FeenoX manual

A free no-fee no-X uniX-like finite-element(ish) computational engineering tool

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Chapter 1

Overview

FeenoX is a computational tool that can solve engineering problems which are usually casted as differential-algebraic equations (DAEs) or partial differential equations (PDEs). It is to finite elements programs and libraries what Markdown is to Word and TeX, respectively. In particular, it can solve

- dynamical systems defined by a set of user-provided DAEs (such as plant control dynamics for example)
- mechanical elasticity
- heat conduction
- structural modal analysis
- neutron diffusion
- neutron transport

FeenoX reads a plain-text input file which contains the problem definition and writes 100%-user defined results in ASCII (through `PRINT` or other user-defined output instructions within the input file). For PDE problems, it needs a reference to at least one Gmsh mesh file for the discretization of the domain. It can write post-processing views in either `.msh` or `.vtk` formats.

Keep in mind that FeenoX is just a back end reading a set of input files and writing a set of output files following the design philosophy of UNIX (separation, composition, representation, economy, extensibility, etc). Think of it as a transfer function between input files and output files:

```
                             +------------+
mesh (*.msh)  }              |            |             { terminal
data (*.dat)  } input ---->  |   FeenoX   |----> output { data files
input (*.fee) }              |            |             { post (vtk/msh)
                             +------------+
```

Following the UNIX programming philosophy, there are no graphical interfaces attached to the FeenoX core, although a wide variety of pre and post-processors can be used with FeenoX. See for example `https://www.caeplex.com` for a web-based interface.

Chapter 2

Introduction

FeenoX is to finite-element software and libraries what Markdown is to word processors and typesetting systems. It can be seen as

- a syntactically-sweetened way of asking the computer to solve engineering-related mathematical problems, and/or
- a finite-element(ish) tool with a particular design basis

Note that some of the problems solved with FeenoX might not actually rely on the finite element method, but on general mathematical models and even on the finite volumes method. That is why we say it is a finite-element(ish) tool.

- FeenoX Overview Presentation, August 2021
  - Recording (audio in Spanish, slides in English)
  - Slides in PDF
  - Markdown examples sources

One of the main features of this allegedly particular design basis is that **simple problems ought to have simple inputs** (*rule of simplicity*). For instance, to solve one-dimensional heat conduction over the domain $x \in [0, 1]$ (which is indeed one of the most simple engineering problems we can find) the following input file is enough:

```
READ_MESH slab.msh                # read mesh in Gmsh's v4.1 format
PROBLEM thermal DIMENSIONS 1      # tell FeenoX what we want to solve
k = 1                             # set uniform conductivity
BC left  T=0                      # set fixed temperatures as BCs
BC right T=1                      # "left" and "right" are defined in the mesh
SOLVE_PROBLEM                     # tell FeenoX we are ready to solve the problem
PRINT T(0.5)                      # ask for the temperature at x=0.5
```

```
$ feenox thermal-1d-dirichlet-constant-k.fee
0.5
$
```

The mesh is assumed to have been already created with Gmsh (or any other pre-processing tool and converted to `.msh` format with Meshio for example). This assumption follows the *rule of composition* and prevents the actual input file to be polluted with mesh-dependent data (such as node coordinates and/or nodal loads) so as to keep it simple and make it Git-friendly (*rule of generation*). The only link between the mesh and the FeenoX input file is through physical groups (in the case above `left` and `right`) used to set boundary conditions and/or material properties.

Another design-basis decision is that **similar problems ought to have similar inputs** (*rule of least surprise*). So in order to have a space-dependent conductivity, we only have to replace one line in the input above: instead of defining a scalar k we define a function of x (we also update the output to show the analytical solution as well):

```
READ_MESH slab.msh
PROBLEM thermal DIMENSIONS 1
k(x) = 1+x                         # space-dependent conductivity
BC left  T=0
BC right T=1
SOLVE_PROBLEM
PRINT T(1/2) log(1+1/2)/log(2)    # print numerical and analytical solutions
```

```
$ feenox thermal-1d-dirichlet-space-k.fee
0.584959        0.584963
$
```

FeenoX has an **everything is an expression** design principle, meaning that any numerical input can be an algebraic expression (e.g. `T(1/2)` is the same as `T(0.5)`). If we want to have a temperature-dependent conductivity (which renders the problem non-linear) we can take advantage of the fact that $T(x)$ is available not only as an argument to `PRINT` but also for the definition of algebraic functions:

```
READ_MESH slab.msh
PROBLEM thermal DIMENSIONS 1
k(x) = 1+T(x)                      # temperature-dependent conductivity
BC left  T=0
BC right T=1
SOLVE_PROBLEM
PRINT T(1/2) sqrt(1+(3*0.5))-1    # print numerical and analytical solutions
```

```
$ feenox thermal-1d-dirichlet-temperature-k.fee
0.581139        0.581139
$
```

For example, we can solve the NAFEMS LE11 “Solid cylinder/Taper/Sphere-Temperature” benchmark like

```
READ_MESH nafems-le11.msh DIMENSIONS 3
PROBLEM mechanical

# linear temperature gradient in the radial and axial direction
T(x,y,z) = sqrt(x^2 + y^2) + z

# Boundary conditions
BC xz     symmetry  # same as v=0 but ”symmetry” follows the statement
BC yz     symmetry  # ide with u=0
BC xy     w=0
BC HIH'I' w=0
```

```
# material properties (isotropic & uniform so we can use scalar constants)
E = 210e3*1e6       # mesh is in meters, so E=210e3 MPa -> Pa
nu = 0.3            # dimensionless
alpha = 2.3e-4      # in 1/°C as in the problem

SOLVE_PROBLEM
WRITE_MESH nafems-le11.vtk VECTOR u v w   T sigma1 sigma2 sigma3 sigma sigmaz
PRINT "sigma_z(A) = " sigmaz(0,1,0)/1e6 "MPa"
```

Another example would be the famous chaotic Lorenz' dynamical system—the one of the butterfly—whose differential equations are

$$\begin{cases} \dot{x} &= \sigma \cdot (y - x) \\ \dot{y} &= x \cdot (r - z) - y \\ \dot{z} &= xy - bz \end{cases}$$

where $\sigma = 10$, $b = 8/3$ and $r = 28$ are the classical parameters that generate the butterfly as presented by Edward Lorenz back in his seminal 1963 paper Deterministic non-periodic flow. We can solve it with FeenoX by writing the equations in the input file as naturally as possible, as illustrated in the input file that follows:

```
PHASE_SPACE x y z     # Lorenz 'attractors phase space is x-y-z
end_time = 40         # we go from t=0 to 40 non-dimensional units

sigma = 10            # the original parameters from the 1963 paper
r = 28
b = 8/3

x_0 = -11             # initial conditions
y_0 = -16
z_0 = 22.5

# the dynamical system's equations written as naturally as possible
x_dot = sigma*(y - x)
y_dot = x*(r - z) - y
z_dot = x*y - b*z

PRINT t x y z        # four-column plain-ASCII output
```

Please note the following two points about both cases above:

1. The input files are very similar to the statements of each problem in plain English words (*rule of clarity*). Take some time to read the problem statement of the NAFEMS LE11 benchmark and the FeenoX input to see how well the latter matches the former. Same for the Lorenz' chaotic system. Those with some experience may want to compare them to the inputs decks (sic) needed for other common FEA programs.
2. By design, 100% of FeenoX' output is controlled by the user. Had there not been any `PRINT` or `WRITE_MESH` instructions, the output would have been empty, following the *rule of silence*. This is a significant change with respect to traditional engineering codes that date back from times when one CPU hour was worth dozens (or even hundreds) of engineering hours. At that time, cognizant engineers had to dig into thousands of lines of data to search for a single individual result. Nowadays, following the *rule of*

economy, it is actually far easier to ask the code to write only what is needed in the particular format that suits the user.

In other words, FeenoX is a computational tool to solve

- dynamical systems written as sets of ODEs/DAEs, or
- steady or quasi-static thermo-mechanical problems, or
- steady or transient heat conduction problems, or
- modal analysis problems,
- neutron diffusion or transport problems
- community-contributed problems

in such a way that the input is a near-English text file that defines the problem to be solved. Some basic rules are

- FeenoX is just a **solver** working as a *transfer function* between input and output files. Following the *rules of separation, parsimony and diversity*, **there is no embedded graphical interface** but means of using generic pre and post processing tools—in particular, Gmsh and Paraview respectively. See also CAEplex.

- The input files should be syntactically sugared so as to be as self-describing as possible.

- Simple problems ought to need simple input files.

- Similar problems ought to need similar input files.

- Everything is an expression. Whenever a number is expected, an algebraic expression can be entered as well. Variables, vectors, matrices and functions are supported. Here is how to replace the boundary condition on the right side of the slab above with a radiation condition:

```
sigma = 1       # non-dimensional stefan-boltzmann constant
e = 0.8         # emissivity
Tinf=1          # non-dimensional reference temperature
BC right q=sigma*e*(Tinf^4-T(x)^4)
```

- FeenoX should run natively in the cloud and be able to massively scale in parallel. See the Software Requirements Specification and the Software Development Specification for details.

Since it is free (as in freedom) and open source, contributions to add features (and to fix bugs) are welcome. In particular, each kind of problem supported by FeenoX (thermal, mechanical, modal, etc.) has a subdirectory of source files which can be used as a template to add new problems, as implied in the "community-contributed problems" bullet above (*rules of modularity and extensibility*). See the documentation for details about how to contribute.

Chapter 3

Running **feenox**

3.1 Invocation

The format for running the `feenox` program is:

```
feenox [options] inputfile [optional_extra_arguments] ...
```

The `feenox` executable supports the following options:

`-h`, **`--help`** display usage and commmand-line help and exit

`-v`, **`--version`** display brief version information and exit

`-V`, **`--versions`** display detailed version information

Instructions will be read from standard input if "-" is passed as inputfile, i.e.

```
$ echo 'PRINT 2+2' | feenox -
4
```

PETSc and SLEPc options can be passed in `[options]` as well, with the difference that two hyphens have to be used instead of only once. For example, to pass the PETSc option `-ksp_view` the actual FeenoX invocation should be

```
$ feenox --ksp_view input.fee
```

The optional `[replacement arguments]` part of the command line mean that each argument after the input file that does not start with an hyphen will be expanded verbatim in the input file in each occurrence of `$1`, `$2`, etc. For example

```
$ echo 'PRINT $1+$2' | feenox - 3 4
7
```

3.2 Compilation

These detailed compilation instructions are aimed at `amd64` Debian-based GNU/Linux distributions. The compilation procedure follows POSIX, so it should work in other operating systems and architectures as well. Distributions not using `apt` for packages (i.e. `yum`) should change the package installation commands (and possibly the package names). The instructions should also work for in MacOS, although the `apt-get` commands should be replaced by `brew` or similar. Same for Windows under Cygwin, the packages should be installed through the Cygwin installer. WSL was not tested, but should work as well.

3.2.1 Quickstart

Note that the quickest way to get started is to get an already-compiled statically-linked binary executable. Follow these instructions if that option is not suitable for your workflow.

On a GNU/Linux box (preferably Debian-based), follow these quick steps. See next section for detailed explanations.

1. Install mandatory dependencies

   ```
   sudo apt-get install gcc make git automake autoconf libgsl-dev
   ```

   If you cannot install `libgsl-dev` but still have `git` and the build toolchain, you can have the `configure` script to download and compile it for you. See point 4 below.

2. Install optional dependencies (of course these are *optional* but recommended)

   ```
   sudo apt-get install libsundials-dev petsc-dev slepc-dev
   ```

3. Clone Github repository

   ```
   git clone https://github.com/seamplex/feenox
   ```

4. Boostrap, configure, compile & make

   ```
   cd feenox
   ./autogen.sh
   ./configure
   make
   ```

   If you cannot (or do not want) to use `libgsl-dev` from a package repository, call `configure` with `--enable ↩ -download-gsl`:

   ```
   ./configure --enable-download-gsl
   ```

   If you do not have Internet access, get the tarball manually, copy it to the same directory as `configure` and run again.

5. Run test suite (optional)

```
make check
```

6. Install the binary system wide (optional)

   ```
   sudo make install
   ```

3.2.2 Detailed configuration and compilation

The main target and development environment is Debian GNU/Linux, although it should be possible to compile FeenoX in any free GNU/Linux variant (and even the in non-free MacOS and Windows). As per the SRS, all dependencies have to be available on mainstream GNU/Linux distributions. But they can also be compiled from source in case the package repositories are not available or customized compilation flags are needed (i.e. optimization or debugging settings).

All the dependencies are free and open source software. PETSc/SLEPc also depend on other mathematical libraries to perform particular operations such as linear algebra. These extra dependencies can be either free (such as LAPACK) or non-free (such as MKL), but there is always at least one combination of a working setup that involves only free and open source software which is compatible with FeenoX licensing terms (GPLv3+). See the documentation of each package for licensing details.

3.2.2.1 Mandatory dependencies

FeenoX has one mandatory dependency for run-time execution and the standard build toolchain for compilation. It is written in C99 so only a C compiler is needed, although `make` is also required. Free and open source compilers are favored. The usual C compiler is `gcc` but `clang` can also be used. Nevertheless, the non-free `icc` has also been tested.

Note that there is no need to have a Fortran nor a C++ compiler to build FeenoX. They might be needed to build other dependencies (such as PETSc), but not to compile FeenoX with all the dependencies installed from package repositories. In case the build toolchain is not already installed, do so with

```
sudo apt-get install gcc make
```

If the source is to be fetched from the Git repository then of course `git` is needed but also `autoconf` and `automake` since the `configure` script is not stored in the Git repository but the `autogen.sh` script that bootstraps the tree and creates it. So if instead of compiling a source tarball one wants to clone from GitHub, these packages are also mandatory:

```
sudo apt-get install git automake autoconf
```

Again, chances are that any existing GNU/Linux box has all these tools already installed.

3.2.2.1.1 The GNU Scientific Library The only run-time dependency is GNU GSL (not to be confused with Microsoft GSL). It can be installed with

```
sudo apt-get install libgsl-dev
```

In case this package is not available or you do not have enough permissions to install system-wide packages, there are two options.

1. Pass the option `--enable-download-gsl` to the `configure` script below.
2. Manually download, compile and install GNU GSL

If the `configure` script cannot find both the headers and the actual library, it will refuse to proceed. Note that the FeenoX binaries already contain a static version of the GSL so it is not needed to have it installed in order to run the statically-linked binaries.

3.2.2.2 Optional dependencies

FeenoX has three optional run-time dependencies. It can be compiled without any of these but functionality will be reduced:

- SUNDIALS provides support for solving systems of ordinary differential equations (ODEs) or differential-algebraic equations (DAEs). This dependency is needed when running inputs with the `PHASE_SPACE` ↩ keyword.

- PETSc provides support for solving partial differential equations (PDEs). This dependency is needed when running inputs with the `PROBLEM` keyword.

- SLEPc provides support for solving eigen-value problems in partial differential equations (PDEs). This dependency is needed for inputs with `PROBLEM` types with eigen-value formulations such as `modal` and `neutron_transport`.

In absence of all these, FeenoX can still be used to

- solve general mathematical problems such as the ones to compute the Fibonacci sequence,
- operate on functions, either algebraically or point-wise interpolated,
- read, operate over and write meshes,
- etc.

These optional dependencies have to be installed separately. There is no option to have `configure` to download them as with `--enable-download-gsl`.

3.2.2.2.1 SUNDIALS SUNDIALS is a SUite of Nonlinear and DIfferential/ALgebraic equation Solvers. It is used by FeenoX to solve dynamical systems casted as DAEs with the keyword `PHASE_SPACE`, like the Lorenz system.

Install either by doing

```
sudo apt-get install libsundials-dev
```

or by following the instructions in the documentation.

3.2.2.2.2 PETSc

PETSc, the Portable, Extensible Toolkit for Scientific Computation, pronounced PET-see (/ˈpɛt-siː/), is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It is used by FeenoX to solve PDEs with the keyword `PROBLEM`, like thermal conduction on a slab.

Install either by doing

```
sudo apt-get install petsc-dev
```

or by following the instructions in the documentation.

Note that

- Configuring and compiling PETSc from scratch might be difficult the first time. It has a lot of dependencies and options. Read the official documentation for a detailed explanation.
- There is a huge difference in efficiency between using PETSc compiled with debugging symbols and with optimization flags. Make sure to configure `--with-debugging=0` for FeenoX production runs and leave the debugging symbols (which is the default) for development only.
- FeenoX needs PETSc to be configured with real double-precision scalars. It will compile but will complain at run-time when using complex and/or single or quad-precision scalars.
- FeenoX honors the `PETSC_DIR` and `PETSC_ARCH` environment variables when executing `configure`. If these two do not exist or are empty, it will try to use the default system-wide locations (i.e. the `petsc-dev` package).

3.2.2.2.3 SLEPc

SLEPc, the Scalable Library for Eigenvalue Problem Computations, is a software library for the solution of large scale sparse eigenvalue problems on parallel computers. It is used by FeenoX to solve PDEs with the keyword `PROBLEM` that need eigen-value computations, such as modal analysis of a cantilevered beam.

Install either by doing

```
sudo apt-get install slepc-dev
```

or by following the instructions in the documentation.

Note that

- SLEPc is an extension of PETSc so the latter has to be already installed and configured.
- FeenoX honors the `SLEPC_DIR` environment variable when executing `configure`. If it does not exist or is empty it will try to use the default system-wide locations (i.e. the `slepc-dev` package).
- If PETSc was configured with `--download-slepc` then the `SLEPC_DIR` variable has to be set to the directory inside `PETSC_DIR` where SLEPc was cloned and compiled.

3.2.2.3 FeenoX source code

There are two ways of getting FeenoX' source code:

1. Cloning the GitHub repository at `https://github.com/seamplex/feenox`
2. Downloading a source tarball from `https://seamplex.com/feenox/dist/src/`

3.2.2.3.1 Git repository

The main Git repository is hosted on GitHub at https://github.com/seamplex/feenox. It is public so it can be cloned either through HTTPS or SSH without needing any particular credentials. It can also be forked freely. See the Programming Guide for details about pull requests and/or write access to the main repository.

Ideally, the `main` branch should have a usable snapshot. All other branches might contain code that might not compile or might not run or might not be tested. If you find a commit in the main branch that does not pass the tests, please report it in the issue tracker ASAP.

After cloning the repository

```
git clone https://github.com/seamplex/feenox
```

the `autogen.sh` script has to be called to bootstrap the working tree, since the `configure` script is not stored in the repository but created from `configure.ac` (which is in the repository) by `autogen`.

Similarly, after updating the working tree with

```
git pull
```

it is recommended to re-run the `autogen.sh` script. It will do a `make clean` and re-compute the version string.

3.2.2.3.2 Source tarballs

When downloading a source tarball, there is no need to run `autogen.sh` since the `configure` script is already included in the tarball. This method cannot update the working tree. For each new FeenoX release, the whole tarball has to be downloaded again.

3.2.2.4 Configuration

To create a proper `Makefile` for the particular architecture, dependencies and compilation options, the script `configure` has to be executed. This procedure follows the GNU Coding Standards.

```
./configure
```

Without any particular options, `configure` will check if the mandatory GNU Scientific Library is available (both its headers and run-time library). If it is not, then the option `--enable-download-gsl` can be used. This option will try to use `wget` (which should be installed) to download a source tarball, uncompress is, configure and compile it. If these steps are successful, this GSL will be statically linked into the resulting FeenoX executable. If there is no internet connection, the `configure` script will say that the download failed. In that case, get the indicated tarball file manually , copy it into the current directory and re-run `./configure`.

The script will also check for the availability of optional dependencies. At the end of the execution, a summary of what was found (or not) is printed in the standard output:

```
$ ./configure
[...]
## ----------------------- ##
## Summary of dependencies ##
## ----------------------- ##
```

```
  GNU Scientific Library  from system
  SUNDIALS IDA            yes
  PETSc                   yes /usr/lib/petsc
  SLEPc                   no
[...]
```

If for some reason one of the optional dependencies is available but FeenoX should not use it, then pass `--without-sundials`, `--without-petsc` and/or `--without-slepc` as arguments. For example

```
$ ./configure --without-sundials --without-petsc
[...]
## ---------------------- ##
## Summary of dependencies ##
## ---------------------- ##
  GNU Scientific Library  from system
  SUNDIALS                no
  PETSc                   no
  SLEPc                   no
[...]
```

If configure complains about contradicting values from the cached ones, run `autogen.sh` again before `configure` or uncompress the source tarball in a fresh location.

