

Overview of Elmer

CSC – IT Center for Science

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1 Introduction

This exposition gives an overview of the Elmer software package. General information on the capabilities of the software, its usage, and how the material of the package is organized is presented. More detailed information is given in the other Elmer manuals, the scopes of which are described in this document.

What is Elmer

Elmer is a finite element software package for the solution of partial differential equations. Elmer can deal with a great number of different equations, which may be coupled in a generic manner making Elmer a versatile tool for multiphysical simulations. As an open source software, Elmer also gives the user the means to modify the existing solution procedures and to develop new solvers for equations of interest to the user.

History of Elmer

The development of Elmer was started in 1995 as part of a national CFD technology program funded by the Finnish funding agency for technology and innovation, Tekes. The original development consortia included partners from CSC – IT Center for Science (formerly known as CSC – Scientific Computing), Helsinki University of Technology TKK, VTT Technical Research Centre of Finland, University of Jyväskylä, and Okmetic Ltd. CSC is a governmental non-profit company fully owned by the Ministry of Education. After the five years initial project ended the development has been continued by CSC in different application fields.

Licensing

In September 2005 Elmer was released under GNU General Public License (GPL). This has widened the user community, particularly the number of international users has grown. However, as the sole owner of the copyright to Elmer source code, CSC may distribute Elmer also under other licensing terms. Therefore, if GPL does not suit your purposes, you may contact the Elmer team for other licensing options.

Distribution

Elmer is distributed only through the Internet. The actual distribution site may vary but the pointer to the location may always be found at <http://www.csc.fi/elmer>.

The distribution of Elmer comes in three different parts: sources, binaries, and documentation. Unix users are encouraged to compile the software themselves. The compilation instructions are given at the www-page. For Windows and Macintosh a precompiled binary version of the code is also provided. The documentation of the software is already quite extensive, but unfortunately still not complete.

Contributing

Everybody is welcome to contribute to the Elmer project. Often the bottle-neck is in case specification, testing and verification which may be done without in-depth knowhow of the code. Also contributions to the code are welcome. However, before granting a permission to commit to the main source file archive a Elmer Contributor Agreement has to be signed. This gives CSC the right to use contributions to Elmer under the current free software license, and also under other licenses we may use. However, this does not limit the contributors right to use the contributed code in any way.

2 Key features of Elmer

Elmer offers a wide range of methods and techniques for the computational modeling of physical phenomena described by partial differential equations. In the following some of the most essential ones are summarized.

Physical models in Elmer

The Elmer package contains solvers for a variety of mathematical models. The following list summarizes the capabilities of Elmer in specialized fields.

- Heat transfer: models for conduction, radiation and phase change
- Fluid flow: the Navier-Stokes, Stokes and Reynolds equations, $k-\epsilon$ model
- Species transport: generic convection-diffusion equation
- Elasticity: general elasticity equations, dimensionally reduced models for plates and shells
- Acoustics: the Helmholtz equation
- Electromagnetism: electrostatics, magnetostatics, induction
- Microfluidics: slip conditions, the Poisson-Boltzmann equation
- Levelset method: Eulerian free boundary problems
- Quantum Mechanics: density functional theory (Kohn-Sham)

Numerical methods in Elmer

For approximation and linear system solution Elmer offers a great number of possibilities. The following list summarizes some of the most essential ones.

- All basic element shapes in 1D, 2D and 3D with the Lagrange shape functions of degree $k \leq 2$
- Higher degree approximation using p -elements
- Time integration schemes for the first and second order equations
- Solution methods for eigenvalue problems
- Direct linear system solvers (Lapack & Umfpack)
- Iterative Krylov subspace solvers for linear systems
- Multigrid solvers (GMG and AMG) for some basic equations
- ILU preconditioning of linear systems
- Parallelization of iterative methods
- The discontinuous Galerkin method
- Stabilized finite element formulations, including the methods of residual free bubbles and SUPG
- Adaptivity, particularly in 2D
- BEM solvers (without multipole acceleration)

Pros and Cons of Elmer

Potential users may find a list of the possible pros and cons of Elmer package useful. The following summary is naturally open to subjective judgment and not complete either.

