The content and usage of ARTS are not only described by this document. An overview of ARTS documentation and help features is given in ARTS User Guide, Section 1.2. For continuous reports on changes of the source code and this user guide, subscribe to the ARTS developers mailing list at https://www.radiativetransfer.org/contact/.

We welcome gladly comments and reports on errors in the document. Send then an e-mail to: patrick.eriksson (at) chalmers.se or sbuehler (at) uni-hamburg.de.

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Stefan Buehler <sbuehler (at) uni-hamburg.de>
Patrick Eriksson <patrick.eriksson (at) chalmers.se>

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Software Foundation, Inc., 59 Temple Place - Suite 330,
Boston, MA 02111-1307, USA.
## Contributing authors

<table>
<thead>
<tr>
<th>Author/email</th>
<th>Main contribution(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stefan Buehler [a] sbuehler (at) uni-hamburg.de</td>
<td>Editor, Sections 1, 2, 3 and 5.</td>
</tr>
<tr>
<td>Mattias Ekström [b]</td>
<td>Section 3.6.</td>
</tr>
<tr>
<td>Claudia Emde [c] claudia.emde (at) dlr.de</td>
<td>Section 7.</td>
</tr>
<tr>
<td>Patrick Eriksson [b] patrick.eriksson (at) chalmers.se</td>
<td>Editor.</td>
</tr>
<tr>
<td>Oliver Lemke [a] olemke (at) core-dump.info</td>
<td>Section 4.</td>
</tr>
<tr>
<td>Sreerekha T.R. [c]</td>
<td>Section 6.</td>
</tr>
</tbody>
</table>

The present address is given for active contributors, while for others the address to the institute where the work was performed is given:

\[a\] Meteorological Institute, University of Hamburg, Bundesstr. 55, 20146 Hamburg, Germany.

\[b\] Department of Space, Earth and Environment, Chalmers University of Technology, SE-41296 Gothenburg, Sweden.

\[c\] Institute of Environmental Physics, University of Bremen, P.O. Box 33044, 28334 Bremen, Germany.
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Chapter 1

The art of developing ARTS

The aim of this section is to describe how the program is organized and to give detailed instructions how to make extensions. That means, it is addressed to the ARTS developers, not the users. If you only want to use ARTS, you should not need to read it. But if you want to make changes or additions, you should definitely read this carefully, since it can save you a lot of work to understand how things are organized.

1.1 Organization

ARTS is written in C++ and uses the cross-platform, open-source build system CMake (http://www.cmake.org/). It is organized in a similar manner as most GNU packages. The top-level ARTS directory is either called arts or arts-x.y, where x.y is the release number. It contains various sub-directories, notably doc for documentation, src for the C++ source code, The document that you are reading right now, the ARTS Developer Guide, is located in doc/uguide.

There are two different versions of the ARTS package: The development version and the end-user version. Both contain the complete source code, the only difference is that the developers version is where active development takes place.

The end-user version contains everything that you need in order to compile and install ARTS in a fairly automatic manner. The only thing you should need is an ANSI-C++ compiler, and the CMake utility. Please see files arts/README and arts/INSTALL for installation instructions. We are aiming to support recent version of the GNU and clang C++ compilers.

1.2 The ARTS build system

As mentioned above, CMave is used to build the ARTS package. A good introduction to the CMave system can be found in:

http://www.cmake.org/cmake/project/about.html

History

020425 Stefan Buehler: Put this part back in the AUG. Updated.
000728 Stefan Buehler: Added stuff about build system and howto cut a release.
000615 Created by Stefan Buehler.
1.2.1 Configure options

For development, it is recommended to build ARTS using the RelWithDebInfo configuration (see below), which aims to provide a reasonable trade-off between debugging capability and performance. To use ARTS in production, however, it is important to perform a release build, which is therefore set as the default configuration.

-DCMAKE_BUILD_TYPE=RelWithDebInfo: This is the build option that should be used for development, as it will make it easier to track down errors in the code. It does, however, not disable all compiler optimization, so as to still provide reasonable performance.

-DCMAKE_BUILD_TYPE=Release: Removes -g from the compiler flags and includes #define NDEBUG 1 in config.h. The central switch to turn off all debugging features (index range checking for vectors, the trace facility, assertions,...).

-DCMAKE_BUILD_TYPE=Debug: This switch turns off all optimizations. This should only be used if the RelWithDebInfo configuration makes debugging a given problem difficult.

-DNO_OPENMP=1: Disables the generation of multi-threaded code. CMake tries to detect if the compiler supports OpenMP and enables it by default.

1.3 Coding conventions

With the aim of improving quality and consistency of the code, all new code that is added to ARTS should adhere to naming and formatting conventions from Google’s C++ programming guidelines (https://google.github.io/styleguide/cppguide.html#Formatting). Adhering to a well-defined coding style will make it much easier for your fellow ARTS developers to understand and work with your code. A brief summary of the most important programming style and formatting conventions is given below.

1.3.1 Naming conventions

Naming things is one of the two hard problems in computer science. Certainly, there is no single best way to do it and even with the best names code can still be bad. Yet still, the consistently naming of objects in your code will make it much easier for other developers to read and understand your code.

In general, the use descriptive names in all your code is recommended. Try to avoid abbreviations except when they are very common. Giving proper names to objects increases the readability of the code and decreases the need for explanatory comments.

Variables

Variable names should use lower-case letters. Words should be separated using underscores:

Index element_index = 0;
Numeric t_surface = 0.0; // common abbreviation
Classes, structs and type names
Classes, structs and user-defined type names should start with a capital letter and use camel case to separate different words.

```cpp
class CovarianceMatrix {};```

Class member variables
Variables that are defined as data members of classes should be suffixed with an underscore (_). This convention has the important advantage that it allows inferring the scope of variables used inside definitions of member functions.

```cpp
class CovarianceMatrix {
  private:
    Numeric *elements_;
};```

Constant names
Names of constants should be prefixed with a lower-case k. Following words should use camel case starting with a capital letter.

```cpp
const Numeric kAlmostPi = 3.0;```

Function names
Function names should start with a capital letter and words should be separated using camel case.

```cpp
void InterpolateTo(const Vector &x_new) {
  ...
}
```

1.3.2 Formatting
The formatting, i.e. the layout of your code, should adhere strictly to the Google guidelines. Google’s indentation style is also supported by the clang-format tool, which provides functionality for automatic formatting. A format file for clang-format is provided in ARTS’ top-level directory. Most development environments provide support for clang-format, which makes following these guidelines extremely easy.

- Line length of 80 characters
- No tabs, only spaces
- 2 spaces per indentation level
- Opening brace { of function/class/struct definition and if/for blocks on the same line
- No spaces on the inner side of the parentheses of the conditional expressions of if statements.
1.3.3 ARTS-specific rules

Numeric types

Never use float or double explicitly, use the type Numeric instead. This is set by CMake (to double by default). In the same way, use Index for all integers. It can take on positive or negative values and defaults to long. To change the default types, run cmake with the options -DINDEX=long or -DNUMERIC=double:

cmake -DINDEX=int --DNUMERIC=float ..

Note that changing the numeric type to a lower precision type than double might have unforeseen impacts on the numerical precision and could lead to wrong results. In a similar way, reducing the index type can make it impossible to handle larger Vectors, Matrices or Tensors. The maximum range of the index type determines the maximum number of elements the container types can handle.

1.3.4 Container types

Use Vector and Matrix for mathematical vectors and matrices (with elements of type Numeric). Use Array<something> to create an array of somethings. Commonly used Arrays have been predefined, they have names like ArrayOfString, ArrayOfMatrix, and so forth.

1.3.5 Terminology

Calculations are carried out in the so called workspace (WS), on workspace variables (WSVs). A WSV is for example the variable containing the absorption coefficients. The WSVs are manipulated by workspace methods (WSMs). The WSMs to use are specified in the controlfile in the same order in which they will be executed.

1.3.6 Global variables

Are not visible by default. To use them you have to declare them like this:

    extern const Numeric PI;

which will make the global constant PI=3.14... available. Other important globals are:

- full_name: Full name of the program, including version.
- parameters: All command line parameters.
- basename: Used to construct output file names.
- out_path: Output path.
- messages: Controls the verbosity level.
- wsv_data: WSV lookup data.
- wsv_group_names: Lookup table for the names of types of WSVs.
- WsvMap: The map associated with wsv_data.
- md_data: WSM lookup data.
- MdMap: The map associated with md_data.
- workspace: The workspace itself.
- species_data: Lookup information for spectroscopic species.
- SpeciesMap: The map associated with species_data.
The only exception from this rule are the output streams `out0` to `out3`, which are visible by default.

### 1.3.7 Files

Always use the `open_output_file` and `open_input_file` functions to open files. This switches on exceptions, so that any error occurring later on with this file will result in an exception. (Currently not really implemented in the GNU compiler, but please use it anyway.)

### 1.3.8 Version numbers

The package version number is set in the `VERSION` file in the top level ARTS directory. It will be incremented by the ARTS maintainers when new features or bug fixes have been added to ARTS, not on every commit. Never change this number when working in your own branch. The major and/or minor version number will be incremented on public releases. The micro version indicates the addition of new features during development or bugfixes for stable releases.

### 1.3.9 Header files

The global header file `arts.h` *must* be included by every file. Apart from that you have to see yourself what header files you need. If you use functions from the C or C++ standard library, you have to also include the appropriate header file.

### 1.3.10 Documentation

Doxygen is used to generate automatic source code documentation. See

http://www.stack.nl/~dimitri/doxygen/

for information. There is a complete User manual there. At the moment we only generate the output as HTML, although latex, man-page, and rtf format is also possible. The HTML version is particularly useful for source code browsing, since it includes the complete source code! You should add Doxygen headers to the following:

1. Files
2. Classes (Including all private and public members)
3. Functions
4. Global Variables

The documentation headers are comment blocks that look like the examples below.

Doxygen supports several different comment block styles. Over the years, probably all of them were used somewhere in ARTS. New code should follow the Doxygen JavaDoc style. If you edit existing documentation, it is recommended to convert it to the current style.
File comment

Each header and source code file should contain a doxygen comment stating the original author, creation date and a short summary of its contents.

```cpp
/**
 * @file dummy.cc
 * @author John Doe <john.doe@example.com>
 * @date 2011-03-02
 * @brief A dummy file.
 * This file has no purpose at all,
 * it just serves as an example...
 */
```

Function comment

Each function should be preceded with a doxygen comment. It starts with a brief description, ending with a dot. Then follows a more detailed description of the function’s purpose and parameters.

The doxygen comment block should be put above the declaration of the function, i.e., in the .h file. If a function is only declared in a .cc file, the comment should be put there instead.

If arguments are modified by the function you should add ‘[out]’ after the @param command, just like for the parameter a in the example below. If a parameter is both input and output, it should say ‘[in,out]’. Parameters that are not modified inside the function, e.g. passed by value or const reference, should carry an ‘[in]’. The documentation for each parameter should start with a capital letter and end with a period, like in the example below.

Author and date tags are not inserted by default, since they would be overkill if you have many small functions. However, you should include them for important functions.

```cpp
/** A dummy function.
 * This function has no purpose at all,
 * it just serves as an example...
 * @param[out] a This parameter is initialized by the function.
 * @param[in,out] b This parameter is modified by the function.
 * @param[in] c This parameter is not changed by the function.
 * @return Dummy value computed from a and b.
 */
int dummy(int& a, int& b, int c);
```

Classes and structs

Classes und structs must be preceded by a doxygen comment describing their intent and purpose. A short description should be provided for each member variable. Member function are documented as described in the previous section.

```cpp
/** Brief description of Foobar.
 */
```
* Long description of Foobar.
*/
class FooBar {
    private:
    /** Number of elements. */
    Index nelem;
}

**Doxymacs for Emacs**

There is an Emacs package (Doxymacs) that makes the insertion of documentation headers particularly easy. You can find documentation of this on the Doxymacs webpage: [http://doxymacs.sourceforge.net/](http://doxymacs.sourceforge.net/). To use it for ARTS (provided you have it), put the following in your Emacs initialization file:

```lisp
(require 'doxymacs)
(setq doxymacs-doxygen-style "JavaDoc")
(defun my-doxymacs-font-lock-hook ()
  (if (or (eq major-mode 'c-mode) (eq major-mode 'c++-mode))
      (progn
       (doxymacs-font-lock)
       (doxymacs-mode))
    (add-hook 'font-lock-mode-hook 'my-doxymacs-font-lock-hook)

    (setq doxymacs-doxygen-root "../doc/doxygen/html/")
    (setq doxymacs-doxygen-tags "../doc/doxygen/arts.tag")

    The only really important lines are the first two, where the second line is the one selecting the style of documentation. The next block just turns on syntax highlighting for the Doxygen headers, which looks nice. The last two lines are needed if you want to use the tag lookup features (see Doxymacs documentation if you want to find out what this is). The package allows you to automatically insert headers. The standard key-bindings are:

- C-c d ? look up documentation for the symbol under the point.
- C-c d r rescan your Doxygen tags file.
- C-c d f insert a Doxygen comment for the next function.
- C-c d i insert a Doxygen comment for the current file.
- C-c d ; insert a Doxygen comment for a member variable on the current line (like M-;).
- C-c d m insert a blank multi-line Doxygen comment.
- C-c d s insert a blank single-line Doxygen comment.
- C-c d @ insert grouping comments around the current region.

You can call macros to insert certain types of doxygen comment by name:

- doxymacs-insert-file-comment
- doxymacs-insert-function-comment
- doxymacs-insert-blank-multiline-comment
- doxymacs-insert-blank-singleline-comment
1.4 Extending ARTS

1.4.1 How to add a workspace variable

You should read Section 2.2 to understand what workspace variables are. Here is just the practical description how a new variable can be added.

1. Create a record entry in file workspace.cc. (Just add another one of the wsv_data.push_back blocks.) Take the already existing entries as templates. The ARTS concept works best if WSVs are only of a rather limited number of different types, so that generic WSMs can be used extensively, for example for IO.

The name must be exactly like you use it in the source code, because this is used to generate interface functions.

Make sure that the documentation string you give explains the variable and its purpose well. In particular, state the dimensions (in the case of matrices) and the units! This string is used for the online documentation. Please take some time to write it carefully. Use the template at the beginning of function define_wsv_data() in file workspace.cc as a guideline.

2. That’s it!

1.4.2 How to add a workspace variable group

You should read Section 2.2 to understand what workspace variable groups are. Here is just the practical description how a new group can be added.

1. Add a wsv_group_names.push_back("your_type") function to the function define_wsv_group_names() in groups.cc. The name must be exactly like you use it in the source code, because this is used to generate interface functions.

2. XML reading/writing routines are mandatory for each workspace variable group. Two steps are necessary to add xml support for the new group:

   (a) Implement an xml_read_from_stream and xml_write_to_stream function. Depending on the type of the group the implementation goes into one of the three files xml_io_basic_types.cc, xml_io_compound_types.cc, or xml_io_array_types.cc. Basic types are for example Index or Numeric. Compound types are structures and classes. And array types are arrays of basic or compound types. Also add the function declaration in the corresponding .h file.

   (b) Add an explicit instantiation for xml_read_from_file<GROUP> and xml_write_to_file<GROUP> to xml_io_instantiation.h.

3. If your new group does not implement the output operator (operator<<), you have to add an explicit implementation of the Print function in m_general.h and m_general.cc.

4. That’s it! (But as stated above, use this feature wisely)
1.4.3 How to add a workspace method

You should read Section 2.3 to understand what workspace methods are. Here is just the practical description how a new method can be added.

