

# arb

code version 0.25

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## 1 What's new?

- 12/4/11 Rewrite of mesh routines, allowing multiple meshes and data input.
- 22/2/11 Installation instructions have been improved.
- 3/2/11 Work has been done to make error messages more helpful.
- 12/12/10 The GNU GPL'd sparse linear solver [UMFPACK](#) written by Tim Davis is now interfaced to arb. An easy download and setup script is included.
- 25/11/10 The run procedure has been simplified for version 0.24. Basically you don't have to run `setup_equations` separately anymore - all meta-programming, compilation and running is handled by the single command `./arb`, run from the working directory.

## 2 What is arb?

arb solves arbitrary partial differential equations on unstructured meshes using the finite volume method. The code is written in fortran95, with some meta-programming done in perl with help from maxima.

The primary strengths of arb are:

- All equations and variables are defined using ‘maths-type’ expressions written by the user, and hence can be easily tailored to each application;
- All equations are solved simultaneously using a Newton-Raphson method, so implicitly discretised equations can be solved efficiently; and
- The unstructured mesh over which the equations are solved can be composed of all sorts of convex polygons/polyhedrons.

arb requires a UNIX type environment to run, and has been tested on both the Apple OsX and ubuntu linux platforms. Certain third party programs are used by arb:

- A fortran compiler; ifort and gfortran are supported;
- The computer algebra system [maxima](#);
- A sparse matrix linear solver: [UMFPACK](#), [pardiso](#) and (currently a single) Harwell Subroutine Library routines are supported; and
- The mesh generator [gmsh](#).

Further details about how to get and install this software are given in section [3.1](#).

arb is copyright Dalton Harvie (2009–2011), but released under the [GNU General Public License \(GPL\)](#). Further details of this license can be found in the license directory once the code has been unpacked.

## 3 Installation

### 3.1 Installing prerequisite software

#### 3.1.1 Minimum setup steps required for ubuntu 10.04:

1. Install the arb files as per section [3.2](#)
2. Install required packages:

```
sudo apt-get install maxima maxima-share gfortran  
liblapack-dev libblas-dev gmsb
```

3. Install the suitesparse solver as per section [3.1.6](#)
4. Run a test simulation as per section [4](#)

On ubuntu 8.04 the versions of `gfortran` and `gmsb` in the standard repositories are too old to be installed via this method.

#### 3.1.2 Minimum setup steps required for OsX:

Installation on OsX is straightforward but takes more time.

1. Install the arb files as per section [3.2](#)
2. Install Apple's Xcode developer package.
3. Install a `gfortran` binary package as per section [3.1.4](#)
4. Install a maxima binary package as per section [3.1.3](#)
5. Install the suitesparse solver as per section [3.1.6](#)
6. Install the `gmsb` package as per section [3.1.10](#)
7. Run a test simulation as per section [4](#)

### 3.1.3 Maxima

Equation generation is performed using the Maxima Computer Algebra system. It is released under the [GNU General Public License \(GPL\)](#) and is available for free. To check whether you have it installed already try typing `maxima`. If the program is installed you will enter a symbolic maths environment. Then check that the command `load(f90);` finds these libraries, and then quit using `quit();`. If you need to install it:

#### Installing maxima on ubuntu:

On ubuntu linux maxima and the f90 package can be installed using

```
sudo apt-get install maxima maxima-share
```

#### Installing maxima on OsX using a binary package:

A precompiled version of maxima for the mac is available from [sourceforge](#). This is a fastest way of getting things going. Download the package and copy the application 'Maxima.app' to your Applications directory as directed. To make it available from the command line place the script `misc/maxima_OsX/maxima` somewhere in your path (for example in a `bin` directory).

#### Installing maxima on OsX using fink/macports:

On OsX maxima can be installed using either [macports](#) or [fink](#) package managers. For fink enable the unstable branch and use

```
sudo fink install maxima
```

For macports replace `fink` with `port` in the above. Compilation will take some time.

### 3.1.4 A fortran compiler and the blas/lapack libraries

Two different compilers have been tested with arb: `ifort` (Intel) and `gfortran`. The [Intel Fortran compiler](#) `ifort` is probably the faster of the two. It also includes the Intel Maths Kernel library which itself includes the excellent Pardiso linear solver routines (see section below): however this compiler is not free except on

linux and even then, only under specific non-commercial circumstances. The GNU compiler gfortran is an easier option to get going, and is freely available on both the OsX and linux platforms. It does not include the Pardiso routines but with the new interface to the UMFPACK routines this isn't a tremendous disadvantage.

Compiler choice is made automatically when the arb script is run (defaulting to ifort if it exists, otherwise using gfortran). These defaults can be overwritten with the arb options `--compiler-gnu` or `--compiler-intel`.

### **Installing ifort:**

The non-commercial download site for ifort on linux is [here](#). For OsX the compiler must be bought. Make sure you install both the compiler and MKL (Math Kernel Libraries). ifort versions of 11.1.069 and newer (including Composer XE which is version 12) have been tested on both linux and OsX.

### **Installing gfortran on ubuntu:**

On ubuntu linux gfortran and the lapack/blas libraries can be installed using

```
sudo apt-get install gfortran liblapack-dev libblas-dev
```

gfortran version 4.2.4 on ubuntu 8.04 doesn't seem to work on some computers (internal compiler error) whereas version 4.4.3 on ubuntu 10.04 does. On ubuntu 8.04 you could try downloading a newer binary version of gfortran but I haven't tried this.

### **Installing gfortran on OsX using a binary package:**

The easiest way to install an up-to-date version of gfortran is via a precompiled package. One that worked for me is found [here](#) - currently (23/2/11) this is version 4.6. Alternatively this [hpc site](#) and this [gcc site](#) gives information about other precompiled versions. Check that once installed the gfortran executable is in your path - that is, typing gfortran at the command line should find the compiler. Version 4.5 of gfortran should also work fine.

### **Installing gfortran on OsX using fink/macports:**

gfortran can also be installed by the package managers but there are some issues with this. gfortran is included as part of fink's gcc packages (for example gcc45) but it will need to be installed as 64bit, otherwise there will be some compatibility problems with UMFPACK (unless this is modified). With macports it is also part of gcc but needs to be specified as a variant:

```
sudo port install gcc46 +gfortran
```

Again, compilation will take some time. I have not tested this fully.

### 3.1.5 Pardiso

The pardiso sparse linear matrix solver is included as part of the Intel Math Kernel Library which is packaged with the [Intel Fortran compiler](#) (see above).

If using the intel compiler then this solver will automatically become available (check the initial output when running `arb` to see if this has been found).

### 3.1.6 UMFPACK

The [UMFPACK](#) sparse linear solver is part of the suitesparse collection of sparse matrix routines written by Prof. Tim Davis. It is written in c and released under the GNU GPL (see [conditions here](#)).

UMFPACK depends on '[METIS - Serial Graph Partitioning and Fill-reducing Matrix Ordering](#)'. METIS is freely available but not free distributable. For more details see the [conditions here](#).

The installation process for the UMFPACK/METIS combination has been automated so that it can be easily used with `arb`. To install these packages and compile them in a form that is suitable for `arb`:

```
cd src/contributed/suitesparse
make
```

The `make` command will download the latest version of UMFPACK and version 4.0 of METIS (using `curl`), and then compile these libraries using the `gcc` compiler. A wrapper script for using UMFPACK from fortran (included with UMFPACK) will also be compiled. The files will be placed in the `src/contributed/suitesparse` directory, so will not overwrite any alternative suitesparse or metis libraries already on your system. You need to have `gcc` installed on your system to build these libraries.

If all goes well the following files will be placed in `src/contributed/suitesparse` to be used by `arb`:

```
libamd.a  
libcamd.a  
libccolamd.a  
libcholmod.a  
libcolamd.a  
libmetis.a  
libumfpack.a  
umf4_f77wrapper.o
```

All of these files are required for UMFPACK to successfully run.

You also need to have a version of the blas libraries available for arb to use UMFPACK. On OsX these should already be installed as part of Xcode (see section 3.1.4). On ubuntu linux they can be installed using `sudo apt-get install libblas-dev` if they're not already present.

To remove the compiled libraries and files type

```
make clean
```

from the suitesparse directory. This will leave only the downloaded files (ready to be reused). To remove the suitesparse and metis downloads as well, type

```
make clean_all
```

Note that UMFPACK library compilation is dependent on the type of machine architecture and the libraries will need to be remade if transferred from one machine to another - do a `make clean` and then a `make` again.

arb has been tested with the following combinations of umfpack and metis:

- UMFPACK.tar.gz 02-Jun-2010 11:46 and metis-4.0.tar.gz (4.0.1)

### 3.1.7 Perl

On ubuntu or OsX you should already have a version of perl installed.