- + Since Elmer is an open source product, it is possible to verify and modify the solution procedures.
- + Elmer has a modern programmable graphical user interface.
- + Elmer can handle the coupling of field equations in a flexible manner and new field variables can be introduced easily.
- + All material parameters may depend on the field variables and other parameters in a free manner.
- + Elmer offers a large selection of modern numerical methods.
- + Elmer enables the user to use most generally used finite elements.
- + Assembly and iterative solution can also be done in parallel. Good scaling has been obtained up to thousands of processors.
- + Elmer has a graphical preprocessing interface for simple problem setups.
- + Elmer is easily compiled for most Unix systems and it is also available for Windows and some Linux distributions in precompiled binaries.
- + Elmer has a steadily growing user community and it has already been used in tens of scientific papers.
- The different aspects of the code (solver, interface, documentation) are not always at the same development phase. For example documentation is not up-to-date and interface lacks many of the more esoteric physical models provided by the solver.
- Getting acquainted with the large package may take time. Previous experience on FEM packages may therefore be useful.
- Elmer itself does not include proper geometry or mesh generation tools for geometrically complicated problems. Only mesh import interfaces are supported.
- As a multiphysical solver Elmer may sometimes lack features in some areas that are standard for established single-field codes. Thus, some users may find the capabilities of Elmer inadequate for their needs.

3 Elmer executables

As most finite element packages, Elmer is divided into a number of separate executables that may also be used independently. The main parts are the preprocessor, solver and postprocessor, but there are also other modules that may be called for specific assignments.

ElmerGUI

ElmerGUI is the graphical user interface for Elmer software based on the Qt cross-platform application framework (see. <http://qt.nokia.com/>). ElmerGUI includes elmergrid, and optionally tetlib and nglib, as finite element mesh generators. Also OpenCASCADE may be included as the CAD import tool. ElmerGUI does not include any geometry definition tools so for defining the original geometry some other software must be used. However, the large number of supported formats should make the mesh import straight-forward. With ElmerGUI the problem setup may be done easily using programmable menu structures that make the modification of the GUI very simple. ElmerGUI also controls the ElmerSolver and ElmerPost binaries and includes a real-time convergence monitor. ElmerGUI is still young as the development was started in early 2008.

ElmerSolver

ElmerSolver is a program executable forming the solver of Elmer. It is the soul of the Elmer software and the part where most of the development work is directed to. ElmerSolver includes a large number of finite element library tools which enable the user to write new equation solvers economically. The specific equation solvers are mainly available as dynamical libraries that have standard interfaces and can be linked to the main program on request.

ElmerPost

ElmerPost is a versatile postprocessor that is expected to be quite sufficient for the usual postprocessing needs. ElmerPost provides a straightforward graphical user interface that is easy to learn. ElmerPost utilizes Mesa and TCL/TK graphics libraries. ElmerPost is quite old and stable and its not much further developed.

ElmerGrid

ElmerGrid provides functionality for the generation of simple structured meshes and may also be used for mesh manipulation and transformation tasks of many kinds. For example, ElmerGrid may be used to partition the mesh for parallel runs or to import meshes written by other mesh generators. The ElmerGrid command file is to be written by a text editor.

ElmerFront

ElmerFront is the old graphical user interface for creating setups for simple problems. ElmerFront is not developed anymore but the codes are still part of the Elmer package. The replacement of ElmerFront is ElmerGUI.

Mesh2D

This is a Delaunay triangulator that is called by ElmerFront but it may also be called independently. It is the default mesh generation tool used for adaptive computations.

ViewFactors

This is a program for the computation of view factors that need to be determined in some radiation problems. Usually there is no need to call this independently as it is automatically called within ElmerSolver.

4 Elmer source code

Elmer development uses the subversion version control system available at sourceforge. The code may be viewed under "Code" and you may obtain a complete snapshot of the source codes, for example with

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

This is the recommended way of obtaining the source codes since it is always up to date.

Elmer source code is also available as tar bundles bearing the suffix `tar.gz` on the following site

```
http://www.nic.funet.fi/pub/sci/physics/elmer/src
```

The code version is best recognized by the svn revision number. This is also printed at the start of ElmerSolver execution.

Elmer code is distributed as partially interdependent modules. Some of them are used for creating program executables while others are only used for creating program libraries. Basically knowing the module interdependencies is unnecessary unless the user wants to setup only a partial system.

eio

Elmer input/output library written in C++ and used for some I/O operations by the ElmerSolver.

elmergrid

ElmerGrid source codes written in C, including also the Metis library from the Karypis Lab.

elmerpost

ElmerPost source codes written in C.

fem

ElmerSolver source codes written mainly in Fortran90.

front

ElmerFront source codes written in C++.

hutiter

The iterative linear algebra solvers written mainly in Fortran90 and called by ElmerSolver.

matc

This library is used in the command file interpreter of ElmerSolver and inside the command window of ElmerPost for evaluating mathematical expressions written in C.

mathlibs

This includes basic mathematical libraries such as Lapack, Blas, Arpack, and Parpack.

meshgen2d

This includes the source code of the 2D Delaunay mesher.

misc

Miscellaneous developments, also the new preprocessor ElmerGUI may be found here under the directory Mesh3D.

umfpack

This includes the source code of the Umfpack (GPL version 4.4) library from University of California.

