)
 - ElmerGrid (~30,000 lines)
 - MATC (~11,000 lines)

Tools for Elmer development



- Programming languages
 - Fortran90 (and newer), C, C++
- Compilation
 - Compiler (e.g. gnu), configure, automake, make, (cmake)
- Editing
 - emacs, vi, notepad++,...
- Code hosting (git)
 - https://github.com/ElmerCSC
- Consistency tests
 - Currently around 450
- Code documentation
 - Doxygen
- Theory documentation
 - Latex
- Community server
 - www.elmerfem.org (forum, wiki, etc.)

Elmer libraries



ElmerSolver

- Required: Matc, Hutlter, 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 proprierity license
 - Note: some optional libraries may constrain this freedom due to use of GPL licences
- Most other parts of Elmer published under GPL
 - Derived work must also be under same license ("copyleft")
- Proprierity modules linked with ElmerSolver may be freely licensed if they are not derived work
 - Note that you must not violete licences of other libraries

Elmer version control at GitHub



- In 2015 the official version control of Elmer was transferred from svn at sf.net to git hosted at GitHub
- Git offers more flexibility over svn
 - Distributed version control system
 - Easier to maintain several development branches
 - More options and hence also steeper learning curve
 - Developed by Linus Torvalds to host Linux kernel development
- GitHub is a portal providing Git and some additional servives
 - Management of user rights
 - Controlling pull requests

Directory listing of elmerfem/trunk with TortoiseGIT

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Consistency tests



- Utilize ctest system to run a set of Elmer cases
 - Upon success each case writes 1 to file TEST.PASSED, and on failure 0, respectively
- There are more than 460 consistency tests (Nov 2016)
 - Located under fem/tests
- Each time a significant commit is made the tests are run with the fresh version
 - Aim: even devel version is a stable
 - 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 resolution

Executing the consistency tests of Elmer

Total Test time (real) = 365.62 sec



```
>ctest -j4 -LE elmerice
       Start 143: mgdyn torus harmonic
       Start 304: ThermalActuator
       Start 344: RotatingBCMagnetoDynamicsGeneric
 1/310 Test #344: RotatingBCMagnetoDynamicsGeneric ...
                                                    Passed
                                                           43.18 sec
       Start 293: mgdyn lamstack lowfreg harmonic
 Passed 59.78 sec
       Start 222: mgdyn transient loss
 3/310 Test #293: mgdyn lamstack lowfreg harmonic ....
                                                            21.80 sec
       Start 322: mgdyn bh
308/310 Test #46: CoupledPoisson7 ..............
                                                    Passed
                                                             0.38 sec
                                                    Passed
309/310 Test #212: CoordinateScaling ............
                                                             0.38 sec
       Start 54: RotatingBCPoisson3DSymmSkev
310/310 Test #54: RotatingBCPoisson3DSymmSkev ......
                                                    Passed
                                                             6.34 sec
100% tests passed, 0 tests failed out of 310
```

Cmake build system



- During 2014-2015 Elmer was migrated from gnu autotools into cmake
- Cmake offers several advantages
 - Enables cross compilation for diffirent platforms (e.g. Intel MICs)
 - More standardizes installation scripts
 - Straight-forward package creation for many systems (using cpack)
 - Great testing utility with ctest now also in parallel
- Transition to cmake required significant code changes
 - ISO C-bindings & many changes in APIs
 - Backward compatibility in compilation lost

Compiling fresh Elmer source from GitHub



```
# clone the git repository. $ git clone <a href="https://www.github.com/ElmerCSC/elmerfem">https://www.github.com/ElmerCSC/elmerfem</a>
```

```
# Switch to devel branch (currently the default branch)
$ cd elmerfem
$ git checkout devel
$ cd ..
```

```
# create build directory
$ mkdir build
$ cd build
```

```
$ cmake -DWITH_ELMERGUI:BOOL=FALSE -
DWITH_MPI:BOOL=FALSE -
DCMAKE_INSTALL_PREFIX=../install ../elmerfem
```

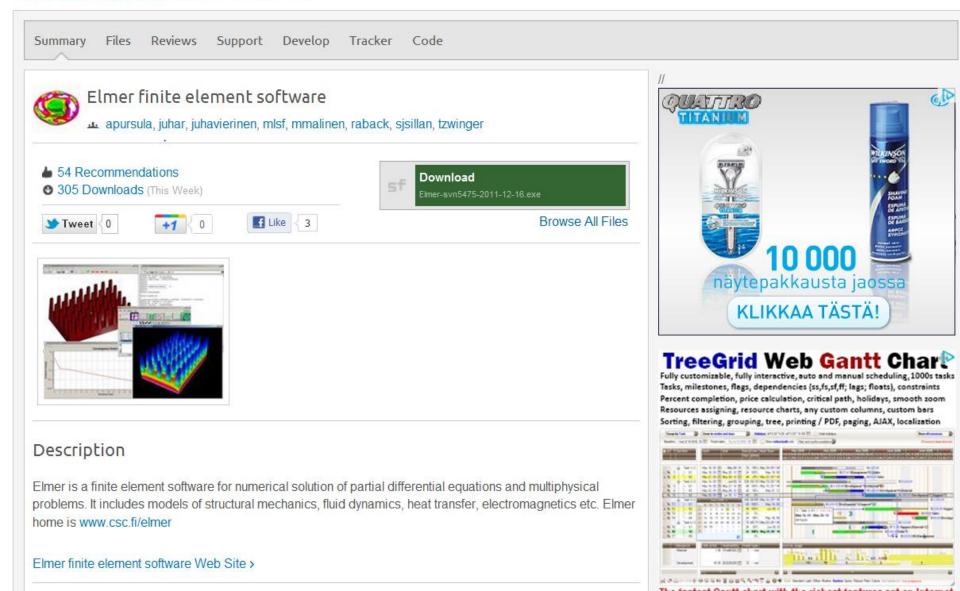
```
$ cmake <flags>
# You can tune the compilation parameters graphically with $ ccmake or $cmake-gu
```