To see all the available options run

```
./configure --help
```

3.2.2.5 Source code compilation

After the successful execution of `configure`, a `Makefile` is created. To compile FeenoX, just execute

```
make
```

Compilation should take a dozen of seconds. It can be even sped up by using the `-j` option

```
make -j8
```

The binary executable will be located in the `src` directory but a copy will be made in the base directory as well. Test it by running without any arguments

```
$ ./feenox
FeenoX v0.1.24-g6cfe063
a free no-fee no-X uniX-like finite-element(ish) computational engineering tool

usage: ./feenox [options] inputfile [replacement arguments]

  -h, --help         display usage and commmand-line help and exit
  -v, --version      display brief version information and exit
  -V, --versions     display detailed version information
  -s, --sumarize     list all symbols in the input file and exit

Instructions will be read from standard input if “”- is passed as
inputfile, i.e.

    $ echo "PRINT 2+2" | feenox -
    4

Report bugs at https://github.com/seamplex/feenox or to jeremy@seamplex.com
Feenox home page: https://www.seamplex.com/feenox/
$
```

The `-v` (or `--version`) option shows the version and a copyright notice:

```
$ ./feenox -v
FeenoX v0.1.24-g6cfe063
a free no-fee no-X uniX-like finite-element(ish) computational engineering tool

Copyright (C) 2009--2021 jeremy theler
GNU General Public License v3+, https://www.gnu.org/licenses/gpl.html.
FeenoX is free software: you are free to change and redistribute it.
There is NO WARRANTY, to the extent permitted by law.
$
```

The `-V` (or `--versions`) option shows the dates of the last commits, the compiler options and the versions of the linked libraries:

```
$ ./feenox -V
FeenoX v0.1.24-g6cfe063
a free no-fee no-X uniX-like finite-element(ish) computational engineering tool

Last commit date   : Sun Aug 29 11:34:04 2021 -0300
Build date         : Sun Aug 29 11:44:50 2021 -0300
Build architecture : linux-gnu x86_64
Compiler           : gcc (Ubuntu 10.3.0-1ubuntu1) 10.3.0
Compiler flags     : -O3
Builder            : gtheler@chalmers
GSL version        : 2.6
SUNDIALS version   : 4.1.0
PETSc version      : Petsc Release Version 3.14.5, Mar 03, 2021
PETSc arch         :
PETSc options      : --build=x86_64-linux-gnu --prefix=/usr --includedir=${prefix}/include --mandir=${prefix ↩
    }/share/man --infodir=${prefix}/share/info --sysconfdir=/etc --localstatedir=/var --with-option- ↩
    checking=0 --with-silent-rules=0 --libdir=${prefix}/lib/x86_64-linux-gnu --runstatedir=/run --with- ↩
    maintainer-mode=0 --with-dependency-tracking=0 --with-debugging=0 --shared-library-extension=_real -- ↩
    with-shared-libraries --with-pic=1 --with-cc=mpicc --with-cxx=mpicxx --with-fc=mpif90 --with-cxx- ↩
    dialect=C++11 --with-opencl=1 --with-blas-lib=-lblas --with-lapack-lib=-llapack --with-scalapack=1 -- ↩
    with-scalapack-lib=-lscalapack-openmpi --with-ptscotch=1 --with-ptscotch-include=/usr/include/scotch -- ↩
    with-ptscotch-lib="-lptesmumps -lptscotch -lptscotcherr" --with-fftw=1 --with-fftw-include="[]" --with- ↩
    fftw-lib="-lfftw3 -lfftw3_mpi" --with-superlu_dist=1 --with-superlu_dist-include=/usr/include/superlu- ↩
    dist --with-superlu_dist-lib=-lsuperlu_dist --with-hdf5-include=/usr/include/hdf5/openmpi --with-hdf5- ↩
    lib="-L/usr/lib/x86_64-linux-gnu/hdf5/openmpi -L/usr/lib/x86_64-linux-gnu/openmpi/lib -lhdf5 -lmpi" -- ↩
```

```
     CXX_LINKER_FLAGS=-Wl,--no-as-needed --with-hypre=1 --with-hypre-include=/usr/include/hypre --with-hypre ↩
     -lib=-lHYPRE_core --with-mumps=1 --with-mumps-include="[]" --with-mumps-lib="-ldmumps -lzmumps -lsmumps ↩
      -lcmumps -lmumps_common -lpord" --with-suitesparse=1 --with-suitesparse-include=/usr/include/ ↩
     suitesparse --with-suitesparse-lib="-lumfpack -lamd -lcholmod -lklu" --with-superlu=1 --with-superlu- ↩
     include=/usr/include/superlu --with-superlu-lib=-lsuperlu --prefix=/usr/lib/petscdir/petsc3.14/x86_64- ↩
     linux-gnu-real --PETSC_ARCH=x86_64-linux-gnu-real CFLAGS="-g -O2 -ffile-prefix-map=/build/petsc-pVufYp/ ↩
     petsc-3.14.5+dfsg1=. -flto=auto -ffat-lto-objects -fstack-protector-strong -Wformat -Werror=format- ↩
     security -fPIC" CXXFLAGS="-g -O2 -ffile-prefix-map=/build/petsc-pVufYp/petsc-3.14.5+dfsg1=. -flto=auto  ↩
     -ffat-lto-objects -fstack-protector-strong -Wformat -Werror=format-security -fPIC" FCFLAGS="-g -O2 - ↩
     ffile-prefix-map=/build/petsc-pVufYp/petsc-3.14.5+dfsg1=. -flto=auto -ffat-lto-objects -fstack- ↩
     protector-strong -fPIC -ffree-line-length-0" FFLAGS="-g -O2 -ffile-prefix-map=/build/petsc-pVufYp/petsc ↩
     -3.14.5+dfsg1=. -flto=auto -ffat-lto-objects -fstack-protector-strong -fPIC -ffree-line-length-0"  ↩
     CPPFLAGS="-Wdate-time -D_FORTIFY_SOURCE=2" LDFLAGS="-Wl,-Bsymbolic-functions -flto=auto -Wl,-z,relro - ↩
     fPIC" MAKEFLAGS=w
SLEPc version      : SLEPc Release Version 3.14.2, Feb 01, 2021
$
```

3.2.2.6 Test suite

To be explained.

3.2.2.7 Installation

To be explained.

3.2.3 Advanced settings

3.2.3.1 Compiling with debug symbols

By default the C flags are `-O3`, without debugging. To add the `-g` flag, just use `CFLAGS` when configuring:

```
./configure CFLAGS="-g -O0"
```

3.2.3.2 Using a different compiler

Without PETSc, FeenoX uses the `CC` environment variable to set the compiler. So configure like

```
./configure CC=clang
```

When PETSc is detected FeenoX uses the `mpicc` executable, which is a wrapper to an actual C compiler with extra flags needed to find the headers and the MPI library. To change the wrapped compiler, you should set `MPICH_CC` or `OMPI_CC`, depending if you are using MPICH or OpenMPI. For example, to force MPICH to use `clang` do

```
./configure MPICH_CC=clang CC=clang
```

To know which is the default MPI implementation, just run `configure` without arguments and pay attention to the "Compiler" line in the "Summary of dependencies" section. For example, for OpenMPI a typical summary would be

```
## ---------------------- ##
## Summary of dependencies ##
## ---------------------- ##
  GNU Scientific Library  from system
  SUNDIALS                yes
  PETSc                   yes /usr/lib/petsc
  SLEPc                   yes /usr/lib/slepc
  Compiler                gcc -I/usr/lib/x86_64-linux-gnu/openmpi/include/openmpi -I/usr/lib/x86_64-linux- ↩
       gnu/openmpi/include -pthread -L/usr/lib/x86_64-linux-gnu/openmpi/lib -lmpi
```

For MPICH:

```
## ---------------------- ##
## Summary of dependencies ##
## ---------------------- ##
  GNU Scientific Library  from system
  SUNDIALS                yes
  PETSc                   yes /home/gtheler/libs/petsc-3.15.0 arch-linux2-c-debug
  SLEPc                   yes /home/gtheler/libs/slepc-3.15.1
  Compiler                gcc -Wl,-z,relro -I/usr/include/x86_64-linux-gnu/mpich -L/usr/lib/x86_64-linux-gnu ↩
        -lmpich
```

Other non-free implementations like Intel MPI might work but were not tested. However, it should be noted that the MPI implementation used to compile FeenoX has to match the one used to compile PETSc. Therefore, if you compiled PETSc on your own, it is up to you to ensure MPI compatibility. If you are using PETSc as provided by your distribution's repositories, you will have to find out which one was used (it is usually OpenMPI) and use the same one when compiling FeenoX.

The FeenoX executable will show the configured compiler and flags when invoked with the `--versions` option:

```
$ feenox --versions
FeenoX v0.1.47-g868dbb7-dirty
a free no-fee no-X uniX-like finite-element(ish) computational engineering tool

Last commit date   : Mon Sep 6 16:39:53 2021 -0300
Build date         : Tue Sep 07 14:29:42 2021 -0300
Build architecture : linux-gnu x86_64
Compiler           : gcc (Debian 10.2.1-6) 10.2.1 20210110
Compiler flags     : -O3
Builder            : gtheler@tom
GSL version        : 2.6
SUNDIALS version   : 5.7.0
PETSc version      : Petsc Release Version 3.15.0, Mar 30, 2021
PETSc arch         : arch-linux2-c-debug
PETSc options      : --download-eigen --download-hdf5 --download-hypre --download-metis --download-mumps -- ↩
     download-parmetis --download-pragmatic --download-scalapack --with-x=0
SLEPc version      : SLEPc Release Version 3.15.1, May 28, 2021
$
```

Note that the reported values are the ones used in `configure` and not in `make`. Thus, the recommended way to set flags is in `configure` and not in `make`.

3.2.3.3 Compiling PETSc

To be explained.

Chapter 4

Examples

To be done.

Chapter 5

Tutorial

To be done.

Chapter 6

Description

Chapter 7

Description

FeenoX solves a problem defined in an plain-text input file and writes user-defined outputs to the standard output and/or files, either also plain-text or with a particular format for further post-processing. The syntax of this input file is designed to be as self-describing as possible, using English keywords that explains FeenoX what problem it has to solve in a way is understandable by both humans and computers. Keywords can work either as

1. Definitions, for instance ”define function $f(x)$ and read its data from file `f.dat`”), or as
2. Instructions, such as “write the stress at point D into the standard output”.

A person can tell if a keyword is a definition or an instruction because the former are nouns (`FUNCTION`) and the latter verbs (`PRINT`). The equal sign `=` is a special keyword that is neither a verb nor a noun, and its meaning changes depending on what is on the left hand side of the assignment.

a. If there is a function, then it is a definition: define an algebraic function to be equal to the expression on the right-hand side, e.g.:

   ```
   f(x,y) = exp(-x^2)*cos(pi*y)
   ```

b. If there is a variable, vector or matrix, it is an instruction: evaluate the expression on the right-hand side and assign it to the varible or vector (or matrix) element indicated in the left-hand side. Strictly speaking, if the variable has not already been defined (and implicit declaration is allowed), then the variable is also defined as well, e.g:

   ```
   VAR a
   VECTOR b[3]
   a = sqrt(2)
   b[i] = a*i^2
   ```

   There is no need to explicitly define the scalar variable `a` with `VAR` since the first assigment also defines it implicitly (if this is allowed by the keyword `IMPLICIT`).

An input file can define its own variables as needed, such as `my_var` or `flag`. But there are some reserved names that are special in the sense that they either

1. can be set to modify the behavior of FeenoX, such as `max_dt` or `dae_tol`
2. can be read to get the internal status or results back from FeenoX, such as `nodes` or `keff`
3. can be either set or read, such as `dt` or `done`

The problem being solved can be static or transient, depending on whether the special variable `end_time` is zero (default) or not. If it is zero and `static_steps` is equal to one (default), the instructions in the input file are executed once and then FeenoX quits. For example

```
VAR x
PRINT %.7f func_min(cos(x)+1,x,0,6)
```

If `static_steps` is larger than one, the special variable `step_static` is increased and they are repeated the number of time indicated by `static_steps`:

```
static_steps = 10
f(n) = n^2 - n + 41
PRINT f(step_static^2-1)
```

If the special variable `end_time` is set to a non-zero value, after computing the static part a transient problem is solved. There are three kinds of transient problems:

1. Plain "standalone" transients
2. Differential-Algebraic equations (DAE) transients
3. Partial Differential equations (PDE) transients

In the first case, after all the instruction in the input file were executed, the special variable `t` is increased by the value of `dt` and then the instructions are executed all over again, until `t` reaches `end_time`:

```
end_time = 2*pi
dt = 1/10

y = lag(heaviside(t-1), 1)
z = random_gauss(0, sqrt(2)/10)

PRINT t sin(t) cos(t) y z HEADER
```

In the second case, the keyword `PHASE_SPACE` sets up DAE system. Then, one initial condition and one differential-algebraic equation has to be given for each element in the phase space. The instructions before the DAE block executed, then the DAE timestep is advanced and finally the instructions after DAE block are executed (there cannot be any instruction between the first and the last DAE):

```
PHASE_SPACE x
end_time = 1
x_0 = 1
x_dot = -x
PRINT t x exp(-t) HEADER
```

The timestep is chosen by the SUNDIALS library in order to keep an estimate of the residual error below `dae_tol` (default is 10^{-6}), although `min_dt` and `max_dt` can be used to control it. See the section of the [Differential-Algebraic Equations subsystem] for more information.

In the third cae, the type of PDE being solved is given by the keyword `PROBLEM`. Some types of PDEs do support transient problems (such as `thermal`) but some others do not (such as `modal`). See the detailed explanation of each problem type for details. Now the transient problem is handled by the TS framework of the PETSc library. In general transient PDEs involve a mesh, material properties, inital conditions, transient boundary conditions, etc. And they create a lot of data since results mean spatial and temporal distributions of one or more scalar fields:

```
# example of a 1D heat transient problem
# from https://www.mcs.anl.gov/petsc/petsc-current/src/ts/tutorials/ex3.c.html
# a non-dimensional slab 0 < x < 1 is kept at T(0) = T(1) = 0
# there is an initial non-trivial T(x)
# the steady-state is T(x) = 0
PROBLEM thermal 1d
READ_MESH slab60.msh

end_time = 1e-1

# initial condition
T_0(x) := sin(6*pi*x) + 3*sin(2*pi*x)
# analytical solution
T_a(x,t) := exp(-36*pi^2*t)*sin(6*pi*x) + 3*exp(-4*pi^2*t)*sin(2*pi*x)

# unitary non-dimensional properties
k = 1
rho = 1
cp = 1

# boundary conditions
BC left  T=0
BC right T=0

SOLVE_PROBLEM

PRINT %e t dt T(0.1) T_a(0.1,t) T(0.7) T_a(0.7,t)
WRITE_MESH temp-slab.msh T

IF done
 PRINT "\# open temp-anim-slab.geo in Gmsh to see the result!"
ENDIF
```

PETSc's TS also honors the `min_dt` and `max_dt` variables, but the time step is controled by the allowed relative error with the special variable `ts_rtol`. Again, see the section of the [Partial Differential Equations subsystem] for more information.

7.1 Algebraic expressions

To be done.

- Everything is an expression.

7.2 Initial conditions

7.3 Expansions of command line arguments

Chapter 8

Reference

This chapter contains a detailed reference of keywords, variables, functions and functionals available in FeenoX. These are used essentially to define the problem that FeenoX needs to solve and to define what the output should be. It should be noted that this chapter is to be used, indeed, as a *reference* and not as a tutorial.

8.1 Differential-Algebraic Equations subsystem

8.1.1 DAE keywords

8.1.1.1 `INITIAL_CONDITIONS`

Define how initial conditions of DAE problems are computed.

```
INITIAL_CONDITIONS { AS_PROVIDED | FROM_VARIABLES | FROM_DERIVATIVES }
```

In DAE problems, initial conditions may be either:

- equal to the provided expressions (`AS_PROVIDED`)
- the derivatives computed from the provided phase-space variables (`FROM_VARIABLES`)
- the phase-space variables computed from the provided derivatives (`FROM_DERIVATIVES`)

In the first case, it is up to the user to fulfill the DAE system at $t = 0$. If the residuals are not small enough, a convergence error will occur. The `FROM_VARIABLES` option means calling IDA's `IDACalcIC` routine with the parameter `IDA_YA_YDP_INIT`. The `FROM_DERIVATIVES` option means calling IDA's `IDACalcIC` routine with the parameter IDA_Y_INIT. Wasora should be able to automatically detect which variables in phase-space are differential and which are purely algebraic. However, the [`DIFFERENTIAL`] keyword may be used to explicitly define them. See the (SUNDIALS documentation)[https://computation.llnl.gov/casc/sundials/documentation/ida_guide.pdf] for further information.

8.1.1.2 `PHASE_SPACE`

Asks FeenoX to solve a set of algebraic-differntial equations and define the variables, vectors and/or matrices that span the phase space.

```
PHASE_SPACE PHASE_SPACE <vars> ... <vectors> ... <matrices> ...
```

8.1.1.3 TIME_PATH

Force time-dependent problems to pass through specific instants of time.

```
TIME_PATH <expr_1> [ <expr_2>  [ ... <expr_n> ] ]
```

The time step `dt` will be reduced whenever the distance between the current time `t` and the next expression in the list is greater than `dt` so as to force `t` to coincide with the expressions given. The list of expresssions should evaluate to a sorted list of values for all times.

8.1.2 DAE variables

8.1.2.1 dae_rtol

Maximum allowed relative error for the solution of DAE systems.

Default value is is 1×10^{-6}. If a fine per-variable error control is needed, special vector `abs_error` should be used.

8.2 Partial Differential Equations subsytem

8.2.1 PDE keywords

8.2.1.1 BC

Define a boundary condition to be applied to faces, edges and/or vertices.

```
BC <name> [ MESH <name> ] [ PHYSICAL_GROUP <name_1>  PHYSICAL_GROUP <name_2> ... ] [ <bc_data1> <bc_data2> ↩
    ... ]
```

If the name of the boundary condition matches a physical group in the mesh, it is automatically linked to that physical group. If there are many meshes, the mesh this keyword refers to has to be given with `MESH`. If the boundary condition applies to more than one physical group in the mesh, they can be added using as many `PHYSICAL_GROUP` keywords as needed. Each `<bc_data>` argument is a single string whose meaning depends on the type of problem being solved. For instance `T=150*sin(x/pi)` prescribes the temperature to depend on space as the provided expression in a thermal problem and `fixed` fixes the displacements in all the directions in a mechanical or modal problem. See the particular section on boundary conditions for further details.

8.2.1.2 DUMP

Dump raw PETSc objects used to solve PDEs into files.

```
DUMP [ FORMAT { binary | ascii | octave } ] [ K |   K_bc |   b |   b_bc |   M |   M_bc |
```

8.2.1.3 FIND_EXTREMA

Find and/or compute the absolute extrema of a function or expression over a mesh (or a subset of it).

```
FIND_EXTREMA { <expression> | <function> } [ OVER <physical_group> ] [ MESH <mesh_identifier> ] [ NODES |  ↩
    CELLS | GAUSS ]
 [ MIN <variable> ] [ MAX <variable> ] [ X_MIN <variable> ] [ X_MAX <variable> ] [ Y_MIN <variable> ] [  ↩
     Y_MAX <variable> ] [ Z_MIN <variable> ] [ Z_MAX <variable> ] [ I_MIN <variable> ] [ I_MAX <variable> ]
```

Either an expression or a function of space x, y and/or z should be given. By default the search is performed over the highest-dimensional elements of the mesh, i.e. over the whole volume, area or length for three, two and one-dimensional meshes, respectively. If the search is to be carried out over just a physical group, it has to be given in `OVER`. If there are more than one mesh defined, an explicit one has to be given with `MESH`. If neither `NODES`, `CELLS` or `GAUSS` is given then the search is performed over the three of them. With `NODES` only the function or expression is evalauted at the mesh nodes. With `CELLS` only the function or expression is evalauted at the element centers. With `GAUSS` only the function or expression is evalauted at the Gauss points. The value of the absolute minimum (maximum) is stored in the variable indicated by `MIN` (`MAX`). If the variable does not exist, it is created. The value of the x-y-z coordinate of the absolute minimum (maximum) is stored in the variable indicated by `X_MIN`-`Y_MIN`-`Z_MIN` (`X_MAX`-`Y_MAX`-`Z_MAX`). If the variable does not exist, it is created. The index (either node or cell) where the absolute minimum (maximum) is found is stored in the variable indicated by `I_MIN` (`I_MAX`).

8.2.1.4 INTEGRATE

Spatially integrate a function or expression over a mesh (or a subset of it).

```
INTEGRATE { <expression> | <function> } [ OVER <physical_group> ] [ MESH <mesh_identifier> ] [ NODES |  ↩
    CELLS ]
 RESULT <variable>
```

Either an expression or a function of space x, y and/or z should be given. If the integrand is a function, do not include the arguments, i.e. instead of `f(x,y,z)` just write `f`. The results should be the same but efficiency will be different (faster for pure functions). By default the integration is performed over the highest-dimensional elements of the mesh, i.e. over the whole volume, area or length for three, two and one-dimensional meshes, respectively. If the integration is to be carried out over just a physical group, it has to be given in `OVER`. If there are more than one mesh defined, an explicit one has to be given with `MESH`. Either `NODES` or `CELLS` define how the integration is to be performed. With `NODES` the integration is performed using the Gauss points and weights associated to each element type. With `CELLS` the integral is computed as the sum of the product of the integrand at the center of each cell (element) and the cell's volume. Do expect differences in the results and efficiency between these two approaches depending on the nature of the integrand. The scalar result of the integration is stored in the variable given by the mandatory keyword `RESULT`. If the variable does not exist, it is created.

8.2.1.5 MATERIAL

Define a material its and properties to be used in volumes.

```
MATERIAL <name> [ MESH <name> ] [ PHYSICAL_GROUP <name_1>  [ PHYSICAL_GROUP <name_2> [ ... ] ] ] [  ↩
    <property_name_1>=<expr_1> [ <property_name_2>=<expr_2> [ ... ] ] ]
```

If the name of the material matches a physical group in the mesh, it is automatically linked to that physical group. If there are many meshes, the mesh this keyword refers to has to be given with `MESH`. If the material applies to more than one physical group in the mesh, they can be added using as many `PHYSICAL_GROUP` keywords as needed. The names of the properties in principle can be arbitrary, but each problem type needs a minimum set of properties defined with particular names. For example, steady-state thermal problems need at least the conductivity which should be named `k`. If the problem is transient, it will also need heat capacity `rhocp` ↩ or diffusivity `alpha`. Mechanical problems need Young modulus `E` and Poisson's ratio `nu`. Modal also needs density `rho`. Check the particular documentation for each problem type. Besides these mandatory properties, any other one can be defined. For instance, if one mandatory property dependend on the concentration of boron in the material, a new per-material property can be added named `boron` and then the function `boron(` ↩ `x,y,z)` can be used in the expression that defines the mandatory property.

8.2.1.6 PHYSICAL_GROUP

Explicitly defines a physical group of elements on a mesh.

```
PHYSICAL_GROUP <name> [ MESH <name> ] [ DIMENSION <expr> ] [ ID <expr> ]
 [ MATERIAL <name> | | BC <name> [ BC ... ] ]
```

This keyword should seldom be needed. Most of the times, a combination of `MATERIAL` and `BC` ought to be enough for most purposes. The name of the `PHYSICAL_GROUP` keyword should match the name of the physical group defined within the input file. If there is no physical group with the provided name in the mesh, this instruction has no effect. If there are many meshes, an explicit mesh can be given with `MESH`. Otherwise, the physical group is defined on the main mesh. An explicit dimension of the physical group can be provided with `DIMENSION`. An explicit id can be given with `ID`. Both dimension and id should match the values in the mesh. For volumetric elements, physical groups can be linked to materials using `MATERIAL`. Note that if a material is created with the same name as a physical group in the mesh, they will be linked automatically, so there is no need to use `PHYSCAL_GROUP` for this. The `MATERIAL` keyword in `PHYSICAL_GROUP` is used to link a physical group in a mesh file and a material in the feenox input file with different names. Likewise, for non-volumetric elements, physical groups can be linked to boundary using `BC`. As in the preceeding case, if a boundary condition is created with the same name as a physical group in the mesh, they will be linked automatically, so there is no need to use `PHYSCAL_GROUP` for this. The `BC` keyword in `PHYSICAL_GROUP` is used to link a physical group in a mesh file and a boundary condition in the feenox input file with different names. Note that while there can be only one `MATERIAL` associated to a physical group, there can be many `BC`s associated to a physical group.

8.2.1.7 PROBLEM

Ask FeenoX to solve a partial-differential equation problem.

```
PROBLEM [ mechanical | thermal | modal | neutron_diffusion ]

 [ 1D |   2D |   3D |   DIMENSIONS <expr> ] [ MESH <identifier> ]

[ AXISYMMETRIC { x | y } | [ PROGRESS ]
 [ TRANSIENT | QUASISTATIC]
 [ LINEAR | NON_LINEAR ] [ MODES <expr> ]
 [ PRECONDITIONER { gamg | mumps | lu | hypre | sor | bjacobi | cholesky | ... } ]
 [ LINEAR_SOLVER { gmres | mumps | bcgs | bicg | richardson | chebyshev | ... } ]
 [ NONLINEAR_SOLVER { newtonls | newtontr | nrichardson | ngmres | qn | ngs | ... } ]
 [ TRANSIENT_SOLVER { bdf | beuler | arkimex | rosw | glee | ... } ]
 [ TIME_ADAPTATION { basic | none | dsp | cfl | glee | ... } ]
 [ EIGEN_SOLVER { krylovschur | lanczos | arnoldi | power | gd | ... } ]
 [ SPECTRAL_TRANSFORMATION { shift | sinvert | cayley | ... } ]
 [ EIGEN_FORMULATION { omega | lambda } ]
```

- `laplace` (or `poisson`) solves the Laplace (or Poisson) equation.
- `mechanical` (or `elastic`) solves the mechanical elastic problem. If the mesh is two-dimensional, and not `AXISYMMETRIC`, either `plane_stress` or `plane_strain` has to be set instead.
- `thermal` (or `heat`) solves the heat conduction problem.
- `modal` computes the natural mechanical frequencies and oscillation modes.
- `neutron_diffusion` multi-group core-level neutron diffusion with a FEM formulation

If you are a programmer and want to contribute with another problem type, please do so! Check out [FeenoX repository](https: for licensing information, programming guides and code of conduct.