1. Create an entry in the function define_md_data in file methods.cc. (Make a copy of an existing entry (one of the md_data.push_back(...) blocks) and edit it to fit your new method.) Don’t forget the documentation string! Please refer to the example at the beginning of the file to see how to format it.

2. Run: make.

3. Look in auto_md.h. There is a new function prototype

   void <YourNewMethod>(...)

4. Add your function to one of the .cc files which contain method functions. Such files must have names starting with m_. (See separate HowTo if you want to create a new source file.) The header of your function must be compatible with the prototype in auto_md.h.

5. Check that everything looks nice by running

   arts -d YourNewMethod

   If necessary, change the documentation string.

6. That’s it!

1.4.4 How to add a source code file

1. Create your file. Names of files containing workspace methods should start with m_.

2. You have to register your file in the file src/CMakeLists.txt. This file states which source files are needed for arts. In the usual case, you just have to add your .cc file to the list of source files of the artscore library. Header files are not added to this list.

3. Go to src and run: git add <my_file> to make your file known to git.

1.4.5 How to add a test case

1. Tests are located in subdirectories in the controlfiles folder. Instrument specific test cases are in the controlfiles/instruments folder, all other cases are located in the controlfiles/artscomponents folder. Create a new subdirectory in the appropriate folder. If your test is closely related to another test case you can skip this step and instead add it to one of the existing subdirectories.

2. Create your own test controlfile. The filename should start with Test followed by the name of the subdirectory it is located in, e.g. controlfiles/artscomponents/doit/TestDOIT.arts.

   If the subdirectory contains more than one test controlfile, append a short descriptive text to the end of the filename like controlfiles/artscomponents/montecarlo/TestMonteCarloGaussian.arts.
3. Copy all required input files into the subdirectory. Input data that is shared among several test cases should be placed in `controlfiles/testdata`.

4. Add an entry for your test case in `controlfiles/CMakeLists.txt`.

### 1.4.6 How to add a particle size distribution

In `mpsdc.c`, add a workspace method `psdPsdName`, where `PsdName` stands for the name or name tag of the new particle size distribution (PSD) parametrization. (see Section 1.4.3 for details). If several `psdPsdName` methods are based on the same algorithm, add the algorithm as an internal function to `psd.cc`.

### 1.5 Version control

ARTS uses git for version control. The central or upstream repository is hosted on github ([https://github.com/atmtools/arts](https://github.com/atmtools/arts)). Contributions to ARTS are handled via pull requests on github. This is the de-facto standard workflow for open source development, so the time required to get familiar with it is certainly a worthy investment. Contributing a new feature or bug-fix to ARTS thus involves the following steps:

1. Fork the upstream repository
2. Clone the ARTS fork from your github account onto your local workstation
3. Implement your changes
4. Commit and push your changes to your ARTS fork
5. Issue a pull request to merge your ARTS fork with the central repository
6. One of the ARTS core developers will review your code and help with the final integration

The required steps are described below in more detail. Note that all of these steps are so common to modern software development, that it is very easy to find tutorials and manuals online that described them in more detail.

#### 1.5.1 Forking the central repository

The forking of the central repository is through the web interface of github.com. This will create a copy of the central repository in your account. This repository is your personal version of the ARTS repository. You can change all you want here without breaking ARTS for anyone else.

#### 1.5.2 Clone your ARTS fork

So far your fork of ARTS exists only in your github account somewhere in the cloud. To really work with the code, you need to obtain a copy of the code on your local workstation. This is done by cloning the repository from your account:

```
git clone https://github.com/<your_username>/arts
```
where your_username is the name of your github account. The important point to note here is that you did not clone the central ARTS repository from github.com/atmtools but the one from your account. As explained above, this is your personal version of the ARTS repository and you can do anything you want with it.

### 1.5.3 Update your fork

One consequence of the forking of the central ARTS repository is that the fork in your own github account will not automatically be updated when changes are made to the upstream repository. Before checking in your changes into your repository it is therefore important that you update your repository with the most recent changes made to the upstream repository. For this two steps are required:

1. Register the upstream repository as remote repository for your local clone of your ARTS fork:
   ```bash
git remote --add upstream https://github.com/atmtools/arts
   ```
2. Rebase your code onto the newest changes from the upstream repository:
   ```bash
git fetch upstream master
   git rebase -i upstream/master
   ```

The first step here needs to be performed only the first time you are going through this process. Afterwards only the second step is required. A detailed description of the rebase step can be found at [https://www.atlassian.com/git/tutorials/rewriting-history/git-rebase](https://www.atlassian.com/git/tutorials/rewriting-history/git-rebase).

### 1.5.4 Commit and push your changes

After implementing your changes, commit and push them to your ARTS fork. The changes are now publicly available from your github account. Note that at this point you can already share your code with others or across different machines. It has, however, not yet been integrated into the upstream repository. That means your changes are not yet affecting regular users of the ARTS development version.

### 1.5.5 Issuing a pull request

Once your changes have been pushed to the ARTS repository in your github account, you can issue a pull request. This is done most easily through the github web interface. This will notify the ARTS core developers that you want to integrate your changes into the upstream repository. On issuing your pull request, the ARTS test-suite will be run on your code. If all tests pass, an ARTS core developer will review your code and finally merge it into the central repository.

### 1.6 Debugging (use of ARTS_ASSERT)

The idea behind ARTS_ASSERT is simple. It exists to stop program execution at times when the precondition or post-condition of the function is not met. Suppose that at a certain
point in your code, you expect two variables to be equal. If this expectation is a precondi-
tion that must be satisfied in order for the subsequent code to execute correctly, you must
 ARTS_ASSERT it with a statement like this:

    ARTS_ASSERT(var1 == var2);

or

    ARTS_ASSERT(var1 == var2, "\(\text{\texttt{\textbackslash (,var1,\texttt{, }}\text{\texttt{\textbackslash ,\texttt{ var2,\texttt{)}}\text{\textbackslash )}}}\)"

In general ARTS_ASSERT takes as argument a boolean expression followed by any
number of arguments that the developer wants to pass along to the output operator in case
the assertion is invoked. If the boolean expression is true, execution continues. Other-
wise a C++ std::runtime_error is invoked and the program execution is stopped. If
a bug prevents the precondition from being true, then you can trace the bug at the point
where the precondition breaks down instead of further down in execution or not at all. The
 ARTS_ASSERT call is implemented as a C preprocessor macro, so it can be enabled or
disabled at will.

In ARTS, you don’t have to do this manually. Instead, assertions are turned on and
off with the global NDEBUG preprocessor macro, which is set or unset automatically by
the cmake build configuration. Assertions are enabled in the default cmake build con-
figuration (-DCMAKE_BUILDTYPE=RelWithDebInfo). They are turned off in the
release configuration (-DCMAKE_BUILDTYPE=Release) and in native configuration
(-DCMAKE_BUILDTYPE=Native).

If your program is stopped by an assertion failure, then the first thing you should do is
to find out where the error happens. To do this, run the program under the GDB debugger.
First invoke the debugger:

    gdb arts

You have to give the full path to the ARTS executable. Then set a breakpoint at the assertion
failure:

    (gdb) break __assert_fail

(Note the two leading underscores!) Now run the program:

    (gdb) run

Instead of just exiting, under the debugger the program will be paused when the asser-
tion fails, and you will get back the debugger prompt. Now type:

    (gdb) where

to see where the assertion failure happened. You can use the print command to look at
the contents of variables and you can use the up and down commands to navigate the stack.
For more information, see the GDB documentation or type help at the prompt of GDB.

For ARTS, the assertion failures mostly happen inside the Tensor / Matrix / Vector
package (usually because you triggered a range check error, i.e., you tried to read or write
beyond array bounds). In this case the up command of GDB is particularly useful. If you
give this a couple of times you will finally end up in the part of your code that caused the
error.

Recommendation: In Emacs there is a special GDB mode. With this you can very
conveniently step through your code.
1.7 Debugging (use of ARTS_USER_ERROR_IF)

The ARTS_USER_ERROR_IF command should be used whenever the validity of the program being able to produce expected output is compromised by direct user input. This helps the user debug their controlfiles, python scripts, or C++ API usage. Developing ARTS, you should use these devotedly to ensure that the user input is correct and can be understood by all internal functions called by a user-facing method. Invocation of ARTS_USER_ERROR_IF is not a bug in ARTS per se but an indication that some calculations will fail at a later stage given the user input.

The interface is exactly the same as for ARTS_ASSERT, however the expectation is that the first boolean argument is false for the program execution to stop. As for the assertions, you can pass any number of arguments to the output operator, however, as opposed to the assertions, you are not allowed to pass no arguments because the user needs to be able to understand what s/he did wrong.

The ARTS_USER_ERROR_IF command is also implemented as a macro and can be turned off manually by passing -DNO_USER_ERRORS=1 to cmake. Note that this is not recommended and that the kinds of errors that it can cause to ARTS execution is beyond the responsibility of the ARTS developers and that we do not even try to understand what might happen. It might speed up execution times, however, so it is provided for users that need all possible speed-ups.
Chapter 2

The workspace

This chapter deals with the main components of ARTS: Workspace variables (WSVs) and workspace methods (WSMs). Furthermore, it explains the use of agendas, a special group of WSVs.

2.1 Implementation files

The most important files are:

- **workspace.cc:**
  Definition and documentation of WSVs.

- **methods.cc:**
  Definition and documentation of WSMs. The implementations of WSMs reside in files named `m_something.cc`.

- **agendas.cc:**
  Definition and documentation of agendas.

It is very likely that you will have to edit these. Less likely, but possibly, you also have to edit:

- **groups.cc:**
  Definition of WSV groups.

When ARTS is built, a number of source code files are generated automatically. They are listed here in the order in which they are generated:

- **auto_workspace.h:**
  Generated from `groups.cc`.

- **auto_md.h, auto_md.cc:**
  Generated from `auto_workspace.h, agendas.cc, groups.cc, and methods.cc`.

**History**

110622 Updated by Oliver Lemke.
020605 Created by Stefan Buehler.
This is achieved by a set of simple C++ programs:

- `make_auto_workspace_h.cc`
- `make_auto_md_h.cc`
- `make_auto_md_cc.cc`

The meaning of the names should be self-explanatory. There is one program for each file to be generated. The generation of the auto_files happens automatically when you do a make. Therefore, never edit any of these files.

Next, there are some files that contain the internal implementation of WSVs and WSMs. These are:

- `wsv_aux.h`:
  Implementation of class WsvRecord, which stores the lookup information for one WSV, plus auxiliary stuff for the workspace.

- `methods.h, methods_aux.cc`:
  Implementation of class MdRecord, which stores the lookup information for one WSM.

Finally, there are some files that contain the internal implementation of agendas. These are:

- `agenda_class.h, agenda_class.cc`:
  Implementation of class MRecord, which stores runtime information for one WSM, and class Agenda, which stores an agenda.

- `agenda_record.h, agenda_record.cc`:
  Implementation of class AgRecord, which is used to store agenda lookup information.

As mentioned above, you will not have to modify any of the implementation files, they are listed here just for reference. Normally, you only have to modify `workspace.cc, methods.cc, and agendas.cc`.

### 2.2 Workspace Variables or WSVs

All important variables in ARTS are WSVs. This means that they can be manipulated by a list of WSMs, which is specified in the ARTS controlfile. There exists a predefined list of possible WSVs. This list defines the workspace. One can think of each WSV as a ‘slot’ in the workspace: The WSV can be either set, or unset. Set means that the WSV has a well-defined content, unset means that it has no well-defined content. At the start of an ARTS job all WSVs are unset.

WSVs are defined in the file `workspace.cc`. A typical definition looks like this:

```cpp
wsv_data.push_back
(WsvRecord
  (NAME( "f_grid" ),
   DESCRIPTION
```
All WSV definitions have the same three elements:

1. The name, exactly the same name has to be used in the code.

2. The description, which is normally much longer than in the example here. It must fully describe the WSV, its purpose, and its normal usage. See file workspace.cc for instructions how to write the documentation.

3. The group to which the WSV belongs. You can think of a group as something similar to a C++ data type. The WSV in the example belongs to the group Vector. The allowed groups are defined in file groups.cc.

See Section 1.4 for explicit instructions how to add a new WSV to ARTS.

2.3 Workspace Methods or WSMs

WSMs manipulate WSVs to produce other WSVs. There are three kinds of WSMs:

1. Specific WSMs.

2. Generic WSMs.

3. Agenda WSMs.

As in the case of WSVs, there is a central place in ARTS where information on the available WSMs is stored. This place is the file methods.cc. It contains a record for each WSM. Here is an example:

```cpp
md_data_raw.push_back
    ( MdRecord
      ( NAME( "r_geoidSpherical" ),
        DESCRIPTION
        ( "Sets the geoid to be a perfect sphere.\n" "\n" "The radius of the sphere is selected by the generic argument r.\n" ),
        AUTHORS( "Patrick Eriksson" ),
        OUT( "r_geoid" ),
        GOUT(),
        GOUT_TYPE(),
        GOUT_DESC(),
        IN( "atmosphere_dim", "lat_grid", "lon_grid" ),
        GIN( "r" ),
```
All WSM definitions have the same elements:

1. The NAME, exactly as in the code.

2. The DESCRIPTION. This must fully describe the WSM, its purpose, and its normal usage. See file methods.cc for instructions how to write the documentation.

3. The OUT. This is a list of WSV names. All these WSVs are set by this WSM.

4. The GOUT. This is a list descriptive names for the generic outputs.

5. The GOUT_TYPE. This is a list of WSV group names. This defines the group to which the generic output arguments must belong (see below).

6. The GOUT_DESC, a list of short descriptions for the generic outputs.

7. The IN. This is a list of WSV names. All these WSVs are required as input by this WSM. This means they must have been set before.

8. The GIN, a list of descriptive names for the generic inputs.

9. The GIN_TYPE. This is a list of WSV group names. This defines the group to which the generic input arguments must belong.

10. The GIN_DEFAULT, a list of default values for the generic inputs. NODEF means that the generic input has no default and the user has to set it in the control file.

11. The GIN_DESC, a list of short descriptions for the generic inputs.

### 2.3.1 Specific WSMs

```cpp
md_data_raw.push_back
  ( MdRecord
    ( NAME( "p_gridFromGasAbsLookup" ),
      DESCRIPTION
        ( "Sets *p_grid* to the frequency grid of *abs_lookup*.
        
      ),
      AUTHORS( "Patrick Eriksson" ),
      OUT( "p_grid" ),
      GOUT(),
      GOUT_TYPE(),
      GOUT_DESC(),
      IN( "abs_lookup" ),
      GIN(),
      GIN_TYPE(),
      GIN_DEFAULT(),
      GIN_DESC()
    )
  );
```
2.4 Agendas

For this type of WSM the output and input is fixed. Fields GIN and GOUT are empty. The example above belongs in this category. It sets the WSV \texttt{p\_grid}, using the WSV \texttt{abs\_lookup} as input.

To call this method in the controlfile, you just have to write \texttt{p\_gridFromGasAbsLookup}.