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

Elmer binaries at sourceforge.net

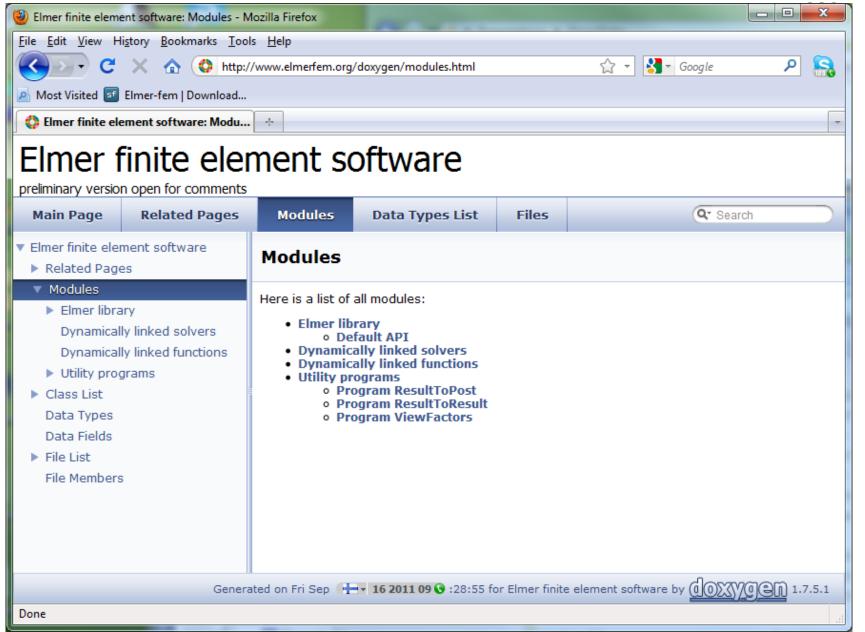


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Doxygen – WWW documentation





Doxygen – Example in code



Special comment indicators: !> and <!</p>

```
!> 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, Bo
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 WWW



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:

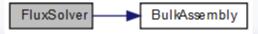
Solver Linear & nonlinear equation solver options

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:



Installers



- 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:elmer-csc-ubuntu/elmer-csc-ppa
 - \$ sudo apt-get update
 - \$ sudo apt-get install elmerfem-csc

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

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)</pre>
  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,...

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

Elmer – High level abstractions



- The quite good success of Elmer as a multiphysics code may be addressed to certain design choices
 - Solver is an asbtract dynamically loaded object
 - Parameter value is an abstract property feethed 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. glaceology)
- MATC a poor man's Matlab adds to flexibility as algebraic expressions may be evalueted 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 ~60 different Solvers, roughly half presenting physical phenomena
 - No upper limit to the number of Solvers
 - Often cases include ~10 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

Code structure



- Elmer code structure has evolved over the years
 - There has been no major restructuring operations
- Ufortunately there is no optimal hierarchy and the number of subroutines is rather large
 - ElmerSolver library consists of more than ~40 modules
 - There are all-in-all around 1050 SUBROUTINES and 650 FUNCTIONS (both internal and external)
- To ease the learning curve the most important routines for basic use have been collected into module DefUtils.F90

DefUtils



- 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	, , , , , , , , , , , , , , , , , , ,
recursive REAL(KIND=dp) function	GetCReal (List, Name, Found)
recursive REAL(KIND=dp)	
function, dimension(:),	
pointer	GetReal (List, Name, Found, UElement)

Modules related to linear algebra



BandMatrix.F90

BandwidthOptimize.F90

BlockSolve.F90

cholmod.c

CircuitUtils.F90

ClusteringMethods.F90

CRSMatrix.F90

DirectSolve.F90

EigenSolve.F90

IterativeMethods.F90

IterSolve.F90

LinearAlgebra.F90

LUDecomposition.F90

MGPrec.F90

Multigrid.F90

Smoothers.F90

SolveBand.F90

SolveHypre.c

SolverUtils.F90

SolveSBand.F90

SolveSuperLU.c

SolveTrilinos.cxx

Modules related to space and time discretization



ElementDescription.F90

ElementUtils.F90

H1ElementBasisFunctions.F90

PElementBase.F90

PElementMaps.F90

TimeIntegrate.F90

Historical modules including physics



Differentials.F90

DiffuseConvectiveAnisotropic.F90

DiffuseConvectiveGeneralAnisotropic.F90

ExchangeCorrelations.F90

MaxwellAxiS.F90

Maxwell.F90

MaxwellGeneral.F90

NavierStokesCylindrical.F90

NavierStokes.F90

NavierStokesGeneral.F90

Stress.F90

StressGeneral.F90

VelocityUpdate.F90

Walls.F90

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, Transient Simulation )
 ·----
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:
   1-----
   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"
Fnd
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 dependeing 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



```
CSC
<?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> "Poisosn" "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
 - Do not 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