The number of spatial dimensions of the problem needs to be given either as `1d`, `2d`, `3d` or with the keyword `DIMENSIONS`. Alternatively, one can define a `MESH` with an explicit `DIMENSIONS` keyword before `PROBLEM`. If there are more than one `MESH`es define, the one over which the problem is to be solved can be defined by giving the explicit mesh name with `MESH`. By default, the first mesh to be defined in the input file is the one over which the problem is solved. If the `AXISYMMETRIC` keyword is given, the mesh is expected to be two-dimensional in the x-y plane and the problem is assumed to be axi-symmetric around the given axis. If the keyword `PROGRESS` is given, three ASCII lines will show in the terminal the progress of the ensamble of the stiffness matrix (or matrices), the solution of the system of equations and the computation of gradients (stresses). If the special variable `end_time` is zero, FeenoX solves a static problem—although the variable `static_steps` is still honored. If `end_time` is non-zero, FeenoX solves a transient or quasistatic problem. This can be controlled by `TRANSIENT` or `QUASISTATIC`. By default FeenoX tries to detect wheter the computation should be linear or non-linear. An explicit mode can be set with either `LINEAR` on `NON_LINEAR`. The number of modes to be computed when solving eigenvalue problems is given by `MODES`. The default value is problem dependent. The preconditioner (`PC`), linear (`KSP`), non-linear (`SNES`) and time-stepper (`TS`) solver types be any of those available in PETSc (first option is the default):

- List of `PRECONDITIONERS` `http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/PC/PCType.html`.

- List of `LINEAR_SOLVERS` `http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/KSP/KSPType.html`.

- List of `NONLINEAR_SOLVERS` `http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/SNES/SNESType.html`.

- List of `TRANSIENT_SOLVERS` `http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/TS/TSType.html`.

- List of `TIME_ADAPTATIONS` `http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/TS/TSAdaptType.html`.

- List of `EIGEN_SOLVERS` <https:

- List of `SPECTRAL_TRANSFORMATIONS` <https: If the `EIGEN_FORMULATION` is `omega` then $K\phi = \omega^2 M\phi$, and $M\phi = \lambda K\phi$$ if it is `lambda`.

8.2.1.8 `READ_MESH`

Read an unstructured mesh and (optionally) functions of space-time from a file.

```
READ_MESH { <file_path> | <file_id> } [ DIMENSIONS <num_expr> ]
 [ SCALE <expr> ] [ OFFSET <expr_x> <expr_y> <expr_z> ]
 [ INTEGRATION { full | reduced } ]
 [ MAIN ] [ UPDATE_EACH_STEP ]
 [ READ_FIELD <name_in_mesh> AS <function_name> ] [ READ_FIELD ... ]
 [ READ_FUNCTION <function_name> ] [READ_FUNCTION ...]
```

Either a file identifier (defined previously with a `FILE` keyword) or a file path should be given. The format is read from the extension, which should be either

- `.msh`, `.msh2` or `.msh4` Gmsh ASCII format, versions 2.2, 4.0 or 4.1
- `.vtk` ASCII legacy VTK
- `.frd` CalculiX's FRD ASCII output)

Note than only MSH is suitable for defining PDE domains, as it is the only one that provides physical groups (a.k.a labels) which are needed in order to define materials and boundary conditions. The other formats are primarily supported to read function data contained in the file and eventually, to operate over these functions (i.e. take differences with other functions contained in other files to compare results). The file path or file id can be used to refer to a particular mesh when reading more than one, for instance in a `WRITE_MESH` or `INTEGRATE` keyword. If a file path is given such as `cool_mesh.msh`, it can be later referred to as either `cool_mesh.msh` or just `cool_mesh`. The spatial dimensions cab be given with `DIMENSION`. If material properties are uniform and given with variables, the number of dimensions are not needed and will be read from the file at runtime. But if either properties are given by spatial functions or if functions are to be read from the mesh with `READ_DATA` or `READ_FUNCTION`, then the number of dimensions ought to be given explicitly because FeenoX needs to know how many arguments these functions take. If either `OFFSET` and/or `SCALE` are given, the node locations are first shifted and then scaled by the provided values. When defining several meshes and solving a PDE problem, the mesh used as the PDE domain is the one marked with `MAIN`. If none of the meshes is explicitly marked as main, the first one is used. If `UPDATE_EACH_STEP` is given, then the mesh data is re-read from the file at each time step. Default is to read the mesh once, except if the file path changes with time. For each `READ_FIELD` keyword, a point-wise defined function of space named `<function_name>` is defined and filled with the scalar data named `<name_in_mesh>` contained in the mesh file. The `READ_FUNCTION` keyword is a shortcut when the scalar name and the to-be-defined function are the same. If no mesh is marked as `MAIN`, the first one is the main one.

8.2.1.9 `SOLVE_PROBLEM`

Explicitly solve the PDE problem.

```
SOLVE_PROBLEM
```

Whenever the instruction `SOLVE_PROBLEM` is executed, FeenoX solves the PDE problem. For static problems, that means solving the equations and filling in the result functions. For transient or quasisstatic problems, that means advancing one time step.

8.2.1.10 WRITE_MESH

Write a mesh and functions of space-time to a file for post-processing.

```
WRITE_MESH { <file_path> | <file_id> } [ MESH <mesh_identifier> ] [ NO_MESH ] [ FILE_FORMAT { gmsh | vtk } ↩
    ] [ NO_PHYSICAL_NAMES ]  [ NODE | CELL ] [ SCALAR_FORMAT <printf_specification>] [ VECTOR <field_x> ↩
    <field_y> <field_z> ] [...] [ <field_1> ] [ <field_2> ] ...
```

Either a file identifier (defined previously with a `FILE` keyword) or a file path should be given. The format is automatically detected from the extension. Otherwise, the keyword `FILE_FORMAT` can be use to give the format explicitly. If there are several meshes defined then which one should be used has to be given explicitly with `MESH`. If the `NO_MESH` keyword is given, only the results are written into the output file. Depending on the output format, this can be used to avoid repeating data and/or creating partial output files which can the be latter assembled by post-processing scripts. When targetting the `.msh` output format, if `NO_PHYSICAL_NAMES` is given then the section that sets the actual names of the physical entities is not written. This can be needed to avoid name clashes when reading multiple `.msh` files. The output is node-based by default. This can be controlled with both the `NODE` and `CELL` keywords. All fields that come after a `NODE` (`CELL`) keyword will be written at the node (cells). These keywords can be used several times and mixed with fields. For example `CELL k(x,y,z)NODE T sqrt(x^2+ ↩ y^2)CELL 1+z` will write the conductivity and the expression $1+z$ as cell-based and the temperature $T(x,y,z)$ and the expression $\sqrt{x^2+y^2}$ as a node-based fields. Also, the `SCALAR_FORMAT` keyword can be used to define the precision of the ASCII representation of the fields that follow. Default is `%g`. The data to be written has to be given as a list of fields, i.e. distributions (such as `k` or `E`), functions of space (such as `T`) and/or expressions (such as `x^2+y^2+z^2`). Each field is written as a scalar, unless the keyword `VECTOR` is given. In this case, there should be exactly three fields following `VECTOR`.

8.2.2 PDE variables

8.3 Laplace's equation

Set `PROBLEM` to `laplace` to solve Laplace's equation

$$\nabla^2 \phi = 0$$

If `end_time` is set, then the transient problem is solved

$$\alpha(\mathbf{x}) \frac{\partial \phi}{\partial t} + \nabla^2 \phi = 0$$

8.3.1 Laplace results

8.3.1.1 phi

The scalar field $\phi(\mathbf{x})$ whose Laplacian is equal to zero or to $f(\mathbf{x})$.

8.3.2 Laplace properties

8.3.2.1 `alpha`

The coefficient of the temporal derivative for the transient equation $\alpha\frac{\partial\phi}{\partial t} + \nabla^2\phi = f(\mathbf{x})$. If not given, default is one.

8.3.2.2 `f`

The right hand side of the equation $\nabla^2\phi = f(\mathbf{x})$. If not given, default is zero (i.e. Laplace).

8.3.3 Laplace boundary conditions

8.3.3.1 `dphidn`

Alias for `phi'`.

```
dphidn=<expr>
```

8.3.3.2 `phi`

Dirichlet essential boundary condition in which the value of ϕ is prescribed.

```
phi=<expr>
```

8.3.3.3 `phi'`

Neumann natural boundary condition in which the value of the normal outward derivative $\frac{\partial\phi}{\partial n}$ is prescribed.

```
phi'=<expr>
```

8.3.4 Laplace keywords

8.3.5 Laplace variables

8.4 The heat conduction equation

Set `PROBLEM` to `thermal` (or `heat`) to solve thermal conduction:

$$\rho p \frac{\partial T}{\partial t} + \text{div}\left[k(\mathbf{x}, \mathbf{T} \cdot \text{grad}T\right] = q'''(\mathbf{x}, T)$$

If `end_time` is zero, only the steady-state problem is solved. If k, q''' or any Neumann boundary condition depends on T, the problem is set to non-linear automatically.

8.4.1 Thermal results

8.4.1.1 `T`

The temperature field $T(\mathbf{x})$. This is the primary unknown of the problem.

8.4.1.2 qx

The heat flux field $q_x(\mathbf{x}) = -k(\mathbf{x}) \cdot \frac{\partial T}{\partial x}$ in the x direction. This is a secondary unknown of the problem.

8.4.1.3 qy

The heat flux field $q_y(\mathbf{x}) = -k(\mathbf{x}) \cdot \frac{\partial T}{\partial y}$ in the x direction. This is a secondary unknown of the problem. Only available for two and three-dimensional problems.

8.4.1.4 qz

The heat flux field $q_z(\mathbf{x}) = -k(\mathbf{x}) \cdot \frac{\partial T}{\partial z}$ in the x direction. This is a secondary unknown of the problem. Only available for three-dimensional problems.

8.4.2 Thermal properties

8.4.2.1 k

The thermal conductivity in units of power per length per degree of temperature.

```
k
```

8.4.2.2 q

Alias for `q'''`

```
q
```

8.4.2.3 q'''

The volumetric power dissipated in the material in units of power per unit of volume. Default is zero (i.e. no power).

```
q'''
```

8.4.3 Thermal boundary conditions

8.4.4 Thermal keywords

8.4.5 Thermal variables

8.4.5.1 T_max

The maximum temperature T_{max}.

8.4.5.2 T_min

The minimum temperature T_{min}.

8.5 General & “standalone” mathematics

8.5.1 Keywords

8.5.1.1 ABORT

Catastrophically abort the execution and quit FeenoX.

```
ABORT
```

Whenever the instruction `ABORT` is executed, FeenoX quits with a non-zero error leve. It does not close files nor unlock shared memory objects. The objective of this instruction is to either debug complex input files by using only parts of them or to conditionally abort the execution using `IF` clauses.

8.5.1.2 ALIAS

Define a scalar alias of an already-defined indentifier.

```
ALIAS { <new_var_name> IS <existing_object> | <existing_object> AS <new_name> }
```

The existing object can be a variable, a vector element or a matrix element. In the first case, the name of the variable should be given as the existing object. In the second case, to alias the second element of vector `v` to the new name `new`, `v(2)` should be given as the existing object. In the third case, to alias second element (2,3) of matrix `M` to the new name `new`, `M(2,3)` should be given as the existing object.

8.5.1.3 CLOSE

Explicitly close a file after input/output.

```
CLOSE <name>
```

The given `<name>` can be either a fixed-string path or an already-defined `FILE`.

8.5.1.4 DEFAULT_ARGUMENT_VALUE

Give a default value for an optional commandline argument.

```
DEFAULT_ARGUMENT_VALUE <constant> <string>
```

If a `$n` construction is found in the input file but the commandline argument was not given, the default behavior is to fail complaining that an extra argument has to be given in the commandline. With this keyword, a default value can be assigned if no argument is given, thus avoiding the failure and making the argument optional. The `<constant>` should be 1, 2, 3, etc. and `<string>` will be expanded character-by-character where the `$n` ↩ construction is. Whether the resulting expression is to be interpreted as a string or as a numerical expression will depend on the context.

8.5.1.5 FILE

Define a file with a particularly formatted name to be used either as input or as output.

```
< FILE | OUTPUT_FILE | INPUT_FILE > <name> PATH <format> expr_1 expr_2 ... expr_n [ INPUT | OUTPUT | MODE ↩
    <fopen_mode> ]
```

For reading or writing into files with a fixed path, this instruction is usually not needed as the `FILE` keyword of other instructions (such as `PRINT` or `MESH`) can take a fixed-string path as an argument. However, if the file name changes as the execution progresses (say because one file for each step is needed), then an explicit `FILE` needs to be defined with this keyword and later referenced by the given name. The path should be given as a `printf`-like format string followed by the expressions which shuold be evaluated in order to obtain the actual file path. The expressions will always be floating-point expressions, but the particular integer specifier `%d` is allowed and internally transformed to `%.0f`. The file can be explicitly defined and `INPUT`, `OUTPUT` or a certain `fopen()` mode can be given (i.e. “a”). If not explicitly given, the nature of the file will be taken from context, i.e. `FILE`s in `PRINT` will be `OUTPUT` and `FILE`s in `FUNCTION` will be `INPUT`. This keyword justs defines the `FILE`, it does not open it. The file will be actually openened (and eventually closed) automatically. In the rare case where the automated opening and closing does not fit the expected workflow, the file can be explicitly opened or closed with the instructions `FILE_OPEN` and `FILE_CLOSE`.

8.5.1.6 FIT

Find parameters to fit an analytical function to a pointwise-defined function.

```
FIT <function_to_be_fitted>  TO <function_with_data> VIA <var_1> <var_2> ... <var_n>
 [ GRADIENT <expr_1> <expr_2> ... <expr_n> ]
 [ RANGE_MIN <expr_1> <expr_2> ... <expr_j> ]
 [ RANGE_MAX <expr_1> <expr_2> ... <expr_n> ]
 [ TOL_REL <expr> ] [ TOL_ABS <expr> ] [ MAX_ITER <expr> ]
 [ VERBOSE ]
```

The function with the data has to be point-wise defined (i.e. a `FUNCTION` read from a file, with inline `DATA` ↩ or defined over a mesh). The function to be fitted has to be parametrized with at least one of the variables provided after the `USING` keyword. For example to fit $f(x,y) = ax^2 + bsqrt(y)$ to a pointwise-defined function $g(x,y)$ one gives `FIT f TO g VIA a b`. Only the names of the functions have to be given, not the arguments. Both functions have to have the same number of arguments. The initial guess of the solution is given by the initial value of the variables after the `VIA` keyword. Analytical expressions for the gradient of the function to be fitted with respect to the parameters to be fitted can be optionally given with the `GRADIENT` keyword. If none is provided, the gradient will be computed numerically using finite differences. A range over which the residuals are to be minimized can be given with `RANGE_MIN` and `RANGE_MAX`. The expressions give the range of the arguments of the functions, not of the parameters. For multidimensional fits, the range is an hypercube. If no range is given, all the definition points of the function with the data are used for the fit. Convergence can be controlled by giving the relative and absolute tolreances with `TOL_REL` (default `DEFAULT_NLIN_FIT_EPSREL`) and `TOL_ABS` (default `DEFAULT_NLIN_FIT_EPSABS`), and with the maximum number of iterations `MAX_ITER` (default DEFAULT_NLIN_FIT_MAX_ITER). If the optional keyword `VERBOSE` is given, some data of the intermediate steps is written in the standard output.

8.5.1.7 **FUNCTION**

Define a function of one or more variables.

```
FUNCTION <function_name>(<var_1>[,var2,...,var_n]) { = <expr> | FILE { <file_path> | <file_id> } | VECTORS ↩
     <vector_1> <vector_2> ... <vector_n> <vector_data> | DATA <num_1> <num_2> ... <num_N> } [  ↩
     INTERPOLATION { linear | polynomial | spline | spline_periodic | akima | akima_periodic | steffen |  ↩
     nearest | shepard | shepard_kd | bilinear } ] [COLUMNS <expr_1> <expr_2> ... <expr_n> <expr_n+1> ] [  ↩
     INTERPOLATION_THRESHOLD <expr> ] [ SHEPARD_RADIUS <expr> ] [ SHEPARD_EXPONENT <expr> ]
```

The number of variables n is given by the number of arguments given between parenthesis after the function name. The arguments are defined as new variables if they had not been already defined explictly as scalar variables. If the function is given as an algebraic expression, the short-hand operator `:=` can be used. That is to say, `FUNCTION f(x)= x^2` is equivalent to `f(x):= x^2`. If a `FILE` is given, an ASCII file containing at least $n+1$ columns is expected. By default, the first n columns are the values of the arguments and the last column is the value of the function at those points. The order of the columns can be changed with the keyword `COLUMNS`, which expects $n+1$ expressions corresponding to the column numbers. If `VECTORS` is given, a set of $n+1$ vectors of the same size is expected. The first n correspond to the arguments and the last one to the function values. The function can be pointwise-defined inline in the input using `DATA`. This should be the last keyword of the line, followed by $N = k\cdot(n+1)$ expresions giving k definition points: n arguments and the value of the function. Multiline continuation using brackets `{` and `}` can be used for a clean data organization. Interpolation schemes can be given for either one or multi-dimensional functions with `INTERPOLATION`. Available schemes for $n=1$ are:

- linear
- polynomial, the grade is equal to the number of data minus one
- spline, cubic (needs at least 3 points)
- spline_periodic
- akima (needs at least 5 points)
- akima_periodic (needs at least 5 points)
- steffen, always-monotonic splines-like interpolator

Default interpolation scheme for one-dimensional functions is `DEFAULT_INTERPOLATION`.

Available schemes for $n>1$ are:

- nearest, $f(\mathbf{x})$ is equal to the value of the closest definition point
- shepard, inverse distance weighted average definition points (might lead to inefficient evaluation)
- shepard_kd, average of definition points within a kd-tree (more efficient evaluation provided `SHEPARD_RADIUS` is set to a proper value)
- bilinear, only available if the definition points configure an structured hypercube-like grid. If $n>3$, `SIZES` should be given.

For $n>1$, if the euclidean distance between the arguments and the definition points is smaller than `INTERPOLATION_THRESHOLD`, the definition point is returned and no interpolation is performed. Default value is square root of `DEFAULT_MULTIDIM_INTERPOLATION_THRESHOLD`. The initial radius of points to take into account in `shepard_kd` is given by `SHEPARD_RADIUS`. If no points are found, the radius is double until at least one definition point is found. The radius is doubled until at least one point is found. Default is `DEFAULT_SHEPARD_RADIUS`. The exponent of the `shepard` method is given by `SHEPARD_EXPONENT`. Default is `DEFAULT_SHEPARD_EXPONENT`.

8.5.1.8 `IF`

Execute a set of instructions if a condition is met.

```
IF expr
  <block_of_instructions_if_expr_is_true>
 [ ELSE
  <block_of_instructions_if_expr_is_false> ]
 ENDIF
```

8.5.1.9 `IMPLICIT`

Define whether implicit definition of variables is allowed or not.

```
IMPLICIT { NONE | ALLOWED }
```

By default, FeenoX allows variables (but not vectors nor matrices) to be implicitly declared. To avoid introducing errors due to typos, explicit declaration of variables can be forced by giving `IMPLICIT NONE`. Whether implicit declaration is allowed or explicit declaration is required depends on the last `IMPLICIT` keyword given, which by default is `ALLOWED`.

8.5.1.10 `INCLUDE`

Include another FeenoX input file.

```
INCLUDE <file_path> [ FROM <num_expr> ] [ TO <num_expr> ]
```

Includes the input file located in the string `file_path` at the current location. The effect is the same as copying and pasting the contents of the included file at the location of the `INCLUDE` keyword. The path can be relative or absolute. Note, however, that when including files inside `IF` blocks that instructions are conditionally-executed but all definitions (such as function definitions) are processed at parse-time independently from the evaluation of the conditional. The included file has to be an actual file path (i.e. it cannot be a FeenoX `FILE`) because it needs to be resolved at parse time. Yet, the name can contain a commandline replacement argument such as `$1` so `INCLUDE $1.fee` will include the file specified after the main input file in the command line. The optional `FROM` and `TO` keywords can be used to include only portions of a file.

8.5.1.11 `MATRIX`

Define a matrix.

```
MATRIX <name> ROWS <expr> COLS <expr> [ DATA <expr_1> <expr_2> ... <expr_n> |
```

A new matrix of the prescribed size is defined. The number of rows and columns can be an expression which will be evaluated the very first time the matrix is used and then kept at those constant values. All elements will be initialized to zero unless `DATA` is given (which should be the last keyword of the line), in which case the expressions will be evaluated the very first time the matrix is used and row-major-assigned to each of the elements. If there are less elements than the matrix size, the remaining values will be zero. If there are more elements than the matrix size, the values will be ignored.

8.5.1.12 OPEN

Explicitly open a file for input/output.

```
OPEN <name> [ MODE <fopen_mode> ]
```

The given `<name>` can be either a fixed-string path or an already-defined `FILE`. The mode is only taken into account if the file is not already defined. Default is write `w`.

