qtcm User's Guide

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Chapter 1

Introduction

1.1 How to Read This Manual

Most users: Just read (1) the installation instructions in Chapter 2, (2) Chapter 3, which tells you all you need to get started using qtcm, and (3) examples in Section 4.10 that give a feel for how you can use the model.

Users having problems: Chapter 5 provides troubleshooting tips for a few problems. The detailed description of how the package functions, in Chapter 4, will probably be more useful.

Developers: If you want to change the source code, please read Chapter 6. Chapter 7 describes all the things I'd like to do to improve the package, but haven't gotten to yet.

1.2 About the Package

The single-baroclinic mode Neelin-Zeng Quasi-Equilibrium Tropical Circulation Model $(QTCM1)^1$ is a primitive equation-based intermediate-level atmospheric model that focuses on simulating the tropical atmosphere. Being more complicated than a simple model, the model has full non-linearity with a basic representation of baroclinic instability, includes a radiative-convective feedback package, and includes a simple land soil moisture routine (but does not include topography). A brief, but more detailed, description of QTCM1 is given in Section 1.6.

Python² is an interpreted, object-oriented, multi-platform, open-source language that is used in a variety of software applications, ranging from game development to bioinformatics. In climate studies, Python has been used as the core language for data analysis (e.g., Climate Data Analysis Tools³), visualization (e.g., Matplotlib⁴),

 $^{^{1}\}rm http://www.atmos.ucla.edu/{\sim}csi$

²http://www.python.org

³http://cdat.sf.net

⁴http://matplotlib.sf.net

and modeling (e.g., $PyCCSM^5$).

In comparison to traditional compiled languages like Fortran, Python's lack of a separate compile step greatly simplifies the debugging and testing phases of development, because code snippets can be testing as code is written. Python's extensive suite of higher-level tools (e.g., statistics, visualization, string and file manipulation) accessible at runtime enables modeling and analysis to occur concurrently.

The qtcm package is an implementation of the Neelin-Zeng QTCM1 in a Python object-oriented environment. The conversion package $f2py^6$ is used to wrap the QTCM1 Fortran model routines and manage model execution using Python datatypes and utilities. The result is a modeling package where order and choice of subroutine execution can be altered at runtime. Model analysis and visualization can also be integrated with model execution at runtime.

1.3 Conventions In This Manual

1.3.1 Audience

In this manual I assume you have a rudimentary knowledge of Python. Thus, I do not describe basic Python data types (e.g., dictionaries, lists), object framework and syntax (e.g., classes, methods, attributes, instantiation), module and package importing. If you need to brush up (or learn) Python, I'd recommend the following resources:

- Python Tutorial:⁷ This tutorial was written by Guido van Rossum, Python's original author.
- Instant Hacking:⁸ Learn how to program with Python.
- Dive Into Python:⁹ Reasonably complete and cohesive. The entire book is available for free online.
- Handbook of the Physics Computing Course:¹⁰ Written for a science audience. Recommended.
- CDAT/Python Tips for Earth Scientists:¹¹ This web site is a FAQ of sorts for people using Python and the Climate Data Analysis Tools (CDAT) in the earth sciences, and thus focuses on using Python to do science rather than the computer science aspects of the language.

⁵http://code.google.com/p/pyccsm/

⁶http://cens.ioc.ee/projects/f2py2e/

⁷http://docs.python.org/tut/

⁸http://www.hetland.org/python/instant-hacking.php

⁹http://diveintopython.org/index.html

¹⁰http://www.pentangle.net/python/handbook/

¹¹http://www.johnny-lin.com/cdat_tips/

1.3. CONVENTIONS IN THIS MANUAL

The purpose of this package is to make the QTCM1 model easier to use. In order to interpret the results, however, you still need to have a robust sense of what climate models can and cannot tell you. A starting point for the QTCM1 model is the brief description of the model in Section 1.6. After that, I would read the original papers describing the model formulation and results [3, 5], and papers citing the model formulation work.¹² Being an intermediate-level model using the quasi-equilibrium assumption, QTCM1 (and thus qtcm) has distinct strengths and limitations; please be aware of them.

commands	to be typed at the command-line are rendered in a blue, serif, fixed-width typewriter font (e.g., make _qtcm_full_365).		
dummy arguments	coupled with code or screen display is rendered		
	in a serif, proportional, italicized font (e.g.,		
	Error-Value too long in $variable).$		
file and directory names	are rendered in a sans-serif, italicized font (e.g.,		
	setbypy.F90).		
screen display	is rendered in a green, serif, fixed-width type-		
	writer font.		
module, method, and	are rendered in a blue, serif, fixed-width type-		
subroutine names	writer font.		
variable and	are rendered in a blue, serif, fixed-width type-		
attribute names	writer font.		
class names	are rendered in a blue, serif, fixed-width type-		
	writer font.		

1.3.2 Typographic Conventions

Blocks of code (usually commands, screen display, and module, variable, and class names) are displayed in a blue, serif, fixed-width typewriter font.

1.3.3 Terminology

- attribute and method references: If there is any possibility of confusion, I will give the class that an attribute or method comes from when that attribute or method is referenced. If no class is mentioned by name or context, assume that the attribute/method comes from the Qtcm class.
- "compiled QTCM1 model": This usually is used to denote when I'm talking about compiled Fortran QTCM1 routines and variables therein, as an extension module to the Python qtcm package.. Thus, "compiled QTCM1 model u1" is

the value of variable **u1** in the Fortran model, not the value at the Pythonlevel. Sometimes I refer to the compiled QTCM1 model as just "QTCM1" or as "compiled QTCM1 Fortran model".