2.3.2 Generic WSMs

This class of WSMs is more powerful, because it can be applied to any WSV that belongs to the right group. A good example is:

\begin{verbatim}
md_data_raw.push_back
 ( MdRecord
   ( NAME( "VectorSetConstant" ),
     DESCRIPTION
     ("Creates a vector and sets all elements to the specified value.\n" "The vector length is determined by \texttt{nelem}.\n" ),
     AUTHORS( "Patrick Eriksson" ),
     OUT(),
     GOUT( "v" ),
     GOUT_TYPE( "Vector" ),
     GOUT_DESC( "Variable to initialize." ),
     IN( "nelem" ),
     GIN( "value" ),
     GIN_TYPE( "Numeric" ),
     GIN_DEFAULT( NODEF ),
     GIN_DESC( "Vector value." )
   ) );
\end{verbatim}

As you probably have guessed, this WSM resizes the output vector to have \texttt{nelem} elements and sets all elements to the given \texttt{value}. You would use it as follows:

\begin{verbatim}
IndexSet(nelem, 10)
VectorCreate(myvector)
VectorSetConstant(myvector, nelem, 0)
\end{verbatim}

This would create the WSV \texttt{myvector} and then fill it with 10 elements set to 1. Note that output arguments always come first, input arguments last. Try \texttt{arts -d VectorSetConstant} to get more information on this method. (See Section 1.2.3 in \textit{ARTS User Guide} for information on the built-in documentation.)

For basic types it is allowed to pass values instead of variables directly to the WSM. In that case, the above example would look like this:

\begin{verbatim}
VectorCreate(myvector)
VectorSetConstant(myvector, 10, 0)
\end{verbatim}

2.3.3 Agenda WSMs

2.4 Agendas
2.4.1 Introduction

Agendas are a special incarnation of a WSM. At runtime an arbitrary number of WSMs can be added to an agenda. On invocation, the agenda will execute its methods one after the other. The inputs and outputs defined for the agenda must be satisfied by the invoked WSMs. E.g., if an agenda has `f_grid` in its list of output WSVs, a WSM which generates `f_grid` must be added to the agenda in the control file.

Agendas run their methods in a separate scope. Although WSMs invoked by an agenda have full access to all workspace variables, only the WSVs defined as output of the agenda will keep their values after the agenda execution. All other WSVs retain the values from before the agenda run.

Even though it is possible to execute agendas directly from the control file with the `AgendaExecute` method, the more common and intended use case is the internal invocation by other WSMs. This adds a considerable amount of flexibility to arts. The `iyEmissionStandard` method for example calculates (besides other components) the emission term. Without the means of an agenda, it would only be possible to use always the same method for the emission calculation. By the use of an agenda the user can choose between different methods to calculate the emission and plug them into the emission agenda in the control file:

```plaintext
AgendaSet( blackbody\_radiation\_agenda ){  
  blackbody\_radiationPlanck
}
```
Chapter 3

Vectors, matrices, tensors, and arrays

This section describes how vectors and matrices are implemented in ARTS and how they are used. Furthermore it describes how arrays of arbitrary type can be constructed and used.

3.1 Implementation files

The Matrix and Vector classes described below reside in the files:

- matpackI.h
- matpackI.cc

Tensors of order 3 to 7 reside in the files:

- matpackIII.h
- matpackIV.h
- matpackV.h
- matpackVI.h
- matpackVII.h

The template class Array (also described below) is implemented in the file:

- array.h

The Sparse class is described in the file:

- matpackII.h

The file test_matpack.cc contains test cases and usage examples. For Sparse there is a separate test file, test_sparse.cc.

History

030807 Sparse added by Mattias Ekström.
030109 Documentation for using jokers without Range added by Stefan Buehler.
020516 Tensors added by Stefan Buehler.
011018 Created and written by Stefan Buehler.
3.2 Vectors

The class Vector implements the mathematical concept of a vector. (Surprise, surprise.) This means that:

- A Vector contains a list of floating point values of type Numeric.
- A Vector can be multiplied with another Vector (scalar product), or with a Matrix.
- Sub-ranges of a Vector can easily be accessed, and used as if they were Vectors.
- Resizing a Vector is expensive and should be avoided.

3.2.1 Constructing a Vector

You can construct an object of class Vector in any of these ways:

```cpp
// By simple initialization
Vector a; // Create empty Vector.
Vector b(3); // Create Vector of length 3, if
    // created like this it will contain
    // arbitrary values.
Vector c(3,0.0); // Create Vector of length 3, and
    // fill it with 0.

// By copy
Vector d=c; // Make d a copy of c.

// By special initialization
Vector e(1,5,1); // 1, 2, 3, 4, 5
Vector f(1,5,.5); // 1, 1.5, 2, 2.5, 3
Vector g(5,5,-1); // 5, 4, 3, 2, 1

// By initialization list
Vector h{1.0,2.0,3.0}; // Creates a vector of length 3
    // containing the values
    // 1.0, 2.0, and 3.0.

// By moving from another target
Vector i=func(...); // func(...) returns a Vector
Vector j=other.reduce_rank<I>(); // Where other is an
    // rvalue matrix or
    // tensor and I is the
    // kept dimension
```

The special initialization examples all use the same constructor, which takes the three arguments ‘start’, ‘extent’, and ‘stride’. It will create a Vector containing ‘extent’ elements, starting with ‘start’, with a step of ‘stride’.

The ‘reduce_rank’ example requires that ‘I’ is less than the rank of the matrix/tensor, and that the dimensions not kept are all 1-long in the higher ranked type. Note that the higher ranked type will be left in a valid to destroy, but not valid to access state.
3.2 VECTORS

3.2.2 VectorViews

An object of class VectorView is, like the name says, just another view on an existing Vector. It does not have its own data. This has the important consequence that it cannot be resized, since that would mess up the original Vector that the view is referring to. You can create VectorViews from Vectors using the index operator ‘[]’, the class Range, and the special joker object. Examples:

```cpp
Vector x{1,2,3,4,5,6,7};
VectorView a = x;          // Now a refers to the
                        // whole of x;
VectorView b = x[Range(joker)]; // Same effect.
VectorView c = x[Range(0,2)]; // Take 2 elements of x,
                        // starting at the
                        // beginning,
                        // in this case: 1,2.
VectorView d = x[Range(0,3,2)]; // In this case: 1,3,5.
VectorView e = x[Range(3,joker)]; // In this case: 4,5,6,7.
```

As you can see, most useful ways to create VectorViews involve the Range class. The general constructor to this class takes three arguments, ‘start’, ‘extent’, and ‘stride’. This means that you will select ‘extent’ elements from the Vector, starting with index ‘start’, with a step-width of stride. Note that indices are 0-based, so 0 refers to the first element. The last argument, ‘stride’, can be omitted, in that case the default of 1 is assumed. As a special case, ‘extent’==joker means ‘to the end’, and calling Range with only one argument joker means ‘all elements’.

Usually, you will not have to use VectorView explicitly, because you can use expressions like:

```cpp
Vector a(1,5,1);          // a = 1,2,3,4,5
Vector b = a[Range(1,3)]; // b = 2,3,4
```

However, VectorView and the related class ConstVectorView are extremely useful as the argument types of functions operating on Vectors. You should define your functions like this:

```cpp
void silly_function(VectorView a,       // Output argument
                    ConstVectorView b // Input argument
                      // (read only)
)
{
    // Do some silly stuff with a and b.
}
```

Note that there must not be any ‘&’ after VectorView or ConstVectorView. In other words they have to be passed by value, not by reference. This is ok, since they do not contain the actual data, so that passing by value is efficient. Passing VectorViews by reference is forbidden.

You should use these kind of arguments for all input Vectors, and also for the output if you have a function that does not resize the output Vector. This has the great advantage that you can call the function with Vector sub-ranges, e.g.,
3.2.3 What you can do with a Vector (or VectorView)

All examples below (except for the first) assume that \( a \) is a Vector or VectorView.

**Resize (only for Vector, not for VectorView!):**

\[ a \text{.resize}(5); \]

This makes \( a \) a 5 element vector. The new Vector is not initialized (i.e., the contents will be unpredictable). Also, note that the previous content will be completely lost. Appending to a Vector is not possible.

**Get the number of elements:**

\[ \text{cout} \ll \text{a.nelem}(); \]

**Sum up all elements:**

\[ \text{cout} \ll \text{a.sum}(); \]

**Element access:**

\[ \text{cout} \ll a[3]; \quad // \text{Print 4th element.} \]
\[ a[0] = 3.5; \quad // \text{Assign 3.5 to first element.} \]

Note that we use 0-based indexing! Furthermore note that the operator ‘[]’ can be also used with `Range`, as explained above.

**Copying Vectors:**

\[ \text{Vector b;} \]
\[ b = a; \]

In this case the size of \( b \) will be adjusted to that of \( a \) automatically. Maybe you have noticed that there is a way to formulate the example above in even shorter fashion:

\[ \text{Vector b = a;} \]

The result is exactly the same. Note, though, that in this case \( b \) is constructed from \( a \), not copied (see section about constructing Vectors above).
Copying in connection with views:

This one is a bit tricky. Obviously, the size of views cannot be adjusted, because a view is just some selection of the underlying object. The ‘=’ operator in this case copies the contents, so the sizes of the left-hand and right-hand argument must match. VectorView internally uses assertions to make sure of this. So, if you get an assertion failure one reason could be that you forgot to make the target the correct size. Here is an example:

```cpp
b[Range(5,5,-1)] = a[Range(3,5)]; // Copy 5 elements from a to b, reversing
   // the order and starting
   // with index 3 in a.
```

Great, isn’t it?

Assigning a scalar:

```cpp
a = 1.0; // Assign 1 to all elements.
```

Mathematical operators:

```cpp
Vector a(1,3,1), b(3,1); // a = 1,2,3; b = 1,1,1
a *= 2; // a = 2,4,6
   // Similarly, /=, +=, -=
a += b; // a = 3,5,7
   // Similarly, -=, *=, /=
a += a; // a = 6,10,14
   // So a can appear on both sides.
```

All these operate element-wise. Note, that there are no return versions of these operators (i.e., expressions like `b = a+1` are not possible). This is again for efficiency reasons. It is currently an active area of research in programming techniques how to make this kind of expression efficient. None of the available solutions works, so ARTS has to live without it.

Maximum, minimum and mean:

```cpp
cout << max(a);
cout << min(a);
cout << mean(a);
```

Scalar product:

```cpp
cout << a*a;
```

This is an exception to the rule not to have return versions of operators. The reason is quite obvious: The return value is only a scalar.

Arbitrary single-argument math functions:

```cpp
Vector b(a.nelem());
transform(b,sin,a); // b = sin(a)
transform(b,cos,b); // b = sin(b)
   // So b can appear on both sides.
```
The transform function operates on each element of `a` with the function you specify and puts the result in `b`. Note that the order of the arguments is swapped compared to the old function `trans` that we had in the pre-Matpack era.

### 3.3 Matrices

The class `Matrix` implements the mathematical concept of a matrix. (Who would have guessed this?) This means that:

- A Matrix contains floating point values of type `Numeric`.
- The values are arranged in rows and columns and can be accessed by indices. The first index is the row, the second the column. In other words, we use *row-major* order, similar to C, Matlab, and most math textbooks. Note, however, that some languages like FORTRAN and IDL use *column-major* order.
- A Matrix can be multiplied with a Vector, or with another Matrix.
- A sub-range of a Matrix in both dimensions (submatrix) can easily be accessed, and used as if it was just a normal matrix.
- Resizing a Matrix is expensive and should be avoided.

#### 3.3.1 Constructing a Matrix

You can construct an object of class `Matrix` in any of these ways:

```cpp
// By simple initialization
Matrix a; // Create empty Matrix.
Matrix b(3,4); // Create Matrix with 3 rows and 4 columns. When created like this it will contain arbitrary values.
Matrix c(3,4,0.0); // Similar, but fill it with 0.

// By copy
Matrix d=c; // Make d a copy of c.

// By moving from another target
Matrix e=func2(...); // func2(...) returns a Matrix
Matrix f=other.reduce_rank<I, J>(); // Where other is an rvalue tensor and I and J are the kept dimensions
```

The ‘reduce_rank’ example requires that ‘I’ and ‘J’ are less than the rank of the tensor, and that the dimensions not kept are all 1-long in the higher ranked type. Note that the higher ranked type will be left in a valid to destroy, but not valid to access state.
3.3 Matrices

3.3.2 MatrixViews

A MatrixView is a view on an existing Matrix, in the same way as a VectorView is a view on an existing Vector. Like a VectorView, a MatrixView cannot be resized and does not contain the actual data. A view is generated by using Ranges:

```cpp
Matrix x(10,20); // Create 10x20 matrix.
MatrixView a = x; // Now a refers to the whole of x;
MatrixView b = x(Range(joker),Range(joker)); // Same effect.
MatrixView c = x[Range(0,2),Range(0,2)]; // 2x2 sub-matrix.
```

You probably get the idea. Note that the second argument of Range gives the number of elements to take, not the index of the last element. See the section about Vectors for more examples how to use Range. You can use joker, and also the third argument of Range to select only every nth row, or column, or reverse the order of the rows or columns.

In analogy to the Vector case, you should use the two classes MatrixView and ConstMatrixView as function arguments. Please refer to the discussion in the Vector section for details. As in the case of VectorViews, all arguments of these types should be passed by value, not by reference. Also, similar to the Vector case, workspace methods are the exception, because they have to use the conventional const Matrix& or Matrix& as input/output arguments.

3.3.3 What you can do with a Matrix (or MatrixView)

All examples below (except for the first) assume that a is a Matrix or MatrixView.

Resize (only for Matrix, not for MatrixView!):

```cpp
a.resize(5,10);
```

This makes a a 5x10 Matrix (5 rows, 10 columns). The new Matrix is not initialized (i.e., the contents will be unpredictable). Also, note that the previous content will be completely lost.

Get the number of rows or columns:

```cpp
cout << a.nrows();
cout << a.ncols();
```

Refer to a row or column:

```cpp
Vector x = a(0,Range(joker)); // First row.
Vector y = a(Range(joker),a.ncols()-1); // Last column.
```

Of course, you can use more complicated Range expressions to refer to only parts of a row or column. However, the case that you want all elements of a given dimension is so much more common than the more sophisticated uses of the Range class, that it is worth to introduce a simplified notation for this case. Therefore, you are allowed to omit the Range and just write:
Vector x = a(0,joker);        // First row.
Vector y = a(joker,a.ncols()-1); // Last column.

Technically, expressions of this kind return the type VectorView. This means, they can be used in all cases where an object of that type is expected, for example with the function defined in Section 3.2.2:

silly_function(a(0,Range(joker)),
               a(1,Range(joker))); // Call silly_function
               // with first and
               // second row of a.

Element access:

cout << a(3,4); // Print that element.
a(0,0) = 3.5;   // Assign 3.5 to the top-left element

Note that we use 0-based indexing! Furthermore note that the operator '(' can be also used with one or two Range arguments, as explained above. To summarize:

- (Index,Index) returns Numeric (element access).
- (Index,Range) or (Range,Index) returns VectorView (row or column access).
- (Range,Range) returns MatrixView (sub-matrix access).

You may find it unlogical, that Matrix uses '(' for indexing, whereas Vector uses '[]'. However, using '[]' for Matrix is not possible, since it can have only one argument. On the other hand, using '(' for Vector element access seemed not a good idea, since that would break with the established use of '[]' for element access in C and C++.

Copying Matrices:

Matrix b;
b = a;

As in the case of Vectors, the '=' operator adjusts the size of the target automatically.

Copying in connection with views:

As in the case of Vectors, the '=' operator copies only the contents for views, so the dimensions must match. An attempt to justify this behavior has been made above in the Section about Vector. As for Vector, you can use '=' with complicated expressions. Here is a more elaborate example:

b(Range(0,3),Range(0,4)) =
a(Range(10,3),Range(3,4,-1)); // Copy a row 10-12,
                             // column 0-3
                             // to b row 0-2,
                             // column 0-3, reversing
                             // the order of columns.

Note that in this case the dimensions must match exactly, as explained in the Section about Vector.

If you do not understand the use of Range here, refer to Section 3.2.2.
Assigning a scalar:

\[ a = 1.0; \]  // Assign 1 to all elements.