8.5.1.13 PRINT

Write plain-text and/or formatted data to the standard output or into an output file.

```
PRINT [ <object_1> <object_2> ... <object_n> ] [ TEXT <string_1> ... TEXT <string_n> ]
 [ FILE { <file_path> | <file_id> } ] [ HEADER ] [ NONEWLINE ] [ SEP <string> ]
 [ SKIP_STEP <expr> ] [ SKIP_STATIC_STEP <expr> ] [ SKIP_TIME <expr> ] [ SKIP_HEADER_STEP <expr> ]
```

Each argument `object` which is not a keyword of the `PRINT` instruction will be part of the output. Objects can be either a matrix, a vector or any valid scalar algebraic expression. If the given object cannot be solved into a valid matrix, vector or expression, it is treated as a string literal if `IMPLICIT` is `ALLOWED`, otherwise a parser error is raised. To explicitly interpret an object as a literal string even if it resolves to a valid numerical expression, it should be prefixed with the `TEXT` keyword such as `PRINT TEXT 1+1` that would print `1+1` instead of `2`. Objects and string literals can be mixed and given in any order. Hashes `#` appearing literal in text strings have to be quoted to prevent the parser to treat them as comments within the FeenoX input file and thus ignoring the rest of the line, like `PRINT "\# this is a printed comment"`. Whenever an argument starts with a porcentage sign `%`, it is treated as a C `printf`-compatible format specifier and all the objects that follow it are printed using the given format until a new format definition is found. The objects are treated as double-precision floating point numbers, so only floating point formats should be given. See the `printf(3)` man page for further details. The default format is `DEFAULT_PRINT_FORMAT`. Matrices, vectors, scalar expressions, format modifiers and string literals can be given in any desired order, and are processed from left to right. Vectors are printed element-by-element in a single row. See `PRINT_VECTOR` to print one or more vectors with one element per line (i.e. vertically). Matrices are printed element-by-element in a single line using row-major ordering if mixed with other objects but in the natural row and column fashion if it is the only given object in the `PRINT` instruction. If the `FILE` keyword is not provided, default is to write to `stdout`. If the `HEADER` keyword is given, a single line containing the literal text given for each object is printed at the very first time the `PRINT` instruction is processed, starting with a hash `#` character. If the `NONEWLINE` keyword is not provided, default is to write a newline `\n` character after all the objects are processed. Otherwise, if the last token to be printed is a numerical value, a separator string will be printed but not the newline `\n` character. If the last token is a string, neither the separator nor the newline will be printed. The `SEP` keyword expects a string used to separate printed objects. To print objects without any separation in between give an empty string like `SEP ""`. The default is a tabulator character 'DEFAULT_PRINT_SEPARATOR' character. To print an empty line write `PRINT` without arguments. By default the `PRINT` instruction is evaluated every step. If the `SKIP_STEP` (`SKIP_STATIC_STEP`) keyword is given, the instruction is processed only every the number of transient (static) steps that results in evaluating the expression, which may not be constant. The SKIP_HEADER_STEP keyword works similarly for the optional HEADER but by default it is only printed once. The SKIP_TIME keyword use time advancements to choose how to skip printing and may be useful for non-constant time-step problems.

8.5.1.14 PRINT_FUNCTION

Print one or more functions as a table of values of dependent and independent variables.

```
PRINT_FUNCTION <function_1> [ { function | expr } ... { function | expr } ]
 [ FILE { <file_path> | <file_id> } ] [ HEADER ]
 [ MIN <expr_1> <expr_2> ... <expr_k> ] [ MAX <expr_1> <expr_2> ... <expr_k> ]
 [ STEP <expr_1> <expr_2> ... <expr_k> ] [ NSTEPs <expr_1> <expr_2> ... <expr_k> ]
 [ FORMAT <print_format> ] <vector_1> [ { vector | expr } ... { vector | expr } ]
```

Each argument should be either a function or an expression. The output of this instruction consists of $n+k$ columns, where n is the number of arguments of the first function of the list and k is the number of functions and expressions given. The first n columns are the arguments (independent variables) and the last k one has the evaluated functions and expressions. The columns are separated by a tabulator, which is the format that most plotting tools understand. Only function names without arguments are expected. All functions should have the same number of arguments. Expressions can involve the arguments of the first function. If the FILE keyword is not provided, default is to write to stdout. If HEADER is given, the output is prepended with a single line containing the names of the arguments and the names of the functions, separated by tabs. The header starts with a hash # that usually acts as a comment and is ignored by most plotting tools. If there is no explicit range where to evaluate the functions and the first function is point-wise defined, they are evalauted at the points of definition of the first one. The range can be explicitly given as a product of n ranges $[x_{i,\text{min}}, x_{i,\text{max}}]$ for $i = 1, \dots, n$. The values $x_{i,\text{min}}$ and $x_{i,\text{max}}$ are given with the MIN *and* MAX keywords. The discretization steps of the ranges are given by either STEP that gives δx *or* NSTEPS that gives the number of steps. If the first function is not point-wise defined, the ranges are mandatory.

8.5.1.15 PRINT_VECTOR

Print the elements of one or more vectors, one element per line.

```
PRINT_VECTOR
 [ FILE { <file_path> | <file_id> } ] [ HEADER ]
 [ FORMAT <print_format> ]
```

Each argument should be either a vector or an expression of the integer i. If the FILE keyword is not provided, default is to write to stdout. If HEADER is given, the output is prepended with a single line containing the names of the arguments and the names of the functions, separated by tabs. The header starts with a hash # that usually acts as a comment and is ignored by most plotting tools.

8.5.1.16 SORT_VECTOR

Sort the elements of a vector, optionally making the same rearrangement in another vector.

```
SORT_VECTOR <vector> [ ASCENDING | DESCENDING ] [ <other_vector> ]
```

This instruction sorts the elements of `<vector>` into either ascending or descending numerical order. If `<` ↩ `other_vector>` is given, the same rearrangement is made on it. Default is ascending order.

8.5.1.17 VAR

Explicitly define one or more scalar variables.

```
VAR <name_1> [ <name_2> ] ... [ <name_n> ]
```

When implicit definition is allowed (see `IMPLICIT`), scalar variables need not to be defined before being used if from the context FeenoX can tell that an scalar variable is needed. For instance, when defining a function like `f(x)= x^2` it is not needed to declare `x` explictly as a scalar variable. But if one wants to define a function like `g(x)= integral(f(x'), x', 0, x)` then the variable `x'` needs to be explicitly defined as `VAR x'` before the integral.

8.5.1.18 VECTOR

Define a vector.

```
VECTOR <name> SIZE <expr> [ FUNCTION_DATA <function> ] [ DATA <expr_1> <expr_2> ... <expr_n> |
```

A new vector of the prescribed size is defined. The size can be an expression which will be evaluated the very first time the vector is used and then kept at that constant value. If the keyword `FUNCTION_DATA` is given, the elements of the vector will be synchronized with the inpedendent values of the function, which should be point-wise defined. The sizes of both the function and the vector should match. All elements will be initialized to zero unless `DATA` is given (which should be the last keyword of the line), in which case the expressions will be evaluated the very first time the vector is used and assigned to each of the elements. If there are less elements than the vector size, the remaining values will be zero. If there are more elements than the vector size, the values will be ignored.

8.5.2 Variables

8.5.2.1 done

Flag that indicates whether the overall calculation is over.

This variable is set to true by FeenoX when the computation finished so it can be checked in an `IF` block to do something only in the last step. But this variable can also be set to true from the input file, indicating that the current step should also be the last one. For example, one can set `end_time = infinite` and then finish the computation at $t = 10$ by setting `done = t > 10`. This `done` variable can also come from (and sent to) other sources, like a shared memory object for coupled calculations.

8.5.2.2 done_static

Flag that indicates whether the static calculation is over or not.

It is set to true (i.e. $\neq 0$) by feenox if `step_static` $\geq$ `static_steps`. If the user sets it to true, the current step is marked as the last static step and the static calculation ends after finishing the step. It can be used in `IF` blocks to check if the static step is finished or not.

8.5.2.3 `done_transient`

Flag that indicates whether the transient calculation is over or not.

It is set to true (i.e. $\neq 0$) by feenox if `t` $\geq$ `end_time`. If the user sets it to true, the current step is marked as the last transient step and the transient calculation ends after finishing the step. It can be used in `IF` blocks to check if the transient steps are finished or not.

8.5.2.4 `dt`

Actual value of the time step for transient calculations.

When solving DAE systems, this variable is set by feenox. It can be written by the user for example by importing it from another transient code by means of shared-memory objects. Care should be taken when solving DAE systems and overwriting `t`. Default value is DEFAULT_DT, which is a power of two and roundoff errors are thus reduced.

8.5.2.5 `end_time`

Final time of the transient calculation, to be set by the user.

The default value is zero, meaning no transient calculation.

8.5.2.6 `i`

Dummy index, used mainly in vector and matrix row subindex expressions.

8.5.2.7 `in_static`

Flag that indicates if FeenoX is solving the iterative static calculation.

This is a read-only variable that is non zero if the static calculation.

8.5.2.8 `in_static_first`

Flag that indicates if feenox is in the first step of the iterative static calculation.

8.5.2.9 `in_static_last`

Flag that indicates if feenox is in the last step of the iterative static calculation.

8.5.2.10 `in_transient`

Flag that indicates if feenox is solving transient calculation.

8.5.2.11 `in_transient_first`

Flag that indicates if feenox is in the first step of the transient calculation.

8.5.2.12 `in_transient_last`

Flag that indicates if feenox is in the last step of the transient calculation.

8.5.2.13 `infinite`

A very big positive number.

It can be used as `end_time = infinite` or to define improper integrals with infinite limits. Default is $2^{50} \approx 1 \times 10^{15}$.

8.5.2.14 `j`

Dummy index, used mainly in matrix column subindex expressions.

8.5.2.15 `max_dt`

Maximum bound for the time step that feenox should take when solving DAE systems.

8.5.2.16 `min_dt`

Minimum bound for the time step that feenox should take when solving DAE systems.

8.5.2.17 `ncores`

The number of online available cores, as returned by `sysconf(_SC_NPROCESSORS_ONLN)`.

This value can be used in the `MAX_DAUGHTERS` expression of the `PARAMETRIC` keyword (i.e `ncores/2`).

8.5.2.18 `on_gsl_error`

This should be set to a mask that indicates how to proceed if an error ir raised in any routine of the GNU Scientific Library.

8.5.2.19 `on_ida_error`

This should be set to a mask that indicates how to proceed if an error ir raised in any routine of the SUNDIALS Library.

8.5.2.20 `on_nan`

This should be set to a mask that indicates how to proceed if Not-A-Number signal (such as a division by zero) is generated when evaluating any expression within feenox.

8.5.2.21 `pi`

A double-precision floating point representaion of the number π

It is equal to the `M_PI` constant in `math.h` .

8.5.2.22 `pid`

The UNIX process id of the FeenoX instance.

8.5.2.23 `realtime_scale`

If this variable is not zero, then the transient problem is run trying to syncrhonize the problem time with realtime, up to a scale given.

For example, if the scale is set to one, then FeenoX will advance the problem time at the same pace that the real wall time advances. If set to two, FeenoX time wil advance twice as fast as real time, and so on. If the calculation time is slower than real time modified by the scale, this variable has no effect on the overall behavior and execution will proceed as quick as possible with no delays.

8.5.2.24 `static_steps`

Number of steps that ought to be taken during the static calculation, to be set by the user.

The default value is one, meaning only one static step.

8.5.2.25 `step_static`

Indicates the current step number of the iterative static calculation.

This is a read-only variable that contains the current step of the static calculation.

8.5.2.26 `step_transient`

Indicates the current step number of the transient static calculation.

This is a read-only variable that contains the current step of the transient calculation.

8.5.2.27 `t`

Actual value of the time for transient calculations.

This variable is set by FeenoX, but can be written by the user for example by importing it from another transient code by means of shared-memory objects. Care should be taken when solving DAE systems and overwriting `t`.

8.5.2.28 `zero`

A very small positive number.

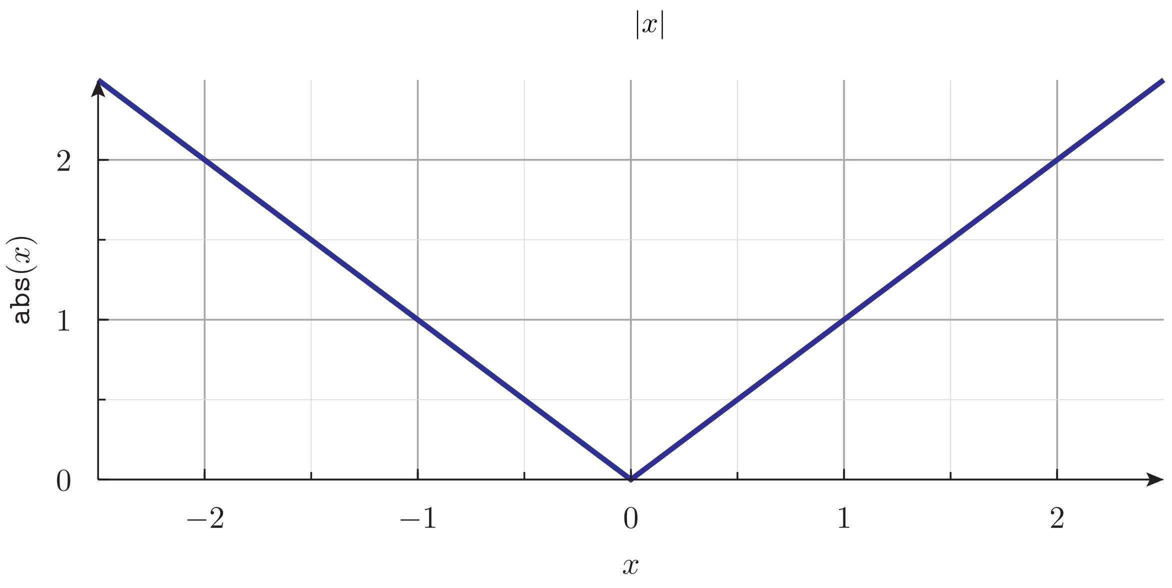
It is taken to avoid roundoff errors when comparing floating point numbers such as replacing $a \leq a_\text{max}$ with $a < a_\text{max}+$ `zero`. Default is $(1/2)^{-50} \approx 9 \times 10^{-16}$.

8.6 Functions

8.6.1 abs

Returns the absolute value of the argument x.

```
abs(x)
```



8.6.1.1 Example #1, abs.fee

```
PRINT sqrt(abs(-2))

# exercise: remove the absolute value from the sqrt argument
```

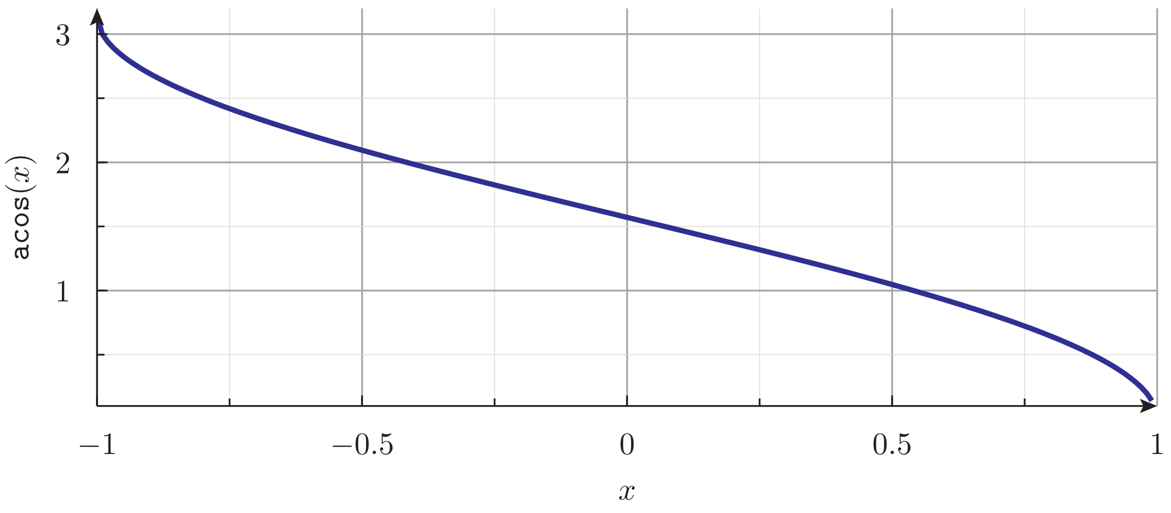
```
$ feenox abs.fee
1.41421
$
```

8.6.2 acos

Computes the arc in radians whose cosine is equal to the argument x. A NaN error is raised if $|x| > 1$.

```
acos(x)
```

$\arccos(x)$



8.6.2.1 Example #1, acos.fee

```
PRINT acos(0)
PRINT acos(1)
PRINT cos(acos(0.5))  acos(cos(0.5))
```

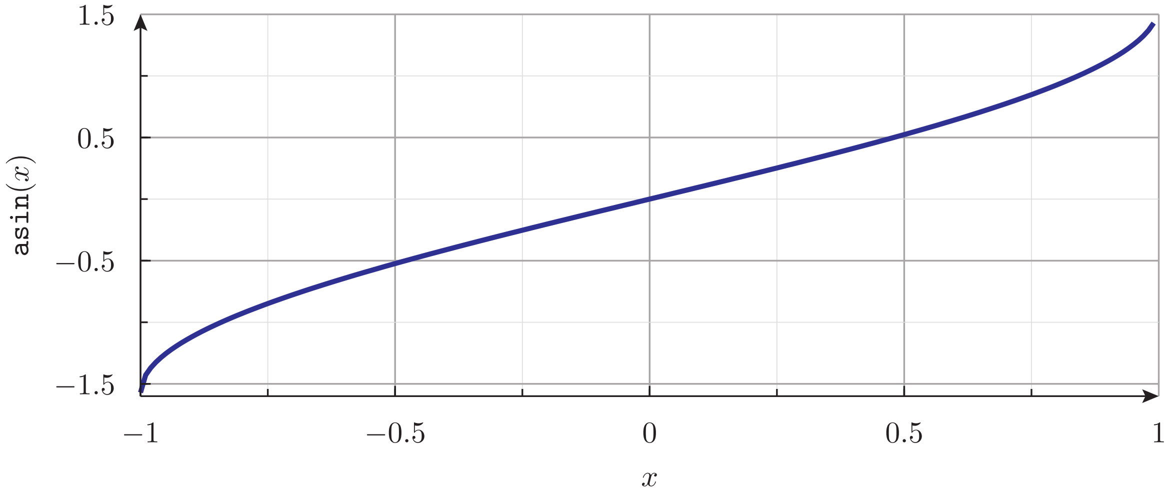
```
$ feenox acos.fee
1.5708
0
0.5     0.5
$
```

8.6.3 `asin`

Computes the arc in radians whose sine is equal to the argument x. A NaN error is raised if $|x| > 1$.

```
asin(x)
```

$$\arcsin(x)$$



8.6.3.1 Example #1, asin.fee

```
PRINT asin(0)
PRINT asin(1)
PRINT sin(asin(0.5))  asin(sin(0.5))
```

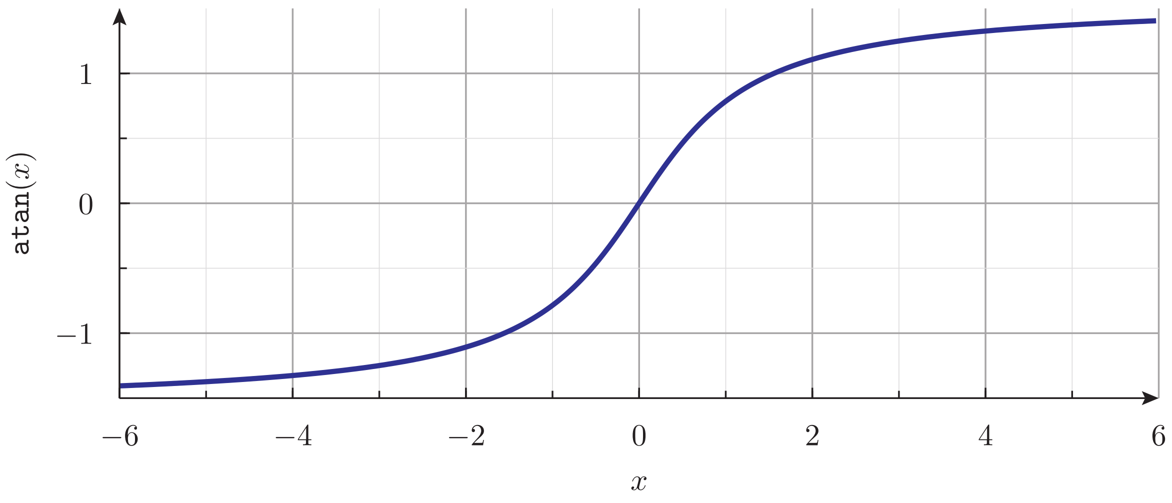
```
$ feenox asin.fee
0
1.5708
0.5     0.5
$
```

8.6.4 atan

Computes, in radians, the arc tangent of the argument x.

```
atan(x)
```

$$\arctan(x)$$



8.6.5 atan2

Computes, in radians, the arc tangent of quotient y/x, using the signs of the two arguments to determine the quadrant of the result, which is in the range $[-\pi, \pi]$.

```
atan2(y,x)
```

$$\arctan(y/x)$$

8.6.5.1 Example #1, atan.fee

```
PRINT atan(-0.5)  mod(atan(-0.5),2*pi)-pi
```

```
$ feenox atan.fee
-0.463648       2.67795
$
```

8.6.5.2 Example #2, atan2.fee

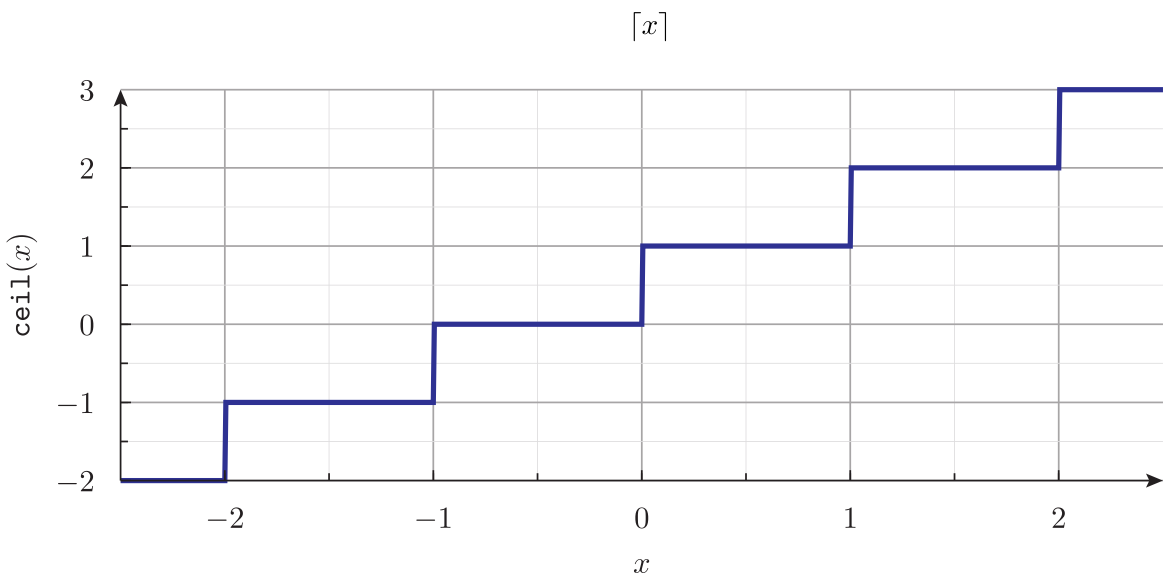
```
PRINT atan2(1,-2) mod(atan(-0.5),2*pi)-pi
```

```
$ feenox atan2.fee
2.67795 2.67795
$
```

8.6.6 ceil

Returns the smallest integral value not less than the argument x.

```
ceil(x)
```



8.6.7 `clock`

Returns the value of a certain clock in seconds measured from a certain (but specific) milestone. The kind of clock and the initial milestone depend on the optional integer argument f. It defaults to one, meaning `CLOCK_MONOTONIC`. The list and the meanings of the other available values for f can be checked in the `clock_gettime (2)` system call manual page.

```
clock([f])
```

8.6.7.1 Example #1, clock.fee

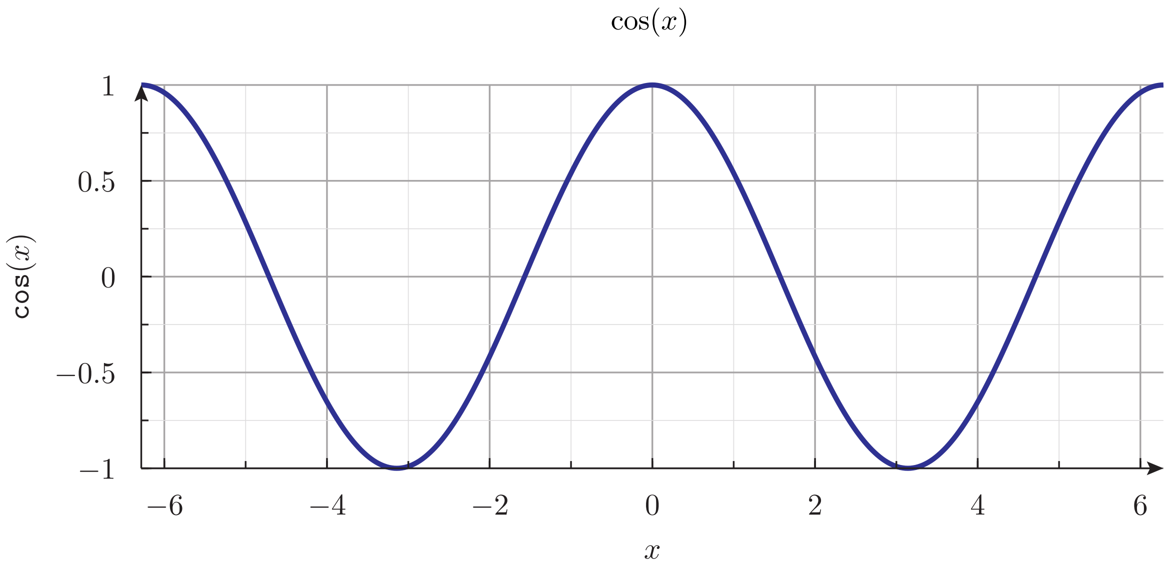
```
t1 = clock()
PRINT "doing something in between"
t2 = clock()
PRINT "difference" t2-t1 "[seconds]"
```

```
$ feenox clock.fee
doing something in between
difference      2.9773e-05      [seconds]
$
```

8.6.8 `cos`

Computes the cosine of the argument x, where x is in radians. A cosine wave can be generated by passing as the argument x a linear function of time such as $\omega t + \phi$, where ω controls the frequency of the wave and ϕ controls its phase.