- "pure-Fortran QTCM1": This refers to the Neelin-Zeng QTCM1 model in it's original Fortran form, not as an extension module to the Python qtcm package.
- "Python-level": This usually denotes the value of a variable as an attribute of a Qtcm instance. This variable is stored at the Python interpreter level.
- Qtcm: This refers to the Python Qtcm class (note the capitalized first letter).
- qtcm: This refers to the Python qtcm package.
- **QTCM1 vs. QTCM:** Although the QTCM1 is currently the only version of a quasiequilibrium tropical circulation model (QTCM), in principle one can construct a QTCM with any number of baroclinic modes. In anticipation of this, the names of the Python package and class do not end in a numeral. In this manual and the qtcm docstrings, QTCM and QTCM1 are used interchangably. Usually either of these phrases mean the quasi-equilibrium tropical circulation model in a generic sense, regardless of its form of implementation.

1.4 Current Version Information and Acknowledgments

This manual describes version 0.1.2 (dated September 12, 2008), of package qtcm. Johnny Lin is the primary author of the package.

The qtcm package is built upon the pure-Fortran QTCM1 model, version 2.3 (August 2002), with a few minor changes. Those changes are described in detail in Section 6.2.

The homepage for the qtcm package is http://www.johnny-lin.com/py_pkgs/qtcm. All Python code in this package, and the Fortran files *setbypy.F90* and *wrapcall.F90*, are © 2003–2008 by Johnny Lin¹³ and constitutes a library that is covered under the GNU Lesser General Public License (LGPL):

This library is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License¹⁴ as published by the Free Software Foundation; either version 2.1 of the License, or (at your option) any later version.

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¹³http://www.johnny-lin.com

¹⁴http://www.gnu.org/copyleft/lesser.html

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You can contact Johnny Lin at his email address or at North Park University, Physics Department, 3225 W. Foster Ave., Chicago, IL 60625, USA.

All other Fortran code in this package, as well as the makefiles, are covered by licenses (if any) chosen by their respective owners.

This manual, in all forms (e.g., HTML, PDF, LATEX), is part of the documentation of the qtcm package and is © 2007–2008 by Johnny Lin. Permission is granted to copy, distribute and/or modify this document under the terms of the GNU Free Documentation License, Version 1.2 or any later version published by the Free Software Foundation; with no Invariant Sections, no Front-Cover Texts, and no Back-Cover Texts. A copy of the license can be found here¹⁵.

Transparent copies of this document are located online in PDF¹⁶ and HTML¹⁷ formats. The $\[mathbb{E}T_EX$ source files are distributed with the qtcm distribution. While the HTML version is nearly identical to the PDF and $\[mathbb{E}T_EX$ versions, not every feature in the manual was successfully converted. This is particularly true with figures, which are unnumbered in the HTML version and may be formatted differently than the authoritative PDF version. Thus, please consider the $\[\]T_EX$ version as the authoritative version.

Acknowledgements: Thanks to David Neelin and Ning Zeng and the Climate Systems Interactions Group at UCLA for their encouragement and help. On the Python side, thanks to Alexis Zubrow, Christian Dieterich, Rodrigo Caballero, Michael Tobis, and Ray Pierrehumbert for steering me straight. Early versions of some of this work was carried out at the University of Chicago Climate Systems Center, funded by the National Science Foundation (NSF) Information Technology Research Program under grant ATM-0121028. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the NSF.

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¹⁵http://www.gnu.org/licenses/fdl.html

¹⁶http://www.johnny-lin.com/py_pkgs/qtcm/doc/manual.pdf

¹⁷http://www.johnny-lin.com/py_pkgs/qtcm/doc/

1.5 Summary of Release History

- 2008 Sep 12: Version 0.1.2 released. Summary of changes:
 - Create Qtcm method get_qtcm1_item. This method is effectively an alias of method get_qtcm_item.
 - Create Qtcm method set_qtcm1_item. This method is effectively an alias of method set_qtcm_item.
 - Update User's Guide to phase out references to the get_qtcm_item and set_qtcm_item methods. Adding the "1" to the method names makes the purpose of the methods clearer.
 - Add unit tests to cover methods get_qtcm1_item and set_qtcm1_item.
- 2008 Jul 30: Updates to the User's Guide (just the online versions, not the copies released with the tarball).
- 2008 Jul 15: First publicly available distribution released (v0.1.1).

1.6 A Brief Description of The QTCM1

This description is copied from Ch. 3 of Lin [2], with minor revisions. Model formulation is fully described in Neelin & Zeng [3] and model results are described in Zeng et al. [5]. Neelin & Zeng [3] is based upon v2.0 of QTCM1 and Zeng et al. [5] is based on QTCM1 v2.1. The QTCM1 manual¹⁸ [4] describes the details of model implementation.

QTCM1 differs from most full-scale GCMs primarily in how the vertical temperature, humidity, and velocity structure of the atmosphere is represented. First, instead of representing the vertical structure by finite-differenced levels, the model uses a Galerkin expansion in the vertical. The vertical basis functions are chosen according to analytical solutions under convective quasi-equilibrium conditions, so only a few need be retained. Temperature and humidity are each described by separate vertical basis functions (a_1 and b_1 , respectively). Low-level variations in the humidity basis are larger than in the temperature basis. For velocity, QTCM1 uses a single baroclinic basis function (V_1) defined consistently with the temperature basis function, as well as a barotropic velocity mode (V_0). The vertical profiles of a_1 , b_1 , and V_1 are given in Figure 1.1. Currently, QTCM1 does not include a separate vertical degree of freedom describing the PBL. The horizontal grid spacing of the model is 5.625° longitude by 3.75° latitude.