### 3.1.8 Harwell Subroutine Library

An interface to the subroutine MA28D has been implemented. With the availability of UMFPACK, there is no real reason to use this, except for development. For more information see the `src/contributed/hs1_ma28d` directory. An interface to MA48D is under development (don't hold your breath though!).

### 3.1.9 Numerical Recipes in Fortran 77

These are an alternative to using some of the lapack routines. There is no reason to use these, except for development. For more information see the `src/contributed/numerical_recipes` directory.

### 3.1.10 Gmsh

While not integral to the arb code, the mesh and data format which arb uses is that developed for gmsh. Gmsh is a mesh element generator which can be run using scripts or via a graphical interface and can be used for post-processing (visualisation) too. Gmsh uses the [GNU General Public License \(GPL\)](#).

There is some great introductory material available on the [gmsh website](#) on the use of this program, particularly these online [screencasts](#).

#### Installing gmsh on ubuntu 10.04:

```
sudo apt-get install gmsh
```

On earlier ubuntu versions the repository version is too old.

#### Installing gmsh on anything else:

Download a version from the [gmsh website](#). Version 2.4 is the minimum required for arb - most importantly the msh file format produced needs to be 2.1 or greater. I have had no problems using development versions that are available.

## 3.2 Installing arb

As arb is distributed as source code that is compiled for each application, arb is not installed in the traditional sense. Instead, for each new simulation a new



self-contained copy of the source files is unpacked from a source tarball. Once created `arb` is run from a working directory which contains a specific structure of files and subdirectories. Two routines, `pack` and `unpack`, are provided to automate the process of managing this required file/subdirectory structure.

### 3.2.1 Unpacking the code

To create a new version of `arb`, a new working directory should be created or [downloaded](#) that contains the four files

```
archive.tar.gz
unpack
README
LICENSE
```

Using the command

```
./unpack
```

from within this directory will unpack the archive ready for use.

In the remainder of this section details the file structure and how to pack up the code again.

### 3.2.2 The working directory and file structure

Once the archive is unpacked the working directory will contain the following subdirectories and files/links:

- `src` directory: contains the main fortran source code of `arb`, and the `makefile` necessary to build everything (except for the contributed libraries). It also contains the meta-programming perl script `setup_equations.pl` and a template file `equations_module.f90` which are used to create the fortran file `equations_module.f90` within `build` which is specific to each problem.

- `src_equations/contributed` directory: This directory may/should/can contain contributed third party code that can be used by `arb`, along with associated interface modules — for example, linear solver routines. There is a separate subdirectory for each package. Each directory contains error handling modules that handle runtime cases where the third party routines are not available, and also some brief installation instructions. Most directories work on the drop-box principle — if the required files are available then they will be included in the `arb` executable.
- `build` directory: all building is done within this directory.
- `tmp` directory: temporary files are stored within this directory, including the file `setup/debug` which is used for debugging the equation setup.
- `output` directory: output files from a simulation are placed in here.
- `misc` directory: contains miscellaneous files — for example a simple script `create_mesh` which builds a `.msh` file from any `.geo` file in the working directory.
- `doc` directory: contains documentation including this manual.
- `examples` directory: example problem-specific files `equations.in`, `constants.in` and any geometry files (structure files with `.geo` extension, and mesh files with `.msh` extension) are stored here. Examples that are detailed in this manual (section 7) are stored in the `examples/manual` subdirectory.
- `packer` directory: contains various files specific to the pack and unpack operations. A history file within this directory records the distribution history of the specific code version.
- `license` directory: contains license details, including the (GNU GPL) license under which `arb` is released.
- `equations.in` and `constants.in` files: these files and an associated `.msh` or `.geo` file contain all the problem-specific information required for a particular simulation. `equations.in` is read by `setup_equations` when creating the equation-specific fortran code `equations_module.f90` within `build`. `constants.in` is read by both `setup_equations` and by the executable fortran code `arb`. It contains constant and numerical simulation data which can be (mainly) edited without requiring `arb` to be recompiled.
- `arb` script: this shell script is a wrapper script for setting-up, making and running `arb`. You can pass options to this script to control the compilation

process — for example choose between the gnu and intel compilers. It also performs simulation restart file management (not implemented!). This script works out when the equation meta-programming has to be redone or not, and when recompilation is necessary. So if in doubt, just type `arb.....`

- `pack` file: this shell script is used to pack up a simulation.

### 3.2.3 Packing the code

To pack a simulation ready to transport or backup, use the command

```
./pack
```

from within the working directory. This will create a subdirectory with a name of the form `arb_[date]_[version]` which contains all files necessary to run `arb`. Following the command with a name, as in

```
./pack a_name
```

will create the archive in a subdirectory named `a_name` instead of the default.

The script `pack` accepts a number of options. By default only files within the `examples` or `gmsh` directories that are specific to this manual are included in the archive. The options `--example`, `--misc` or `--all` specify that all files within either the `example`, `misc` or both directories are contained within the archive. By default only source code within the `src/contributed` directory that is not subject to a non-free third party license is included in the archive. Using the options `--contributed` or `--all` causes all files in these directories to be archived (including the build suitesparse libraries). Using `--distribute` means that no third party software is included in the archive. The option `--build` means that all files in the build directory will be included in the archive. This may be useful if you want to transport the simulation to another machine that may not have maxima installed (for example).

Other options to `pack` include `--notar` and `--help`.

## 4 Running simulations

### 4.1 A super-quick example: A heat conduction simulation

Once the code is unpacked you should be left in the working directory. If this version has been downloaded from the homepage then the three files

```
constants.in  
equations.in  
surface.msh
```

that exist in the working directory specify a simple heat conduction problem. If they don't exist for whatever reason they can be copied from `examples/manual/heat_conduction.ar` to the working directory.

Check that the file `constants.in` specifies your choice of linear solver. If you are using the gnu compiler with the UMFPACK routines then this file should already contain the line

```
LINEAR_SOLVER "SUITESPARSE_UMF" # suitesparse umf solver  
      (UMFPACK) by Timothy A. Davis
```

so you don't need to change anything. If you are using the intel compiler with MKL libraries then change this line to

```
LINEAR_SOLVER "INTEL_PARDISO" # pardiso solver contained  
      in intel mkl library
```

Now run the simulation using

```
./arb
```

If all goes well the code will be metaprogrammed and compiled, the simulation will run and output will be produced in the directory `output`. To view the output type

```
gmsht output/output.msh
```

You should see the temperature field around a heated ellipse.

## 4.2 Other examples:

Other example simulation files are included in the subdirectories of `examples/manual`. To run any of these first copy the relevant `.in` and `.geo` files to the working directory. Next create the `.msh` file via the included `create_mesh` script:

```
misc/create_msh/create_msh d 1
```

replacing 'd' with the dimension of the problem (i.e. 1, 2 or 3). Note that the second argument controls the relative cell size — the smaller the parameter, the smaller the mesh element size and greater the number. Finally run `arb` using `./arb` and view the results.

Right now the examples include:

- `1d_nonuniform_diffusion`: diffusion along a line containing two diffusion coefficients (1D)
- `heat_conduction_around_ellipse`: diffusion (nominally heat) around an ellipse within a box (2D)
- `heat_conduction_with_linked_regions`: similar to the above but demonstrating the use of linked regions (2D)
- `laplacian_in_square`: comparison between the numerical and analytical solution for a laplacian problem (2D)
- `steady_state_channel_flow_with_cylinder`: CFD benchmark problem of fluid flow around a slightly offset cylinder at  $Re = 20$  (2D)

## 4.3 The arb run script:

This shell script handles the perl meta-programming, fortran compiling, linking and running of `arb`. It uses a makefile (`src/makefile`) to determine when various components have to be remade. All code building is done in the directory `build`.