Mathematical operators:

You can use the operators `+=`, `-=``, `*=``, and `/=`, which operate element-wise, just as for Vector.

Maximum, minimum and mean:

\[
\text{cout} \ll \text{max}(a);
\]
\[
\text{cout} \ll \text{min}(a);
\]
\[
\text{cout} \ll \text{mean}(a);
\]

These operations act on the complete matrix. Hence, the output is a scalar value.

Arbitrary single-argument math functions:

The function `transform` works just like for Vector.

Transpose:

\[
\text{Matrix } b = \text{transpose}(a); \]  // Make b the transpose of a.

The function `transpose` creates a MatrixView, for which rows and columns are interchanged. Note, that only the way the data is accessed is changed, not the data itself. So Matrix a in the example above is not changed. For this reason, transposing is very efficient. You can use `transpose(a)` instead of a in any matrix expression practically without additional cost. (This is not strictly true, after all, the view has to be generated and passed. But that cost should be negligible except for very small matrices.)

Matrix multiplication:

\[
\text{// Matrix-Vector:}
\]
\[
\text{Vector } b(a.nrows()), c(a.ncols());
\]
\[
\text{mult}(b,a,c); \]  // b = a * c

\[
\text{// Matrix-Matrix:}
\]
\[
\text{Matrix } d(a.nrows(),5), e(a.ncols(),5);
\]
\[
\text{mult}(d,a,e); \]  // d = a * e

Note, that the result is put in the first argument, consistent with the general ARTS policy, but different from the old MTL based multiplication function. Furthermore note, that as you can see from the first example, a Vector is always considered to be a 1-column Matrix.

Important: The matrices or vectors that you give for the three arguments must not overlap, or you will get garbage. In particular, this means that

\[
\text{mult}(x,y,x); \]  // x = y * x FORBIDDEN!!!
does not work. No, even worse: It works, but it gives the wrong result. The reason for this behavior is that the result is constructed in the first argument variable. If that is also an input variable it will change while it is multiplied, which will lead to a different result. There is no efficient way to detect overlap, so the only way to allow input and output arguments to be identical would be to use another internal dummy variable to store the result. However, this would be much less efficient.

Another thing: You can use transpose, of course. These two examples should obviously give the same result:

```
// Define b and c as in first example above.
mult(c,transpose(a),b); // c = a' * b

// Vector-Matrix:
mult(transpose(c),transpose(b),a); // c' = b' * a
```

### 3.4 Tensors

ARTS has tensors with rank 3 to 7. They are called Tensor3, Tensor4, Tensor5, Tensor6, Tensor7, and work very much like matrices, just with more dimensions. Some properties:

- A Tensor contains floating point values of type Numeric.

- The rank of a tensor means the number of dimensions, so a Tensor4 has 4 dimensions. Tensors of different rank are different classes. That means, the rank is fixed at compile time and cannot be changed at runtime. We will use rank and dimension as synonyms.

- The different dimensions are named:
  - Library
  - Vitrine
  - Shelf
  - Book
  - Page
  - Row
  - Column

For example, Tensor3 \( b(2,4,3) \) defines a third order tensor with 2 pages, 4 rows, and 3 columns. Note that the column dimension is always last. (Incidentally, a Matrix behaves exactly like a second order tensor, except that it has some additional features.)

- A sub-range of a tensor in all dimensions (sub tensor) can easily be accessed, and used as if it was just a normal tensor.

- More importantly, you can easily access lower dimensional ‘slices’ of a tensor.

- Resizing a tensor is expensive and should be avoided.
3.4 Tensors

3.4.1 Constructing a tensor

You can construct an object of a tensor class like this:

```cpp
// By simple initialization
Tensor7 a; // Create empty tensor of rank 7
Tensor3 b(2,4,3); // 2 pages, 4 rows, 3 columns
Tensor3 c(2,4,3,0.0); // Similar, but
// fill it with 0.

// By copy
Tensor3 d=c; // Make d a copy of c.

// By moving from another target
Tensor3 e3=func3(...); // func3(...) returns a Tensor3
Tensor4 e4=func4(...); // func4(...) returns a Tensor4
Tensor4 e5=func5(...); // func5(...) returns a Tensor5
Tensor4 e6=func6(...); // func6(...) returns a Tensor6
Tensor4 e7=func7(...); // func7(...) returns a Tensor7

Tensor3 f=other.reduce_rank<I, J, K>(); // Where other is an
// rvalue tensor of
// higher order than 3
// and I-K are the
// kept dimensions

Tensor4 f=other.reduce_rank<I, J, K, L>(); // Where other is an
// rvalue tensor of
// higher order than 4
// and I-L are the
// kept dimensions

Tensor5 f=other.reduce_rank<I, J, K, L, M>()); // Where other is an
// rvalue tensor of
// higher order than 5
// and I-L are the
// kept dimensions

Tensor6 f=other.reduce_rank<I, J, K, L, M, N>()); // Where other is an
// rvalue Tensor7 and
// I-N are the kept
// dimensions
```

The ‘reduce_rank’ examples require that ‘I’ to ‘N’ are all less than the rank of the higher ranked tensor, and that the dimensions not kept are all 1-long of this tensor. Note that the higher ranked tensor will be left in a valid to destroy, but not valid to access state.

3.4.2 Tensor views

Tensor views work exactly like matrix and vector views. Example:

```cpp
Tensor4 a(10,20,5,4);
Tensor3View b = a(3,Range(1,3),joker,joker);
```

If you have read the previous sections carefully, it should be clear what this expression does.

This is what is meant by slicing: You can easily create a view of a tensor that picks out an object of lower dimension. Note that you can use either an `Index` or a `Range` argument\(^1\)

\(^1\)Using just `joker` is equivalent to using `Range(joker)`, as explained in Section 3.3.
for any of the dimensions. The dimensionality of the result will adjust accordingly, as in the example above.

Everything that was said about matrix and vector views holds also here. In particular, please always use views as function arguments.

### 3.4.3 What you can do with a tensor (or tensor view)

All examples below (except for the first) assume that \( a \) is a Tensor7 or Tensor7View.

**Resize (only for tensors, not for views):**

\[
a\text{.resize}(5, 10, 4, 5, 3, 6, 8);
\]

This makes \( a \) the requested size. The new tensor is not initialized (i.e., the contents will be unpredictable). Also, note that the previous content will be completely lost.

**Get the extent of the various dimensions:**

\[
\begin{align*}
\text{Index } nl & = a\text{.nlibraries}(); \\
\text{Index } nv & = a\text{.nvitrines}(); \\
\text{Index } ns & = a\text{.nshelves}(); \\
\text{Index } nb & = a\text{.nbooks}(); \\
\text{Index } np & = a\text{.npages}(); \\
\text{Index } nr & = a\text{.nrows}(); \\
\text{Index } nc & = a\text{.ncols}();
\end{align*}
\]

Which of these functions are available depends on the dimension of your tensor. For example, `nlibraries()` is only available for Tensor7. Note, that I took care that the first letters of the dimension names are unique, which is very convenient if you prefer short names for your variables that refer so some dimension of a tensor.

**Slicing:**

\[
\text{Vector } x = a(0, 2, 1, 8, 3, 4, \text{joker});
\]

// Select row 4
// on page 3
// in book 8
// on shelf 1
// in vitrine 2
// in library 0
// and copy it to the Vector x.

Any `Range` or `Index` expression is allowed in any of the arguments, of course.

**Element access:**

\[
\begin{align*}
\text{cout } & \ll a(3, 4, 0, 0, 0, 0, 0); \quad / / \text{ Print that element.} \\
a(0, 0, 0, 0, 0, 0, 0) & = 3.5; \quad / / \text{ Assign 3.5 to this element.}
\end{align*}
\]

**Copying tensors:**

Works exactly like copying matrices. Size of output argument is adjusted for Tensors, but must already have the correct size for TensorViews.
Assigning a scalar:

\[ a = 1.0; \quad \text{// Assign 1 to all elements.} \]

Mathematical operators:

You can use the operators `+=`, `-=`, `*=` and `/=` which operate element-wise, just as for Vector.

Maximum and minimum:

```cpp
cout << max(a);
cout << min(a);
```

Arbitrary single-argument math functions:

The function `transform` works just like for Vector.

### 3.4.4 Making things appear larger than they are

Assume that you have written a function that performs some calculation for a `Tensor5`:

```cpp
void my_function(Tensor5View x);
```

Can you call this function with a `Tensor4`? Yes, you can:

```cpp
Tensor4 a;
Tensor5View b = a; \quad \text{// The extent of the first}
\quad \text{// dimension of b will be 1.}
my_function(b); \quad \text{// Call the function.}
```

In general, you can always create a view that is one dimension bigger than what you have. The leading dimension then has extent 1. There is one important exception: If you interpret a Vector as a Matrix, the trailing dimension will be 1, not the leading dimension. This is necessary, because the vector has to act like a column vector, so that matrix-vector products work in the normal way. Of course you can use telescoping to blow up anything to `Tensor7`:

```cpp
Numeric b = 3.1415; \quad \text{// Just any number here.}
Tensor7View bt7 =
\quad \text{// All dimensions of bt7 will be 1!}
```

This kind of conversion works also implicitly. So, instead of the first example, you could have simply written:
my_function(a);

The purpose of this feature is to avoid having to make special versions of auxiliary functions for all different tensor dimensions. Use it wisely! There is very little runtime overhead for this, since the data itself is not copied.

### 3.4.5 Summary

This is all. In particular, we have no tensor products, since they are not needed. So, tensors are mostly used to store things, notably atmospheric field and so on. There is a set of sophisticated interpolation routines, though, which are described separately in Chapter 5.

### 3.5 Arrays

The template class `Array` can be used to make arrays out of anything. I do not know a good definition for 'array', but I guess anybody who has written a computer program in any programming language is familiar with the concept. Of course, it is rather similar to the concept of a Vector, just missing all the mathematical functionality like Matrix-Vector multiplication and sub-range access.

The implementation of our `Array` class is based on the STL class `std::vector`, whereas the implementation of our `Vector` class is done from scratch. So the two implementations are completely independent. Nevertheless, I tried to make `Array` behave consistently with `Vector`, as much as possible. There are a number of important differences, though, hopefully sufficiently explained in this part. A short summary of important differences:

- An Array can contain elements of any type, whereas a Vector always contains elements of type Numeric.
- No mathematical functionality for Array (no sub-ranges (nothing like VectorView); no +=, -=, *=, /=; no scalar product; no transform function; no mult function; no transpose function).
- On the other hand, resizing (for example adding to the end) of an Array is ok. (See the `push_back` method below.) It is still rather expensive, though, at least for large Arrays.

#### 3.5.1 Constructing an Array

You can construct an object of an Array class like this:

```cpp
Array<Index> a; // Empty Array of class Index.
Array<String> b(5); // String Array with 5 elements. Without initialization, elements contain random values.
Array<String> c(5, "x"); // The same, but fill with "x".
Array<Index> d = a; // Make d a copy of a;
Array<String> a("ARTS", "is", "is", "is", "is");
```
There are already a lot of predefined Array classes. The naming convention for them is: ArrayOfIndex, ArrayOfString, etc. Normally you should use these predefined classes. But if you want to define an Array of some uncommon type, you can do it with ‘<<’ , as in the above examples.

3.5.2 What you can do with an Array

All examples below assume that a is an ArrayOfString.

Resize:

a.resize(5);  

This adjusts the size of a to 5. Resizing is more efficiently implemented than for Vector, but still expensive.

Get the number of elements:

cout << a.nelem();  // Just as for Vector.

In particular, note that the return type of this method is Index, just as for Vector. This is an extension compared to std::vector, which just has a method size() that returns the positive integer type size_t.

Element access:

cout << a[3];  // Print 4th element.
a[0] = "Hello";  // Assign string "Hello" to first element.

In other words, this works just like for Vector.

Copying Arrays:

This works also the same as for Vector. The size of the target must match! In this respect, I have modified the behavior with respect to the underlying std::vector, which has different copy semantics.

Assigning a scalar of the base type:

a = "Hello";  // Assign string "Hello" to all elements.
Append to the end:

```cpp
a.push_back("Hello"); // Adds this new element at the
// end of a.
```

This can be an expensive operation, especially for large Arrays. Therefore, use it with care. Actually, the `push_back` method comes from the `std::vector` class that `Array` is based on. You can do a lot more with `std::vector`, all of which also works with `Array`. However, to explain the Standard Template Library is beyond the scope of this text. You can read about it in C++ or even dedicated STL textbooks.

### 3.6 Sparse matrices

The class `Sparse` implements the mathematical concept of a matrix, same as `Matrix` does, but the data is stored in a different manner. `Sparse` offers a memory saving storage when most of the matrix is filled with zeros. This means that:

- A `Sparse` contains floating point values of type `Numeric`.
- The values are arranged in rows and columns in the same ways as for ordinary matrices, in *row-major* order.
- A `Sparse` can be multiplied with a Vector, a Matrix or with another Sparse.
- There exist no views for Sparse.
- Resizing a Sparse is expensive and should be avoided.

To calculate the maximum number of non-zero elements for efficient storage, take the product of number of columns and number of rows, subtract the number of columns plus one and then divide by two, \( nnz \leq 0.5 \times (\text{ncols} \times \text{nrows} - (\text{ncols} + 1)) \).

#### 3.6.1 Constructing a Sparse

You can construct an object of class `Sparse` in any of these ways:

```cpp
Sparse a; // Create empty Sparse.
Sparse b(3,4); // Create Sparse with 3 rows
// and 4 columns. When
// created like this it will
// contain only zeros, i.e.
// be an empty Sparse.

Sparse d=c; // Make d a copy of c.
```

#### 3.6.2 What you can do with a Sparse

All examples below assume that `a` is a Sparse.
Identity matrix:

```cpp
a.resize(10,10);
id_mat(a);
```

This sets `a` to be the identity matrix of size $10 \times 10$ (10 rows and 10 columns). Using this function is much faster than setting the diagonal elements to one by yourself. Note that `a` must be a square matrix.

Resize:

```cpp
a.resize(5,10);
```

This makes `a` a $5 \times 10$ Sparse (5 rows, 10 columns). Note that the previous content will be completely lost. The new Sparse will be empty.

Get the number of rows, columns or non-zero elements:

```cpp
cout << a.nrows();
cout << a.ncols();
cout << a.nnz();
```

Element access:

There are two different ways to access individual elements. One used for read only and one for read and write. The distinction is necessary since the read and write method creates elements if they don’t already exist. Note that we use 0-based indexing. For reading only use:

```cpp
cout << a.ro(3,4); // Print that element. If it
data doesn’t exist a zero will // be printed.
cout << a(0,0); // Short version of the above.
```

For reading and writing, such as assigning values to elements, use:

```cpp
a.rw(0,0) = 1.5; // Assigns the value 1.5 to the // first row and first column.
cout << a.rw(0,0); // Also returns the value of the // first row and first column, // if the element doesn’t exist // it will be created and set // to zero.
```

Copying Matrices:

```cpp
Sparse b;
b = a;
```

The copying of matrices is implemented as deep copy. That means that the complete object is duplicated including all elements in the matrix. The resulting matrices are completely independent of each other, but depending on `a` this may require considerable amount time and memory.
Transpose:

The function `transpose` works a bit differently for Sparse than for Vector and Matrix. This is due to the fact that we don’t have any views for Sparse. Thus, `transpose` for a Sparse creates a new Sparse variable that contains the transpose of the original Sparse, whereas `transpose` for a Matrix just creates a transposed view of the original Matrix.