These modes are chosen to accurately capture deep convective regions. Outside deep convective regions the mode is simply a highly truncated Galerkin representation. The system is much more tightly constrained than a full-scale GCM, yet

 $^{^{18}} http://www.atmos.ucla.edu/\sim\!csi/qtcm_man/v2.3/qtcm_manv2.3.pdf$

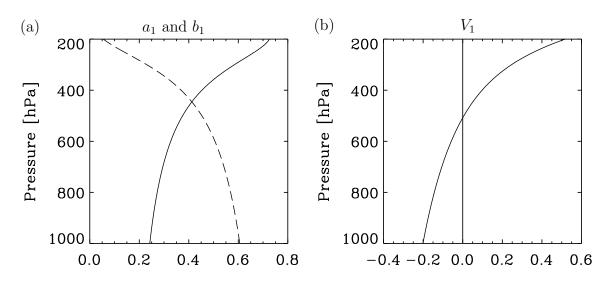


Figure 1.1: Vertical profiles of basis functions for (a) temperature a_1 (solid) and humidity b_1 (dashed) and (b) baroclinic component of horizontal velocity V_1 .

hopefully retains the essential dynamics and nonlinear feedbacks. The result is that QTCM1 is easier to diagnose than a GCM, and is computationally fast (about 8 minutes per year on a Sun Ultra 2 workstation). Zeng et al. [5] show results indicating this intermediate-level model does a reasonable job simulating tropical climatology and ENSO variability.

Below is a summary of the main model equations [3]:

$$\partial_t \mathbf{v}_1 + \mathcal{D}_{V1}(\mathbf{v}_0, \mathbf{v}_1) + f \mathbf{k} \times \mathbf{v}_1 = -\kappa \nabla T_1 - \epsilon_1 \mathbf{v}_1 - \epsilon_{01} \mathbf{v}_0 \tag{1.1}$$

$$\partial_t \zeta_0 + \operatorname{curl}_z(\mathcal{D}_{V0}(\mathbf{v}_0, \mathbf{v}_1)) + \beta v_0 = -\operatorname{curl}_z(\epsilon_0 \mathbf{v}_0) - \operatorname{curl}_z(\epsilon_{10} \mathbf{v}_1)$$
(1.2)

$$\widehat{a_1}(\partial_t + \mathcal{D}_{T1})T_1 + M_{S1}\nabla \cdot \mathbf{v}_1 = \langle Q_c \rangle + (g/p_T)(-R_t^{\dagger} - R_s^{\downarrow} + R_s^{\uparrow} + S_t - S_s + H) \quad (1.3)$$

$$\widehat{b}_1(\partial_t + \mathcal{D}_{q1})q_1 - M_{q1}\nabla \cdot \mathbf{v}_1 = \langle Q_q \rangle + (g/p_T)E \tag{1.4}$$

where (1.1) describes the baroclinic wind component, (1.2) describes the barotropic wind component, (1.3) is the temperature equation, and (1.4) is the moisture equation.

In the simplest formulation, the vertically integrated convective heating and moisture sink are assumed to be equal and opposite, so:

$$-\langle Q_q \rangle = \langle Q_c \rangle = \epsilon_c^* (q_1 - T_1) \tag{1.5}$$

For its convective parameterization for Q_c , this model uses the Betts-Miller [1] moist convective adjustment scheme, a scheme that is also used in some GCMs. In the convective parameterization, the coefficient ϵ_c^* is defined as:

$$\epsilon_c^* \equiv \widehat{a_1}\widehat{b_1}(\widehat{a_1} + \widehat{b_1})^{-1}\tau_c^{-1}\mathcal{H}(C_1) \tag{1.6}$$

where $\mathcal{H}(C_1)$ is zero for $C_1 \leq 0$, and one for $C_1 > 0$, and C_1 is a measure of the convective available potential energy (CAPE), projected onto the model's temperature and moisture basis functions.

Sensible heat (H) and evaporation (E) are given as bulk-aerodynamic formulations:

$$H = \rho_a C_D V_s (T_s - (T_{rs} + a_{1s}T_1))$$
(1.7)

$$E = \rho_a C_D V_s (q_{sat}(T_s) - (q_{rs} + b_{1s}q_1))$$
(1.8)

Longwave radiation components are denoted by R, and net shortwave radiation is denoted by S. The terms \mathcal{D}_{V1} and \mathcal{D}_{V0} are the advection-diffusion operators for the momentum equations (projected onto V_0 and $V_1(p)$, respectively). The terms \mathcal{D}_{T1} and \mathcal{D}_{q1} are the advection-diffusion operators for the temperature and moisture equations, respectively, using a vertical average projection. The $\langle X \rangle$ and \widehat{X} operators are equivalent and denote vertically integration over the troposphere. Please see Neelin & Zeng [3] and Zeng et al. [5] for a more complete description of equations and coefficients.

Chapter 2 Installation and Configuration

2.1 Summary and Conventions

This section provides a summary of the steps needed to install qtcm, and a description of the naming conventions used in this chapter. If you have had a decent amount of experience with Python and installing software on a Unix system, this section will probably be all you need to read. The installation steps are:

- 1. Install a Fortran compiler (see Section 2.2 for a list of compilers known to work). This compiler should be in a directory listed in your system path (e.g., */usr/bin*, etc.).
- 2. Install all required packages (see Section 2.3 for details): Python, matplotlib (plus the basemap toolkit), NumPy (which includes f2py), Scientific Python, LATEX, and netCDF.

Python packages are required to be installed on your system in a directory listed in your sys.path, and the other packages/libraries are required to be in standard directories listed in your system path (e.g., */usr/bin*, */sw/include*, etc.).

Make sure the executable for Python can be called at the Unix command line by typing both python. You might need to define a Unix alias that maps python2.4 (or whichever version of Python you are using) to python.

3. Download¹ the qtcm tarball and extract the distribution into a temporary directory for building purposes. qtcm-0.1.2 is the name of the qtcm distribution directory; the number following the hyphen is the version number of the distribution.

¹http://www.johnny-lin.com/py_pkgs/qtcm/

In this manual, the path to *qtcm-0.1.2* will be called the "qtcm build path" and be given as */buildpath*. When you see */buildpath*, please substitute the actual temporary directory you created for building purposes.