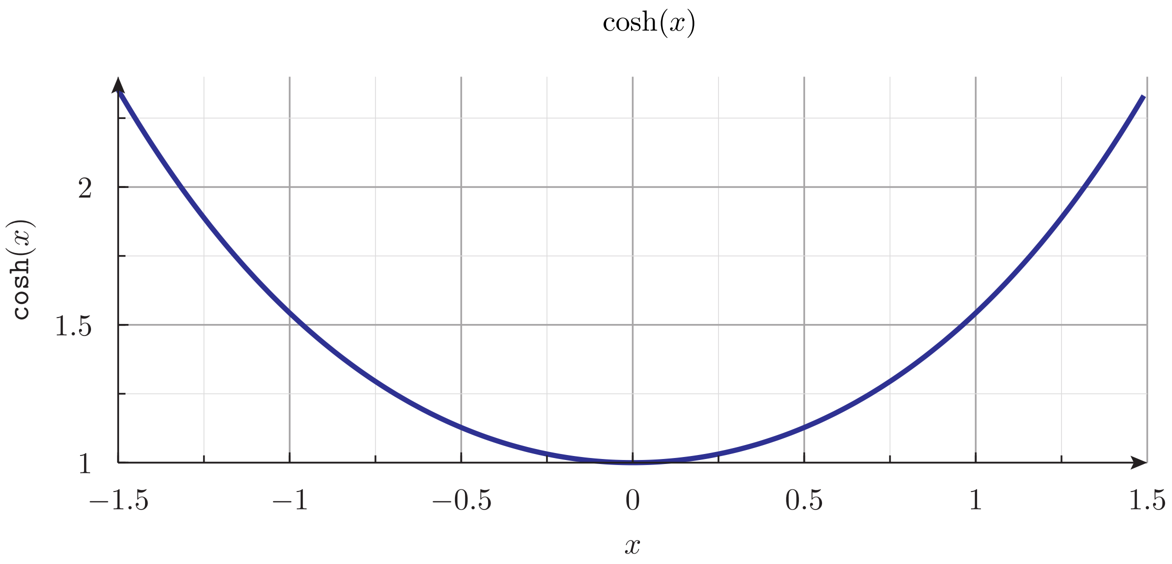
```
cos(x)
```



8.6.9 `cosh`

Computes the hyperbolic cosine of the argument x, where x is in radians.

```
cosh(x)
```



8.6.10 `cpu_time`

Returns the CPU time used by FeenoX, in seconds. If the optional argument `f` is not provided or it is zero (default), the sum of times for both user-space and kernel-space usage is returned. For `f=1` only user time is returned. For `f=2` only system time is returned.

```
cpu_time([f])
```

8.6.11 d_dt

Computes the time derivative of the expression given in the argument x during a transient problem using the difference between the value of the signal in the previous time step and the actual value divided by the time step δt stored in `dt`. The argument x does not neet to be a variable, it can be an expression involving one or more variables that change in time. For $t = 0$, the return value is zero. Unlike the functional `derivative`, the full dependence of these variables with time does not need to be known beforehand, i.e. the expression `x` might involve variables read from a shared-memory object at each time step.

```
d_dt(x)
```

$$\frac{x(t) - x(t - \Delta t)}{\Delta t} \approx \frac{d}{dt}\Big(x(t)\Big)$$

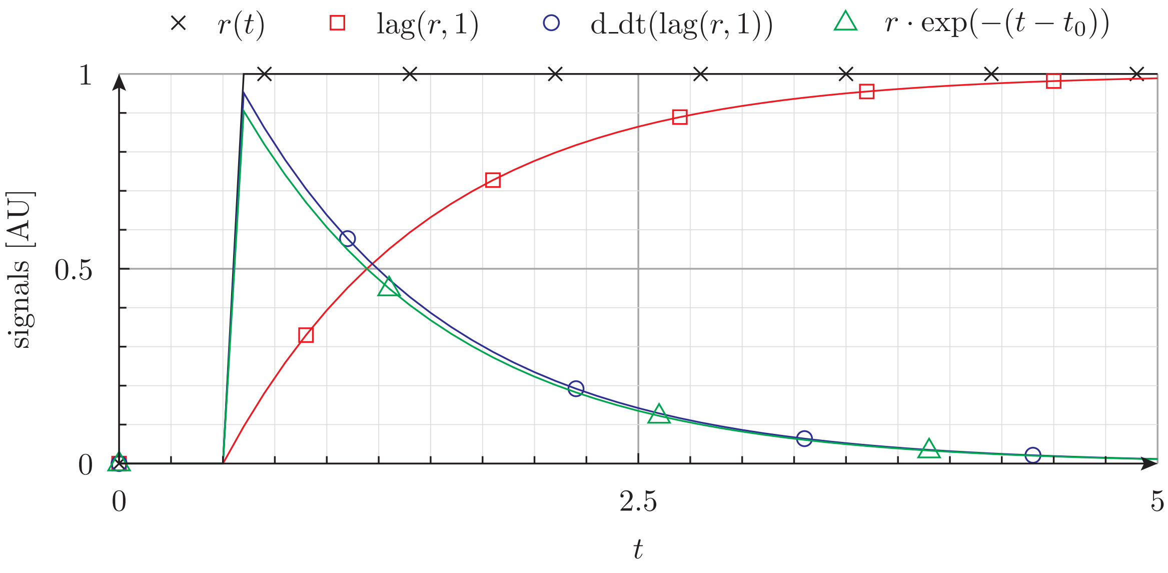
8.6.11.1 Example #1, d_dt.fee

```
end_time = 5
dt = 1/10
t0 = 0.5
r = heaviside(t-t0)

PRINT t r lag(r,1) d_dt(lag(r,1)) r*exp(-(t-t0)) HEADER

# exercise: plot output for different values of dt
```

```
$ feenox d_dt.fee > d_dt.dat
$
```



8.6.12 `deadband`

Filters the first argument x with a deadband centered at zero with an amplitude given by the second argument a.

```
deadband(x, a)
```

$$\begin{cases} 0 & \text{if } |x| \leq a \\ x + a & \text{if } x < a \\ x - a & \text{if } x > a \end{cases}$$

8.6.13 `equal`

Checks if the two first expressions a and b are equal, up to the tolerance given by the third optional argument ϵ. If either $|a| > 1$ or $|b| > 1$, the arguments are compared using GSL's `gsl_fcmp`, otherwise the absolute value of their difference is compared against ϵ. This function returns zero if the arguments are not equal and one otherwise. Default value for $\epsilon = 10^{-9}$.

```
equal(a, b, [eps])
```

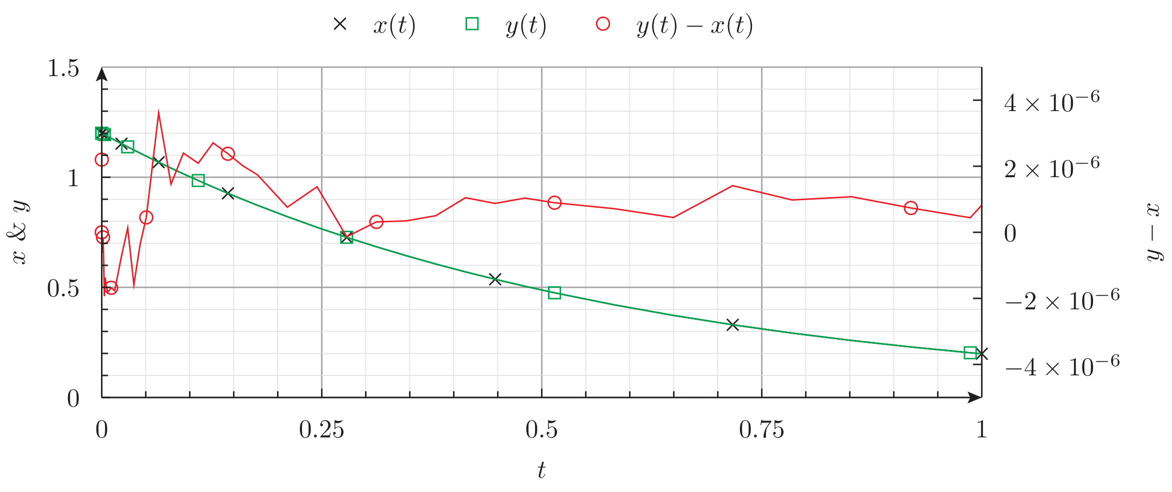
$$\begin{cases} 1 & \text{if } a = b \\ 0 & \text{if } a \neq b \end{cases}$$

8.6.14 `exp`

Computes the exponential function the argument x, i.e. the base of the natural logarithm e raised to the x-th power.

```
exp(x)
```

$$e^x$$



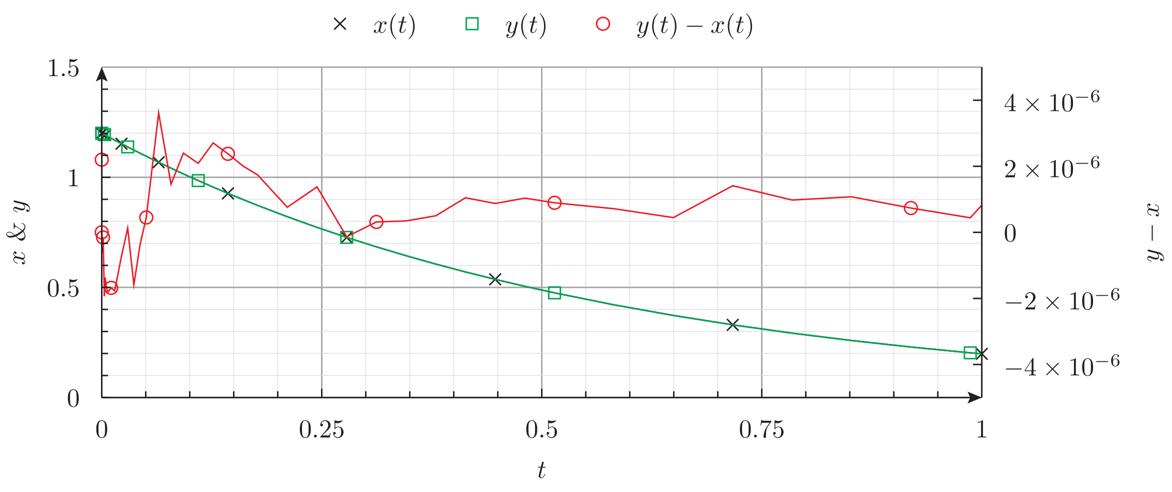
8.6.14.1 Example #1, exp.fee

```
PHASE_SPACE x
end_time = 1
alpha = 1.8
x_0 = 1.2
y(t) := x_0 * exp(-alpha*t)

x_dot .= -alpha*x

PRINT t x y(t) y(t)-x
```

```
$ feenox exp.fee > exp.dat
$
```

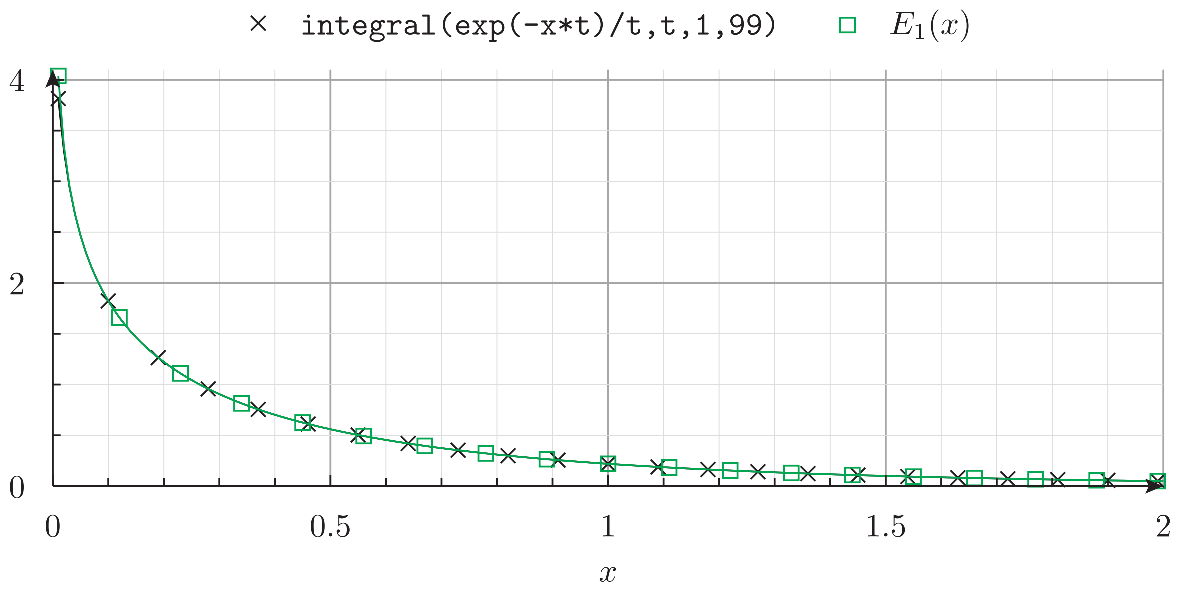


8.6.15 `expint1`

Computes the first exponential integral function of the argument x. If x is zero, a NaN error is issued.

```
expint1(x)
```

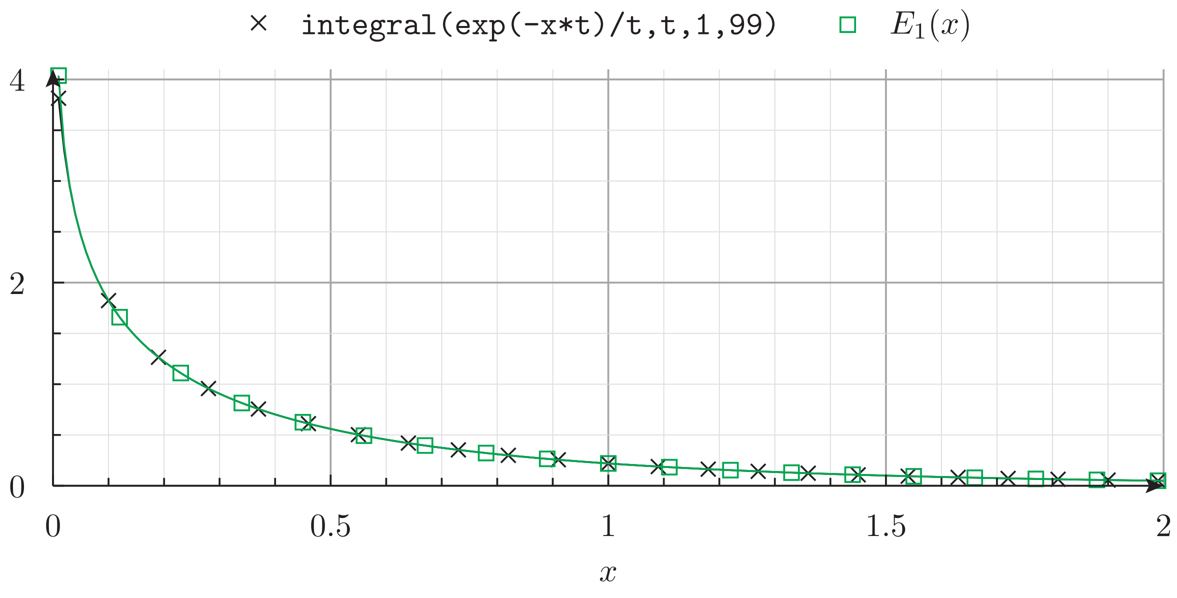
$$\text{Re}\left[\int_1^\infty \frac{\exp(-xt)}{t}\,dt\right]$$



8.6.15.1 Example #1, expint1.fee

```
Def(x) := integral(exp(-x*t)/t,t,1,99)
PRINT_FUNCTION Def expint1(x) MIN 1e-2 MAX 2.0 STEP 1e-2 HEADER
```

```
$ feenox expint1.fee > expint1.dat
$
```

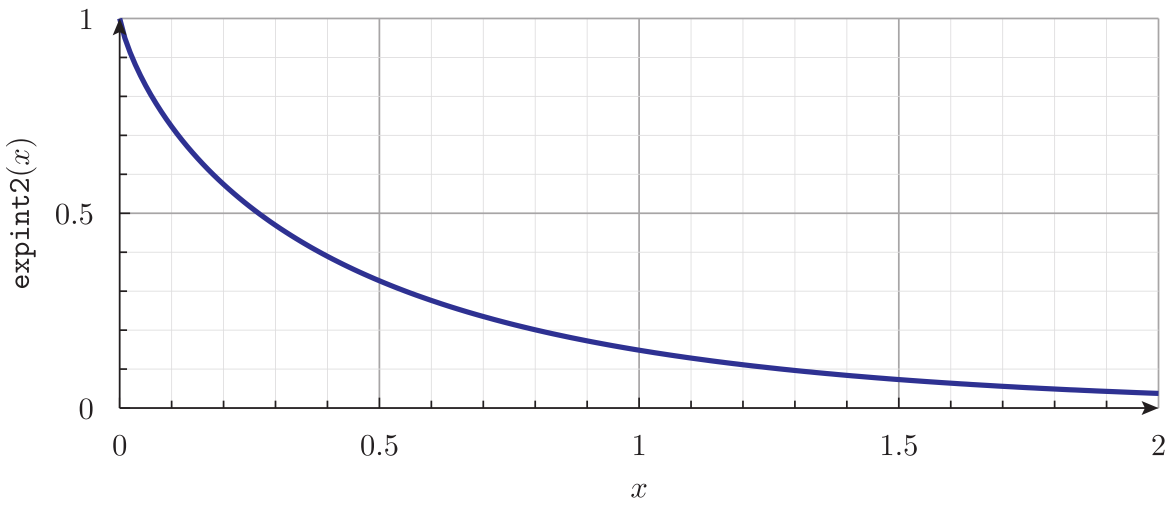


8.6.16 expint2

Computes the second exponential integral function of the argument x.

```
expint2(x)
```

$$\mathrm{Re}\left[\int_1^\infty \frac{\exp(-xt)}{t^2}\,dt\right]$$

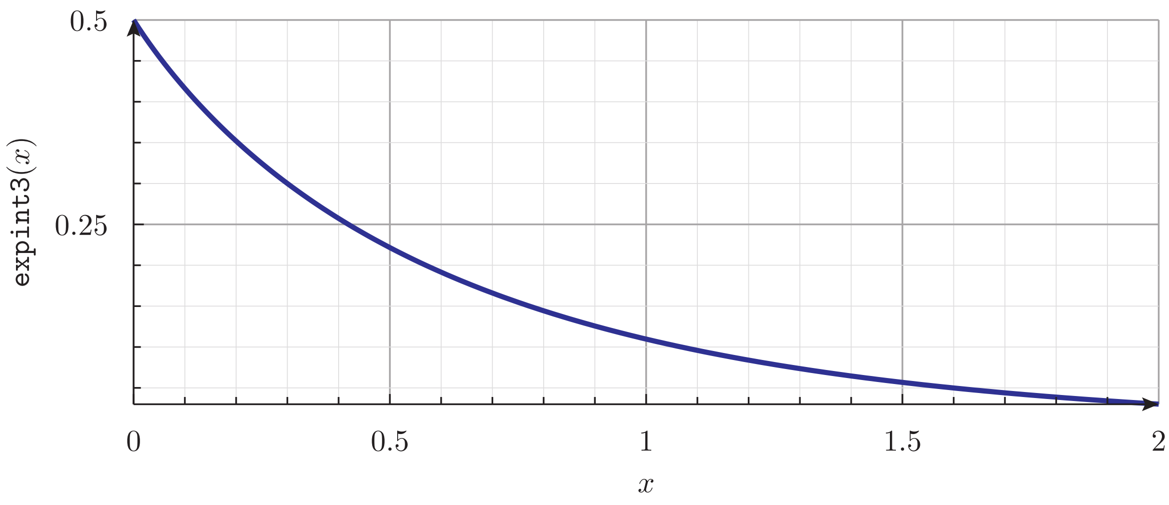


8.6.17 expint3

Computes the third exponential integral function of the argument x.

```
expint3(x)
```

$$\mathrm{Re}\left[\int_1^\infty \frac{\exp(-xt)}{t^3}\,dt\right]$$



8.6.18 expintn

Computes the n-th exponential integral function of the argument x. If n is zero or one and x is zero, a NaN error is issued.

```
expintn(n,x)
```