The target variable for the transposed Sparse has to have the right dimensions before the function is called.

```cpp
Sparse b(a.ncols(),a.nrows());
transpose(b,a); // Make b the transpose of a.
// Note the argument order!
```

Matrix addition and subtraction:

The sums and differences of sparse matrices **with the same dimensions** can be computed as follows:

```cpp
Sparse b(a.nrows(),a.ncols());
Sparse c(a.nrows(),a.ncols());
add( c, a, b ); // c = a + b
a += b; // a = a + b
sub( c, a, b ); // c = a - b
a -= b; // a = a - b
```

Scaling of sparse matrices:

Sparse matrices can be scaled by scalar factors as follows:

```cpp
a *= 2.0; // a = 2.0 * a
a /= 2.0; // a = 0.5 * a
```

Note that the `/=` scales the matrix by the reciprocal of the given scalar factor.

Matrix multiplication:

```cpp
// Sparse-Vector
Vector b(a.nrows()), c(a.ncols());
mult(b,a,c); // b = a * c

// Sparse-Matrix
Matrix d(a.nrows(),5), e(a.ncols(),5);
mult(d,a,e); // d = a * e

// Sparse-Sparse
Sparse f(a.nrows(),5), g(a.ncols(),5);
mult(f,a,g); // f = a * g
```

The result is put in the first argument, consistent with the Matrix class. Note that for the Sparse – Matrix multiplication the output is a Matrix. **Important:** As for Matrix, the matrices or vectors that you give for the three arguments must not overlap, or you will get garbage.
Chapter 4

Gridded Fields

This section describes how gridded fields are implemented in ARTS and how they are used. Gridded fields consist of a data object like a Vector, Matrix, or Tensor and a grid for each dimension of its data. For example, a GriddedField1 consists of one grid and a Vector, whereas a GriddedField3 contains three grids and a Tensor3. Grids can be either numeric, like a pressure grid, or strings, like channel names.

4.1 Implementation files

The GriddedField1, GriddedField2, GriddedField3, GriddedField4 classes and their common base class GriddedField described below reside in the files:

- gridded_fields.h
- gridded_fields.cc

4.2 Design

4.2.1 The abstract base class GriddedField

The abstract base class GriddedField implements the properties all gridded fields have in common. These are mostly the methods to create, set, and access the grids. A GriddedField is never instantiated directly.

4.2.2 Inheritance

The GriddedFieldX classes use indirect inheritance to combine a data object with the grids, see Figure 4.1.

History
2010-09-28 Oliver Lemke: Updated for implementation changes.
2010-04-12 Created and written by Oliver Lemke.
4.3 Constructing Gridded Fields

4.3.1 Creation

Each \texttt{GriddedField} offers two constructors. One default constructor that creates an unnamed gridded field and a second constructor that takes a string with the name of the gridded field as an argument.

\begin{verbatim}
GriddedField1 gfone("I’m a GriddedField1");
GriddedField2 gftwo;
gftwo.set_name("I’m a GriddedField2");
\end{verbatim}

4.3.2 Initializing the grids

Once a gridded field has been created, we can start setting up the grids. There are two different types of grids, a numeric grid and a string grid. In the following example we set up two gridded fields: A \texttt{GriddedField1} with a numeric grid and a \texttt{GriddedField2} with a numeric grid for the rows and a string grid for the columns. Each grid can be assigned a name to describe its contents or unit.

\begin{verbatim}
Vector gfonegrid(1,5,1); // gfonegrid = [1,2,3,4,5]
gfone.set_grid(0, gfonegrid); // Set grid for the vector elements.

Vector gftwogrid0(1,5,1); // gftwogrid0 = [1,2,3,4,5]
ArrayOfString gftwogrid1{"Chan1", "Chan2", "Chan3"};
gftwo.set_grid(0, gftwogrid0); // Set grid for the matrix rows.
gftwo.set_grid(1, gftwogrid1); // Set grid for the matrix columns.

gfone.set_grid_name (0, "Pressure");
gftwo.set_grid_name (0, "Pressure");
gftwo.set_grid_name (1, "Channel");
\end{verbatim}

4.3.3 Initializing the data

The data of a \texttt{GriddedFieldX} can be accessed through its \texttt{data} member. For a \texttt{GriddedField1} data is a \texttt{Vector}, for a \texttt{GriddedField2} a \texttt{Matrix}, for a \texttt{GriddedField3} a \texttt{Tensor3},
and so on.

The following code shows how to fill the gridded fields from the previous example with data:

```cpp
Vector avector(1,4,0.5); // avector = [1,1.5,2,2.5]
gfone.data = avector;

Matrix amatrix(5,3,4.); // amatrix = [[4,4,4],[4,4,4],...]
gftwo.data = amatrix;
```

### 4.3.4 Consistency check

After initializing or changing either the grids or the data, it can happen that the size of the grids does not match the size of the data anymore. Each gridded field provides a convenience function which can be called to perform a consistency check.

```cpp
if (!gfone.checksize())
    cout << gfone.get_name() << " : Sizes of grid and data don't match" << endl;

// This should fail!
if (!gftwo.checksize())
    cout << gftwo.get_name() << " : Sizes of grids and data don't match" << endl;
```

The complete source code of the examples from this chapter can be found in `src/test_gridded_fields.cc`. 
Chapter 5

Interpolation

There are no general single-step interpolation functions in ARTS. Instead, there is a set of useful utility functions that can be used to achieve interpolation. Roughly, you can separate these into functions determining grid position arrays, functions determining interpolation weight tensors, and functions applying the interpolation. Doing an interpolation thus requires a chain of function calls:

1. gridpos (one for each interpolation dimension)
2. interpweights
3. interp

Currently implemented in ARTS is multilinear interpolation in up to 6 dimensions. (Is the 6D case called hexa-linear interpolation?) The necessary functions and their interaction will be explained in this chapter.

5.1 Implementation files

Variables and functions related to interpolation are defined in the files:

- interpolation.h
- interpolation.cc
- test_interpolation.cc

The first two files contain the declarations and implementation, the last file some usage examples.

5.2 Green and blue interpolation

There are two different types of interpolation in ARTS:

<table>
<thead>
<tr>
<th>History</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>100204</td>
<td>Added documentation of grid checking functions by Stefan Buehler.</td>
</tr>
<tr>
<td>020528</td>
<td>Created by Stefan Buehler.</td>
</tr>
</tbody>
</table>
Green Interpolation: Interpolation of a gridded field to a new grid.

Blue Interpolation: Interpolation of a gridded field to a sequence of positions.

Figure 5.1 illustrates the different types for a 2D example.

The first step of an interpolation always consists in determining where your new points are, relative to the original grid. You can do this separately for each dimension. The positions have to be stored somehow, which is described in the next section.

5.3 Grid checking functions

Before you do an interpolation, you should check that the new grid is inside the old grid. (Or only slightly outside.) You can use the convenience function \texttt{chk\_interpolation\_grids} for this purpose, which resides in file \texttt{check\_input.cc}. The function has the following parameters:

\begin{verbatim}
const String& which\_interpolation A string describing the interpolation for which the grids are intended.
ConstVectorView old\_grid The original grid.
ConstVectorView new\_grid The new grid.
const Numeric& extpolfac The extrapolation fraction. See gridpos function for details. Has a default value, which is consistent with gridpos.
\end{verbatim}

There is also a special version for the case that the new grid is just a scalar. What the function does is check if old and new grid for an interpolation are ok. If not, it throws a detailed runtime error message.

The parameter extpolfac determines how much extrapolation is tolerated. Its default value is 0.5, which means that we allow extrapolation as far out as half the spacing of the last two grid points on that edge of the grid.

The \texttt{chk\_interpolation\_grids} function is quite thorough. It checks not only the grid range, but also the proper sorting, whether there are duplicate values, etc.. It is not
completely cheap computationally. Its intended use is at the beginning of workspace methods, when you check the input variables and issue runtime errors if there are any problems. The runtime error thrown also explains in quite a lot of detail what is actually wrong with the grids.

5.4 Grid positions

A grid position specifies where an interpolation point is, relative to the original grid. It consists of three parts, an Index giving the original grid index below the interpolation point, a Numeric giving the fractional distance to the next original grid point, and a Numeric giving 1 minus this number. Of course, the last element is redundant. However, it is efficient to store this, since it is used many times over. We store the two numerics in a plain C array of dimension 2. (No need to use a fancy Array or Vector for this, since the dimension is fixed.) So the structure GridPos looks like:

```c
struct GridPos {
  Index idx;    /* Original grid index below interpolation point. */
  Numeric fd[2]; /* Fractional distance to next point
                   (0<=fd[0]<=1), fd[1] = 1-fd[0]. */
};
```

For example, idx=3 and fd=0.5 means that this interpolation point is half-way between index 3 and 4 of the original grid. Note, that ‘below’ in the first paragraph means ‘with a lower index’. If the original grid is sorted in descending order, the value at the grid point below the interpolation point will be numerically higher than the interpolation point. In other words, grid positions and fractional distances are defined relative to the order of the original grid. Examples:

- **old grid = 2 3**
  - new grid = 2.25
  - idx = 0
  - fd[0] = 0.25

- **old grid = 3 2**
  - new grid = 2.25
  - idx = 0
  - fd[0] = 0.75

Note that fd[0] is different in the second case, because the old grid is sorted in descending order. Note also that idx is the same in both cases.

Grid positions for a whole new grid are stored in an `ArrayOfGridPos` (called `ArrayOfGridPos`).

5.5 Setting up grid position arrays

There is only one function to set up grid position arrays, namely `gridpos`:

```c
void gridpos( ArrayOfGridPos& gp,
              ConstVectorView old_grid,
              ConstVectorView new_grid,
              const Numeric& extpolfac=0.5 );
```
Some points to remember:

- As usual, the output \( g \) has to have the right dimension.
- The old grid has to be strictly sorted. It can be in ascending or descending order. But there must not be any duplicate values. Furthermore, the old grid must contain at least two points.
- The new grid does not have to be sorted, but the function will be faster if it is sorted or mostly sorted. It is ok if the new grid contains only one point.
- The beauty is, that this is all it needs to do also interpolation in higher dimensions: You just have to call gridpos for all the dimensions that you want to interpolate.
- Note also, that for this step you do not need the field itself at all!
- If you want to use the returned \( g \) object for something else than interpolation, you should know that gridpos guarantees the following:
  For the ascending old grid case:
  \[
  \text{old_grid}[\text{tgp.idx}] \leq \text{tng} \quad \text{or} \quad \text{tgp.idx} = 0
  \]
  And for the descending old grid case:
  \[
  \text{old_grid}[\text{tgp.idx}] \geq \text{tng} \quad \text{or} \quad \text{tgp.idx} = 0
  \]
- Finally, note that parameter \( \text{extpolfac} \) plays the same role as explained above in Section 5.3.

5.6 Interpolation weights

As explained in the ‘Numerical Recipes’ [Press et al., 1997], 2D bi-linear interpolation means, that the interpolated value is a weighted average of the original field at the four corner points of the grid square in which the interpolation point is located. Taking the corner points in the order indicated in Figure 5.2, the interpolated value is given by:

\[
y(t,u) = (1-t) \cdot (1-u) \cdot y_1 + t \cdot (1-u) \cdot y_2 + (1-t) \cdot u \cdot y_3 + t \cdot u \cdot y_4
\]

where \( t \) and \( u \) are the fractional distances between the corner points in the two dimensions, \( y_i \) are the field values at the corner points, and \( w_i \) are the interpolation weights.

(By the way, I have discovered that this is exactly the result that you get if you first interpolate linearly in one dimension, then in the other. I was playing around with this a bit, but it is the more efficient way to pre-calculate the \( w_i \) and do all dimensions at once.

How many interpolation weights one needs for a multilinear interpolation depends on the dimension of the interpolation: There are exactly \( 2^n \) interpolation weights for an \( n \) dimensional interpolation. These weights have to be computed for each interpolation point (each grid point of the new grid, if we do a ‘green’ type interpolation. Or each point in the sequence, if we do a ‘blue’ type interpolation).
This means, calculating the interpolation weights is not exactly cheap, especially if one interpolates simultaneously in many dimensions. On the other hand, one can save a lot by re-using the weights. Therefore, interpolation weights in ARTS are stored in a tensor which has one more dimension than the output field. The last dimension is for the weight, so this last dimension has the extent 4 in the 2D case, 8 in the 3D case, and so on (always $2^n$).

In the case of a ‘blue’ type interpolation, the weights are always stored in a matrix, since the output field is always 1D (a vector).

5.7 Setting up interpolation weight tensors

Interpolation weight tensors can be computed by a family of functions, which are all called interpweights. Which function is actually used depends on the dimension of the input and output quantities. For this step we still do not need the actual fields, just the grid positions.

5.7.1 Blue interpolation

In this case the functions are:

```cpp
void interpweights( MatrixView itw,
                    const ArrayOfGridPos& cgp );
void interpweights( MatrixView itw,
                    const ArrayOfGridPos& rgp,
                    const ArrayOfGridPos& cgp );
void interpweights( MatrixView itw,
                    const ArrayOfGridPos& pgp,
                    const ArrayOfGridPos& rgp,
                    const ArrayOfGridPos& cgp );
void interpweights( MatrixView itw,
                    const ArrayOfGridPos& vgp,
                    const ArrayOfGridPos& sgp,
                    const ArrayOfGridPos& bgp,
                    const ArrayOfGridPos& pgp,
                    const ArrayOfGridPos& rgp,
                    const ArrayOfGridPos& cgp );
```

In all cases, the dimension of itw must be consistent with the given grid position arrays and the dimension of the interpolation (last dimension $2^n$). Because the grid position arrays are interpreted as defining a sequence of positions they must all have the same length.
5.7.2 Green interpolation

In this case the functions are:

```c
void interpweights( Tensor3View itw,
                   const ArrayOfGridPos& rgp,
                   const ArrayOfGridPos& cgp );
void interpweights( Tensor4View itw,
                   const ArrayOfGridPos& pgp,
                   const ArrayOfGridPos& rgp,
                   const ArrayOfGridPos& cgp );
void interpweights( Tensor5View itw,
                   const ArrayOfGridPos& bgp,
                   const ArrayOfGridPos& pgp,
                   const ArrayOfGridPos& rgp,
                   const ArrayOfGridPos& cgp );
void interpweights( Tensor6View itw,
                   const ArrayOfGridPos& sgp,
                   const ArrayOfGridPos& bgp,
                   const ArrayOfGridPos& pgp,
                   const ArrayOfGridPos& rgp,
                   const ArrayOfGridPos& cgp );
void interpweights( Tensor7View itw,
                   const ArrayOfGridPos& vgp,
                   const ArrayOfGridPos& sgp,
                   const ArrayOfGridPos& bgp,
                   const ArrayOfGridPos& pgp,
                   const ArrayOfGridPos& rgp,
                   const ArrayOfGridPos& cgp );
```

In this case the grid position arrays are interpreted as defining the grids for the interpolated field, therefore they can have different lengths. Of course, \( \text{itw} \) must be consistent with the length of all the grid position arrays, and with the dimension of the interpolation (last dimension \( 2^n \)).

5.8 The actual interpolation

For this final step we need the grid positions, the interpolation weights, and the actual fields. For each interpolated value, the weights are applied to the appropriate original field values and the sum is taken (see Equation 5.1). The \text{interp} family of functions performs this step.