- 4. The qtcm distribution directory qtcm-0.1.2 contains the following principal subdirectories: doc, lib, src, test. Documentation is in doc, all the package modules are in lib, building of extension modules will take place in src, and testing of the package is done in test.
- 5. Compile qtcm extension modules in *src*: Go to *src*, copy the makefile from *src/Makefiles* corresponding to your system into *src*, rename to *makefile*, make changes to the makefile as needed, and execute:

make clean
make _qtcm_full_365.so
make _qtcm_parts_365.so

If you executed the make commands in *src*, the extension modules will be automatically placed in *lib* in the *qtcm-0.1.2* directory. See Section 2.4 for details.

- 6. Copy the entire contents of *lib* in *qtcm-0.1.2* (not *lib* itself) to a directory named *qtcm* that is on your sys.path. For instance, for Mac OS X using Fink, many Python packages are located in a directory named */sw/lib/python2.4/site-packages*, or something similar, and this directory is on the system sys.path. If this is the case for your system, copy the contents of *lib* into */sw/lib/python2.4/site-packages/qtcm*. (For Unix systems, the equivalent directory is usually */usr/local/lib/python2.4/site-packages*.)
- 7. Test the qtcm distribution in *test*: This step is optional and can take a while. Testing requires you to first generate a suite of benchmarks using the pure-Fortran QTCM1 model, then running the tests of qtcm by typing:

python test_all.py

at the Unix command line while in *test*. See Section 2.5 for details.

At some point, I will automate the installation using Python's distutils² utilities.

²http://docs.python.org/dist/dist.html

2.2 Fortran Compiler

You must have a Fortran compiler installed on your system in order to compile qtcm. The compiler must be able to interface with a pre-processor, as QTCM1 makes copious use of pre-processor directives. qtcm is known to work with the following Fortran compilers on the following platforms:

-	Compiler Web Site	Platform(s)		
g95	http://www.g95.org/	Mac OS X		

It will probably work with other platforms, but I haven't been able to test platforms besides those listed above. Note that g95 is not GNU Fortran (gfortran), the Fortran 95 compiler included with the more recent versions of GCC.

2.3 Required Packages

The following Python packages are required to be installed on your system in a directory listed in your sys.path:

- Python³: The Python programming language and interpreter. Make sure you have a version recent enough to be compatible with all the needed Python packages.
- matplotlib⁴: Scientific plotting package, using Matlab-like syntax. The basemap toolkit for matplotlib must also be installed.
- NumPy⁵: The standard array package for Python. The module name of NumPy imported in a Python session is numpy.
- Scientific Python⁶: Has netCDF file operators, in addition to other routines of use in scientific computing. The module name of Scientific Python imported in a Python session is Scientific.

One other required Python package, f2py, is now a part of the NumPy package, and so installation of NumPy is sufficient to give you both.

The package SciPy⁷, which includes several Python-accessible scientific libraries, also includes NumPy (and thus f2py), so if you install SciPy, you don't have to install NumPy again. Note that SciPy is not the same as Scientific Python; the names are confusing.

A few non-Python packages are also required:

³http://www.python.org/

⁴http://matplotlib.sourceforge.net/

⁵http://numpy.scipy.org/

⁶http://dirac.cnrs-orleans.fr/plone/software/scientificpython/

⁷http://www.scipy.org

- netCDF: This set of libraries enables one to write datasets into a platform independent, binary format, with metdata attached. The netCDF 3.6.2 library⁹ source code can be downloaded from UCAR¹⁰.

For most Unix installations, the easiest way to install all the above is via a package manager, for instance apt-get in Debian GNU/Linux, aptitude or synaptic in Ubuntu GNU/Linux, and fink in Mac OS X. Of course, you can also download a package's source code and build direct and/or install using Python's distutils¹¹ utilities.

2.4 Compiling Extension Modules

The extension modules (.*so* files) are imported and used by qtcm objects, and contain the Fortran QTCM1 model that is called by the qtcm Python wrappers. These extension modules are located in the *lib* directory of the qtcm distribution, and, in general, need to be created only when the qtcm package is installed.

Two extension modules are created: _qtcm_full_365.so and _qtcm_parts_365.so. Both modules define QTCM1 models where:

- A year is 365 days long (makefile macro YEAR360 is off).
- Model output is written to netCDF files (makefile macro NETCDFOUT is on).
- The atmospheric boundary layer model is used (makefile macro NO_ABL is off).
- A global domain is used (makefile macro **SPONGES** is off).
- Topography effects due to induced divergence are not included (makefile macro TOPO is off).
- Coupling between atmosphere and ocean is through mean fluxes (makefile macro CPLMEAN is off).
- The mixed layer ocean model is not used (makefile macros MXL_OCEAN and BLEND_SST are both off).

⁸http://www.tug.org/teTeX

⁹http://www.unidata.ucar.edu/software/netcdf/

¹⁰http://www.unidata.ucar.edu/downloads/netcdf/netcdf-3_6_2/

¹¹http://docs.python.org/dist/dist.html

2.4. COMPILING EXTENSION MODULES

(All other makefile macros not listed are also turned off.) The only difference between these two extension modules is that the "full" module is used by Qtcm instances where compiled_form is set to 'full', and the "parts" module is used by Qtcm instances where compiled_form is set to 'parts'. See Section 4.4 for details about the compiled_form attribute.

