Elmer

Software Development Practices
APIs for Solver and UDF

ElmerTeam

CSC – IT Center for Science Ltd.

PATC Elmer Course
CSC, August 2012

Elmer programming languages

- Fortran90 (and newer)
  - ElmerSolver (~200,000 lines of which ~50% in DLLs)
- C++
  - ElmerGUI (~18,000 lines)
  - ElmerSolver (~10,000 lines)
- C
  - ElmerPost
  - ElmerGrid (~30,000 lines)
  - MATC (~11,000 lines)

Elmer libraries

- ElmerSolver
  - Required: matc, hutiter, eio, lapack, blas, umfpack
  - Optional: Arpack, mumps, Hypre, Pardiso, …
- ElmerGUI
  - Required: Qt, elmergrid, netgen
  - Optional: tetgen, OpenCASCADE, VTK, QVT

Elmer licenses

- ElmerSolver library is published under LGPL
  - Enables linking with all license types
- Rest of Elmer is published under GPL
  - Derived work must also be under same license

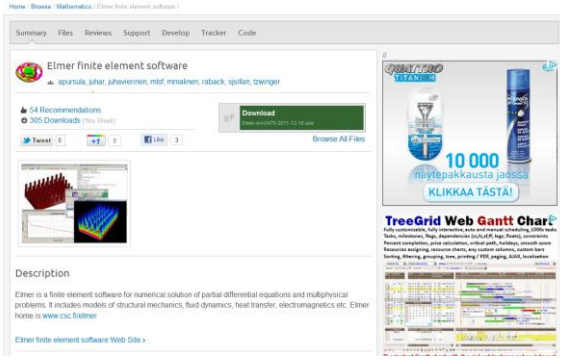
SVN - Version control system

- Elmer uses svn version control system for the code repository
  - Hosted at sourgeforge.net (aka sf.net)
  - Development version in ”trunk” is considered stable
  - To obtain the whole source code

```
svn co https://elmerfem.svn.sourceforge.net/
svnroot/elmerfem/trunk elmerfem
```

  - svn client available in command line in unix systems
  - In Windows systems a nice graphical client is “TortoiseSVN”

Elmer at sourceforge.net



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 (obsolite)
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 obsolite)
misc	16.8.2011 13:26	File folder	Miscallenous 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

Consistency tests

- There are about 200 consistency tests (Feb 2012)
- The tests are located under fem/tests
- Each time a significant commit is made the tests are run with the fresh version
- When new feature is added a corresponding consistency test is usually created
- 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
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
```

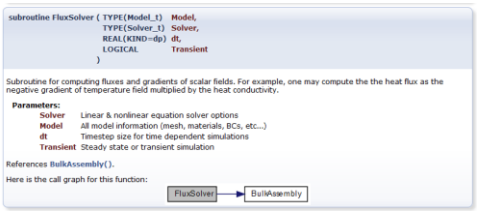
Doxygen – WWW documentation

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 option
TYPE(Model_t) :: Model    !< All model information (mesh, materials, B
REAL(KIND=dp) :: dt       !< Timestep size for time dependent simulati
LOGICAL :: Transient      !< Steady state or transient simulation
!------------------------------------------------------------------------
!    Local variables
!------------------------------------------------------------------------
TYPE(ValueList_t),POINTER :: SolverParams
```

Doxygen – Example in WWW



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
```

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

- 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. "`DefaulSolve()`" 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 …
```

User defined function API

```
!------------------------------------------------------------
!> Standard API for UDF
!------------------------------------------------------------
FUNCTION Source( 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 …
```

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 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

```
<?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
  - …