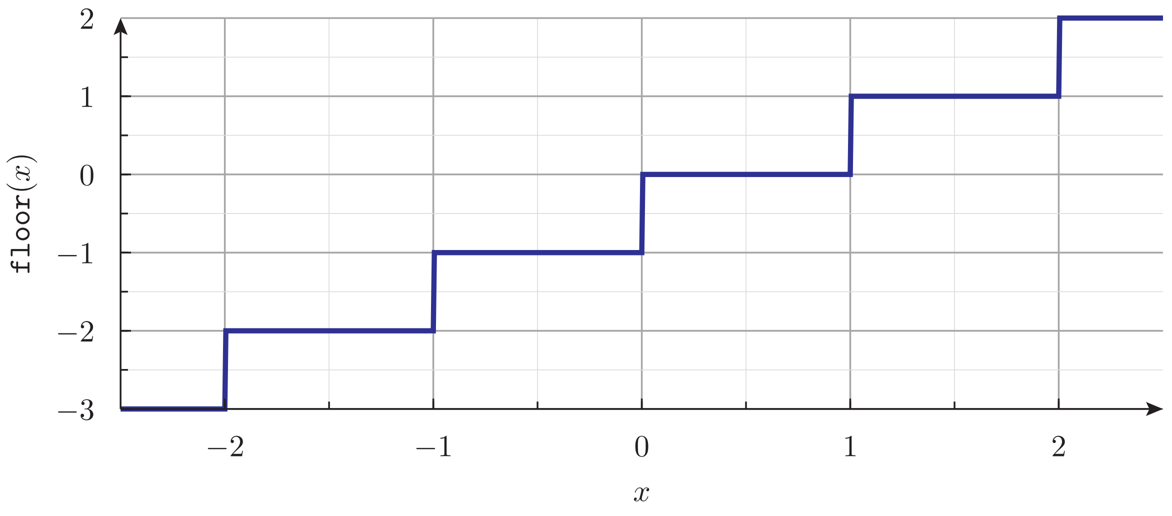
$$\mathrm{Re}\left[\int_1^\infty \frac{\exp(-xt)}{t^n}\,dt\right]$$

8.6.19 floor

Returns the largest integral value not greater than the argument x.

```
floor(x)
```

$$\lfloor x \rfloor$$

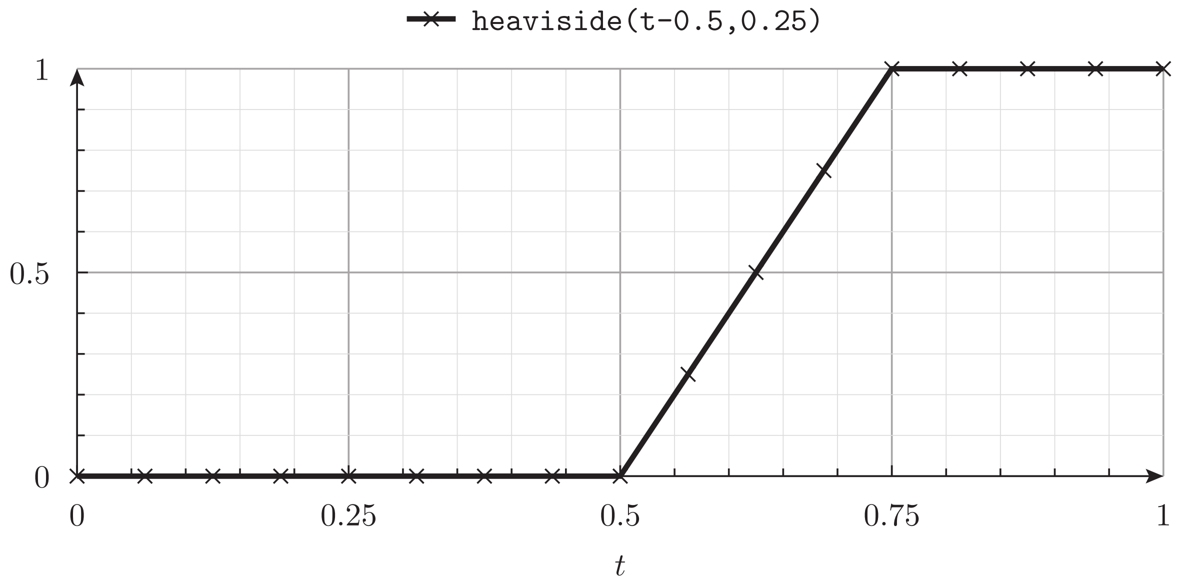


8.6.20 **heaviside**

Computes the zero-centered Heaviside step function of the argument x. If the optional second argument δ is provided, the discontinuous step at $x = 0$ is replaced by a ramp starting at $x = 0$ and finishing at $x = \delta$.

```
heaviside(x, [delta])
```

$$\begin{cases} 0 & \text{if } x < 0 \\ x/\delta & \text{if } 0 < x < \delta \\ 1 & \text{if } x > \delta \end{cases}$$



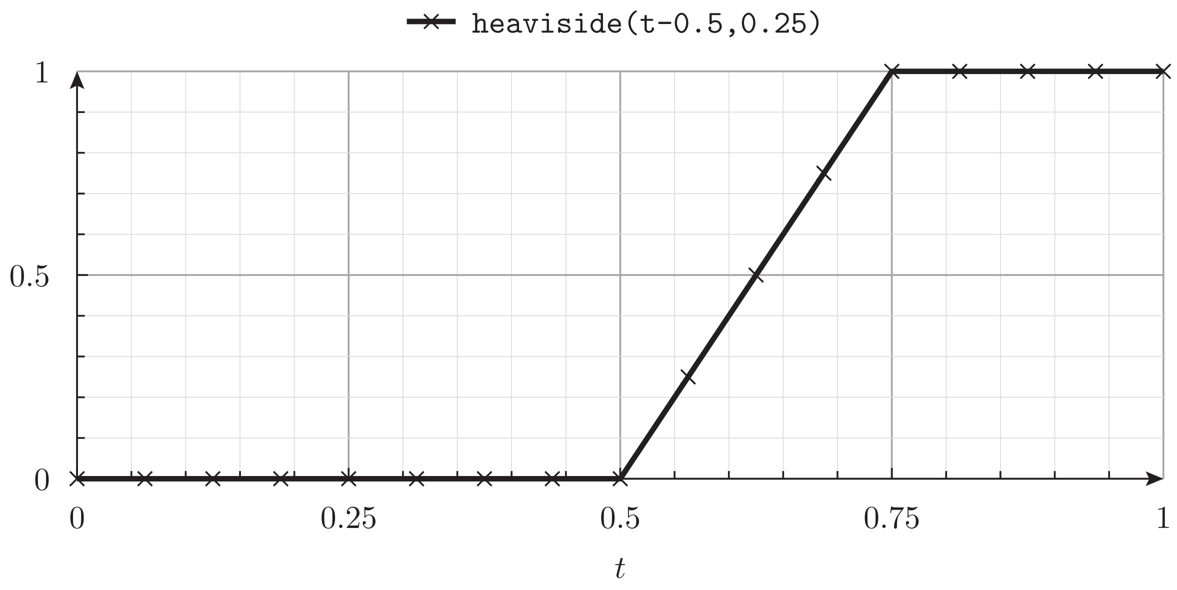
8.6.20.1 Example #1, heaviside.fee

```
end_time = 1

PRINT t heaviside(t-0.5,0.25)

# exercise: what happens if the second argument is negative?
```

```
$ feenox heaviside.fee > heaviside.dat
$
```



8.6.21 `if`

Performs a conditional testing of the first argument a, and returns either the second optional argument b if a is different from zero or the third optional argument c if a evaluates to zero. The comparison of the condition a with zero is performed within the precision given by the optional fourth argument ϵ. If the second argument c is not given and a is not zero, the function returns one. If the third argument c is not given and a is zero, the function returns zero. The default precision is $\epsilon = 10^{-9}$. Even though `if` is a logical operation, all the arguments and the returned value are double-precision floating point numbers.

```
if(a, [b], [c], [eps])
```

$$\begin{cases} b & \text{if } |a| < \epsilon \\ c & \text{otherwise} \end{cases}$$

8.6.22 `integral_dt`

Computes the time integral of the expression given in the argument x during a transient problem with the trapezoidal rule using the value of the signal in the previous time step and the current value. At $t = 0$ the integral is initialized to zero. Unlike the functional `integral`, the full dependence of these variables with time does not need to be known beforehand, i.e. the expression `x` might involve variables read from a shared-memory object at each time step.

```
integral_dt(x)
```

$$z^{-1}\left[\int_0^{t-\Delta t} x(t')\,dt'\right] + \frac{x(t)+x(t-\Delta t)}{2}\,\Delta t \approx \int_0^t x(t')\,dt'$$

8.6.22.1 Example #1, integral_dt.fee

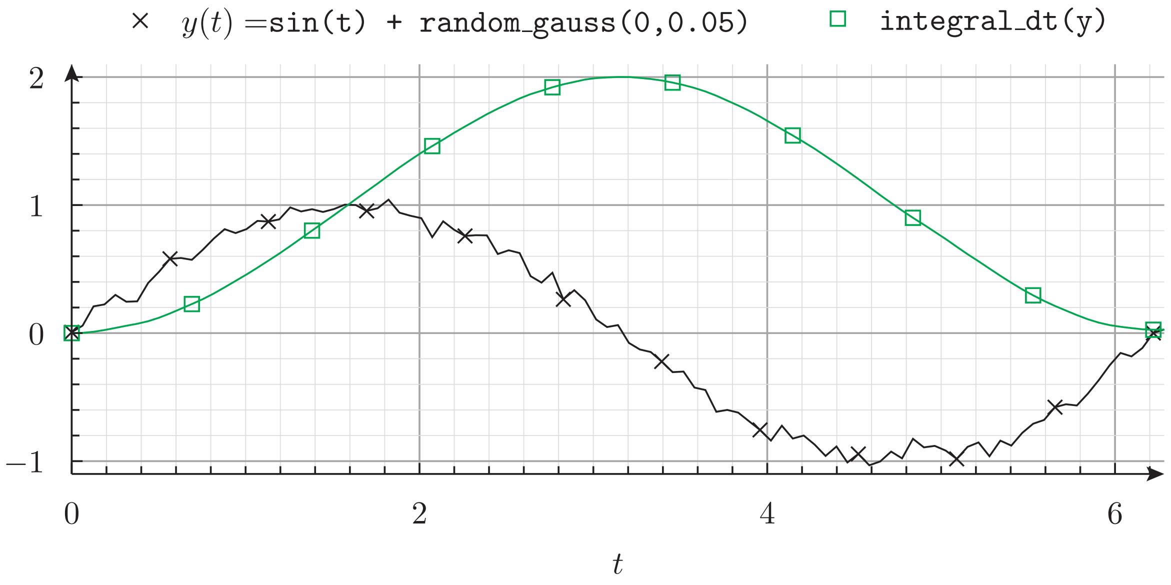
```
end_time = 2*pi
dt = end_time/100

y = sin(t) + random_gauss(0,0.05,0)

PRINT t y integral_dt(y)

# exercise: compute also  the instantaneous
# mean value of the signal y(t)
```

```
$ feenox integral_dt.fee > integral_dt.dat
$
```



8.6.23 `integral_euler_dt`

Idem as `integral_dt` but uses the backward Euler rule to update the instantaenous integral value. This function is provided in case this particular way of approximating time integrals is needed, for instance to compare FeenoX solutions with other computer codes. In general, it is recommended to use `integral_dt`.

```
integral_euler_dt(x)
```

$$z^{-1}\left[\int_0^{t-\Delta t} x(t')\,dt'\right] + x(t)\,\Delta t \approx \int_0^t x(t')\,dt'$$

8.6.24 `is_even`

Returns one if the argument x rounded to the nearest integer is even.

```
is_even(x)
```

$$\begin{cases} 1 & \text{if } x \text{ is even} \\ 0 & \text{if } x \text{ is odd} \end{cases}$$

8.6.25 `is_in_interval`

Returns true if the argument x is in the interval $[a, b)$, i.e. including a but excluding b.

```
is_in_interval(x, a, b)
```

$$\begin{cases} 1 & \text{if } a \le x < b \\ 0 & \text{otherwise} \end{cases}$$

8.6.26 `is_odd`

Returns one if the argument x rounded to the nearest integer is odd.

```
is_odd(x)
```

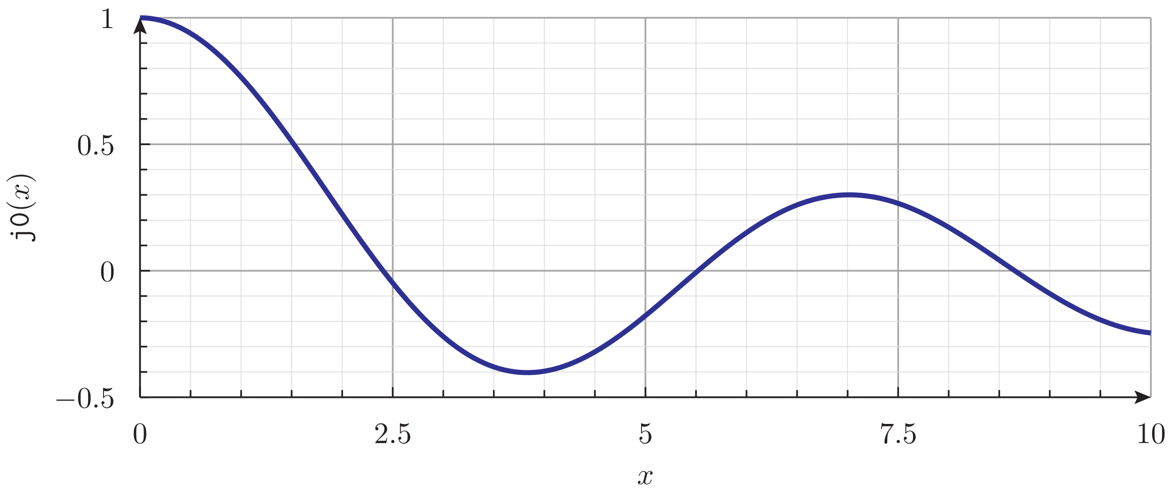
$$\begin{cases} 1 & \text{if } x \text{ is odd} \\ 0 & \text{if } x \text{ is even} \end{cases}$$

8.6.27 `j0`

Computes the regular cylindrical Bessel function of zeroth order evaluated at the argument x.

```
j0(x)
```

$$J_0(x)$$



8.6.27.1 Example #1, j0.fee

```
VAR nu
nu0 = root(j0(nu), nu, 0, 3)
PRINT "J0's first zero is" nu0 SEP " "
PRINT "Indeed, J0(nu0) is equal to" j0(nu0) SEP " "
```

```
$ feenox j0.fee
J0's first zero is 2.40483
Indeed, J0(nu0) is equal to 2.32985e-10
$
```

8.6.28 lag

Filters the first argument $x(t)$ with a first-order lag of characteristic time τ, i.e. this function applies the transfer function $G(s) = \frac{1}{1+s\tau}$ to the time-dependent signal $x(t)$ to obtain a filtered signal $y(t)$, by assuming that it is constant during the time interval $[t - \Delta t, t]$ and using the analytical solution of the differential equation for that case at $t = \Delta t$ with the initial condition $y(0) = y(t - \Delta t)$.

```
lag(x, tau)
```

$$x(t) - \Big[x(t) - y(t - \Delta t)\Big] \cdot \exp\left(-\frac{\Delta t}{\tau}\right)$$

8.6.29 lag_bilinear

Filters the first argument $x(t)$ with a first-order lag of characteristic time τ to the time-dependent signal $x(t)$ by using the bilinear transformation formula.

```
lag_bilinear(x, tau)
```

$$x(t-\Delta t)\cdot\left[1-\frac{\Delta t}{2\tau}\right]+\left[\frac{x(t)+x(t-\Delta t)}{1+\frac{\Delta t}{2\tau}}\right]\cdot\frac{\Delta t}{2\tau}$$

8.6.30 `lag_euler`

Filters the first argument $x(t)$ with a first-order lag of characteristic time τ to the time-dependent signal $x(t)$ by using the Euler forward rule.

```
lag_euler(x, tau)
```

$$x(t-\Delta t)+\Big[x(t)-x(t-\Delta t)\Big]\cdot\frac{\Delta t}{\tau}$$

8.6.31 `last`

Returns the value the variable x had in the previous time step. This function is equivalent to the Z-transform operator "delay" denoted by $z^{-1}[x]$. For $t=0$ the function returns the actual value of x. The optional flag p should be set to one if the reference to `last` is done in an assignment over a variable that already appears inside expression x such as `x = last(x)`. See example number 2.

```
last(x,[p])
```

$$z^{-1}[x]=x(t-\Delta t)$$

8.6.31.1 Example #1, last1.fee

```
static_steps = 5
end_time = 1
dt = 0.1

IF in_static
  PRINT step_static last(step_static) last(last(step_static))
ENDIF
IF done_static
  PRINT t last(t) last(last(1-t))
ENDIF
```

```
$ feenox last1.fee
1       1       1
2       1       1
3       2       1
4       3       2
5       4       3
0       0       1
0.1     0       1
0.2     0.1     1
0.3     0.2     0.9
0.4     0.3     0.8
```

```
0.5     0.4     0.7
0.6     0.5     0.6
0.7     0.6     0.5
0.8     0.7     0.4
0.9     0.8     0.3
1       0.9     0.2
$
```

8.6.31.2 Example #2, last2.fee

```
end_time = 1
dt = 0.1

y = y + 1
z  = last(z,1) + 1
z' = last(z')  + 1

PRINT t %g y z z'
```

```
$ feenox last2.fee
0       1       1       1
0.1     2       2       1
0.2     3       3       2
0.3     4       4       2
0.4     5       5       3
0.5     6       6       3
0.6     7       7       4
0.7     8       8       4
0.8     9       9       5
0.9     10      10      5
1       11      11      6
$
```

8.6.32 `limit`

Limits the first argument x to the interval $[a, b]$. The second argument a should be less than the third argument b.

```
limit(x, a, b)
```

$$\begin{cases} a & \text{if } x < a \\ x & \text{if } a \leq x \leq b \\ b & \text{if } x > b \end{cases}$$

8.6.33 `limit_dt`

Limits the value of the first argument $x(t)$ so to that its time derivative is bounded to the interval $[a, b]$. The second argument a should be less than the third argument b.

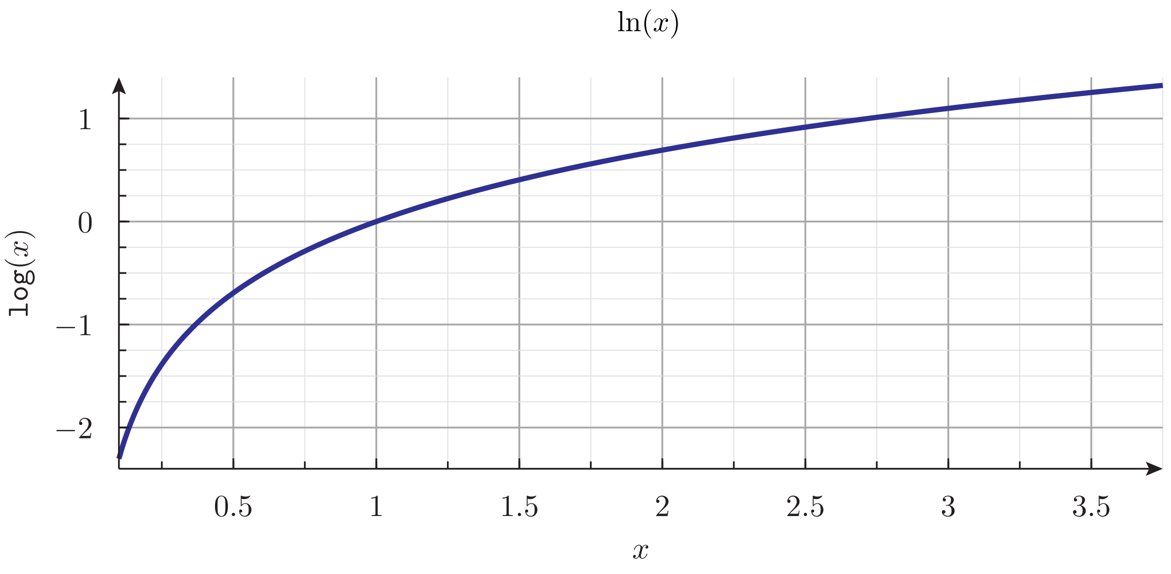
```
limit_dt(x, a, b)
```

$$\begin{cases} x(t) & \text{if } a \leq dx/dt \leq b \\ x(t-\Delta t) + a \cdot \Delta t & \text{if } dx/dt < a \\ x(t-\Delta t) + b \cdot \Delta t & \text{if } dx/dt > b \end{cases}$$

8.6.34 log

Computes the natural logarithm of the argument x. If x is zero or negative, a NaN error is issued.

```
log(x)
```



8.6.34.1 Example #1, log1.fee

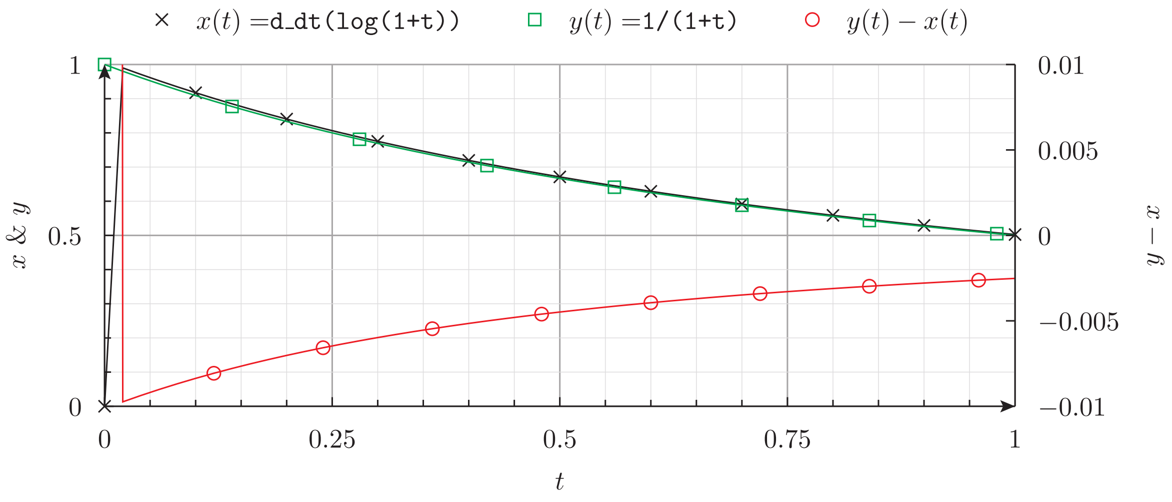
```
end_time = 1
dt = 1/50

x = d_dt(log(1+t))
y = 1/(1+t)

PRINT t x y y-x

# exercise: why does this example give a bigger error than the exp.fee example?
```

```
$ feenox log1.fee > log1.dat
$
```