5 Elmer documentation

The Elmer documentation is constantly under development. The date of the manual version is printed in the cover of the manual. The current set of Elmer manuals is as follows.

ElmerguiManual.pdf

ElmerGUI manual gives a detailed description of the new graphical user interface of Elmer suite. The tutorials includes some technical details and is complemented by the walk-through tutorials.

ElmerSolverManual.pdf

ElmerSolver Manual gives an overview of the general capabilities of the solver, focusing on the utilities that are of use to several physical models. It follows from this organization of material that information specific to a certain physical model is not included in this manual.

ElmerModelsManual.pdf

The Models Manual describes the different physical models which the solver of Elmer can handle. The specific options for controlling the corresponding equation solvers are also documented. In addition, this manual describes certain utilities for other tasks, such as computing derived quantities.

ElmerTutorials.pdf

The tutorials of the Elmer software have two different approaches. The tutorials utilizing the graphical user interface are walk-through examples that guide to choose the right menus and write the right values. The tutorials that do not rely on the graphical user interface are basically just example files with documentation. The files related to the tutorials are contained in `ElmerTutorialFiles.tar.gz` which can be found at the same site where the manuals are located.

ElmerGridManual.pdf

This is the manual of ElmerGrid utility. The examples related to the ElmerGrid documentation are provided in the file `ElmerGridExamples.tar.gz` which can be found at the same site where the manuals are located.

MATCManual.pdf M

annual of the MATC language built in ElmerSolver and ElmerPost.

ElmerOverview.pdf T
his paper.

In addition to these manuals there are separate documentation for some input interfaces (GiD) and for visualization tasks (making animations). Look at the www-pages for more information on these documents. The following documents are now more or less obsolete but may still contain some information not found in the above.

ElmerFrontUserGuide.pdf

This is the manual for the graphical user interface ElmerFront. ElmerFront is not actively developed and this might be the final documentation of the program.

OldElmerUserGuide.pdf

This is the original user guide of Elmer software (1999). Particularly some appendices defining some of the file formats may still be useful.

OldElmerTutorial.pdf

A graphical user interface oriented tutorial guide of the Elmer software (2000).

6 Strategies for using the Elmer package

The modularity of the Elmer package enables the users to have different strategies for using Elmer. Here the possible ways of using the package are outlined. How the input and output data of the software components are organized into files is also summarized.

6.1 Elmer file system

The following list summarizes how the input and output data are organized into files. These are the native files of Elmer. Additionally Elmer suite is capable of handling a large number of mesh and geometry formats as input, and able to produce many postprocessing formats as output.

ElmerSolver command file *.sif

The file with the sif-suffix is the command file which is read by ElmerSolver. It contains user-prepared input data that controls the selection of physical models, boundary conditions, and so on. In the case of simple problem setups this command file may be written automatically by ElmerFront. More complicated setups require that this file is edited using a text editor. The documentation of the software includes several example files that may be used as starting points when editing the command file. For the keyword syntax of the command file the ElmerSolver Manual and Models Manual are the best sources of information.

ElmerSolver mesh files mesh.*

The solver of Elmer reads the mesh from four different files `mesh.nodes`, `mesh.elements`, `mesh.boundary`, and `mesh.header`, which all should be located in a single mesh directory. The mesh files may be created using ElmerFront, ElmerGrid, or by enhanced versions of Netgen and GiD. A program executable Mesh2D which is the mesh generator used by ElmerFront may also be called independently. The file format of the mesh files is compatible with ElmerSolver, ElmerFront and ElmerGrid.

ElmerSolver result file *.result

This result file is written by ElmerSolver and may be used to make a simulation restart from a previous set of results. ElmerSolver by default writes this file to the mesh directory. The file format is compatible only with ElmerSolver.

ElmerPost file *.ep

This file is written by ElmerSolver and can be read by ElmerPost. ElmerSolver by default writes this file to the mesh directory. The file is used mainly for visualization purposes.

ElmerGrid mesh definition file *.grd

This file is used to define 1D, 2D or 3D structured meshes. The file can only be read by ElmerGrid.

ElmerGrid command file *.eg

This file is used to make mesh manipulation operations with ElmerGrid. The same functionality may be achieved by using command line arguments.

ELMERSOLVER_STARTINFO

This file is used by ElmerSolver and simply includes the name of the command file. The other possibility to transfer the command file name to ElmerSolver is to use a command line parameter.