By default the `arb` script will try to do all that is necessary to run a simulation from scratch (except make the suitesparse libraries), however its behaviour can be altered by the following options:

- `--clean`: remove all meta-programmed fortran source and executable objects before building again.
- `--clean-compile`: remove all executable objects before building again. This may be handy if you want to run a simulation on a machine that has a fortran compiler, but not say maxima.
- `--clean-setup`: remove all meta-programmed fortran source before building again.
- `--setup`: create perl meta-programmed fortran source (default).
- `--no-setup`: do not recreate perl meta-programmed fortran source.
- `--compile`: create executable objects by compiling fortran source (default).
- `--no-compile`: do not recreate executable objects by compiling fortran source. If both `--no-setup` and `--no-compile` are specified, the existing arb executable will be rerun regardless of changes to the `.in` files.
- `--run`: run the arb executable once it is built (default).
- `--no-run`: do not run the arb executable.
- `-q|--quiet`: send screen output to `output/output.scr`.
- `-c|--continue`: continue on from a previous simulation. This is not the default behaviour. Unless this is specified the contents of output will be cleared out before each simulation. Note that a copy of the previous output files are placed in `output/previous` so if you accidentally run arb without the continue flag (once) you can get the old files back from this directory.
- `-d|--debug`: compile the fortran using debug flags, and run the executable within the gdb environment.
- `--compiler-gnu`: compile the fortran using gfortran (default if ifort is not present).
- `--compiler-intel`: compile the fortran using ifort (default if ifort is present).

## 4.4 A more detailed guide: Newtonian fluid flow

To discuss the working method in more detail we use the example of the steady-state flow of a Newtonian fluid around a cylinder that is provided in `examples/manual/steady_state_` (listings are also given in section 7.1 of this manual).

There are 5 basic steps to setting up, running and debugging an arb simulation:

1. **Create a mesh:** Geometry definition and mesh creation can be performed in gmsh. The domain geometry details are stored in a `.geo` file, which can be created by hand (file editing) or with the help of the gmsh GUI. Once a geometry (`.geo` file) has been created, gmsh can mesh this to produce a `.msh` file which is the file that is read in by arb. You can either do this via the gmsh GUI, or via the simple `create_mesh` script (mentioned above) which calls gmsh. When creating a 3D mesh be sure to optimise the mesh after creation (greatly improves mesh quality - `create_mesh` does this for 3D meshes).

arb uses the concept of 'regions' to locate various equations (for example boundary conditions, domain equations etc) and these must be defined in the `.geo` file prior to meshing. Regions have names that are delimited by the `<` and `>` signs: for example `<inlet>` and `<outlet>` (generally any user-defined names are delimited this way in arb).

In the example geometry file the boundary regions `<inlet>`, `<outlet>` and `<cylinder>` have all been defined as physical entities. The area region of `<flow domain>` which contains all mesh cells within the flow domain has also been created. This region is necessary as by default, gmsh does not write out mesh cells to a mesh file unless they are part of a physical entity. Note that certain region names are reserved: see section 5.2 for more details.

2. **Edit equations.in and constants.in:** Aside from the mesh file, all information that is specific to a simulation is contained in these two `.in` files. `equations.in` is read only when the perl meta-programming is conducted to create the fortran source. `constants.in` is read both during this meta-programming step and also each time the resulting arb executable is run. Hence, all equations that are processed via maxima during the meta-programming step must be defined in `equations.in`, while physical constants that do not involve equations and may change regularly between similar simulations can be defined in `constants.in`. Any change to `equations.in` or the form or options for the constants in `constants.in` requires the meta-programming step to be redone.

Note that some simulation specific information such as mesh file names and simulation parameters (newton solver convergence tolerance and number of newton iteration steps right now) are defined in the `constants.in` file and read directly by the `arb` executable: Hence these can be changed without requiring the meta-programming to be redone. Similarly any region definitions contained in `constants.in` are only read by the `arb` executable and do not require meta-programming.

Section 7.1 gives example `equations.in` and `constants.in` files for the considered test case of steady-state fluid flow around a cylinder. Physical constants such as the fluid density and viscosity are defined in the `constants.in` file.

Further details regarding the syntax of both `equations.in` and `constants.in` can be found in Sections 5 and 6.

### 3. **Run** `arb`: From the working directory

```
./arb
```

will run `arb`.

The first thing that happens is that the `makefile` checks what libraries/software are available and prints diagnostic messages to the screen.

The perl script `setup_equations.pl` is then called. It reads both `equations.in` and `constants.in`, and using `maxima`, creates the fortran source code file `build/equations_module.f90`. `setup_equations` writes plenty of progress information to the screen - if all goes well this output will end with the statement 'success'. Otherwise errors in the `equations.in` and `constants.in` files will need to be found and corrected. Aside from the screen output, more debugging information is written by `setup_equations` to the file `tmp/setup/debug`. Other files in the `tmp/setup` directory trace the interaction between the perl script and `maxima`.

Next the fortran code is compiled. If the debugging option has been requested (`./arb --debug`) the any error messages will be contained in `build/make.log`.

If all goes well the resulting executable will be run. Alongside the `.msh` and `output.stat` (statistics) files written to the directory `output`, other files in this directory can be used to diagnose problems. If these don't help, there are many `debug`, `debug_sparse` and `details_file` logicals scattered through the code (particularly `src/setup_module.f90`) that can be used.



4. **View results:** arb produces a file `output/output.msh` which can be opened by `gmsh` for viewing.
5. **Rerun the simulation:** The `output/output.msh` file produced by `arb` includes both the mesh information as well as variable data, so can be passed back to `arb` as an input `.msh` file for subsequent simulations. To do this replace the existing `MSH_FILE` line in the `constants.in` file with

```
MSH_FILE "output/output.msh" input
```

and rerun `arb`, without first removing this file via

```
./arb --continue
```

If you forget the `--continue` flag then you can recover the previous output files that are saved in `output/previous` for just this emergency.

## 5 Inside arb

### 5.1 Meshes

arb uses an unstructured mesh composed of cell elements that are separated by face elements. Multiple `.msh` files may be read in. Each `.msh` file has a dimension which is defined as the maximum dimension of domain cell elements it contains. arb can only (successfully) read in `.msh` files which have elements of the same dimension: If multiple dimensions are required, separate `.msh` files should be used for input and output. The dimension of the face elements is always 1 less than that of the adjacent domain cell elements. arb has been coded to be able to handle any poly-sided cells, however in practice it has only been tested to date (v0.25) with tetrahedron in 3D, triangles in 2D and lines in 1D: these are the default element geometries created by gmsh.

Boundary cells are created by arb after a mesh has been imported. They have a dimension that is 1 less than that of the domain cells, so have no volume/area/width in 3D/2D/1D, respectively. Each boundary cell has the same geometry, and is coincident with, a boundary face. Hence, a mesh has the same number of boundary faces as boundary cells.

The `.msh` files written by arb can contain data. Variables associated with cell elements can be written in either `ElementData` (a uniform value for each cell) or `ElementNodeData` (values vary linearly within each cell) gmsh formats. Variables associated with face elements can only be written in `ElementData` format. Variables which are none centred are written using a special Data format which gmsh won't display. When reimporting data files note that variable values can only refer to mesh elements that are specified in the same data file (unless some fancy `facelink` magic is worked).

Mesh and data input and output is specified by `MSH_FILE` statements within the `constants.in` file:

```
MSH_FILE "msh_file_name_including_path" comma,separated,
list,of,options # comments
```

The file name refers to the read location. If a `.msh` file is to be written it will always be written to the output directory. As a result, all file basenames must be unique.

Three types of options are available for each `.msh` file:

### *Output options:*

These options specify what information is to be written to the `.msh` file.

- `output`: Both a mesh and all specified variables will be written.
- `centringoutput`: Both a mesh and all specified variables will be written. Output will be split between three files, each containing variables of only a single centring (cell, face and none). This can be handy for gmsh compatibility when doing cutgrid and streamtrace operations for example.
- `centringmeshoutput`: Only the mesh is written, split between three files as above.
- `meshoutput`: Only the mesh is written.
- `nooutput`: Neither the mesh or any data will be written.

### *Input options:*

These options specify what information is to be read from the `.msh` file.

- `input`: Both a mesh and all relevant data will be read.
- `centringinput`: Both a mesh and all relevant data will be read. In this case the existing `.msh` is split into three, each containing variables of only a single centring (cell, face and none) as output from a previous simulation employing `centringoutput`. In this case the filename should be specified without the centring, for example `output/output.msh` (rather than `output/output.cell.msh`).
- `centringmeshinput`: Only the mesh is read, split between three files as above.
- `meshinput`: Only the mesh is read.
- `noinput`: Neither the mesh or any data will be read.

### *Data format options:*

These options specify how cell centred data will be written to the `.msh` file. These options overwrite any data format options specific to individual variables.

- `elementdata`: All cell data will be written using the `ElementData` format.
- `elementnodedata`: All cell data will be written using the `ElementNodeData` format.
- `elementnodelimiteddata`: All cell data will be written using the `ElementNodeData` format, but with gradients limited (not implemented).