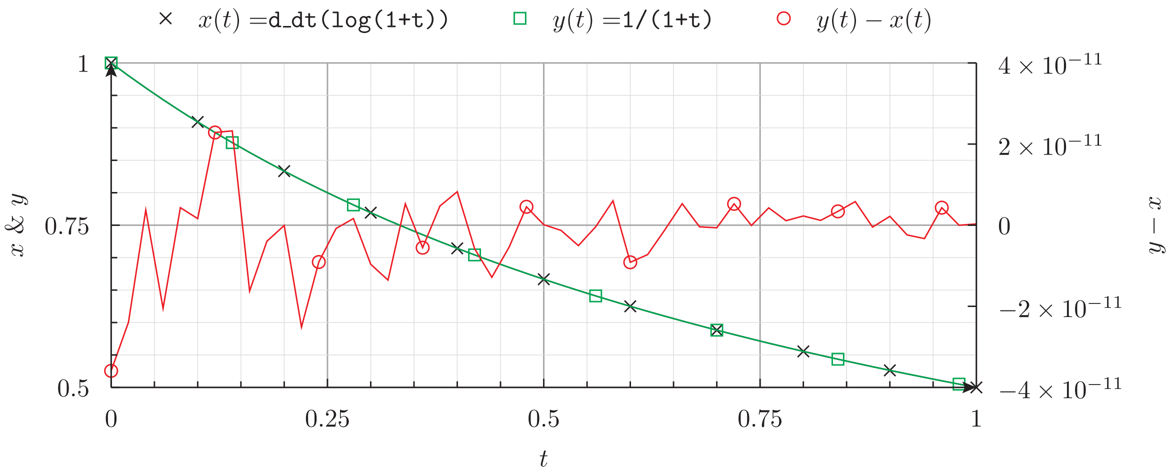
8.6.34.2 Example #2, log2.fee

```
VAR t'
x(t) := derivative(log(1+t'), t', t)
y(t) := 1/(1+t)

PRINT_FUNCTION x y y(t)-x(t) MIN 0 MAX 1 NSTEPS 50

# exercise: why does this example give a smaller error than the exp.fee example?
```

```
$ feenox log2.fee > log2.dat
$
```



8.6.35 `mark_max`

Returns the integer index i of the maximum of the arguments x_i provided. Currently only maximum of ten arguments can be provided.

```
mark_max(x1, x2, [...], [x10])
```

$$i / \max\left(x_1, x_2, \dots, x_{10}\right) = x_i$$

8.6.36 `mark_min`

Returns the integer index i of the minimum of the arguments x_i provided. Currently only maximum of ten arguments can be provided.

```
mark_max(x1, x2, [...], [x10])
```

$$i / \min\left(x_1, x_2, \dots, x_{10}\right) = x_i$$

8.6.37 `max`

Returns the maximum of the arguments x_i provided. Currently only maximum of ten arguments can be given.

```
max(x1, x2, [...], [x10])
```

$$\max\left(x_1, x_2, \dots, x_{10}\right)$$

8.6.38 `memory`

Returns the maximum memory (resident set size) used by FeenoX, in Gigabytes.

```
memory()
```

8.6.39 `min`

Returns the minimum of the arguments x_i provided. Currently only maximum of ten arguments can be given.

```
min(x1, x2, [...], [x10])
```

$$\min\left(x_1, x_2, \dots, x_{10}\right)$$

8.6.40 `mod`

Returns the remainder of the division between the first argument a and the second one b. Both arguments may be non-integral.

```
mod(a, b)
```

$$a - \left\lfloor \frac{a}{b} \right\rfloor \cdot b$$

8.6.41 `not`

Returns one if the first argument x is zero and zero otherwise. The second optional argument ϵ gives the precision of the "zero" evaluation. If not given, default is $\epsilon = 10^{-9}$.

```
not(x, [eps])
```

$$\begin{cases} 1 & \text{if } |x| < \epsilon \\ 0 & \text{otherwise} \end{cases}$$

8.6.42 `random`

Returns a random real number uniformly distributed between the first real argument x_1 and the second one x_2. If the third integer argument s is given, it is used as the seed and thus repetitive sequences can be obtained. If no seed is provided, the current time (in seconds) plus the internal address of the expression is used. Therefore, two successive calls to the function without seed (hopefully) do not give the same result. This function uses a second-order multiple recursive generator described by Knuth in Seminumerical Algorithms, 3rd Ed., Section 3.6.

```
random(x1, x2, [s])
```

$$x_1 + r \cdot (x_2 - x_1) \qquad 0 \leq r < 1$$

8.6.43 `random_gauss`

Returns a random real number with a Gaussian distribution with a mean equal to the first argument x_1 and a standard deviation equatl to the second one x_2. If the third integer argument s is given, it is used as the seed and thus repetitive sequences can be obtained. If no seed is provided, the current time (in seconds) plus the internal address of the expression is used. Therefore, two successive calls to the function without seed (hopefully) do not give the same result. This function uses a second-order multiple recursive generator described by Knuth in Seminumerical Algorithms, 3rd Ed., Section 3.6.

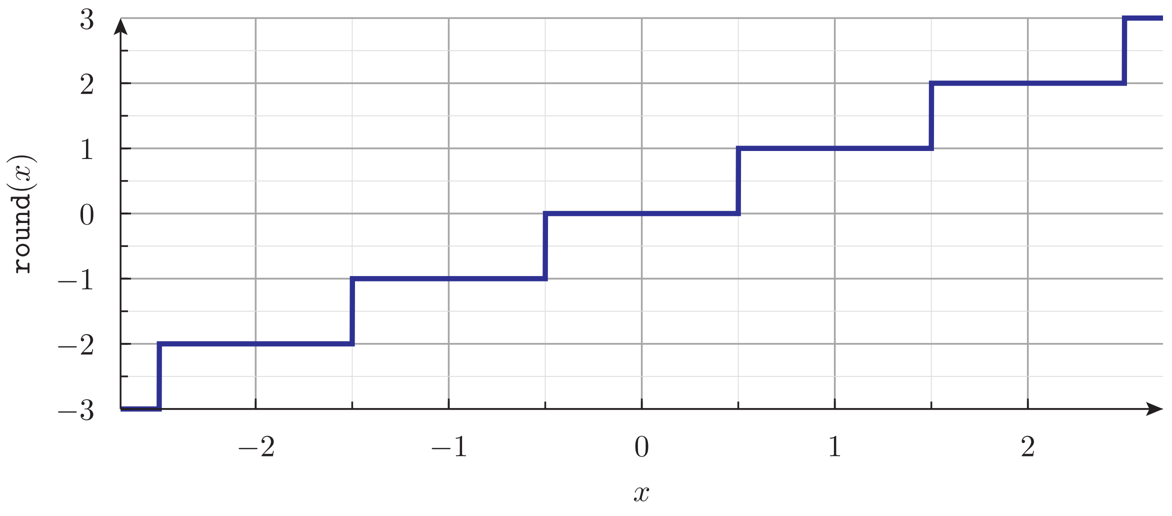
```
random_gauss(x1, x2, [s])
```

8.6.44 `round`

Rounds the argument x to the nearest integer. Halfway cases are rounded away from zero.

```
round(x)
```

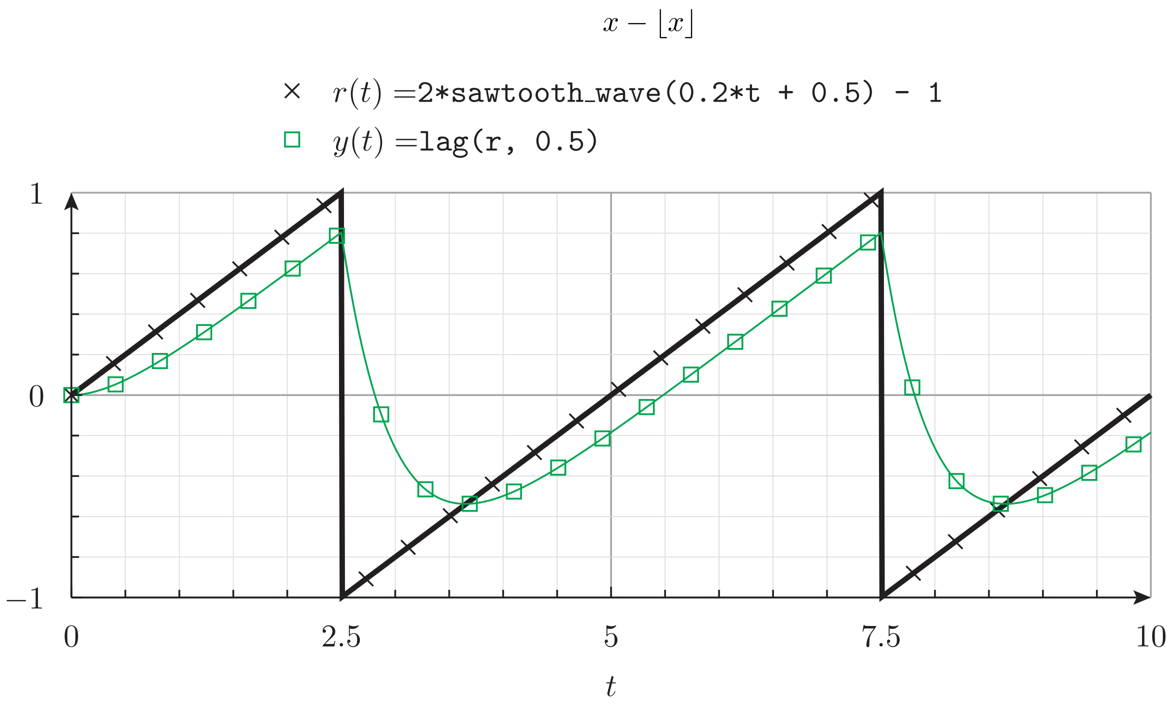
$$\begin{cases} \lceil x \rceil & \text{if } \lceil x \rceil - x < 0.5 \\ \lceil x \rceil & \text{if } \lceil x \rceil - x = 0.5 \wedge x > 0 \\ \lfloor x \rfloor & \text{if } x - \lfloor x \rfloor < 0.5 \\ \lfloor x \rfloor & \text{if } x - \lfloor x \rfloor = 0.5 \wedge x < 0 \end{cases}$$



8.6.45 `sawtooth_wave`

Computes a sawtooth wave between zero and one with a period equal to one. As with the sine wave, a sawtooh wave can be generated by passing as the argument x a linear function of time such as $\omega t + \phi$, where ω controls the frequency of the wave and ϕ controls its phase.

```
sawtooth_wave(x)
```



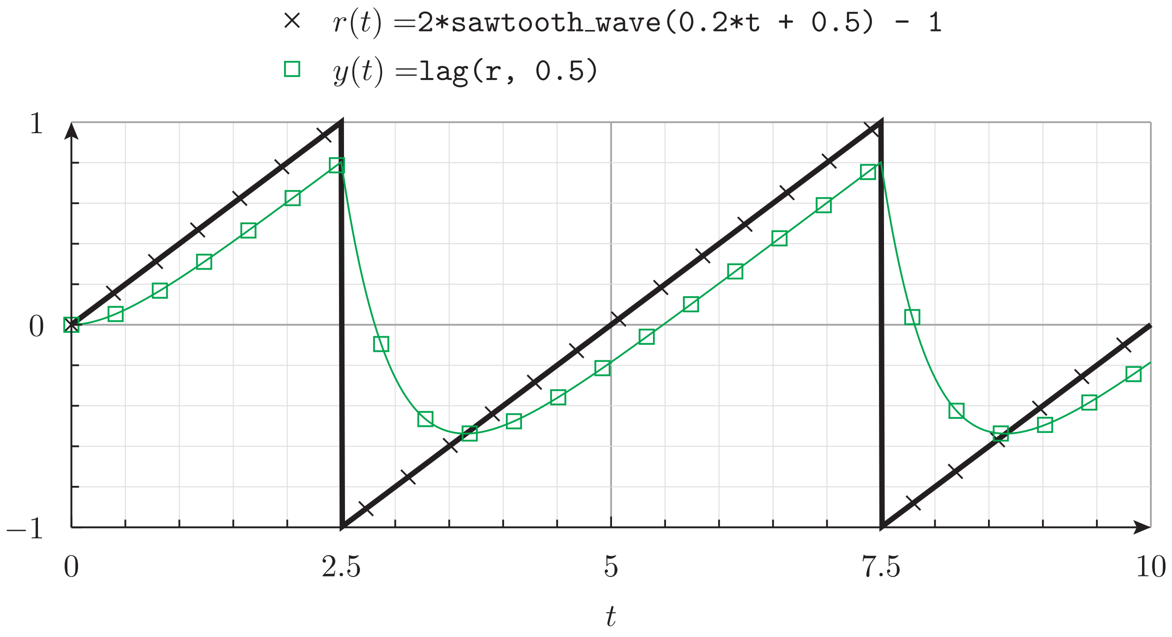
8.6.45.1 Example #1, sawtooth_wave.fee

```
end_time = 10
dt = 1e-2

r = 2*sawtooth_wave(0.2*t + 0.5) - 1
y = lag(r, 0.5)

PRINT t r y
```

```
$ feenox sawtooth_wave.fee > sawtooth_wave.dat
$
```

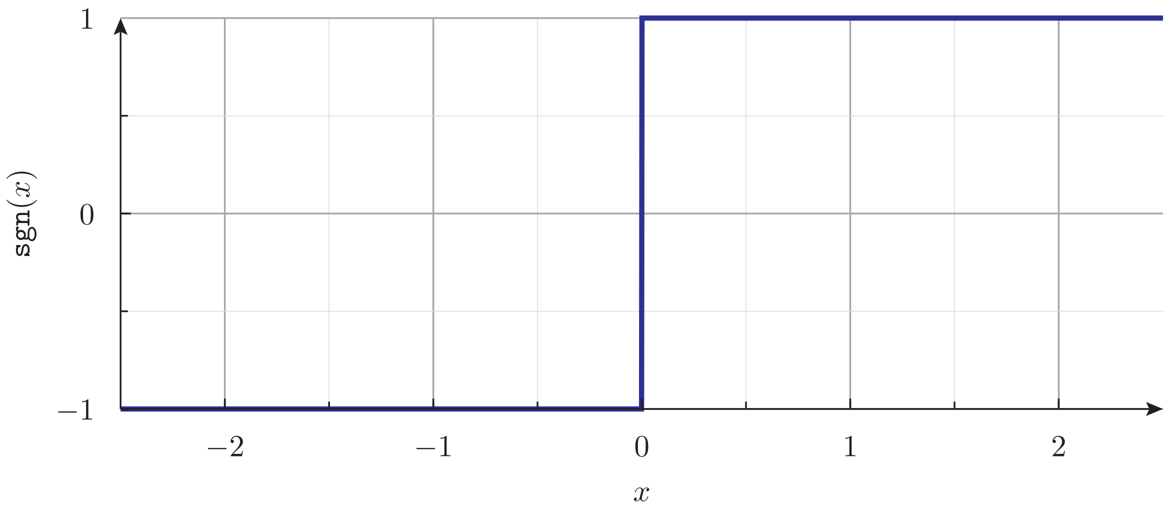


8.6.46 sgn

Returns minus one, zero or plus one depending on the sign of the first argument x. The second optional argument ϵ gives the precision of the "zero" evaluation. If not given, default is $\epsilon = 10^{-9}$.

```
sgn(x, [eps])
```

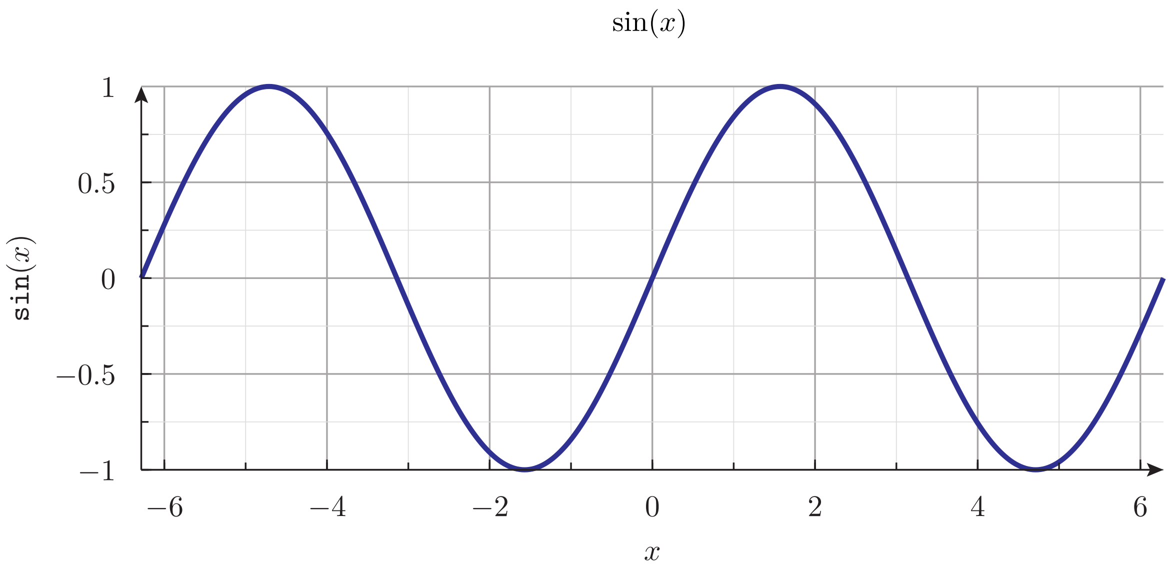
$$\begin{cases} -1 & \text{if } x \leq -\epsilon \\ 0 & \text{if } |x| < \epsilon \\ +1 & \text{if } x \geq +\epsilon \end{cases}$$



8.6.47 `sin`

Computes the sine of the argument x, where x is in radians. A sine wave can be generated by passing as the argument x a linear function of time such as $\omega t + \phi$, where ω controls the frequency of the wave and ϕ controls its phase.

```
sin(x)
```



8.6.47.1 Example #1, sin.fee

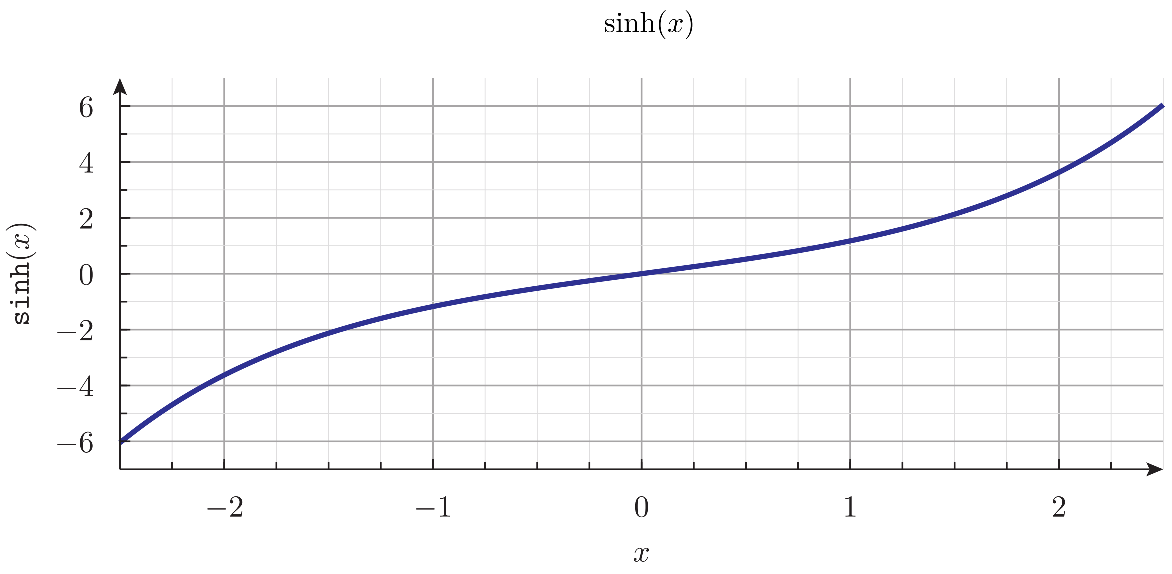
```
PRINT sin(1)
PRINT sqrt(1-cos(1)^2)
```

```
$ feenox sin.fee
0.841471
0.841471
$
```

8.6.48 `sinh`

Computes the hyperbolic sine of the argument x, where x is in radians.

```
sinh(x)
```

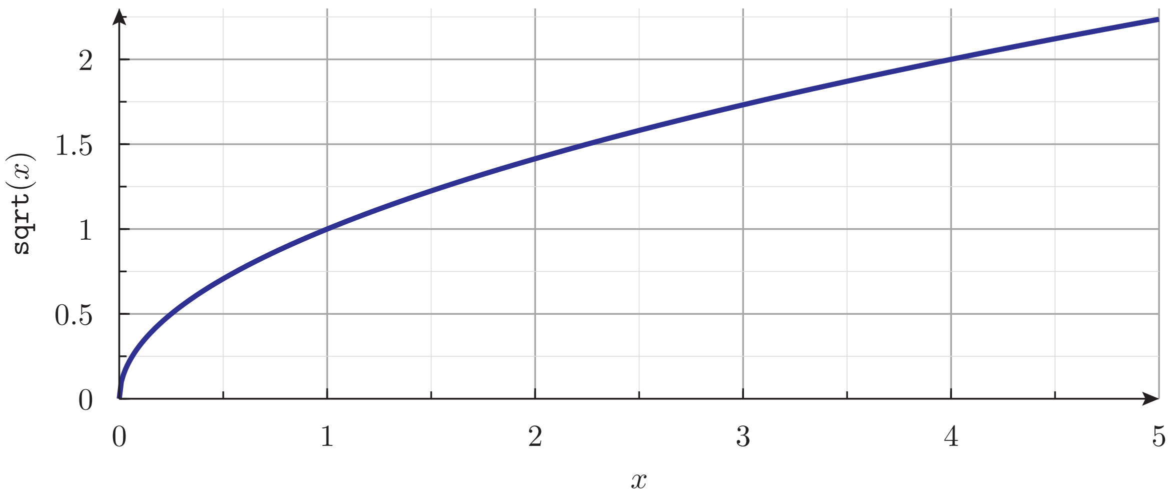


8.6.49 `sqrt`

Computes the positive square root of the argument x. If x is negative, a NaN error is issued.

```
sqrt(x)
```

$$+\sqrt{x}$$

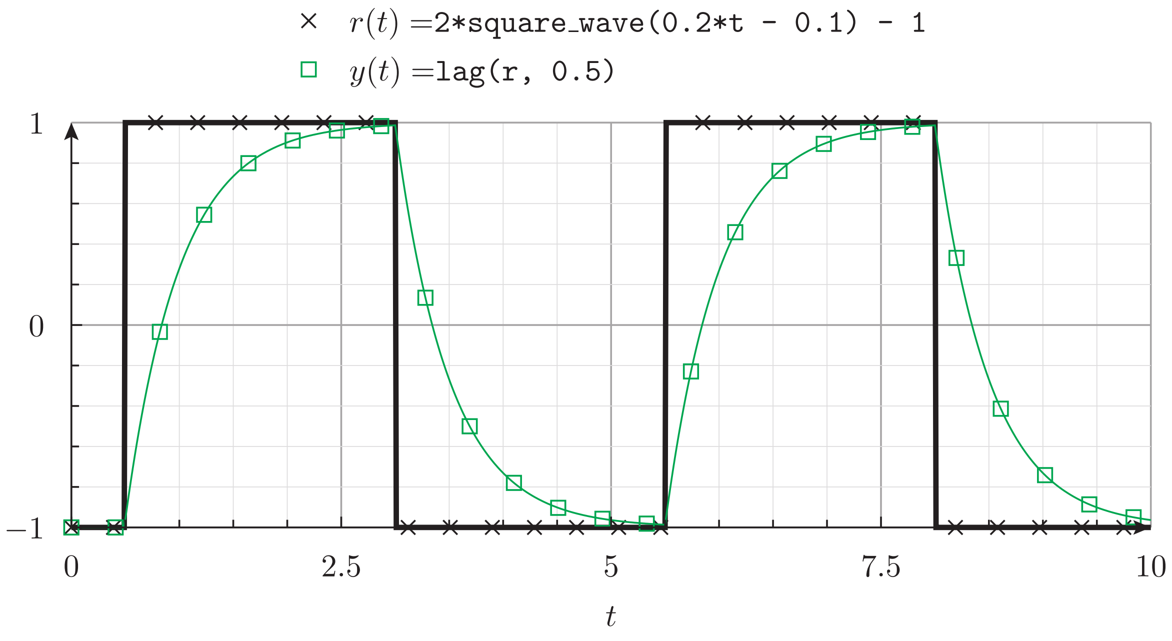


8.6.50 `square_wave`

Computes a square function between zero and one with a period equal to one. The output is one for $0 < x < 1/2$ and zero for $1/2 \leq x < 1$. As with the sine wave, a square wave can be generated by passing as the argument x a linear function of time such as $\omega t + \phi$, where ω controls the frequency of the wave and ϕ controls its phase.

```
square_wave(x)
```

$$\begin{cases} 1 & \text{if } x - \lfloor x \rfloor < 0.5 \\ 0 & \text{otherwise} \end{cases}$$