5.8.1 Blue interpolation

```c
void interp( VectorView ia,
             ConstMatrixView itw,
             ConstVectorView a,
             const ArrayOfGridPos& cgp);
void interp( VectorView ia,
             ConstMatrixView itw,
             ConstMatrixView a,
             const ArrayOfGridPos& rgp,
             const ArrayOfGridPos& cgp);
```
void interp( VectorView ia,
    ConstMatrixView itw,
    ConstTensor3View a,
    const ArrayOfGridPos& pgp,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

void interp( VectorView ia,
    ConstMatrixView itw,
    ConstTensor4View a,
    const ArrayOfGridPos& bgp,
    const ArrayOfGridPos& pgp,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

void interp( VectorView ia,
    ConstMatrixView itw,
    ConstTensor5View a,
    const ArrayOfGridPos& sgp,
    const ArrayOfGridPos& bgp,
    const ArrayOfGridPos& pgp,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

void interp( VectorView ia,
    ConstMatrixView itw,
    ConstTensor6View a,
    const ArrayOfGridPos& vgp,
    const ArrayOfGridPos& sgp,
    const ArrayOfGridPos& bgp,
    const ArrayOfGridPos& pgp,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

5.8.2 Green interpolation

void interp( MatrixView ia,
    ConstTensor3View itw,
    ConstMatrixView a,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

void interp( Tensor3View ia,
    ConstTensor4View itw,
    ConstTensor3View a,
    const ArrayOfGridPos& pgp,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

void interp( Tensor4View ia,
    ConstTensor5View itw,
    ConstTensor4View a,
    const ArrayOfGridPos& bgp,
    const ArrayOfGridPos& pgp,
    const ArrayOfGridPos& rgp,
    const ArrayOfGridPos& cgp);

void interp( Tensor5View ia,
    ConstTensor6View itw,
    ConstTensor5View a,
5.9 Examples

5.9.1 A simple example

This example is contained in file test_interpolation.cc.

```cpp
void test05()
{
    cout << "Very simple interpolation case\n";

    Vector og(1,5,+1); // 1, 2, 3, 4, 5
    Vector ng(2,5,0.25); // 2.0, 2.25, 2.5, 2.75, 3.0

    cout << "Original grid:\n" << og << "\n";
    cout << "New grid:\n" << ng << "\n";

    // To store the grid positions:
    ArrayOfGridPos gp(ng.nelem());
    gridpos(gp,og,ng);
    cout << "Grid positions:\n" << gp;

    // To store interpolation weights:
    Matrix itw(gp.nelem(),2);
    interpweights(itw,gp);
    cout << "Interpolation weights:\n" << itw << "\n";

    // Original field:
    Vector of(og.nelem(),0);
    of[2] = 10; // 0, 0, 10, 0, 0
    cout << "Original field:\n" << of << "\n";

    // Interpolated field:
    Vector nf(ng.nelem());
    interp(nf, itw, of, gp);
}
```
5.9 Examples

cout << "New field:\n" << nf << "\n";
}

Ok, maybe you think this is not so simple, but a large part of the code is either setting up the example grids and fields, or output. And here is how the output looks like:

Very simple interpolation case
Original grid:
  1  2  3  4  5
New grid:
  2  2.25 2.5 2.75 3
Grid positions:
  1  0  1
  1  0.25 0.75
  1  0.5  0.5
  1  0.75 0.25
  1  1  0
Interpolation weights:
  1  0
  0.75 0.25
  0.5  0.5
  0.25 0.75
  0  1
Original field:
  0  0  10  0  0
New field:
  0  2.5  5  7.5  10

5.9.2 A more elaborate example

What if you want to interpolate only some dimensions of a tensor, while retaining others? — You have to make a loop yourself, but it is very easy. Below is an explicit example for a more complicated interpolation case. (Green type interpolation of all pages of a Tensor3.) This example is also contained in file test_interpolation.cc.

void test04()
{
  cout << "Green type interpolation of all "
    << "pages of a Tensor3\n";

  // The original Tensor is called a, the new one n.

  // 10 pages, 20 rows, 30 columns, all grids are: 1,2,3
  Vector a_pgrid(1,3,1), a_rgrid(1,3,1), a_cgrid(1,3,1);
  Tensor3 a( a_pgrid.nelem(),
    a_rgrid.nelem(),
    a_cgrid.nelem() );
  a = 0;
  // Put some simple numbers in the middle of each page:
  a(0,1,1) = 10;
  a(1,1,1) = 20;
  a(2,1,1) = 30;

  // New row and column grids:
// 1, 1.5, 2, 2.5, 3
Vector n_rgrid(1,5,.5), n_cgrid(1,5,.5);
Tensor3 n( a_pgrid.nelem(),
    n_rgrid.nelem(),
    n_cgrid.nelem() );

// So, n has the same number of pages as a,
// but more rows and columns.

// Get the grid position arrays:
ArrayOfGridPos n_rgp(n_rgrid.nelem()); // For rows.
ArrayOfGridPos n_cgp(n_cgrid.nelem()); // For columns.

gridpos( n_rgp, a_rgrid, n_rgrid );
gridpos( n_cgp, a_cgrid, n_cgrid );

// Get the interpolation weights:
Tensor3 itw( n_rgrid.nelem(), n_cgrid.nelem(), 4 );
interpweights( itw, n_rgp, n_cgp );

// Do a "green" interpolation for all pages of a:
for ( Index i=0; i<a.npages(); ++i )
{
    // Select the current page of both a and n:
    ConstMatrixView ap = a( i,
                     Range(joker), Range(joker) );
    MatrixView np = n( i,
                     Range(joker), Range(joker) );

    // Do the interpolation:
    interp( np, itw, ap, n_rgp, n_cgp );

    // Note that this is efficient, because interpolation
    // weights and grid positions are re-used.
}

cout << "Original field:\n";
for ( Index i=0; i<a.npages(); ++i )
    cout << "page " << i << "\n"
            << a(i,Range(joker),Range(joker)) << "\n";

cout << "Interpolated field:\n";
for ( Index i=0; i<n.npages(); ++i )
    cout << "page " << i << "\n"
            << n(i,Range(joker),Range(joker)) << "\n";
}

The output is:

Green type interpolation of all pages of a Tensor3
Original field:
page 0:
  0  0  0
  0 10  0
5.10 Higher order interpolation

Everything that was written so far in this chapter referred to linear interpolation, which uses two neighboring data points in the 1D case. But ARTS also has a framework for higher order polynomial interpolation. It is defined in the two files

- interpolation_lagrange.h
- interpolation_lagrange.cc

We define interpolation order $O$ as the order of the polynomial that is used. Linear interpolation, the ARTS standard case, corresponds to $O = 1$. $O = 2$ is quadratic interpolation, $O = 3$ cubic interpolation. The number of interpolation points (and weights) for a 1D interpolation is $O + 1$ for each point in the new grid. So, linear interpolation uses 2 points, quadratic 3, and cubic 4.

As a special case, interpolation order $O = 0$ is also implemented, which means ‘nearest neighbor interpolation’. In other words, the value at the closest neighboring point is chosen, so there is no real interpolation at all. This case is particularly useful if you have a field that may be interpolated in several dimensions, but you do not really want to do all dimensions all the time. With $O = 0$ interpolation and a grid that matches the original grid, interpolation can be effectively ‘turned off’ for that dimension.
Note, that if you use even interpolation orders, you will have an unequal number of interpolation points ‘to the left’ and ‘to the right’ of your new point. This is an argument for preferring $O = 3$ as the basic higher order polynomial interpolation, instead of $O = 2$.

Overall, higher order interpolation works rather similarly to the linear case. The main difference is that grid positions for higher order interpolation are stored in an object of type LagrangeInterpolation, instead of GridPos. A LagrangeInterpolation object contains the grids first index, interpolation weights for all interpolation points, and on demand the linear derivative of the interpolation at the grid position. For each point in the new grid, there is 1 index, $O + 1$ weights, and 0 or $O + 1$ weight derivatives.

In contrast to GridPos, LagrangeInterpolation stores weights $\ell x$ rather than fractional distances $fd$. For the linear case:

$$\ell x[0] = fd[1]$$
$$\ell x[1] = fd[0]$$

So the two concepts are almost the same. Because the $\ell x$ are associated with each interpolation point, they work also for higher interpolation order, whereas the concept of fractional distance does not.

The weights are calculated according to

$$l_j(x) = \prod_{0 \leq m \leq O} \left\{ \begin{array}{ll}
    \frac{f(x) - f(x_m)}{f(x_j) - f(x_m)} & \text{if } m \neq j \\
    1 & \text{if } m = j \end{array} \right. 0 \leq j \leq O, \quad (5.2)$$

where $f$ is a grid scaling function. This can be a logarithm, reverse cosine, circular constraints, or, most commonly, just the input. The provided options are part of the Interpolation::GridType enum class and are:

- **Standard** $f(t) = t$
- **Cyclic** $f(t) = t + n (t_1 - t_0)$, where $c_0 \leq t + n (c_1 - c_0) < c_1$, with $n$ as an integer and $[c_0, c_1]$ as the cyclic limits so that $g(c_0) \equiv g(c_0 + m [c_1 - c_0])$ holds true for a valid function $g(t)$ and any integer $m$
- **Log** $f(t) = \ln(t)$, where $t > 0$
- **Log10** $f(t) = \log_{10}(t)$, where $t > 0$
- **Log2** $f(t) = \log_2(t)$, where $t > 0$
- **SinDeg** $f(t) = \sin\left(\frac{\pi}{180}t\right)$, where $-90 \leq t \leq 90$
- **SinRad** $f(t) = \sin(t)$, where $-\pi/2 \leq t \leq \pi/2$
- **CosDeg** $f(t) = \cos\left(\frac{\pi}{180} [180 - t]\right)$, where $0 \leq t \leq 180$
- **CosRad** $f(t) = \cos(\pi - t)$, where $0 \leq t \leq \pi$

These are for the 1D case. For 2D and higher dimensional cases, the weights of the individual dimensions have to be multiplied, just as in the linear interpolation case. The derivatives are computed as

$$\frac{\partial l_j(x)}{\partial x} = \sum_{i=0}^{O} \left\{ \begin{array}{ll}
    \frac{l_j(x)}{x_j - x_i} & \text{if } x \neq x_i \\
    \frac{1}{x_j - x_i} \prod_{m=0}^{O} \left\{ \begin{array}{ll}
        \frac{x - x_m}{x_j - x_m} & \text{if } m \neq i, j \\
        1 & \text{if } m \in i, j \end{array} \right. \end{array} \right. \quad (5.3)$$
Note that the upper branch speedup is only available for Standard and for Cyclic code. Other cases must use the lower branch to get linear derivatives. These are again for the 1D case. For 2D and higher dimensional cases, the weights of the individual dimensions have to be multiplied with the weights of the derivative along the dimension of interest.

Instead of gridpos, you have to use the constructor LagrangeInterpolation for higher order interpolation with a single interpolation point, and Interpolation::LagrangeVector for multiple outputs. The single constructor needs an initial guess of the position. Other than that they need the new grid, the old grid, the interpolation order, the extrapolation factor allowed, whether the derivative should be computed, the type of f, and, if needed, the c0 and c1 pair of cyclic limits.

After setting up the LagrangeInterpolation object with either of the constructors, you have to call interpweights and interp, as in the linear case for single-point interpolation, or reinterp for multiple interpolations. (The actual functions used are not the same, since the name is overloaded. The interpweights and interp functions for use with LagrangeInterpolation are implemented in interpolation_lagrange.cc.) So, a complete interpolation chain involves:

\[
\text{LagrangeInterpolation or Interpolation::LagrangeVector}
\]
\[
\text{interpweights}
\]
\[
\text{interp or reinterp}
\]

Note that reinterp is used as the function name for the green interpolations of the linear interpolation routines. They demand all arrays of interpolation points and returns only the same type as was originally interpolated from. For example Tensor7 → Tensor7. There is no blue interpolation routine for the Lagrange interpolation routine.

The way to emulate blue interpolation using the Lagrange interpolation routines is by computing the LagrangeInterpolation for each grid one-by-one before using them in a standard for-loop to get the Blue vector output by calling interpweights, dinterpweights and then interp for each new grid point manually. The function Interpolation::LagrangeVector can conveniently be used for computing all necessary LagrangeInterpolation. This function speeds up the search routine significantly for new grids with relatively small differences between neighboring grid points (relative to the spacing of the original grid). Note that it might be faster to not use Interpolation::LagrangeVector but instead manually remembering the past grid position for the search of the next LagrangeInterpolation. We cannot judge this at this time.

For \( O = 1 \) the result of the interpolation chain will be the same as for the linear interpolation routines. Below are two simple complete examples, first for interp and then for reinterp+reduce_rank. Both examples taken from the file test_interpolation.cc in the arts source directory.

Example 1:

```c
void test09() {
    // Original and new grid
    Vector og(1, 5, +1); // 1, 2, 3, 4, 5
    Vector ng(2, 9, 0.25); // 2.0, 2.25, 2.5, 2.75, 3.0 ... 4.0

    // Original data
    Vector yi{5, -2, 50, 2, 1};
```
std::cout << og << ‘\n’ << yi << ‘\n’ << ‘\n’;

// Do the fit point-by-point:
for (auto x : ng) {
    // Simple linear interpolation:
    GridPos gp;
    gridpos(gp, og, x);

    // General Lagrange interpolation, special case interpolation order 1:
    const LagrangeInterpolation lag(0, x, og);

    std::cout << "gp point: " << gp << "lag point:\n" << lag;

    // Linear interpolation weights:
    Vector iwgp(2);
    interpweights(iwgp, gp);

    // General Lagrange interpolation weights:
    const Vector iwlag = interpweights(lag);

    std::cout << "gp iw: " << iwgp << "\nlag iw: " << iwlag << ‘\n’;

    std::cout << "gp res: " << interp(iwgp, yi, gp)
                "\nlag res: " << interp(yi, iwlag, lag) << ‘\n’
                ‘\n’;
}

// Linear interpolation of all points
ArrayOfGridPos gp(ng.nelem());
gridpos(gp, og, ng);
Matrix gp_iw(gp.nelem(), 2);
interpweights(gp_iw, gp);
Vector gp_y(ng.nelem());
interp(gp_y, gp_iw, yi, gp);
std::cout << "gp: " << gp_y << ‘\n’;

// General Lagrange interpolation, special case interpolation order 1:
const auto lag = Interpolation::LagrangeVector(ng, og, 1);
std::cout << "lag: " << reinterp(yi, interpweights(lag), lag) << ‘\n’;
}

Example 2:

void test28() {
    using Constant::pow2;
    using Constant::pow3;
    using Conversion::sind;
    using Conversion::cosd;

    // Old Grid of pressure, latitude, and longitude
    Vector pre; VectorNLogSpace(pre, 10, 1e5, 1e-1, Verbosity());
    Vector lat; VectorNLinSpace(lat, 5, -80, 80, Verbosity());
    Vector lon; VectorNLinSpace(lon, 4, -170, 170, Verbosity());

    // New Grids (pressure will be reduced)
Vector newpre(1, pre[pre.nelem()/2]);
Vector newlat; VectorNLinSpace(newlat, 4, -90, 90, Verbosity());
Vector newlon; VectorNLinSpace(newlon, 3, -180, 180, Verbosity());

// Old Data given some values
Tensor3 data(pre.nelem(), lat.nelem(), lon.nelem());
for (Index i=0; i<pre.nelem(); i++) {
  for (Index j=0; j<lat.nelem(); j++) {
    for (Index k=0; k<lon.nelem(); k++) {
      data(i, j, k) =
      std::log(pre[i]) * sind(lat[j]) * pow3(cosd(lon[k]));
    }
  }
}