## 5.2 Regions

Regions are sets of mesh elements that are used to locate user-defined variables and equations. Each region may contain only mesh elements of the same centring (that is, either cell or face elements, but not both). Regions can be defined by the user directly in `gmsh` when the mesh is generated, or via statements in the `constants.in` file that are interpreted when `arb` is run. There are also several generic system generated regions. Region names must be delimited by the `<>` characters, but apart from these two characters their names may contain any non-alphanumeric characters.

### 5.2.1 Defining regions via `gmsh`

Regions are specified in `gmsh` by defining and then naming physical entities. To do this via the `gmsh` GUI:

- Add a physical entity (under the physical groups tab) by selecting various elemental entities.
- Edit the geometry file (using the edit tab) and change the physical entity's name from the numerical name given by `gmsh` to the required `<>` delimited name suitable for `arb`.
- Save the `.geo` file.
- Reload the `.geo` file again (using the reload tab). If you now check under the visibility menu the physical entity will be visible.

### 5.2.2 Defining regions within the constants.in file

Currently there are three types of region specification statements that can be used in the constants.in file:

*Compound region:*

```
CELL_REGION <name> "COMPOUND +<region1>+<region2>-<
    region3>" # comments
FACE_REGION <name> "COMPOUND <region1>-<region2>" #
    comments
```

A compound region is defined using other existing regions. All regions that are used in the definition (ie, <region1>, <region2> and <region3> in the above examples) must have the (same) centring that is specified by the REGION keyword. If a + sign precedes a region name in the list of regions, then all the mesh elements that are in the following region are added to the new compound region, if they are not already members. If a - sign precedes a region name in the list of regions, then all the mesh elements that are in the following region are removed from the new compound region, if they are (at that stage) members of the new compound region. If no sign immediately precedes a region name in the defining list then a + sign is assumed. When constructing a compound region arb deals with each region in the defining list sequentially; so whether a mesh element is included in the compound region or not may depend on the order that the regions are listed.

*At region:*

```
CELL_REGION <name> "AT x1 x2 x3" # comments
FACE_REGION <name> "AT x1 x2 x3" # comments
```

This statement defines a region that contains one cell or one face mesh element. The element chosen lies closest to the point (x1,x2,x3). The values x1, x2 and x3 can be real or double precision floats.

*Boundary of region:*

```
CELL_REGION <name> "BOUNDARY OF <region>" # comments
FACE_REGION <name> "BOUNDARY OF <region>" # comments
```

This statement defines a region that contains *only* the boundary elements (either

cell or face) that border the region <region>.

### 5.2.3 System generated regions

The following regions are generated by arb at the start of a simulation. The names cannot be used for user-defined regions:

region name	description
<all cells>	all cells
<domain>	internal domain cells
<boundary cells>	cells located on the boundary
<all faces>	all faces
<domain faces>	internal domain faces
<boundaries>	faces located on the boundary

Additionally, there are a number of system regions which may be used in user-written expressions (see section 6) which specify sets of mesh elements relative to the current position. These names cannot be used for user-defined regions either:

region name	rel. to	description
<celljfaces>	cell	faces that surround the current cell
<nobcelljfaces>	cell	faces that surround the current cell, unless the current cell is on a boundary. In that instance move to the neighbouring domain cell and then cycle around the surrounding face cells.
<cellicells>	cell	cells that are local to the current cell (more than just the adjacent cells)
<faceicells>	face	cells that are local to the current face (more than just the adjacent cells)
<adjacentcellicells>	cell	cells that are strictly adjacent to the current cell
<adjacentfaceicells>	face	cells that are strictly adjacent to the current face (always two)
<upwindfaceicells>	face	the cell that is upwind of the face, used when performing faceave[advection] averaging (see section 6. Not really a user region.

<code>&lt;downwindfaceicells&gt;</code>	face	the cell that is downwind of the face, used when performing <code>faceave[advection]</code> averaging (see section 6. Not really a user region.
<code>&lt;cellkernel[l=0]&gt;</code>	cell	surrounding faces used in a cell averaging kernel (see section 6. Not really a user region.
<code>&lt;cellkernel[l=1-3]&gt;</code>	cell	surrounding cells used in cell derivative kernels (see section 6. Not really a user region.
<code>&lt;cellkernel[l=4]&gt;</code>	cell	surrounding nodes used in a cell averaging kernels (see section 6. Not really a user region.
<code>&lt;facekernel[l=0-6]&gt;</code>	face	surrounding cells used in face averaging and derivative kernels (see section 6. Not really a user region.
<code>&lt;noloop&gt;</code>	face/cell	dummy region which specifies no elements.

---

## 5.3 Variables

There are six types of user defined variables: constant, transient, derived, unknown, equation and output. Each of these are stored in `arb` using the same general data structure (fortran type `var`). Any of these variables can be defined by a user-written expression in `equations.in` which is read by `setup.equations` and interpreted by `maxima`. Additionally, the constant type may be defined in `constants.in` and there given (only) a numerical value. Along with the user defined variables, there are also system defined variables which can be used in user-written expressions.

All variables have an associated compound variable type (scalar, vector or tensor) which is used mainly for output purposes.

Details of both the user and system defined variables are given in this section.

### 5.3.1 Constant type variable defined in `equations.in`

*Synopsis:*

Constant variables are evaluated once at the start of a simulation. If defined in `equations.in` they are defined using an expression which may contain only system variables and other constants — in the latter case the constants must have been defined in either the `constants.in` file or previously (above) in the `equations.in` file.

### Defining statements:

```
CELL_CONSTANT <name> [multiplier*units] "expression" ON
    <region> options # comments
FACE_CONSTANT <name> [multiplier*units] "expression" ON
    <region> options # comments
NONE_CONSTANT <name> [multiplier*units] "expression"
    options # comments
CONSTANT <name> [multiplier*units] "expression" options
    # comments
```

### Statement components:

- (CELL\_|FACE\_|NONE\_|)CONSTANT (*required*): This keyword specifies the centring of the variable. Constants that have cell or face centring vary over the simulation domain, and have values associated with each cell or face, respectively (subject to the region statement, below). None centred constants have one value that is not linked to any spatial location. If the centring specifier is omitted from the keyword (as in CONSTANT) then none centring is assumed (ie., keyword CONSTANT is equivalent to keyword NONE\_CONSTANT).
- <name> (*required*): Each variable must have a unique name, delimited by the < and > characters. Besides these characters, the variable may contain spaces and any other non-alphanumeric characters. If the name ends with a direction index, as in <u[l=1]> or <gradp [l=3]>, then the variable is considered to be a component of a three dimensional vector compound. Similarly, if the name ends with a double direction index, as in <tau[l=1,3]>, the variable is considered to be a component of a three by three tensor compound. Components of compounds that are not explicitly defined are given a zero value (when used in dot and double dot products for example). All defined components that are members of the same compound must be of the same variable type, have the same centring, be defined over the same region and have the same units and multiplier. Certain names are reserved for system variables (see section 5.3.9).
- multiplier (*optional*): When reading in numerical constants, each value is multiplied by this value. At present not in use in equations.in.
- units (*optional*): A string which specifies the units for the variable. At present this string is not interpreted by the code at all and the user must ensure that the units used are consistent.



- "expression" (*required*): When a constant is defined in `equations.in`, this double-quoted expression is used to specify the value of the constant. As they may contain system variables and also other constants, they may vary throughout the domain. For more details regarding the syntax of these expressions, see section 6.
- ON <region> (*optional*): This part of the statement determines over what region the variable should be defined. It is only applicable for cell and face centred variables, and must in these cases refer to a region that has the same centring as the variable. If omitted then by default a cell centred constant will be defined on <all cells> and a face centred constant on <all faces>. Note that referring to a variable value outside of its region of definition will produce an error when running `arb`.
- options (*optional*): This is a comma separated list of options. Valid options for the constant variable type include:
  - output: The compound variable that is component is a member of to be written to each applicable `.msh` file. The opposite option `nooutput` exists. Default is `output` for unknown and `output` variables and `nooutput` for everything else.
  - componentoutput: This component to be written to each applicable `.msh` file. Default is `nocomponentoutput` for all variables.
  - input: The compound variable that is component is a member will be read from each applicable `.msh` file. The opposite option `noinput` exists. Default is `input` for all unknown variables and `noinput` for everything else.
  - componentinput: This component to be read from each applicable `.msh` file. Default is `nocomponentinput` for all variables.
  - elementdata: This compound will be written using the `gmsh ElementData` format. Any data format options specified for each `.msh` file will overwrite this option. Other options include `elementnodedata`, `elementnodelimiteddata`, `componentelementdata`, `componentelementnodedata` and `componentelementnodelimiteddata`. Default is `elementnodedata` and `componentelementdata`.
- comments (*optional*): Anything written beyond the `#` is regarded as a comment.