The extension modules are created through the following steps:

- 1. Go to the qtcm distribution directory qtcm-0.1.2 located in your build path */buildpath*. Go to the *src* sub-directory. This is where all the building of the extension modules will take place.
- 2. Copy the makefile that corresponds to your platform to the *src* directory, and rename it *makefile*. The *Makefiles* sub-directory of *src* contains makefiles for various platforms.
- 3. In *makefile*, make the following changes:
 - (a) Change the FC environment variable as needed, if your Fortran compiler is different.
 - (b) Change the FFLAGSM environment variable, if the compiler flags listed are not supported by your compiler.
 - (c) Change the -I and -L parts of the NCINC and NCLIB environment variables so that the paths for the netCDF library and include files match your system's installation:

NCINC=-I/yourpath/netcdf/include NCLIB=-L/yourpath/netcdf/lib -lnetcdf

Set *yourpath* to the full path to the *netcdf* directory where the *include* and *lib* sub-directories are that hold the netCDF libraries and include files. (You shouldn't have to change the -1 part of NCLIB, since it is standard to name the netCDF library *libnetcdf.a*. But if you have a non-standard installation, change the -1 part too.)

4. At the Unix prompt, type:

make clean && make _qtcm_full_365.so && make _qtcm_parts_365.so

to clean up leftover files from previous compilations, and to compile the extension module shared object files _qtcm_full_365.so and _qtcm_parts_365.so.

The makefile will automatically move the shared object files into ../*lib*, overwriting any pre-existing files of the same name. A detailed description of the makefile and using f2py is given in Section 6.6, if you wish to create a different extension module.

2.5 Testing the Installation

The qtcm distribution comes with a set of tests for the package, using Python's unittest package. Just to warn you, the tests take around an hour to run. The tests will not work if the contents of *lib* after you've finished building qtcm have not been copied to a directory named *qtcm* that is on your sys.path path, so make sure you've gone through all the install steps (summarized in Section 2.1) before you do these tests.

NB: For these tests to work, both **python** and **python2.4** must refer to the executable for the Python installation on your system that you are using for running **qtcm**.

The tests require a set of benchmark output files in the *test/benchmarks* directory in the *qtcm-0.1.2* directory (the output will be in directories whose names begin with "aquaplanet" or "landon"). These output files are not included with the qtcm distribution, and must be created, by doing the following:

- Goto the directory test/benchmarks/create/src in the qtcm-0.1.2 qtcm distribution directory, and copy the makefile from sub-directory Makesfiles, that corresponds to your system to the test/benchmarks/create/src directory. Rename the makefile in test/benchmarks/create/src to makefile.
- 2. In *makefile*, make the following changes:
 - (a) Change the FC environment variable as needed, if your Fortran compiler is different.
 - (b) Change the FFLAGSM environment variable, if the compiler flags listed are not supported by your compiler.
 - (c) Change the -I and -L parts of the NCINC and NCLIB environment variables so that the paths for the netCDF library and include files match your system's installation:

```
NCINC=-I/yourpath/netcdf/include
NCLIB=-L/yourpath/netcdf/lib -lnetcdf
```

Set *yourpath* to the full path to the *netcdf* directory where the *include* and *lib* sub-directories are that hold the netCDF libraries and include files. (You shouldn't have to change the -1 part of NCLIB, since it is standard to name the netCDF library *libnetcdf.a*. But if you have a non-standard installation, change the -1 part too.)

- 3. Go to the directory *test/benchmarks/create* in the *qtcm-0.1.2* qtcm distribution directory.
- 4. Type python create_benchmarks.py at the Unix command line to run the benchmark creation script.

2.6. MODEL PERFORMANCE

The created benchmarks will be located in *test/benchmarks*, in directories with names related to the run that was done, as described earlier. The benchmarks are created using the pure-Fortran QTCM1 model code, version 2.3 (August 2002), with an altered makefile (described above) and the following code change: In all *.F90* files, occurrences of:

Character(len=130)

are changed to:

Character(len=305)

This enables the model to properly deal with longer filenames. The number "305" is chosen to make search and replace easier.

Once the benchmarks are created, you can test the qtcm package by doing the following:

- 1. Go to the *test* directory in the *qtcm-0.1.2* directory.
- 2. Type python test_all.py at the Unix command line.

If at the end of the test runs you see this message (or something similar):

```
------
```

Ran 93 tests in 1244.205s

OK

then everything worked fine! If you get any other message, the test(s) have failed.

2.6 Model Performance

The wall-clock time values below give the mean over three separate 365 day aquaplanet runs, using climatological sea surface temperature for lower boundary forcing. NetCDF output is written daily, for both instantaneous and mean values. The time step is 1200 sec, and the version of qtcm used is 0.1.1. The horizontal grid spacing of all model versions is 5.625° longitude by 3.75° latitude. Values are in seconds:

System	Pure	Full	Parts
Mac OS X: MacBook 1.83 GHz Intel Core	152.59	153.63	158.94
Duo running Mac OS X 10.4.10 with 1 GB $$			
RAM (Python 2.4.3, NumPy 1.0.3, f2py			
$2_{-}3816).$			
Ubuntu GNU/Linux: Dell PowerEdge 860	43.73	44.79	47.45
with 2.66 GHz Quad Core Intel Xeon pro-			
cessors (64 bit) running Ubuntu $8.04.1 \text{ LTS}$			
(Python 2.5.2, NumPy 1.1.0, f2py 2_5237).			

"Pure" refers to the pure-Fortran version of QTCM1. "Full" refers to a qtcm run session with compiled_form set to 'full'. "Parts" refers to a qtcm run session with compiled_form set to 'parts'. (Section 4.4 has details about the difference between compiled forms.)

The 'parts' version of qtcm gives Python the maximum flexibility in accessing compiled QTCM1 model subroutines and variables. The price of that flexibility is an increase in run time of approximately 4–9% over the pure-Fortran version. The difference in performance between the 'full' version of qtcm and the pure-Fortran version of QTCM1 is between negligible and 3% longer.

To make a timing for the pure-Fortran model, go to *test/benchmarks/timing/work* in */buildpath* and run the *timing_365.sh* script in that directory. That script runs the QTCM1 model using /usr/bin/time, which at the end of the script will output the amount of time it took to make the model run. Run the timing script three times and average the values to obtain a time comparable to the above.