// Create Lagrange interpolation values
const ArrayOfLagrangeInterpolation lag_pre =
  Interpolation::LagrangeVector(newpre, pre, 2, 1e9, false,
  Interpolation::GridType::Log);
const ArrayOfLagrangeInterpolation lag_lat =
  Interpolation::LagrangeVector(newlat, lat, 3, 1e9, false,
  Interpolation::GridType::SinDeg);
const ArrayOfLagrangeInterpolation lag_lon =
  Interpolation::LagrangeVector(newlon, lon, 1, 1e9, false,
  Interpolation::GridType::Cyclic, {-180, 180});

// Create the interpolation weights
const auto lag_iw = interpweights(lag_pre, lag_lat, lag_lon);

// Create and reduce the new data
const Matrix newdata = reinterp(data,
  lag_iw, lag_pre, lag_lat, lag_lon).reduce_rank<1, 2>();

// Print the data
std::cout << data(pre.nelem()/2, joker, joker)
  << ‘\n’ << ‘\n’ << newdata << ‘\n’;

Note that we also provide fixed interpolation higher order calculations where the
weights are stored in types of FixedLagrangeInterpolation<O>. These offers
significant speed-ups compared to the runtime code. Internally, they do the same calcula-
tions as the normal LagrangeInterpolation, but since the fixed cases are known at
compile time, there is no allocations when using the fixed calculations. Below is a sim-
ple complete example, taken from the file test_interpolation.cc in the arts source
directory for the fixed calculations:

void test13() {
  constexpr int N = 10;
  constexpr std::array<Numeric, N> y{1, 2, 3, 4, 5, 6, 7, 8, 9, 10};
  constexpr std::array<Numeric, N> y2{1, 2 * 2, 3 * 3, 4 * 4, 5 * 5,
                                  6 * 6, 7 * 7, 8 * 8, 9 * 9, 10 * 10};
  constexpr std::array<Numeric, N> y3{
    1, 2 * 2 * 2, 3 * 3 * 3, 4 * 4 * 4, 5 * 5 * 5,
    6 * 6 * 6, 7 * 7 * 7, 8 * 8 * 8, 9 * 9 * 9, 10 * 10 * 10};
constexpr Numeric x = 2;
constexpr Numeric dx = 1e-2;

// Set up the interpolation Lagranges
constexpr FixedLagrangeInterpolation<1> lin(0, x, std::array<Numeric, 2>{1, 2}, true);
constexpr FixedLagrangeInterpolation<2> sqr(0, x, std::array<Numeric, 3>{1, 2, 3}, true);
constexpr FixedLagrangeInterpolation<3> cub(0, x, std::array<Numeric, 4>{1, 2, 3, 4}, true);
constexpr FixedLagrangeInterpolation<1> dlin(0, x + dx, std::array<Numeric, 2>{1, 2}, true);
constexpr FixedLagrangeInterpolation<2> dsqr(0, x + dx, std::array<Numeric, 3>{1, 2, 3}, true);
constexpr FixedLagrangeInterpolation<3> dcub(0, x + dx, std::array<Numeric, 4>{1, 2, 3, 4}, true);

// Set up the interpolation weights
constexpr auto lin_iw = interpweights(lin);
constexpr auto sqr_iw = interpweights(sqr);
constexpr auto cub_iw = interpweights(cub);
constexpr auto dlin_iw = dinterpweights(lin);
constexpr auto dsqr_iw = dinterpweights(sqr);
constexpr auto dcub_iw = dinterpweights(cub);
constexpr auto alt_lin_iw = interpweights(dlin);
constexpr auto alt_sqr_iw = interpweights(dsqr);
constexpr auto alt_cub_iw = interpweights(dcub);

// Get interpolation value
constexpr auto lin_lin = interp(y, lin_iw, lin);
constexpr auto sqr_sqr = interp(y2, sqr_iw, sqr);
constexpr auto cub_cub = interp(y3, cub_iw, cub);
constexpr auto dlin_lin = interp(y, dlin_iw, dlin);
constexpr auto dsqr_sqr = interp(y2, dsqr_iw, dsqr);
constexpr auto dcub_cub = interp(y3, dcub_iw, dcub);
constexpr auto alt_lin_lin = interp(y, alt_lin_iw, dlin);
constexpr auto alt_sqr_sqr = interp(y2, alt_sqr_iw, dsqr);
constexpr auto alt_cub_cub = interp(y3, alt_cub_iw, dcub);

// Compile-time check that these values are good
static_assert(is_around(lin_lin, x));
static_assert(is_around(sqr_sqr, x * x));
static_assert(is_around(cub_cub, x * x * x));
static_assert(is_around(dlin_lin, 1));
static_assert(is_around(dsqr_sqr, 2 * x));
static_assert(is_around(dcub_cub, 3 * x * x));

std::cout << lin_lin << ' ' << sqr_sqr << ' ' << cub_cub << '
' << dlin_lin << ' ' << dsqr_sqr << ' ' << dcub_cub << '
' << alt_lin_lin << ' ' << alt_sqr_sqr << ' ' << alt_cub_cub << '
' << (alt_lin_lin - lin_lin) / dx << ' ' << (alt_sqr_sqr - sqr_sqr) / dx;
5.11 Summary

Now you probably understand better what was written at the very beginning of this chapter, namely that doing an interpolation always requires the chain of function calls:

1. `gridpos` or `LagrangeInterpolation` or `Interpolation::LagrangeVector` or `FixedLagrangeInterpolation<O>` or `Interpolation::FixedLagrangeVector<O>` (one for each interpolation dimension)

2. `interpweights`

3. `interp` or `reinterp`

If you are interested in how the functions really work, look in file `interpolation.cc` or `interpolation_lagrange.cc/h`. The documentation there is quite detailed. When you are using interpolation, you should always give some thought to whether you can re-use grid positions or even interpolation weights. This can really save you a lot of computation time. For example, if you want to interpolate several fields — which are all on the same grids — to some position, you only have to compute the weights once. However, also be aware that sometimes reallocating might be preferred to passing views.
Chapter 6
Integration functions

A radiative transfer model which takes into account the effect of scattering involves integration of certain quantities over the angles of observation. For example, from Section ?? it is clear that computing scattering cross-section and scattering integral term requires integration over zenith and azimuth directions. There are a wide range of methods that can be used for numerical integration. They can be used depending on various factors starting from how accurate the result should be to the behaviour of the function. The one which is implemented in ARTS is the trapezoidal integration method.

6.1 Implementation files

The integration functions can be found in the files:
- math_funcs.h
- math_funcs.cc

The implementation function AngIntegrate_trapezoid is discussed in the second file.

6.2 Trapezoidal Integration

Trapezoidal Integration method comes under the Newton-Cotes formulas where integration of a function is approximated by the area under the curve described by the function. Trapezoidal integration assumes that the area under the curve is trapezoid.

Trapezoidal rule:

$$\int_{x_1}^{x_2} f(x)dx = \frac{1}{2}h(f_1 + f_2) + O(h^3 f'')$$

(6.1)

This is a two-point formula ($x_1$ and $x_2$). It is exact for polynomials upto and including degree 1, i.e., $f(x) = x$. $O(h^3 f'')$ signifies how far is the true answer from the estimate.

History
220802 Created and written by Sreerekha T.R.
220103 Included mathematical description for implemented integration method(CE).
If we use eq. 6.1 $N - 1$ times, to do the integration in the intervals $(x_1, x_2), (x_2, x_3), \ldots, (x_{N-1}, x_N)$, and then add the results, we obtain extended formula for the integral from $x_1$ to $x_N$.

Extended Trapezoidal rule:

$$\int_{x_1}^{x_N} f(x)dx = \frac{1}{2} h [f_1 + 2(f_2 + f_3 + \ldots + f_{N-1}) + f_N] + O\left(\frac{(b-a)^3 f''}{N^2}\right) \quad (6.2)$$

The last term tells how much the error will be decreased by taking more number of steps.

### 6.3 Solid Angle Integration

In our scattering problem, we are often encountered with a double integration of functions over zenith and azimuth angles (see Chapter ??). One way to achieve double integration is to use repeated one-dimensional trapezoidal integration. This is effective of course only if the boundary is simple and the function is very smooth. If the function is strongly peaked and if know where it occurs, integral should be broken into smaller regions so that the integrand is smooth in each. Another thing is to take into account the symmetry of the function as well as the boundary. For example in our case, if the radiation is symmetric about the azimuth, the integration in that direction returns constant value of $2\pi$ and we need to do only integration over zenith directions.

The general form of a solid angle integration is

$$S = \int_{4\pi} f(\omega)d\omega \quad (6.3)$$

In spherical coordinates we can write:

$$S = \int_0^{\pi} \int_0^{2\pi} f(\theta, \phi) \sin \theta \ d\theta d\phi \quad (6.4)$$

A double integration can be split into two single integrations:

$$S = \int_0^{\pi} \left( \int_0^{2\pi} f(\theta, \phi) \sin \theta d\phi \right) d\theta \quad (6.5)$$

$$= \int_0^{\pi} g(\theta) d\theta \quad (6.6)$$

If we have to integrate a vector, we can apply this method componentwise.

To solve the integral numerically we discretize $\theta$ and $\phi$ and obtain two angular grids $(\theta_0, \theta_1, \ldots, \theta_n)$ and $(\phi_0, \phi_1, \ldots, \phi_m)$. Then we can first calculate $g(\theta_j)$ for all $\theta_j$ using the trapezoidal method.

$$g(\theta_j) = \sum_{i=1}^{m} \sin \theta_j \frac{f(\theta_j, \phi_i) + f(\theta_j, \phi_{i+1})}{2} \cdot (\phi_{i+1} - \phi_i) \quad (6.7)$$

The final step is to sum up all $g(\theta_j)$, again applying the trapezoidal method.

$$S = \sum_{j=1}^{n} \frac{g(\theta_j) + g(\theta_{j+1})}{2} \cdot (\theta_{j+1} - \theta_j) \quad (6.8)$$
If the radiation is symmetric about the azimuth we just calculate:

$$S_{\text{sym}} = 2\pi \int_0^\pi f(\theta) \sin(\theta) d\theta$$  \hspace{1cm} (6.9)

Using the trapezoidal method this can be written as:

$$S_{\text{sym}} = 2\pi \sum_{j=1}^n \frac{h(\theta_j) + h(\theta_{j+1})}{2} \cdot (\theta_{j+1} - \theta_j)$$  \hspace{1cm} (6.10)

where $h(\theta) = \sin \theta \cdot f(\theta)$.

The function `AngIntegrate_trapezoid` takes as input the integrand and the angles over which the integration has to be done. For example in this case it can be the zenith and azimuth angle grid.

```
Numeric AngIntegrate_trapezoid(MatrixView Integrand,
                               ConstVectorView za_grid,
                               ConstVectorView aa_grid)
```

The integrand has the same number of rows as zenith angle grid and columns as azimuth angle grid. The inner loop does trapezoidal integration of the integrand over all azimuth angles and the result is stored in a Vector `res1[i]`. Note that the integrand at every point has to be multiplied with $\sin (\text{za} \_\text{grid}[i] \ast \text{DEG2RAD})$ since we are integrating over solid angles. The outer loop does an integration of `res1[i]` over all zenith angles. The result of this is returned back to the calling function.
Chapter 7

Linear algebra functions

Solving the vector radiative transfer equation requires the computation of linear equation systems and the matrix exponential. This section describes the functions which are implemented in ARTS and it gives instructions how these functions can be used, also for other purposes than the radiative transfer calculations.

7.1 Implementation files

All the functions described below can be found in the files:

- lin_alg.h
- lin_alg.cc

The template class Array and the classes Matrix and Vector are used, therefore the linear algebra functions require the files:

- matpackI.h
- make_vector.h
- array.h
- matpackI.cc
- make_vector.cc
- array.cc

Furthermore logical functions contained in

- logic.h
- logic.cc

are used to check the dimensions of input matrices for various functions.

History

020502 Created and written by Claudia Emde.
7.2 Linear Equation Systems

For solving a set of linear equations

\[ Ax = b \]  \quad (7.1)

the LU decomposition method is implemented. A slightly modified version of the algorithm described in [Press et al. [1997]] is used here. An alternative method is the Gauss-Jordan elimination, but this method is three times slower than the LU decomposition method [Press et al. [1997], p.36]. The LU decomposition method requires two functions, `ludcmp` and `lubacksub`, which will be described below.

The following example for a three dimensional equation system demonstrates how to solve a linear equation system of the type (7.1):

- Create matrix A, vector b:
  
  ```
  A = Matrix(3,3);
  A(1,1) = 4;
  A(2,1) = 3;
  ...
  b = Vector(3);
  b(1) = 7;
  ...
  ```

- Initialize solution vector x and two other variables needed for storing intermediate results:
  ```
  x = Vector(3);
  LU = Matrix(3,3);
  indx = ArrayOfIndex(3);
  ```

- Call LU decomposition function (see Section 7.2.1):
  ```
  ludcmp(LU, indx, A);
  ```

- Call LU backsubstitution function (see Section 7.2.2):
  ```
  lubacksub(x, LU, b, indx);
  ```

- Print the solution vector:
  ```
  cout << x;
  ```

7.2.1 LU Decomposition

A LU decomposition is a procedure for decomposing a square matrix A with dimension n into a product of a lower triangular matrix L (has elements only on the diagonal elements and below) and an upper triangular matrix U (has elements only on the diagonal and above):

\[ L \cdot U = A \]  \quad (7.2)

For a 3 x 3 matrix equation 7.2 would look like this:

\[
\begin{pmatrix}
  l_{11} & 0 & 0 \\
  l_{21} & l_{22} & 0 \\
  l_{31} & l_{32} & l_{33}
\end{pmatrix}
\cdot
\begin{pmatrix}
  u_{11} & u_{12} & u_{13} \\
  0 & u_{22} & u_{23} \\
  0 & 0 & u_{33}
\end{pmatrix}
= 
\begin{pmatrix}
  a_{11} & a_{12} & a_{13} \\
  a_{21} & a_{22} & a_{23} \\
  a_{31} & a_{32} & a_{33}
\end{pmatrix}
\]
The decomposition can be used to rewrite the linear set of equations (7.1) in the following way:

\[ A \cdot x = (L \cdot U) \cdot x = L \cdot (U \cdot x) = b \]  

(7.3)

First

\[ L \cdot y = b \]  

(7.4)
is solved for the vector \( y \) which can be done by forward substitution (see section 7.2.2). Then

\[ U \cdot x = y \]  

(7.5)
is solved again by backsubstitution. The advantage in breaking up one linear set into two successive ones is that the solution of a triangular set of equations is quite trivial.

The function \texttt{ludcmp} requires a square matrix of arbitrary dimension \( n \) as input and performs the LU decomposition. It returns one matrix which contains both matrices, \( L \) and \( U \). For the lower triangular matrix \( L \) the diagonal elements are chosen to be 1, then the other elements of \( L \) and \( U \) are determined. This is possible, as the LU decomposition is an under determined equation system with \( n^2 \) equations for \( n^2 + n \) unknowns. The output matrix does not include the diagonal of \( L \), in the three-dimensional case it has the following elements:

\[
\begin{pmatrix}
  u_{11} & u_{12} & u_{13} \\
  l_{21} & u_{22} & u_{23} \\
  l_{31} & l_{32} & u_{33}
\end{pmatrix}
\]

This special arrangement of the LU decomposition is named \textit{Crout’s algorithm} and a matrix arranged in this form is named \textit{Crout matrix} in this context.

Another output variable of the function \texttt{ludcmp} is an index vector which contains information about pivoting which is absolutely essential for the stability of Crout’s algorithm. Here partial pivoting, i.e. interchange of rows is implemented. That means that not \( A \) is decomposed into \( LU \)-form but a rowwise permutation of \( A \). If the index vector contains for example the elements \((2, 1, 0)\) the first and the last row of a three dimensional matrix would be exchanged.