*Examples:*

```
CELL_CONSTANT <test constant> "<cellx[1=1]>^2" ON <
    boundaries> # a test
FACE_CONSTANT <test constant 2> [m] "<facex[1=2]>" #
    another test
```

### 5.3.2 Constant type variable defined in constants.in

*Synopsis:*

Constant variables defined in `constants.in` are set to numerical values read directly by the `arb` executable, rather than expressions interpreted by `maxima`.

*Defining statements:*

```
CELL_CONSTANT <name> [multiplier*units] value ON <region
    > options # comments
FACE_CONSTANT <name> [multiplier*units] value ON <region
    > options # comments
NONE_CONSTANT <name> [multiplier*units] value options #
    comments
CONSTANT <name> [multiplier*units] value options #
    comments
```

*Statement components:*

The components of these statements are the same as in section 5.3.1 with the exception of:

- *value (required):* A numerical value of real or double precision type.

*Examples:*

```
CONSTANT <mu> [Pa.s] 1.0d-3 # fluid viscosity
NONE_CONSTANT <rho> [997*kg/m^3] 1.0 # fluid density
```

### 5.3.3 Constant type variable defined per region in constants.in

*Synopsis:*

This definition can be used in the `constants.in` file to assign different numerical values to either a cell or face centred constant in specific regions. Two statements are required for this type of constant definition: The first defines the list of regions where the next constant will be set (`REGION_LIST`) and the second defines the constant and sets/lists the corresponding numerical values (`(CELL_|FACE_)REGION_CONSTANT`). The region names in the `REGION_LIST` statement must have the same centring as the following `REGION_CONSTANT` statement. Furthermore, the `<region>` over which the constant is defined must include all of the regions listed within the previous `REGION_LIST` statement.

*Defining statements:*

```
REGION_LIST <region1> <region2> ... <regionN> # comments
CELL_REGION_CONSTANT <name> [multiplier*units] value1
    value2 ... valueN ON <region> options # comments
FACE_REGION_CONSTANT <name> [multiplier*units] value1
    value2 ... valueN ON <region> options # comments
```

*Statement components:*

The components of these statements are the same as in section 5.3.1 with the exception of:

- `<region1> <region2> ... <regionN>` (*required*): A list of regions that have the same centring as the following `REGION_CONSTANT` statement.
- `value1 value2 ... valueN` (*required*): A list of numerical values for the constant, corresponding in a one-to-one fashion with the list of regions given in the previous `REGION_LIST` statement.

*Examples:*

```
REGION_LIST <inlet> <outlet> # some face regions
FACE_REGION_CONSTANT <electric field> [V/m] 10 20. ON <
    boundaries>
```

#### 5.3.4 Transient type variable defined in `equations.in`

*Synopsis:*

These will be implemented for version 0.3 (transient).

### 5.3.5 Derived type variable defined in equations.in

#### *Synopsis:*

Derived variables depend on the unknown variables and other previously defined (ie, above in the file) derived variables.

#### *Defining statements:*

```
CELL_DERIVED <name> [multiplier*units] "expression" ON <
    region> options # comments
FACE_DERIVED <name> [multiplier*units] "expression" ON <
    region> options # comments
NONE_DERIVED <name> [multiplier*units] "expression"
    options # comments
DERIVED <name> [multiplier*units] "expression" options #
    comments
```

#### *Statement components:*

Along with the information presented in section 5.3.1, the following applies to derived variables:

- (CELL\_|FACE\_|NONE\_|)DERIVED (*required*): If no centring is specified then none centring is assumed.
- "expression" (*required*): This is an expression for the derived variable in terms of constant, transient, unknown, previously defined derived (appearing above in equations.in) and system variables.
- ON <region> (*optional*): If omitted then by default a cell centred derived will be defined on <all cells> and a face centred derived on <all faces>.
- options (*optional*): This is a comma separated list of options. Valid options for derived variables (as well as those given in section 5.3.1) include:
  - noderivative: Normally the derivative of this variable's expression is calculated with respect to each unknown variable (the Jacobian) when performing the Newton-Raphson solution procedure. Including this option sets this derivative to zero. This may be required for functions for which the derivative cannot be calculated or for functions that

undergo step changes (not continuous) which are not ammeniable to solution via the Newton-Raphson procedure. Using this option will usually slow convergence.

- positive/negative: Including one of these options causes the code to check the sign of the derived variable. This is particularly useful for quantities like concentrations that are only physically meaningful when being positive. By using an expression such as "1-<con>" and including the option positive an upper limit for a variable can also be enforced.

*Examples:*

```
FACE_DERIVED <tau[l=1,1]> "<p> - <mu>*2.d0*facegrad[l
=1](<u[l=1]>)" output
CELL_DERIVED <graddivp[l=1]> "celldivgrad[l=1](<p>)" #
divergence based pressure gradient
```

### 5.3.6 Unknown type variable defined in equations.in

*Synopsis:*

Unknown variables are those upon which the equations and derived variables ultimately depend.

*Defining statements:*

```
CELL_UNKNOWN <name> [multiplier*units] magnitude "
expression" ON <region> options # comments
FACE_UNKNOWN <name> [multiplier*units] magnitude "
expression" ON <region> options # comments
NONE_UNKNOWN <name> [multiplier*units] magnitude "
expression" options # comments
UNKNOWN <name> [multiplier*units] magnitude "expression"
ON <region> options # comments
```

*Statement components:*

Along with the information presented in section 5.3.5, the following applies to unknown variables:

- (CELL\_|FACE\_|NONE\_|)UNKNOWN (*required*): If no centring is specified then cell centring is assumed.
- magnitude (*required*): An order of magnitude estimate (positive and greater than zero real or double precision value) must be specified for all unknown variables. This magnitude is used when checking on the convergence of the solution.
- "expression" (*required*): For an unknown variable the expression specifies the variable's initial value. The expression may contain constants, previously defined (initial) derived values (those appearing above in `equations.in`) and system variables.
- ON <region> (*optional*): If omitted then by default a cell centred unknown will be defined on <all cells> and a face centred unknown on <all faces>.
- options (*optional*): The `noderivative` option is not applicable for unknown variables.

*Examples:*

```
CELL_UNKNOWN <u[l=1]> 1.d0 "<u_av>" # a velocity
             component
CELL_UNKNOWN <p> [] 1.d0 "1.d0-<cellx[l=1]>" # pressure
NONE_UNKNOWN <p_in> [Pa] 1.d0 "1.d0" # the pressure at
             the inlet
```

### 5.3.7 Equation type variable defined in `equations.in`

*Synopsis:*

Equation variables represent the equations to be satisfied. The equation expressions should be formulated so that when the equation is satisfied, the expression equals zero. The number of equations must equal the number of unknown variables. Furthermore, for the system to be well posed the equations must be unknown (no single equation can be made from a combination of the other equations).

*Defining statements:*

```

CELL_EQUATION <name> [multiplier*units] "expression" ON
    <region> options # comments
FACE_EQUATION <name> [multiplier*units] "expression" ON
    <region> options # comments
NONE_EQUATION <name> [multiplier*units] "expression"
    options # comments
EQUATION <name> [multiplier*units] "expression" options
    # comments

```

*Statement components:*

Along with the information presented in section 5.3.5, the following applies to equation variables:

- (CELL\_|FACE\_|NONE\_|)EQUATION (*required*): If no centring is specified then none centring is assumed.
- "expression" (*required*): For an equation variable the expression should equal zero when the equation is satisfied. The expression may contain constant, transient, derived, unknown and system variables.
- ON <region> (*optional*): If omitted then by default a cell centred equation will be defined on <domain> and a face centred equation on <boundaries>.

*Examples:*

```

CELL_EQUATION <continuity> "celldiv(<u_f>)" ON <domain>
    # continuity
FACE_EQUATION <outlet noslip> "dot(<u[l=:]>,<facetang1[l=:]>)" ON <outlet> # no component tangential to
    outlet
NONE_EQUATION <p_in for flowrate> "<u_av_calc>-<u_av>" #
    set flowrate through inlet to give required average
    velocity

```

### 5.3.8 Output type variable defined in equations.in

*Synopsis:*

Output variables are evaluated once convergence of the solution has been reached: They are only for output purposes.