To make a timing for the qtcm model, type python timing_365.py while in the *test* directory in */buildpath*. Three run sessions will be made for compiled_form equal to 'full' and 'parts', the times are averaged, and the value are output at the end of the script.

2.7 Installing in Mac OS X

2.7.1 Introduction

This section describes issues and a summary of the installation steps I followed to install qtcm on a Mac running OS X. It is a specific realization of the general installation instructions found in Sections 2.1–2.5. I first worked through these installation steps during June–July 2007, with updates during July 2008. The best way to go through this section is to go through the summary of the installation steps in Section 2.7.6, and looking back to other sections as needed.

2.7.2 Platform and Unix Dependencies

This work was done on a MacBook 1.83 GHz Intel Core Duo running Mac OS X 10.4.11. My machine has 1 GB RAM and 64 GB of disk in its main partition.

I recommend you turn-off your antivirus software before you do the installs. Problems have been reported by Fink users¹² using the Fink package manager with antivirus software enabled.

There are a variety of dependencies that are required to get your Mac up-andrunning as a scientific computing platform. The most basic is installing Apple's

 $^{^{12}} http://finkproject.org/faq/usage-fink.php?phpLang=en\#kernel-panics$

XCode¹³ developer tools.¹⁴ This set of tools contains compilers and libraries needed to do anything further. You have to be a member of Apple's Developer Connection, but registration is free.

Besides XCode, there are a variety of Unix libraries and utilities that you need. I first tried installing them by myself, from scratch, into */usr/local*, but it was hard to keep track of all the dependencies. A few that did work, and that I installed from their disk images, are: MacTeX¹⁵, MAMP¹⁶, and Tcl/Tk Aqua BI (Batteries Included)¹⁷.¹⁸

For everything else, thankfully, there's the Fink $Project^{19}$ which uses a package manager built upon Debian tools to install ports of Unix programs onto a Mac. I just downloaded²⁰ a binary version of the Fink 0.8.1 installer for Intel Macs, installed Fink, and used its package management tools to install (almost) everything else I needed.²¹

Although you do not need anything besides a Fortran compiler and the netCDF libraries to run QTCM1 in its pure-Fortran form, in order to manipulate the model and use this Python version qtcm, you need to have Python installed. The default Python that comes with the Mac is a little old, so I used Fink to also install Python 2.5 and related packages, including matplotlib²³, ScientificPython²⁴, and SciPy²⁵ (see Section ?? for details).

2.7.3 Fortran Compiler

There are a variety of high-quality, commercial Fortran compilers. Unfortunately, because I do not have a research budget, I am not able to use those compilers. The GNU Compiler Collection²⁶ (GCC) provides a suite of open-source compilers, some of

¹³http://developer.apple.com/tools/xcode/

¹⁴The package should work in Mac OS X 10.4 with XCode 2.4.1 and higher; I've tried it with both 2.4.1 and XCode 2.5. Note that XCode 3.1 only works on Mac OS X 10.5.

¹⁵http://www.tug.org/mactex/

¹⁶http://www.mamp.info/

¹⁷http://tcltkaqua.sourceforge.net/

 $^{^{18}}$ Theoretically you can use Fink to install the equivalent of these packages, but I like the specific collection found in these packages. For instance, Tcl/Tk Aqua BI runs natively on the Mac.

¹⁹http://www.finkproject.org/

²⁰http://www.finkproject.org/download/index.php?phpLang=en

²¹The one drawback of Fink is that it sometimes has stability problems. In those cases, Fink provides command line suggestions to fix the problems, which sometimes will work. If not, sometimes deleting Fink and everything it installed,²² and starting afresh, will do the trick. It also appeared to me that sometimes when I installed multiple packages via one fink install call, the installation did not work as well as when I installed only one package per call.

²³http://matplotlib.sourceforge.net/

²⁴http://dirac.cnrs-orleans.fr/plone/software/scientificpython/

²⁵http://www.scipy.org

²⁶http://gcc.gnu.org/

which are the standards of their language. Most of the GCC compilers are installed on your Mac when you install XCode.

GNU Fortran²⁷ (gfortran), is the Fortran 95 compiler included with the more recent versions of GCC. Unfortunately, I was not able to get it to compile QTCM1. There is a second open-source Fortran compiler, $G95^{28}$ (g95), which some feel is farther along in its development than gfortran. I was able to successfully compile QTCM1 with g95 on my Mac. I used Fink to install G95 (see Section ?? for details).

2.7.4 NetCDF Libraries

For some reason, the netCDF libraries and include files installed by Fink didn't correspond to the files needed by the calling routines in qtcm. To solve this, I compiled my own set of netCDF 3.6.2 libraries²⁹ using the tarball downloaded from UCAR³⁰.

Once I uncompressed and untarred the package, and went into the top-level directory of the package, I built the package by typing the following at the Unix prompt:

./configure --prefix=/Users/jlin/extra/netcdf make check make install

This installed the netCDF binaries, libraries, and include files into sub-directories *bin*, *lib*, and *include* in the directory specified by --prefix. If you want to install the netCDF libraries in the default (usually */usr/local*), just leave out the --prefix option.

Note: When you build netCDF, make sure the build directory is not in the directory tree of --prefix (or the default directory /usr/local).

2.7.5 Makefile Configuration

NetCDF

In the *src* directory in the qtcm distribution, there is a sub-directory *Makefiles* that contains the makefiles for a variety of platforms. Edit the file *makefile.osx_g95* so that the lines specifying the environment variables for the netCDF libraries and include files:

NCINC=-I/Users/jlin/extra/netcdf/include NCLIB=-L/Users/jlin/extra/netcdf/lib -lnetcdf

 $^{^{27} \}rm http://gcc.gnu.org/fortran/$

²⁸http://www.g95.org/

²⁹http://www.unidata.ucar.edu/software/netcdf/

³⁰http://www.unidata.ucar.edu/downloads/netcdf/netcdf-3_6_2/

are changed to the path where your *manually compiled* netCDF libraries and include files are.