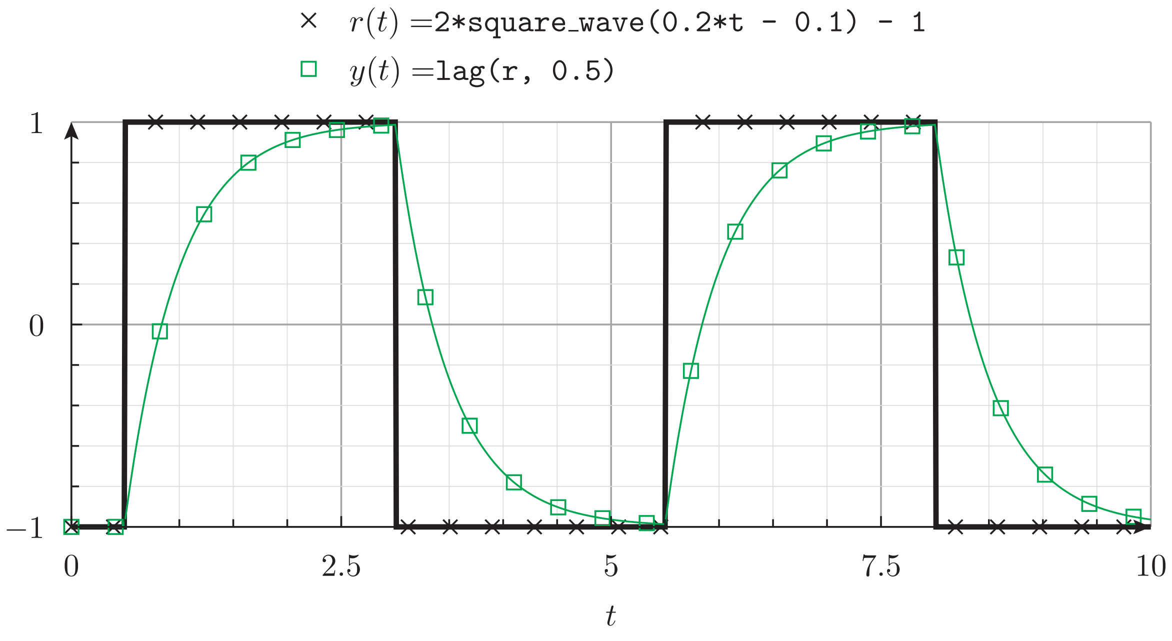
8.6.50.1 Example #1, square_wave.fee

```
end_time = 10
dt = 1e-2

r = 2*square_wave(0.2*t - 0.1) - 1
y = lag(r, 0.5)

PRINT t r y
```

```
$ feenox square_wave.fee > square_wave.dat
$
```

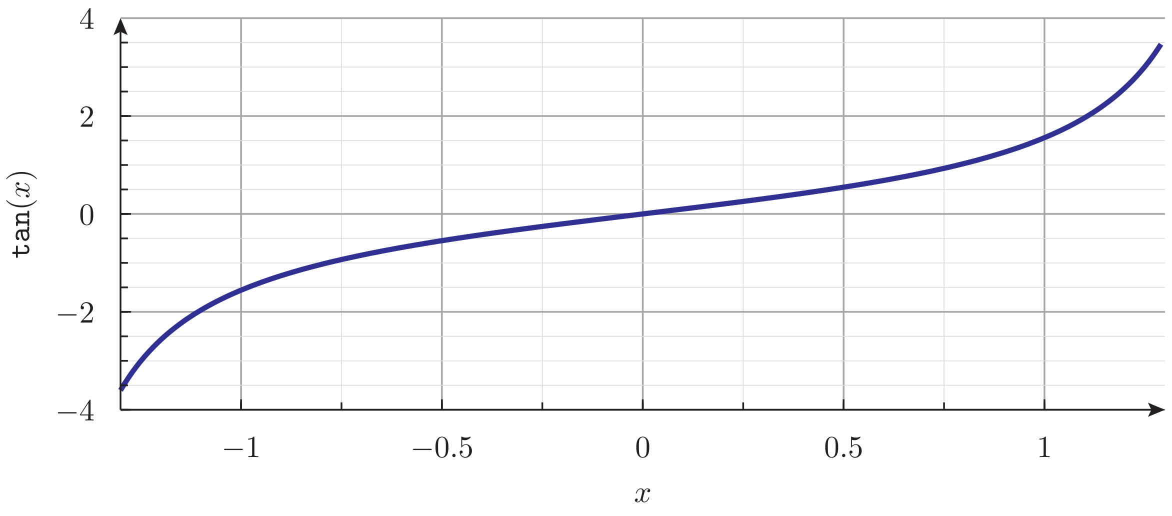


8.6.51 tan

Computes the tangent of the argument x, where x is in radians.

```
tan(x)
```

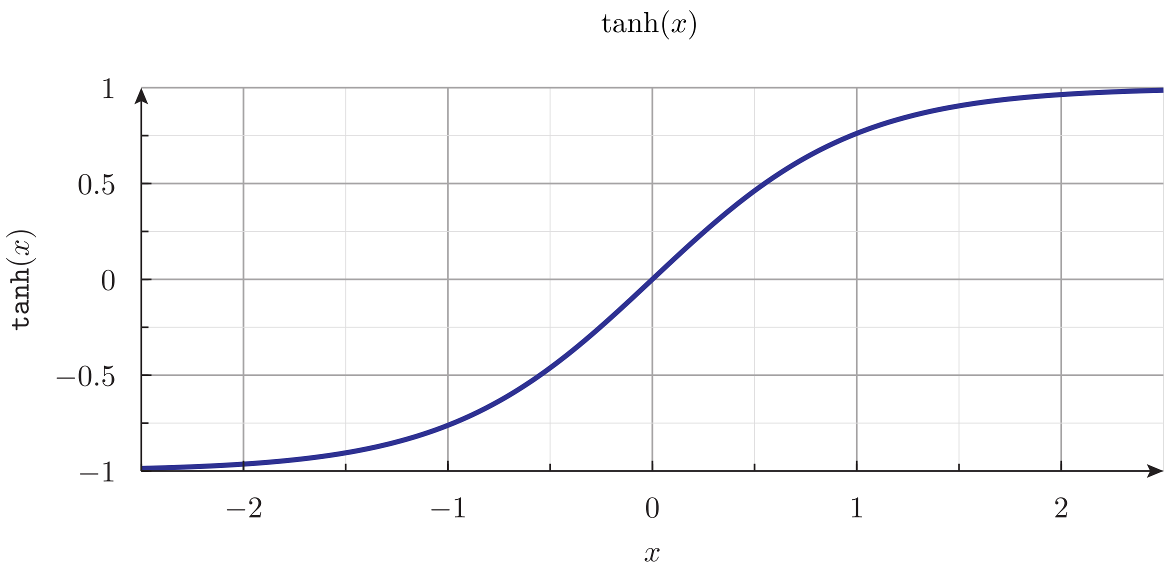
$$\tan(x)$$



8.6.52 `tanh`

Computes the hyperbolic tangent of the argument x, where x is in radians.

```
tanh(x)
```



8.6.53 `threshold_max`

Returns one if the first argument x is greater than the threshold given by the second argument a, and *exactly* zero otherwise. If the optional third argument b is provided, an hysteresis of width b is needed in order to reset the function value. Default is no hysteresis, i.e. $b = 0$.

```
threshold_max(x, a, [b])
```

$$\begin{cases} 1 & \text{if } x > a \\ 0 & \text{if } x < a - b \\ \text{last value of } y & \text{otherwise} \end{cases}$$

8.6.54 `threshold_min`

Returns one if the first argument x is less than the threshold given by the second argument a, and *exactly* zero otherwise. If the optional third argument b is provided, an hysteresis of width b is needed in order to reset the function value. Default is no hysteresis, i.e. $b = 0$.

```
threshold_min(x, a, [b])
```

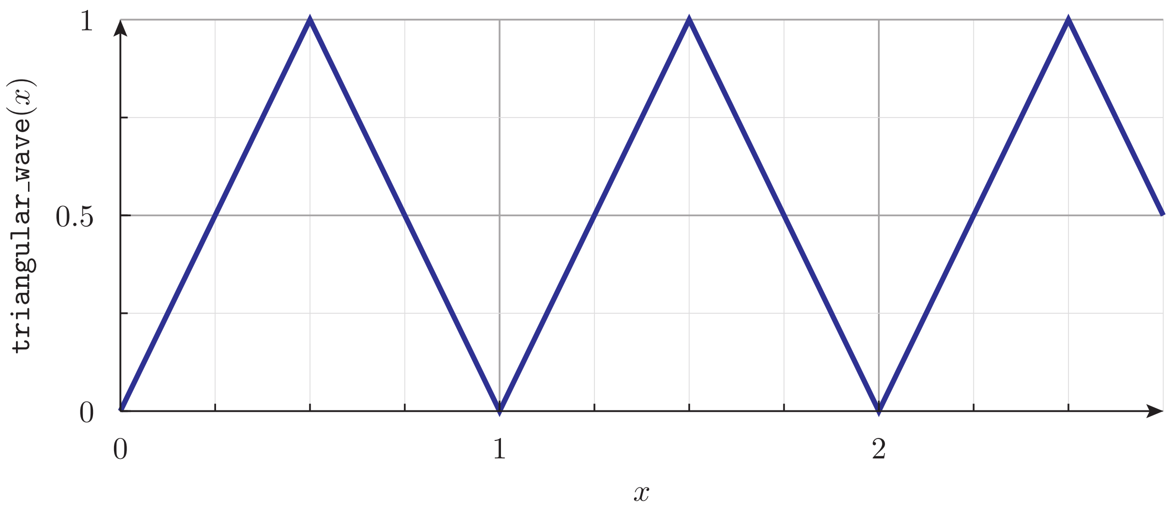
$$\begin{cases} 1 & \text{if } x < a \\ 0 & \text{if } x > a + b \\ \text{last value of } y & \text{otherwise} \end{cases}$$

8.6.55 `triangular_wave`

Computes a triangular wave between zero and one with a period equal to one. As with the sine wave, a triangular wave can be generated by passing as the argument x a linear function of time such as $\omega t + \phi$, where ω controls the frequency of the wave and ϕ controls its phase.

```
triangular_wave(x)
```

$$\begin{cases} 2(x - \lfloor x \rfloor) & \text{if } x - \lfloor x \rfloor < 0.5 \\ 2[1 - (x - \lfloor x \rfloor)] & \text{otherwise} \end{cases}$$



8.6.56 `wall_time`

Returns the time ellapsed since the invocation of FeenoX, in seconds.

```
wall_time()
```

8.7 Functionals

8.7.1 `derivative`

Computes the derivative of the expression $f(x)$ given in the first argument with respect to the variable x given in the second argument at the point $x = a$ given in the third argument using an adaptive scheme. The fourth optional argument h is the initial width of the range the adaptive derivation method starts with. The fifth optional argument p is a flag that indicates whether a backward ($p < 0$), centered ($p = 0$) or forward ($p > 0$) stencil is to be used. This functional calls the GSL functions `gsl_deriv_backward`, `gsl_deriv_central` or `gsl_deriv_forward` according to the indicated flag p. Defaults are $h = (1/2)^{-10} \approx 9.8 \times 10^{-4}$ and $p = 0$.

```
derivative(f(x), x, a, [h], [p])
```

$$\frac{d}{dx}\Big[f(x)\Big]\Big|_{x=a}$$

8.8 Vector functions

8.8.1 `derivative`

Computes the derivative of the expression $f(x)$ given in the first argument with respect to the variable x given in the second argument at the point $x = a$ given in the third argument using an adaptive scheme. The fourth optional argument h is the initial width of the range the adaptive derivation method starts with. The fifth optional argument p is a flag that indicates whether a backward ($p < 0$), centered ($p = 0$) or forward ($p > 0$) stencil is to be used. This functional calls the GSL functions `gsl_deriv_backward`, `gsl_deriv_central` or `gsl_deriv_forward` according to the indicated flag p. Defaults are $h = (1/2)^{-10} \approx 9.8 \times 10^{-4}$ and $p = 0$.

```
derivative(f(x), x, a, [h], [p])
```

$$\frac{d}{dx}\Big[f(x)\Big]\Big|_{x=a}$$

Appendix A

FeenoX & the UNIX Philospohy

A.1 Rule of Modularity

Developers should build a program out of simple parts connected by well defined interfaces, so problems are local, and parts of the program can be replaced in future versions to support new features. This rule aims to save time on debugging code that is complex, long, and unreadable.

- FeenoX uses third-party high-quality libraries
  - GNU Scientific Library
  - SUNDIALS
  - PETSc
  - SLEPc

A.2 Rule of Clarity

Developers should write programs as if the most important communication is to the developer who will read and maintain the program, rather than the computer. This rule aims to make code as readable and comprehensible as possible for whoever works on the code in the future.

- Example two squares in thermal contact.
- LE10 & LE11: a one-to-one correspondence between the problem text and the FeenoX input.

A.3 Rule of Composition

Developers should write programs that can communicate easily with other programs. This rule aims to allow developers to break down projects into small, simple programs rather than overly complex monolithic programs.

- FeenoX uses meshes created by a separate mesher (i.e. Gmsh).
- FeenoX writes data that has to be plotted or post-processed by other tools (Gnuplot, Gmsh, Paraview, etc.).

- ASCII output is 100% controlled by the user so it can be tailored to suit any other programs' input needs such as AWK filters to create LaTeXtables.

A.4 Rule of Separation

Developers should separate the mechanisms of the programs from the policies of the programs; one method is to divide a program into a front-end interface and a back-end engine with which that interface communicates. This rule aims to prevent bug introduction by allowing policies to be changed with minimum likelihood of destabilizing operational mechanisms.

- FeenoX does not include a GUI, but it is GUI-friendly.

A.5 Rule of Simplicity

Developers should design for simplicity by looking for ways to break up program systems into small, straightforward cooperating pieces. This rule aims to discourage developers' affection for writing "intricate and beautiful complexities" that are in reality bug prone programs.

- Simple problems need simple input.
- Similar problems need similar inputs.
- English-like self-evident input files matching as close as possible the problem text.
- If there is a single material there is no need to link volumes to properties.

A.6 Rule of Parsimony

Developers should avoid writing big programs. This rule aims to prevent overinvestment of development time in failed or suboptimal approaches caused by the owners of the program's reluctance to throw away visibly large pieces of work. Smaller programs are not only easier to write, optimize, and maintain; they are easier to delete when deprecated.

- Parametric and/or optimization runs have to be driven from an outer script (Bash, Python, etc.)

A.7 Rule of Transparency

Developers should design for visibility and discoverability by writing in a way that their thought process can lucidly be seen by future developers working on the project and using input and output formats that make it easy to identify valid input and correct output. This rule aims to reduce debugging time and extend the lifespan of programs.

- Written in C99

A.8 Rule of Robustness

Developers should design robust programs by designing for transparency and discoverability, because code that is easy to understand is easier to stress test for unexpected conditions that may not be foreseeable in complex programs. This rule aims to help developers build robust, reliable products.

A.9 Rule of Representation

Developers should choose to make data more complicated rather than the procedural logic of the program when faced with the choice, because it is easier for humans to understand complex data compared with complex logic. This rule aims to make programs more readable for any developer working on the project, which allows the program to be maintained.

A.10 Rule of Least Surprise

Developers should design programs that build on top of the potential users' expected knowledge; for example, '+' in a calculator program should always mean 'addition'. This rule aims to encourage developers to build intuitive products that are easy to use.

- If one needs a problem where the conductivity depends on x as $k(x) = 1 + x$ then the input is

```
k(x) = 1+x
```

- If a problem needs a temperature distribution given by an algebraic expression $T(x, y, z) = \sqrt{x^2 + y^2} + z$ then do

```
T(x,y,z) = sqrt(x^2+y^2) + z
```

A.11 Rule of Silence

Developers should design programs so that they do not print unnecessary output. This rule aims to allow other programs and developers to pick out the information they need from a program's output without having to parse verbosity.

- No `PRINT` no output.

A.12 Rule of Repair

Developers should design programs that fail in a manner that is easy to localize and diagnose or in other words "fail noisily". This rule aims to prevent incorrect output from a program from becoming an input and corrupting the output of other code undetected.

Input errors are detected before the computation is started and run-time errors (i.e. a division by zero) con be user controled, they can be fatal or ignored.

A.13 Rule of Economy

Developers should value developer time over machine time, because machine cycles today are relatively inexpensive compared to prices in the 1970s. This rule aims to reduce development costs of projects.

- Output is 100% user-defined so the desired results is directly obtained instead of needing further digging into tons of undesired data.The approach of "compute and write everything you can in one single run" made sense in 1970 where CPU time was more expensive than human time, but not anymore.
- Example: LE10 & LE11.

A.14 Rule of Generation

Developers should avoid writing code by hand and instead write abstract high-level programs that generate code. This rule aims to reduce human errors and save time.

- Inputs are M4-friendly.
- Parametric runs can be done from scripts through command line arguments expansion.
- Documentation is created out of simple Markdown sources and assembled as needed.

A.15 Rule of Optimization

Developers should prototype software before polishing it. This rule aims to prevent developers from spending too much time for marginal gains.

- Premature optimization is the root of all evil
- We are still building. We will optimize later.
  - Code optimization: TODO
  - Parallelization: TODO
  - Comparison with other tools: TODO

A.16 Rule of Diversity

Developers should design their programs to be flexible and open. This rule aims to make programs flexible, allowing them to be used in ways other than those their developers intended.

- Either Gmsh or Paraview can be used to post-process results.
- Other formats can be added.

A.17 Rule of Extensibility

Developers should design for the future by making their protocols extensible, allowing for easy plugins without modification to the program's architecture by other developers, noting the version of the program, and more. This rule aims to extend the lifespan and enhance the utility of the code the developer writes.

- FeenoX is GPLv3+. The '+' is for the future.
- Each PDE has a separate source directory. Any of them can be used as a template for new PDEs, especially `laplace` for elliptic operators.

Appendix B

History

Very much like UNIX in the late 1960s, FeenoX is a third-system effect: I wrote a first hack that seemed to work better than I had expected. Then I tried to add a lot of features and complexities which I felt the code needed. After ten years of actual usage, I then realized what was worth keeping, what needed to be rewritten and what had to be discarded. The first version was called wasora, the second was "The wasora suite" (i.e. a generic framework plus a bunch of "plugins", including a thermo-mechanical one named Fino) and then finally FeenoX. The story that follows explains why I wrote the first hack to begin with.

It was at the movies when I first heard about dynamical systems, non-linear equations and chaos theory. The year was 1993, I was ten years old and the movie was Jurassic Park. Dr. Ian Malcolm (the character portrayed by Jeff Goldblum) explained sensitivity to initial conditions in a memorable scene, which is worth watching again and again. Since then, the fact that tiny variations may lead to unexpected results has always fascinated me. During high school I attended a very interesting course on fractals and chaos that made me think further about complexity and its mathematical description. Nevertheless, it was not not until college that I was able to really model and solve the differential equations that give rise to chaotic behavior.

In fact, initial-value ordinary differential equations arise in a great variety of subjects in science and engineering. Classical mechanics, chemical kinetics, structural dynamics, heat transfer analysis and dynamical systems, among other disciplines, heavily rely on equations of the form

$$\dot{\mathbf{x}} = F(\mathbf{x}, t)$$

During my years of undergraduate student (circa 2004–2007), whenever I had to solve these kind of equations I had to choose one of the following three options:

1. to program an *ad-hoc* numerical method such as Euler or Runge-Kutta, matching the requirements of the system of equations to solve, or
2. to use a standard numerical library such as the GNU Scientific Library and code the equations to solve into a C program (or maybe in Python), or
3. to use a high-level system such as Octave, Maxima, or some non-free (and worse, see below) programs.

Of course, each option had its pros and its cons. But none provided the combination of advantages I was looking for, namely flexibility (option one), efficiency (option two) and reduced input work (partially given by option three). Back in those days I ended up wandering between options one and two, depending on the type of problem I had to solve. However, even though one can, with some effort, make the code read some parameters from a text file, any other drastic change usually requires a modification in the source code—some times involving a substantial amount of work—and a further recompilation of the code. This was what I most disliked about this way of working, but I could nevertheless live with it.

Regardless of this situation, during my last year of Nuclear Engineering, the tipping point came along. Here's a slightly-fictionalized of a dialog between myself and the teacher at the computer lab, as it might have happened (or not):

> — (Prof.) Open MATLAB.™
> — (Me) It's not installed here. I type `mathlab` and it does not work.
> — (Prof.) It's spelled `matlab`.
> — (Me) Ok, working. (A screen with blocks and lines connecting them appears)
> — (Me) What's this?
> — (Prof.) The point reactor equations.
> — (Me) It's not. These are the point reactor equations:
>
> $$\begin{cases} \dot{\phi}(t) = \dfrac{\rho(t) - \beta}{\Lambda} \cdot \phi(t) + \displaystyle\sum_{i=1}^{N} \lambda_i \cdot c_i \\ \dot{c}_i(t) = \dfrac{\beta_i}{\Lambda} \cdot \phi(t) - \lambda_i \cdot c_i \end{cases}$$
>
> — (Me) And in any case, I'd write them like this in a computer:
>
> ```
> phi_dot = (rho-Beta)/Lambda * phi + sum(lambda[i], c[i], i, 1, N)
> c_dot[i] = beta[i]/Lambda * phi - lambda[i]*c[i]
> ```

This conversation forced me to re-think the ODE-solving issue. I could not (and still cannot) understand why somebody would prefer to solve a very simple set of differential equations by drawing blocks and connecting them with a mouse with no mathematical sense whatsoever. Fast forward fifteen years, and what I wrote above is essentially how one would solve the point kinetics equations with FeenoX.