*Defining statements:*

```
CELL_OUTPUT <name> [multiplier*units] "expression" ON <
    region> options # comments
FACE_OUTPUT <name> [multiplier*units] "expression" ON <
    region> options # comments
NONE_OUTPUT <name> [multiplier*units] "expression"
    options # comments
OUTPUT <name> [multiplier*units] "expression" options #
    comments
```

*Statement components:*

Along with the information presented in section 5.3.5, the following applies to output variables:

- (CELL\_|FACE\_|NONE\_|)OUTPUT (*required*): If no centring is specified then none centring is assumed.
- "expression" (*required*): For an output variable the expression may contain constant, transient, derived, unknown, equation and system variables.
- ON <region> (*optional*): If omitted then by default a cell centred output variable will be defined on <all cells> and a face centred output variable on <all faces>.
- options (*optional*): The noderivative option is not applicable for output variables (this option is implicitly set anyway for these variables).

*Examples:*

```
NONE_OUTPUT <F_drag> [N] "facesum(<facearea>*dot(<
    facenorm[l=:]>,<tau[l=:,1]>),<cylinder>)" # force on
    object in axial direction
```

### 5.3.9 System variables



## 6 Expression language reference

*Sorry - there's lots missing in this section!*

### 6.1 Operators

#### 6.1.1 celldiv: Divergence

*Summary:* Uses Gauss' theorem to calculate the divergence of a face centred vector component around a cell.

*Statement:*

`celldiv[options](face_centred_expression)`

*Centring:*

Operator is cell centred, contents of operator is face centred.

*Details:*

Using Gauss' theorem to evaluate divergences around cells is probably the defining characteristic of Finite Volume methods. `celldiv` performs this operation.

Specifically, to discretise the divergence of a face centred vector  $\mathbf{u}_j$  over a cell  $i$  that sits within the domain, Gauss' theorem gives

$$\begin{aligned} \frac{1}{V_i} \int_{V_i} \nabla \cdot \mathbf{u} dV &\Rightarrow \frac{1}{V_i} \sum_{j \in \mathbb{J}_{\text{nobcellfaces},i}} \frac{1}{S_j} \int_{S_j} \mathbf{N}_{i,j} \cdot \mathbf{u}_j dS \\ &= \underbrace{\sum_{j \in \mathbb{J}_{\text{nobcellfaces},i}} \frac{\mathbf{N}_{i,j} \cdot \mathbf{n}_j}{V_i} \frac{1}{S_j} \int_{S_j} \mathbf{n}_j \cdot \mathbf{u}_j dS}_{\text{celldiv}} \\ &\Rightarrow \text{celldiv}(\text{dot}(\langle \mathbf{u}[1=:] \rangle, \langle \mathbf{facenorm}[1=:] \rangle)) \end{aligned}$$

where  $V_i$  and  $S_j$  are the volume and total surface area of the cell  $i$  and face  $j$ , respectively,  $\mathbf{N}_{i,j}$  is a unit normal pointing outward from cell  $i$  but located at face  $j$ ,  $\mathbf{n}_j$  is a normal associated with face  $j$ , and the sum is conducted over the set of all face elements that surround cell  $i$ , denoted by  $\mathbb{J}_{\text{nobcellfaces},i}$ . In the equivalent coding the face centred vector  $\mathbf{u}_j$  is represented by the three component variables  $\langle \mathbf{u}[1=1] \rangle$ ,  $\langle \mathbf{u}[1=2] \rangle$  and  $\langle \mathbf{u}[1=3] \rangle$ , and the unit normal

associated with the face  $j$ ,  $\mathbf{n}_j$ , is given by the system component variables  $\langle \text{facenorm}[1=1] \rangle$ ,  $\langle \text{facenorm}[1=2] \rangle$  and  $\langle \text{facenorm}[1=3] \rangle$ . Note that as the divergence of a vector results in a scalar, the above operation produces a scalar for each cell it is performed in.

The region used by `arb` in performing the above sum as represented by  $\mathbb{J}_{\text{nobcellfaces},i}$  is  $\langle \text{nobcelljfaces} \rangle$  ('no-boundary-cell-faces'). This relative region specifies all faces that surround a given cell, unless that cell is a boundary cell. As boundary cells are not fully surrounded by faces Gauss' theorem can not be applied. Hence, if the operator `celldiv` is used at a boundary cell then the region  $\langle \text{nobcelljfaces} \rangle$  is taken relative (moved) to the closest domain cell that is adjacent the boundary cell, so this is where `celldiv` becomes evaluated. Physically it is inadvisable to use an equation that involves a divergence at a boundary cell anyway.

*Options:*

- `noderivative`: No derivatives with respect to the unknown variables for the Newton-Raphson Jacobian are calculated for this operator (and its contents).

*Examples:*

```
CELL_EQUATION <continuity> "celldiv(<u_f>)" ON <domain>
# continuity equation
CELL_EQUATION <momentum[1=1]> "celldiv(<J_f[1=1]>)" ON <
domain> # momentum conservation in direction 1=1
CELL_EQUATION <momentum[1=2]> "celldiv(<J_f[1=2]>)" ON <
domain> # momentum conservation in direction 1=2
```

### 6.1.2 `cellgrad` or `facegrad`: Gradient

*Summary:* Calculates a scalar component of a gradient over a cell or face.

*Statement:*

```
cellgrad[options](cell_centred_expression)
facegrad[options](cell_centred_expression)
```

*Centring:*

cellgrad is cell centred and facegrad is face centred. Contents of both are cell centred.

*Details:*

To calculate the gradient of a cell centred scalar  $\phi_i$  in coordinate direction 2 in cell  $i$ ,

$$\frac{1}{V_i} \int_{V_i} \mathbf{e}_2 \cdot \nabla \phi dV \Rightarrow \sum_{i' \in \mathbb{I}_{\text{cellcells},i}} \overset{\bullet(2)}{k}_{i,i'} \phi_{i'} \Rightarrow \text{cellgrad}[1=2](\phi_i)$$

where  $\mathbf{e}_2$  is a unit vector in coordinate direction 2,  $\overset{\bullet(2)}{k}_{i,i'}$  is a predetermined kernel for this operation, and  $\mathbb{I}_{\text{cellcells},i}$  is the set of all cells in the vicinity of cell  $i$  that are used by this kernel. Kernels to calculate the cell gradient in the other coordinate directions, that is  $\overset{\bullet(1)}{k}_{i,i'}$  and  $\overset{\bullet(3)}{k}_{i,i'}$  also exist.

A gradient of a cell centred quantity evaluated at a face can be calculated similarly, for example

$$\frac{1}{S_j} \int_{S_j} \mathbf{e}_3 \cdot \nabla \phi dS \Rightarrow \sum_{i \in \mathbb{I}_{\text{facecells},j}} \overset{\circ(3)}{k}_{j,i} \phi_i \Rightarrow \text{facegrad}[1=3](\phi_i)$$

Gradients taken in directions relative to the face orientation are also available using the facegrad operator. Index 4 gives the gradient relative to the face's normal, that is

$$\frac{1}{S_j} \int_{S_j} \mathbf{n}_j \cdot \nabla \phi dS \Rightarrow \sum_{i \in \mathbb{I}_{\text{facecells},j}} \overset{\circ(4)}{k}_{j,i} \phi_i \Rightarrow \text{facegrad}[1=4](\phi_i)$$

In computational terms the face normal is represented by ( $\langle \text{facenorm}[1=1] \rangle, \langle \text{facenorm}[1=2] \rangle, \langle \text{facenorm}[1=3] \rangle$ ). Indices 5 and 6 give gradients in the directions of the first and second tangents for each face, respectively, that is

$$\frac{1}{S_j} \int_{S_j} \mathbf{t}_j^{(1)} \cdot \nabla \phi dS \Rightarrow \sum_{i \in \mathbb{I}_{\text{facecells},j}} \overset{\circ(5)}{k}_{j,i} \phi_i \Rightarrow \text{facegrad}[1=5](\phi_i)$$

and

$$\frac{1}{S_j} \int_{S_j} \mathbf{t}_j^{(2)} \cdot \nabla \phi dS \Rightarrow \sum_{i \in \mathbb{I}_{\text{facecells},j}} \overset{\circ(6)}{k}_{j,i} \phi_i \Rightarrow \text{facegrad}[1=6](\phi_i)$$

Computationally  $t_j^{(1)}$  is represented by ( $\langle \text{facetang1}[1=1] \rangle, \langle \text{facetang1}[1=2] \rangle, \langle \text{facetang1}[1=3] \rangle$ ) and  $t_j^{(2)}$  by ( $\langle \text{facetang2}[1=1] \rangle, \langle \text{facetang2}[1=2] \rangle, \langle \text{facetang2}[1=3] \rangle$ ), respectively. If the face has one dimension then  $t_j^{(1)}$  will be directed along the face, and  $t_j^{(2)}$  will be normal to both  $t_j^{(1)}$  and  $\text{vecti}[j]n$ . If the face has no or two dimensions (a point or a plane) then there are no preferential directions for these tangents. If no index is specified on the facegrad operator then 1=4 is assumed.