### 7.2.2 Forward- and Backsubstitution

An equation system of the form

\[
\begin{pmatrix}
  a_{11} & a_{12} & a_{13} \\
  0 & a_{22} & a_{23} \\
  0 & 0 & a_{33}
\end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}
\]

can be solved very easy. The last element, here \( x_3 \), is already isolated, namely

\[ x_3 = b_3/a_{33} \]  

(7.6)

As \( x_3 \) is known \( x_2 \) can be calculated using the second row of the equations. Then, finally, \( x_1 \) can be calculated as well using the first row. This procedure is called backsubstitution. The same method applied for an equation system including a lower triangular matrix is named forward substitution.

The function \texttt{lubacksub} does forward and backward substitution to solve the equation system described in 7.2.1. As input it requires the output variables of \texttt{ludcmp} which are the \textit{Crout matrix} and the index vector. Output of the function is the solution vector \( x \) to the equation system.
7.2.3 More Applications of the LU Decomposition

- Inverse of a matrix:
  To compute \((K)^{-1} \cdot b\), which is a part of the solution to the vector radiative transfer equation (Equation ?? in ARTS User Guide) the LU decomposition method can be used. The following equations show, that the problem is equivalent to solving a linear equation system of the type 7.1.

\[
K^{-1} \cdot b = x \quad (7.7)
\]
\[
\iff \quad K \cdot x = b \quad (7.8)
\]

- To solve the equation system
\[
A \cdot X = B \quad (7.9)
\]
where \(A\), \(B\) and \(X\) are matrices of dimension \(n\), the LU decomposition functions can be applied as well. Assume that \(A\) and \(B\) are known and you want to solve for \(X\). First you should do a LU decomposition of \(A\) and then backsubstitute with the columns of \(B\) and you get the columns of \(X\) as solution vectors.

7.3 Matrix Exponential Function

A very important function for solving differential equations is the matrix exponential:

\[
e^{A_s} = \sum_{k=0}^{\infty} \frac{(A_s)^k}{k!} \quad (7.10)
\]

In principle it could be computed using the Taylor power series but this method is not efficient. Moler and Van Loan have shown for the simple example [Moler and Loan [1979]]

\[
A = \begin{pmatrix}
-49 & 24 \\
-64 & 31
\end{pmatrix}
\]

that convergence is obtained not until 59 terms. And if a relative accuracy of only \(10^{-5}\) is taken, the method even leads to a wrong result due to rounding errors.

7.3.1 Padé Approximation

One of the better algorithms for computing the matrix exponential is the Padé approximation which is also shortly described in [Moler and Loan [1979]] and outlined in the book “Matrix Computations” by Golub and Loan [1991]. The method uses perturbation theory as well as the so called Padé functions. It is possible to derive an algorithm which calculates

\[
F = e^{A+E} \quad (7.11)
\]

where

\[
\|E\|_\infty \leq \delta \|A\| \quad (7.12)
\]
The accuracy of the computation given by \( \delta \) can be chosen. The parameter \( q \) has to be the smallest non-negative integer such that \( \epsilon(q, q) \leq \delta \) where

\[
\epsilon(p, q) = 2^{3-(p+q)} \frac{p!q!}{(p+q)!(p+q+1)!}.
\] (7.13)

The following table shows values of epsilon for different values of \( q \).

<table>
<thead>
<tr>
<th>( q )</th>
<th>( \epsilon(q,q) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1667</td>
</tr>
<tr>
<td>2</td>
<td>6.9444 \cdot 10^{-4}</td>
</tr>
<tr>
<td>3</td>
<td>1.2401 \cdot 10^{-6}</td>
</tr>
<tr>
<td>4</td>
<td>1.2302 \cdot 10^{-9}</td>
</tr>
<tr>
<td>5</td>
<td>7.7667 \cdot 10^{-13}</td>
</tr>
<tr>
<td>6</td>
<td>3.3945 \cdot 10^{-16}</td>
</tr>
</tbody>
</table>

The algorithm is implemented in the function \texttt{matrix\_exp}. Input to this function is the matrix \( A \) and the parameter \( q \). As output it gives the matrix \( F \) which is defined above. The following example shows how to use the \texttt{matrix\_exp} function:

- Initialize \( A \) and assign values:
  
  ```
  Matrix A(3,3);
  A(1,1) = 45;
  A(1,2) = 3;
  ...
  ```

- Initialize \( F \):

  ```
  Matrix F(3,3);
  ```

- Give a parameter for the accuracy:

  ```
  Index q=6;
  ```

- Call the matrix exponential function:

  ```
  matrix\_exp(F,A,q);
  ```

- Print the result:

  ```
  cout << "exp(A) = " << F;
  ```
Chapter 8

Include ARTS in third-party C++

It is possible to include ARTS in another C++ program using the `public_arts_interface` and linking to `autoarts.h`. This will pull in the ARTS public API defined in `agendas.cc`, `groups.cc`, `methods.cc`, `workspace.cc` as well as an automatically generated ARTS namespace to your project.

FIXME: a private Module that imports only the ARTS namespace should be added as soon as soon as C++20 becomes norm.

8.1 Linking the public interface

To link the public interface, you need to `add_subdirectory(arts)` anywhere in your CMake project, where the `arts` directory should contain a current version of ARTS.

An example (in your projects `CMakeLists.txt`):

```
# ARTS Custom Executable
add_executable(arts_interface interface.cpp)
target_link_libraries(arts_interface PUBLIC
    public_arts_interface)
```

At this point, your `interface.cpp` must have `#include <autoarts.h>` as one of its headers and you are good to go.

8.2 Using the C++ namespace interface

The ARTS namespace contains all the interfaces you will need to perform all operations supported by ARTS. The namespace defines only a single top level function call, the `init(...)` function and a single top-level type, the ARTS Workspace. The function is used to generate the ARTS Workspace upon which all your function calls are made. The ARTS namespace has several sub-namespaces for various purposes. These are in short:

- **Group** Defines the ARTS public type-system.

---

**History**

2020-10-06 Created and written by Richard Larsson.
Internal  Defines the ARTS internal type-system.

Var  Defines the ARTS interface type-system, create variables for the ARTS interface, and access automatic variables that are defined in the ARTS Workspace from the start.

Method  Defines the ARTS methods. The ARTS methods can only be called using their generic inputs and outputs.

AgendaMethod  Defines the ARTS methods that can be used by agendas. They return an internal type and are best used directly, with no manual modification.

AgendaDefine  Defines methods to set the different ARTS agendas. The agendas are checked and ready to be used after these methods are called.

AgendaExecute  Executes an agenda.

If you are using the public interface, you need not be concerned with the types in the sub-namespaces Group and Internal. FIXME: Otherwise, these define the basic types you need to use ARTS easily. These sub-namespaces are used the same as any other C++ type-system. The other namespaces are domain specific.

An interface will generally start with a call to the initialize function. This could look like:

```cpp
auto ws = init();
```

After this the order and set of commands that are placed is up to the user. For sake of ease, `ws` will be used below to indicate a defined Workspace. Also, the access to each sub-namespace will be written as if operating in the ARTS namespace itself.

### 8.2.1 Var

The Var namespace, short for Variable namespace, have three purposes

1. Type the Method and Agenda interface
2. Access common Workspace variables
3. Create new variables on the Workspace

The types that are defined correspond to the types in Group. The purpose of these types is to pass input to the functions of Method and AgendaMethod. The main way to generate instances of these variables is by their corresponding `Create` function or by simply accessing them via their common Workspace names. The only constructor that is recommended to use is the construction from the corresponding Group, as this can simplify the access to several methods. The other two constructors risk accessing out-of-bound memory, or to deference a null-pointer.

It is highly recommended to not discard created variables, as they will still occupy memory in the Workspace until the end of the program and they become impossible to access once discarded.

Examples:
// Define an index that is not in the workspace
Var::Index x(Var::Group::Index(1));

// Access an index that is in the workspace
Var::Index y = Var::stokes_dim(ws);

// Create a new index on the workspace
Var::Index z{Var::IndexCreate(ws, Var::Group::Index{1},
    "new_index_name")};

Note that x will not work as an input to AgendaMethod functions but it will work as an input to Method functions. It does not append to the Workspace. The other two will work both as inputs to AgendaMethod and to Method functions.

8.2.2 Method

The Method namespace contains all but the Agenda manipulating methods defined in methods.cc. These can all be called using the generic input and outputs. The inputs and outputs are not guaranteed to be the same as in the ARTS methods however, because C++ requires inputs with default values be placed last in the calling order. Note that all standard inputs and outputs taken from the Workspace must be set on the Workspace itself and cannot be passed as inputs. This creates a few idiosyncrasies compared to how ARTS is used in python or in a normal controlfile.

Examples:

// Call yCalc (no GIN/GOUT)
Method::yCalc(ws);

// Call Touch on the wind field (Pure GOUT)
Method::Touch(ws, Var::wind_u_field(ws));
Method::Touch(ws, Var::wind_v_field(ws));
Method::Touch(ws, Var::wind_w_field(ws));

// Set p_grid by VectorNLogSpace
Var::nelem(ws) = 51;
Method::VectorNLogSpace(ws, Var::p_grid(ws), 1e+05, 1e-4);

// Save x, y, z from the Var example
Var::output_file_format(ws) = Group::String("ascii");
Method::WriteXML(ws, x);
Method::WriteXML(ws, y, Group::String("extra.xml"));
Method::WriteXML(ws, z);

All methods requires a Workspace (ws) to work. The first case of the examples calls a function with neither generic input nor generic output — it cannot take anything other than the Workspace. The second triplet case of the examples calls Touch on all wind-field variables. They will have been default-initialized after this process. The third example shows the idiosyncrasies to other methods of using ARTS. The Workspace variable nelem has been used instead of a generic input index to define VectorNLogSpace — thus nelem
must be set manually by the user of the interface. The last examples uses the fact that many of WriteXML’s inputs are default defined. Since the default value of filename is empty and since the interface then infers it has the variable name input, the first call to WriteXML will generate a file called arts.in.xml, the second call will generate a file called extra.xml, and the last call will generate a file called arts.new_index_name.xml. The first part of the name can be changed by calling init() with the corresponding arguments.

As a last note. Several inputs above automatically generates inputs from standard C++ types, such as VectorNLogSpace generating two Var::Numeric from two doubles. This is a convenient way to use the methods but the user should be aware that these methods will end up deleting variables in the end, so some care has to be taken when the scope of such automatic variables is long.

8.2.3 AgendaMethod, AgendaDefine, and AgendaExecute

The Agenda namespaces deal with setting and defining Workspace Agendas. It is only possible to set Workspace Agendas that have been defined as part of the Workspace at compilation time. The AgendaMethod namespace contains the same functions as the Method namespace but returns an Internal::MRecord. The user of this interface is expected to never manually construct an MRecord. Instead, this type is meant to only be used when Agendas are defined in the AgendaDefine namespace. The AgendaDefine namespace defines a variadic function per Agenda in the common Workspace and expects a list of MRecord to set this Agenda’s methods. Finally, AgendaExecute exists to execute a single Agenda. Normally, this is not preferred since Agendas should generally just be used inside methods, but the option still exists.

Examples:

```cpp
// Define the basic iy_main_agenda emission agenda
AgendaDefine::iy_main_agenda(ws,
   AgendaMethod::ppathCalc(ws),
   AgendaMethod::iyEmissionStandard(ws));

// Define an empty geo positioning agenda
AgendaDefine::geo_pos_agenda(ws,
   AgendaMethod::Ignore(ws, Var::ppath(ws)),
   AgendaMethod::VectorSet(ws, Var::geo_pos(ws),
                          Var::VectorCreate(ws, {}, "Default")));```

The first example simply sets its agenda by using two functions that complete the inputs/outputs expected of the agenda. The second example does not need or want to use Var::ppath(ws) so it ignores it. It also has the need of a default empty Var::Vector. This variable has to first be created onto the Workspace before it can be used as an input. Had a pure vector been used instead of the create-function, a runtime error would occur. The create function is only invoked once, since the internal workings of the Agenda just need to have defined the variable.

Lastly, each AgendaMethod function that has a default generic input will create a static const Workspace variable of this type upon first call to the method. This means that calling such a method will incur a memory cost that lasts until the end of the program.
Chapter 9

GUI — simple plotting

ARTS provides a simple debug plotting tool for developers to see their results in-place. To build and use the plotting tool you need to activate `-DENABLE_GUI=1` in your cmake settings. The plotting debug tool is now available by using `#include <gui/plot.h>` in your desired file. The plotting routines that are available are quite simple. You get these interfaces:

```cpp
plot(const Vector& y) // Plots y evenly spaced
plot(const Vector& x, const Vector& y)
plot(...) // Plots any number of pairs of X-Y
```

These are all available via the `ARTSGUI` namespace. Figure 9.1 shows a fullscreen example produced by the templated version of `plot` on Ubuntu.

The features of the plotting tool is limited but intuitive enough to access and view the data.

There are three components to the plotting tool. The plot frame is where your data is displayed. The plot axis shows the scales of the data. The menu bar offers some options to manipulate the window. Each of these have limited operations listed below.

- **Menu bar**
  - File — access meta information about the window and data
    * Fullscreen (shortcut F11) takes the plotting window fullscreen. The exit fullscreen mode, use escape, F11, quit the application or press the fullscreen menu item again.
    * Export Data (shortcut Ctrl+S) saves the Y-axis data to an XML-file. In the templated code, the new file will be an `ArrayOfVector`, in the non-templated code it will be a simple `Vector`.
    * Quit (shortcut Ctrl+X) quits the application.

- **Plot axis**
  - Double left-click: Resets the clicked axis to the maximum possible value. Note that for values very small or very large, this might fail and you need to manually fix the axis.

---

**History**

201203 First version Richard Larsson
Figure 9.1: Example plot. Here we show the absorption versus frequency for some O\textsubscript{2} absorption models.

- Double right-click: Opens the axis dropdown-menu with the following options:
  - Min: Select the minimum value by writing the number in the text box, or lock the axis by ticking the checkbox.
  - Max: Select the maximum value by writing the number in the text box, or lock the axis by ticking the checkbox.
  - Invert: Check the box to switch the order of high-and-low along the respective axis.
  - Log Scale: Check the box to show the axis in logarithmic scale.
  - Time (X-axis only): Check the box to interpret the X axis as Unix time and display the relevant as dates.
  - Grid Lines: Uncheck the box to remove grid lines in the plot frame for the axis.
  - Tick Marks: Uncheck the box to remove tick marks in the plot frame for the axis.
  - Labels: Uncheck the box to remove the labels from the axis.
- Left-click and drag: Moves the axis in the direction dragged.
- Vertical scroll: Extends or contracts the axis range around the value where the scroll began.

- Plot frame
  - Double left-click: Scales both X-and-Y to a best-fit scenario (still with the caveat that very small and very large numbers might not work properly)
  - Double right-click: Opens a dropdown-menu with access to the plot axis dropdown-menus and some settings
  - Scroll: Extend or contract both axis around the point where the scroll began
– Left-click and drag: Moves the axis around
– Right-click and drag: Selects a region and zooms in when the right-click is let go. If Shift is held, the zoom window is modified to include the entire Y-axis. If Alt held, the zoom window is modified to include the entire X-axis.
– Legends: In the upper left corner of the plot frame are the legends of the plot. If hovered, the hovered line will be enlarged inside the plot frame. If the colored check box is pressed, the line will be removed from the plot frame.

The debug GUI is based on the Dear ImGui GUI framework, with ImPlot drawing the plots and uses imgui-filebrowser to deal with the filesystem.
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Part II

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