SOLVER.KEYWORDS

The keywords that may be used in the ElmerSolver command file are listed in this file, located in the directory of the shared library files of ElmerSolver. This list may not be complete as new keywords are always popping up due to the development work. Therefore the user may create a local file and add the missing keywords to this file. Note that it does not really matter if a keyword is not listed as long as the type of the keyword value is given in the command file and ElmerSolver is not asked to do a strict checking of keywords.

Elmer geometry file *.egf

This file defines a 2D geometry using primitives such as points and lines. It is read by the now obsolete ElmerFront program.

Elmer mesh generator input file *.mif

This is the file that Mesh2D uses to create Delaunay triangulations. It is usually written by ElmerFront but it may easily be modified using an editor.

6.2 Strategies for preprocessing

The purpose of the preprocessing phase is to create the ElmerSolver input files, which are at the minimum the command file and the mesh files. Before the introduction of ElmerGUI the strategies for using Elmer were rather mixed since power users tended to avoid ElmerFront which was still used by many in the introductory phase. It is hoped that with the ElmerGUI the different strategies will be more unified.

Existing mesh definition file + ElmerGUI

ElmerGUI includes ElmerGrid, and optionally tetlib and nglib, as finite element mesh generators. When a suitable mesh definition file for these software exists the mesh is created on-the-fly before reading it into ElmerGUI. ElmerGUI can also be used to pass inline parameters to the mesh generators which often allows sufficient control over the mesh generators. However, full control of the mesh generation process with complicated geometries is not possible with the provided interface. However, still this approach provides maybe the easiest way to start using Elmer.

Existing mesh + ElmerGUI

ElmerGUI is also able to read many existing mesh formats. These include .FDNEUT (Gambit), .msh (gmsh), .mphtxt (Comsol Multiphysics), and .unv (Ideas universal) file formats. Additionally there is a small number of third party mesh generators that can directly write meshes in Elmer format provided that some interfaces are used. Currently interfaces for GiD and Netgen are provided. For more information on the interfaces see the Elmer www-pages. This approach is not limited by the mesh generation possibilities of ElmerGUI and is therefore suitable even for the most complicated cases, provided that a good mesh generation software is at disposal.

Existing mesh and command file + editor

ElmerGUI is often used as the first-step tool in the simulations. However, if in following simulations only minor modifications to the initial setup are needed it is often most practical to edit the command file (*.sif) by some text editor (e.g. emacs). A good place to start may be one of the minimal test cases provided in the source distribution. The more than one hundred tests often provides a close-enough starting point for consecutive simulations particularly if the geometry is rather simple. Also it may be that some new solvers are not implemented in the ElmerGUI and hence adding them manually is the only option. In adding the keywords in the command file, the Models Manual is of great help. In this approach ElmerSolver and ElmerPost are to be executed from the command line.

ElmerGrid + editor

An easy way to make simple 2D and 3D meshes is to use ElmerGrid. The mesh definition file of ElmerGrid also defines the geometry. However, the structured format of ElmerGrid favors box-like forms and making more complicated shapes may be difficult. In this approach the solver command file must be created using a text editor. Previous command files provide a good starting point also in this case.

This approach is most suited for making academic tests using simple structured meshes. It is easy to test different things in this approach as the mesh is basically fully parameterized. Many of the provided tests of ElmerSolver are defined using this approach. Trying to push this approach to more complicated shapes may turn out to be cumbersome.

Sometimes ElmerGrid needs also to be used as an intermediate tool, for example in the partitioning of the mesh. Then the changes to the command file are often quite minimal.

6.3 Strategies for postprocessing

There are also several strategies for visualizing the numerical results.

ElmerPost

The easiest way for visualization is to use ElmerPost. ElmerPost does not pose any severe limitations and has good features in exporting data in raster formats or animations. However, if you want to draw line graphs, or want to have several data sets available at the same time, you need other file formats as well.

VTK widget of ElmerGUI

ElmerGUI also includes a set of visualization techniques that come from the VTK library (if compiled with it). The functionality is almost the same as that of ElmerPost but the look and feel of the code is more concurrent. ElmerPost may still be favored for speed and stability.

VTK, GiD etc.

ElmerSolver can write the results also in formats understood by some third party visualization software. Use the `ResultOutputSolve` keyword (see Elmer Models Manual) for outputting in VTK and VTU (Paraview, VisIt,...) or GiD format.

Matlab, gnuplot, etc.

Ascii data for producing line graphs can be written automatically by saving the solution data along predefined lines, or lines that are created on-the-fly. For this purpose use the `SaveScalars` or `SaveLine` keyword (see Elmer Models Manual).

Contact info

For questions concerning the use and capabilities of Elmer, please use preferably the Elmer discussion mailing list at www.elmerforum.org/forum. If you have some question concerning collaboration of some sort, you may direct your mail to elmeradm@csc.fi, or to some of the Elmer developers directly.