*Options:*

- 1=1, 1=2, etc: This index specifies the direction that the gradient will be taken in. For cellgrad this index represents the dimension the gradient is taken in and must be specified. For facegrad if the index is specified and is  $\leq 3$ , this specifies the dimension the gradient is taken in. For an index  $\geq 4$ , the direction is taken relative to the face orientation. 1=4 specifies a gradient taken in the direction of the face normal, 1=5 a gradient taken in the direction of the first tangent to the face and 1=6 in the direction of the second tangent to the face. If the index is not specified for facegrad then 1=4 is assumed — that is, a gradient taken normal to the face.
- noderivative: As previously.

*Examples:*

```
FACE_DERIVED <T flux> "-<D>*facegrad(<T>)" ON <all faces
> # some type of heat flux occuring across each face
CELL_DERIVED <dpx[1=1]> "cellgrad[1=1](<p>)" # gradient
of pressure in first dimension
```

### 6.1.3 cellave or faceave: Interpolation

*Summary:* Interpolates or averages an expression from one centring to another.

*Statement:*

```
cellave[options](face_centred_expression)
faceave[options](cell_centred_expression)

faceave[advection,options](cell_centred_expression,
face_centred_flux_expression)
```

```
faceave[advection,options](cell_centred_expression,  
    face_centred_flux_expression,cell_centred_limiter_expression)
```

*Centring:*

cellave takes a face centred expression and returns a cell centred result. faceave does the opposite.

*Details:*

TODO

*Options:*

- harmonic:
- advection:
- lastface and lastcell:
- noderivative: As previously.

#### 6.1.4 cellsum or facesum: **Sum**

*Summary:* Performs a sum over a region of either cell or face elements.

*Statement:*

```
cellsum[options](cell_centred_expression)  
cellsum[options](cell_centred_expression),<cell_centred_region>  
facesum[options](face_centred_expression)  
facesum[options](face_centred_expression),<face_centred_region>
```

*Centring:*

Operators may be cell, face or none centred. Contents of cellsum is cell centred, contents of facesum is face centred.

*Details:*

This operator sums the contained expression over a region of cell or face elements. If no region is specified, then default regions are applied, defined by:

*Options:*

- noderivative: As previously.

Operator centring	Expression centring	Default region
cell	face	<celljfaces>
cell	cell	<adjacentcellicells>
face	cell	<adjacentfaceicells>
	all else	<noloop>

- 6.1.5** `celldivgrad`: **Gradient evaluated at a cell calculated via a divergence**
- 6.1.6** `celllimiter`: **Gradient limiter for ensuring advection stability**
- 6.1.7** `celllif`, `faceif` **or** `noneif`: **If conditional statement**
- 6.1.8** `cellproduct` **or** `faceproduct`: **Product performed over a region of elements**
- 6.1.9** `cellmin/max`, `facemin/max` **or** `nonemin/max`: **Picks the minimum/-maximum from a region of elements**
- 6.1.10** `celldelta` **or** `facedelta`: **A delta function to identify specific regions**
- 6.1.11** `celllink` **or** `facelink`: **Link to other regions**

## 7 Example applications

### 7.1 Incompressible steady-state Newtonian flow through a 2D channel containing a cylinder with set inlet velocities

Listing 1: ../../examples/manual/steady\_state\_channel\_flow\_with\_cylinder/surface.geo

```
// 2d_channel_with_cylinder

lc = 0.05; // charateristic mesh length variable

// setup domain boundaries
Point(1) = {0, 0, 0, lc/2};
Point(15) = {0.2, 0, 0, lc/4};
Point(2) = {2.2, 0, 0, lc} ;
Point(3) = {2.2, 0.41, 0, lc} ;
Point(16) = {0.2, 0.41, 0, lc/4};
Point(4) = {0, 0.41, 0, lc/2} ;

Line(1) = {1,15} ;
Line(15) = {15,2} ;
Line(2) = {2,3} ;
Line(3) = {3,16} ;
Line(16) = {16,4} ;
Line(4) = {4,1} ;

// create an elementary entity that is the domain
boundary
Line Loop(5) = {1,15,2,3,16,4} ;

// create the physical entities for the inlet and output
which become the arb regions
Physical Line("<inlet>") = {4};
Physical Line("<outlet>") = {2};

// create the cylinder
Point(5) = {0.2, 0.15, 0, lc/4};
Point(6) = {0.25, 0.2, 0, lc/4};
Point(7) = {0.2, 0.25, 0, lc/4};
Point(8) = {0.15, 0.2, 0, lc/4};
Point(9) = {0.2, 0.2, 0, lc/4};
```

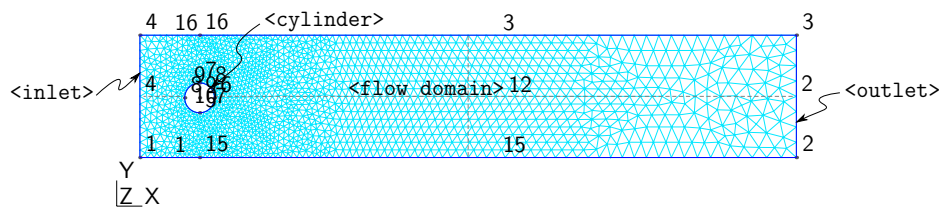


Figure 1: Geometry and resulting mesh from the `surface.geo` file for the flow through a 2d channel containing a cylinder problem.

```

Ellipse(7) = {5, 9, 9, 6};
Ellipse(8) = {6, 9, 9, 7};
Ellipse(9) = {7, 9, 9, 8};
Ellipse(10) = {8, 9, 9, 5};

// create an elementary entity that is the cylinder
boundary
Line Loop(11) = {7, 8, 9, 10};

// create the physical entity for the cylinder boundary
which becomes the arb region
Physical Line("<cylinder>") = {7, 8, 9, 10};

// all of the flow domain must be included as a physical
entity to be output under gmsh
Plane Surface(12) = {5, 11};
Physical Surface("<flow domain>") = {12};

```

Listing 2: `../examples/manual/steady_state_channel_flow_with_cylinder/constants.in`

```

# arb finite volume solver
# Copyright 2009,2010 Dalton Harvie (daltonh@unimelb.edu
  .au)
#
# arb is released under the GNU GPL. For full details
  see the license directory.
#
#
-----

# file constants.in
VERSION 0.25

```



```

#
-----

# user-defined constants

# REGION_LIST line has the ordered names of any regions
  (quoted)
# (CELL_|FACE_)REGION_CONSTANT sets a constant that
  varies with region and has the form: <name> [
  multiplier*units] value_for_region_1 ..
  value_for_region_n options # comments
# (CELL_|FACE_|NONE_|)CONSTANT sets a constant specific
  to one region or no regions and has the form: <name>
  [multiplier*units] value ON <region> options #
  comments

# physical data
CONSTANT <mu> [Pa.s] 1.d-3 # viscosity of liquid
CONSTANT <rho> [kg/m^3] 1.d0 # density
CONSTANT <u_av> [m/s] 0.2d0 # average inlet velocity

# numerical data
CONSTANT <C_{Rhie-Chow}> [] 1.0d+0 # multiplier for Rhie
  -Chow-type pressure oscillation control
CONSTANT <adv_limiter> [] 1.d0 # multiplier used to
  limit gradients when calculating advection fluxes

#
-----

# system constants

NEWTRESTOL 1.d-12 # convergence criterion for newton
  solver
NEWTSTEPMAX 20 # maximum number of steps for newton
  solver

#
-----

# geometry

# CELL_REGION/FACE_REGION specified by: <name> "location

```

```

    string" # comments
# where location string could be: "AT x1 x2 x3" for a
  single point closest to these coordinates
# where location string could be: "COMPOUND +<a region
  >-<another region>" for a + and - compound region
  list

FACE_REGION <walls> "COMPOUND <boundaries>-<inlet>-<
  outlet>"

# MSH_FILE instructs arb to read or write a gmsh file (
  location is read location - write location will
  always be within the output directory)
# output options are: output,centringoutput,meshoutput,
  centringmeshoutput,nooutput
# input options are: input,centringinput,meshinput,
  centringmeshinput,noinput
# data output format options for CELL centred data (
  which overwrite individual variable options if
  specified): elementdata,elementnodedata,
  elementnodelimiteddata
MSH_FILE "surface.msh"

# linear solver that is used to invert jacobian
#LINEAR_SOLVER "HSL_MA28" # hsl archive direct solver
#LINEAR_SOLVER "INTEL_PARDISO" # pardiso solver
  contained in intel mkl library
#LINEAR_SOLVER "INTEL_PARDISO_OOC" # pardiso solver
  contained in intel mkl library
LINEAR_SOLVER "SUITESPARSE_UMF" # suitesparse umf solver
  (UMFPACK) by Timothy A. Davis

#
  -----