Copy makefile.osx_g95 from the Makefiles sub-directory in src into src. In other words, from the qtcm distribution directory (i.e., /buildpath), at the Unix prompt execute:

cp src/Makefiles/makefile.osx_g95 src/makefile

Linking Order

Compilers in the GNU Compiler Collection (GCC) search libraries and object files in the order they are listed in the command-line, from left-to-right³¹. Thus, if routines in b.o call routines in a.o, you must list the files in the order a.o b.o.

For some reason, that isn't the case for g95. Thus, you will find g95 makefile rules structured like the following (below is part of the rule to create an executable (*qtcm*) for benchmark runs):

```
qtcm: main.o
$(FC) -0 $(NCINC) -0 $@ main.o $(QTCMLIB) $(NCLIB)
```

even though *main.o* depends on the QTCM library (specified in macro setting \$(QTCMLIB)), which in turn depends on the netCDF library (specified in macro setting \$(NCLIB)).

2.7.6 Summary of Steps

The following summarizes all the steps I took to install qtcm in Mac OS X:

- 1. Install XCode 2.5^{32} .
- 2. Install MacTeX³³, MAMP³⁴, and TCL/Tk Aqua BI (Batteries Included)³⁵.
- 3. Install Fink 0.8.1³⁶. Make sure you set up your environment to enable you to use the packages you install with Fink (e.g. PATH settings, etc.). Most of the time, that just means adding the line source /sw/bin/init.csh to your .cshrc file (or the equivalent in your .bashrc).

Note that for many of the packages needed to run qtcm, you need to configure Fink to download packages from the unstable trees. To do that, add unstable/main and unstable/crypto to the Trees: line in /sw/etc/fink.conf, and run:

 $^{^{31}} http://gcc.gnu.org/onlinedocs/gcc-4.1.2/gcc/Link-Options.html\#index-l-670$

 $^{^{32}}$ http://developer.apple.com/tools/xcode/

³³http://www.tug.org/mactex/

³⁴http://www.mamp.info/

³⁵http://tcltkaqua.sourceforge.net/

³⁶http://www.finkproject.org/download/index.php?phpLang=en

fink selfupdate
fink index
fink scanpackages
fink update-all

When **selfupdate** runs, choose **rsync** for the self update method. If you do not, Fink will not look in the unstable trees for packages.

4. Use Fink to install the g95 Fortran compiler. From a Unix prompt, type:

fink --use-binary-dist install g95

5. Use Fink to install Python and the NumPy package (which f2py is a part of). From a Unix prompt, type:

```
fink --use-binary-dist install python25
fink --use-binary-dist install scipy-core-py25
```

(Numpy used to be called SciPy Core.) If you want to install Python 2.4 instead, just change the "25" and "py25" above (and in later occurrences) to "24" and "py24", respectively. Note that Fink does not have a version of epydoc for Python 2.4, so if you wish to create documentation using epydoc, you will need to install Python 2.5.

6. Install teTeX and LATEX2HTML using Fink. From a Unix prompt, type:

```
fink --use-binary-dist install tetex
fink --use-binary-dist install latex2html
```

When prompted, choose ghostscript and ghostscript-fonts to satisfy the dependency (which should be the default options). I tried choosing systemghostscript8, but Fink looks for ghostscript 8.51 and didn't recognize ghostscript 8.57 that was already installed in /usr/local (via my MacTeX install). LaTEX2HTML has a package required by the qtcm manual LATEX file.

7. Install additional programming and scientific packages and libraries using Fink. From a Unix prompt, type:

```
fink --use-binary-dist install scientificpython-py25
fink --use-binary-dist install matplotlib-py25
fink --use-binary-dist install matplotlib-basemap-py25
fink --use-binary-dist install xaw3d
fink --use-binary-dist install fftw fftw3
fink --use-binary-dist install epydoc-py25
fink --use-binary-dist install graphviz
fink --use-binary-dist install scipy-py25
```

- 8. Manually install netCDF 3.6.2 (see Section 2.7.4).
- 9. From this point on, you can follow the general instructions given in Section 2.1, starting with step 3. Please do not ignore, however, Section 2.7's Mac-specific details.

2.8 Installing in Ubuntu

2.8.1 Introduction

This section describes installation issues I followed to install qtcm on my Dell PowerEdge 860 running Ubuntu GNU/Linux 8.04.1 LTS (Hardy). The machine has 2.66 GHz Quad Core Intel Xeon processors (64 bit), 4 GB RAM, and 677 GB of disk in its main partition. This section is a specific realization of the general installation instructions found in Sections 2.1–2.5. I worked through these installation steps during July 2008. The best way to go through this section is to go through the summary of the installation steps in Section 2.8.5, and looking back to other sections as needed.

2.8.2 Fortran Compiler

The easiest Fortran compiler to install in Ubuntu 8.04.1 is GNU Fortran³⁷ (gfortran), the Fortran 95 compiler included with the more recent versions of the GNU Compiler Collection (GCC); you can use any package manager (e.g., apt-get, aptitude) to install it. Unfortunately, I was not able to get it to compile QTCM1. I was, however, able to successfully compile QTCM1 using the second open-source Fortran compiler, G95³⁸ (g95), which some feel is farther along in its development than gfortran. G95, however, is not supported as an Ubuntu package, and so I had to manually install it.

I downloaded the binary version of G95 v0.91 (the Linux $x86_64$ /EMT64 with 32 bit default integers) using the following curl command:³⁹

curl -o g95.tgz http://ftp.g95.org/v0.91/g95-x86_64-32-linux.tgz

which saves the .tgz file as the local file g95.tgz. After that, I followed the G95 project's standard installation instructions⁴⁰ to finish the install.⁴¹ The regular Linux

sudo ln -s ../g95-install_64/bin/x86_64-suse-linux-gnu-g95 g95.