```

Listing 3: ../../examples/manual/steady\_state\_channel\_flow\_with\_cylinder/equations.in

```

# arb finite volume solver
# Copyright 2009,2010 Dalton Harvie (daltonh@unimelb.edu
  .au)
#
# arb is released under the GNU GPL. For full details

```

```

    see the license directory.
#
#
-----

# file equations.in
VERSION 0.25
#
-----

# statement reference
# (CELL_|FACE_|NONE|)CONSTANT <name> [units] "expression
    (involving only constants)" ON <region> options #
    comments
# (CELL_|FACE_|NONE|)TRANSIENT <name> [units] magnitude
    "expression" ON <region> options # comments
# (CELL_|FACE_|NONE|)DERIVED <name> [units] magnitude "
    expression" ON <region> options # comments
# (CELL_|FACE_|NONE|)UNKNOWN <name> [units] "expression
    (initial value)" ON <region> options # comments
# (CELL_|FACE_|NONE|)EQUATION <name> [units] "expression
    (equation equaling zero)" ON <region> options #
    comments
# (CELL_|FACE_|NONE|)OUTPUT <name> [units] "expression"
    ON <region> options # comments

# options include:
# noderivative - for DERIVED, EQUATION : do not
    calculate Jacobian derivatives for this variable
# positive,negative - for DERIVED, UNKNOWN, EQUATION :
    check at each iteration that variable is positive/
    negative
# output/nooutput - for ALL : output compound to msh
    files
# componentoutput/nocomponentoutput - for ALL : output
    just this component to msh files
# input/noinput - for ALL : read in compound from msh
    files
# componentinput/nocomponentinput - for ALL : read in
    just this component from msh files
# elementdata,elementnodedata,elementnodelimiteddata -
    for CELL centred var : data type when writing this

```

```

    compound (unless gmesh override is specified) (also
    same for components with prefix component)

# unknown variables used for flow problems
CELL_UNKNOWN <u[l=1]> [] 1.d0 "<u_av>" # velocity
    component
CELL_UNKNOWN <u[l=2]> [] 1.d0 "0.d0" # velocity
    component
CELL_UNKNOWN <p> [] 1.d0 "1.d0-<cellx[l=1]>" # pressure

# total stress tensor
FACE_DERIVED <tau[l=1,1]> "<p> - <mu>*2.d0*facegrad[l
=1](<u[l=1]>)" output
FACE_DERIVED <tau[l=1,2]> "- <mu>*(facegrad[l=2](<u[l
=1]>)+facegrad[l=1](<u[l=2]>))"
FACE_DERIVED <tau[l=2,2]> "<p> - <mu>*2.d0*facegrad[l
=2](<u[l=2]>)"
FACE_DERIVED <tau[l=2,1]> "<tau[l=1,2]>"

# a Rhie-Chow-type correction is applied to the face
velocities
CELL_DERIVED <graddivp[l=1]> "celldivgrad[l=1](<p>)" #
    pressure gradient calculated via a divergence (
    consistent with momentum conservation)
CELL_DERIVED <graddivp[l=2]> "celldivgrad[l=2](<p>)" #
    pressure gradient calculated via a divergence (
    consistent with momentum conservation)
FACE_DERIVED <p_error> "facegrad(<p>) - dot(<graddivp[l
=:]>,<facenorm[l=:]>)" # difference between face
    centred and cell divergence type gradient at face and
    normal to the face
FACE_DERIVED <u_f_{correction}> "-<C_{Rhie-Chow}>*
    facedelta(<domain faces>)*facemin(<facedx>^2/<mu>,
    sqrt(<facedx>/(<rho>*facemax(abs(<p_error>),1.d-6)))
    )*<p_error>" compoundoutput # the Rhie-Chow type
    velocity correction, only applied (nonzero) on the
    domain faces

# flux of mass (volume) and momentum components over
each face
FACE_DERIVED <u_f> "dot(<u[l=:]>,<facenorm[l=:]>) + <
    u_f_{correction}>" # volume (velocity) transport
FACE_DERIVED <J_f[l=1]> "dot(<facenorm[l=:]>,<tau[l

```

```

    =:,1]>)+<rho>*faceave[advection](<u[l=1]>,<u_f>,<
    adv_limiter>)*<u_f>" output # component of momentum
    transport from stress and advection
FACE_DERIVED <J_f[l=2]> "dot(<facenorm[l=:]>,<tau[l
    =:,2]>)+<rho>*faceave[advection](<u[l=2]>,<u_f>,<
    adv_limiter>)*<u_f>" # component of momentum
    transport from stress and advection

# conservation equations solved over each domain cell (
    finite volume method)
CELL_EQUATION <continuity> "celldiv(<u_f>)" ON <domain>
    # continuity
CELL_EQUATION <momentum[l=1]> "celldiv(<J_f[l=1]>)" ON <
    domain> # momentum component
CELL_EQUATION <momentum[l=2]> "celldiv(<J_f[l=2]>)" ON <
    domain> # momentum component

# boundary conditions on nonslip walls
FACE_EQUATION <wall noflux> "<u_f>" ON <walls> # no flux
    normal to walls
FACE_EQUATION <wall noslip> "dot(<u[l=:]>,<facetang1[l
    =:]>)" ON <walls> # nonslip
FACE_EQUATION <wall p extrapolation> "dot(<graddivp[l
    =:]>,<facenorm[l=:]>)" ON <walls> # extrapolate
    pressure to the wall using zero gradient normal to
    wall

# boundary conditions on outlet - fully developed flow
FACE_EQUATION <outlet fully developed> "facegrad(dot(<u[
    l=:]>,cellave[lastface](<facenorm[l=:]>)))" ON <
    outlet> # normal velocity component is fully
    developed
FACE_EQUATION <outlet noslip> "dot(<u[l=:]>,<facetang1[l
    =:]>)" ON <outlet> # no component tangential to
    outlet
FACE_EQUATION <outlet p> "<p>" ON <outlet> # specified
    uniform (zero) pressure

# boundary conditions on inlet - fully developed flow
FACE_EQUATION <inlet fully developed> "facegrad(dot(<u[
    l=:]>,cellave[lastface](<facenorm[l=:]>)))" ON <inlet>
    # normal velocity component is fully developed
FACE_EQUATION <inlet noslip> "dot(<u[l=:]>,<facetang1[l

```

```

=:]>)" ON <inlet> # no component tangential to inlet

# set velocity distribution corresponding to fully
  developed Cartesian flow
FACE_EQUATION <inlet flowrate> "<u_f>+6.d0*<u_av>*<cellx
  [1=2]>*(0.41d0-<cellx[1=2]>)/(0.41d0^2)" ON <inlet> #
  specified velocity distribution

# alternatively, set uniform inlet pressure giving
  required average velocity
#NONE_DERIVED <u_av_calc> "facesum(-<u_f>*<facearea>,<
  inlet>)/facesum(<facearea>,<inlet>)" # calculate
  average velocity directed into the domain
#NONE_UNKNOWN <p_in> [Pa] 1.d0 "1.d0" # define the
  pressure at inlet
#NONE_EQUATION <p_in for flowrate> "<u_av_calc>-<u_av>"
  # set flowrate through inlet to give required average
  velocity
#FACE_EQUATION <inlet flowrate> "<p>-<p_in>" ON <inlet>
  # apply specified pressure over inlet

# calculate drag and lift on object
NONE_OUTPUT <F_drag> [N] "facesum(<facearea>*dot(<
  facenorm[1=:]>,<tau[1=:,1]>),<cylinder>)" # force on
  object in axial direction
NONE_OUTPUT <F_lift> [N] "facesum(<facearea>*dot(<
  facenorm[1=:]>,<tau[1=:,2]>),<cylinder>)" # force on
  object in vertical direction
NONE_OUTPUT <C_drag> "2.d0*<F_drag>/(<rho>*<u_av>^2*0.1
  d0)" # drag coefficient
NONE_OUTPUT <C_lift> "2.d0*<F_lift>/(<rho>*<u_av>^2*0.1
  d0)" # lift coefficient

#

```

---