³⁷http://gcc.gnu.org/fortran/

³⁸http://www.g95.org/

³⁹I use curl because I usually access my Ubuntu server via a terminal session.

 $^{^{40}} http://g95.sourceforge.net/docs.html\#starting$

⁴¹The G95 installation instructions say you can put g95-install anywhere, and make a link to the executable g95 in \sim/bin . I put g95-install in /usr/local, and while in /usr/local/bin, I put a link to the G95 executable using the command:

x86 version of G95 (in g95-x86-linux.tgz from the G95 website) did not work on my machine.

2.8.3 NetCDF Libraries

For some reason, the netCDF libraries and include files installed from the Ubuntu packages do not correspond to the files needed by the calling routines in qtcm. To solve this, I compiled my own set of netCDF 3.6.2 libraries⁴² using the tarball downloaded from UCAR⁴³.

Once I uncompressed and untarred the package, and went into the top-level directory of the package, I built the package by typing the following at the Unix prompt:

```
export FC=g95
export FFLAGS="-0 -fPIC"
export FFLAGS="-fPIC"
export F90FLAGS="-fPIC"
export CFLAGS="-fPIC"
export CXXFLAGS="-fPIC"
./configure
make check
sudo make install
```

(The export commands set environment variables for the Fortran compiler and Fortran and other compiler flags. The -fPIC flag enables the compilers to create position independent code, needed for shared libraries in Ubuntu on a 64 bit Intel processor.)

The above installs the netCDF binaries, libraries, and include files into subdirectories *bin*, *lib*, and *include* in */usr/local*, the default. The include files for this netCDF installation are thus located in */usr/local/include*, and the libraries for this netCDF installation are location in */usr/local/lib*. (If you want to specify a different installation location, use the --prefix option in configure.) While you don't have to have root privileges during the configuration and check steps, you do during the installation step if you're installing into */usr/local* (thus the sudo in the last step).⁴⁴

2.8.4 Makefile Configuration

NetCDF

In the *src* directory in the qtcm distribution, there is a sub-directory *Makefiles* that contains the makefiles for a variety of platforms. Edit the file *makefile.ubuntu_64_g95*

⁴²http://www.unidata.ucar.edu/software/netcdf/

 $^{^{43}} http://www.unidata.ucar.edu/downloads/netcdf/netcdf-3_6_2/$

⁴⁴Note that when you build netCDF, make sure the build directory is not in the directory tree of --prefix or the default directory /usr/local.

so that the lines specifying the environment variables for the netCDF libraries and include files:

NCINC=-I/usr/local/include NCLIB=-L/usr/local/lib -lnetcdf

are changed to the path where your manually compiled netCDF libraries and include files are.

Copy makefile.ubuntu_64_g95 from the Makefiles sub-directory in src into src. In other words, from the qtcm distribution directory (i.e., /buildpath), at the Unix prompt execute:

cp src/Makefiles/makefile.ubuntu_64_g95 src/makefile

Linking Order

Compilers in the GNU Compiler Collection (GCC) search libraries and object files in the order they are listed in the command-line, from left-to-right⁴⁵. Thus, if routines in b.o call routines in a.o, you must list the files in the order a.o b.o.

For some reason, that isn't the case for g95. Thus, you will find g95 makefile rules structured like the following (below is part of the rule to create an executable (*qtcm*) for benchmark runs):

qtcm: main.o \$(FC) -O \$(NCINC) -o \$@ main.o \$(QTCMLIB) \$(NCLIB)

even though *main.o* depends on the QTCM library (specified in macro setting QTCMLIB), which in turn depends on the netCDF library (specified in macro setting NCLIB).

Shared Object PIC

In order to compile the model in Ubuntu on a 64 bit Intel processor, the model and the netCDF library it is linked to needs to be compiled to be position independent code (PIC).⁴⁶ This is accomplished with the -fPIC flag⁴⁷.

In the qtcm makefiles, the -fPIC flag is introduced in the macro FFLAGSM, for instance:

FFLAGSM = -0 - fPIC

For makefiles used in creating extension modules, -fPIC must be passed into the f2py call. To do so, put the flags:

⁴⁵http://gcc.gnu.org/onlinedocs/gcc-4.1.2/gcc/Link-Options.html#index-l-670

⁴⁶http://www.gentoo.org/proj/en/base/amd64/howtos/index.xml?part=1&chap=3

⁴⁷http://www.fortran-2000.com/ArnaudRecipes/sharedlib.html

--f90flags="-fPIC" --f77flags="-fPIC"

after the --fcompiler flag in the f2py calling line.

The -fPIC flag must also be used when compiling the netCDF libraries, as described in Section 2.8.3. Failure to create PIC libraries in 64 bit Ubuntu can result in errors like the following when creating the qtcm extension modules:

ld: /usr/local/lib/libnetcdf.a(fort-attio.o): relocation
R_X86_64_32 against 'a local symbol' can not be used
when making a shared object; recompile with -fPIC
/usr/local/lib/libnetcdf.a: could not read symbols: Bad value

2.8.5 Summary of Steps

The following summarizes all the steps I took to install qtcm in Ubuntu 8.04.1 LTS (Hardy) running on a Quad Core Intel Xeon (64 bit) machine. Note that while I use the aptitude package manager, you are free to use any manager of your choice (e.g., apt-get, synaptic, etc.):

- 1. Install the G95 Fortran compiler from the binary distribution. See Section 2.8.2 for details.
- 2. Use an Ubuntu package manager to install the following packages, by typing:

```
sudo aptitude update
sudo aptitude install curl
sudo aptitude install python-epydoc
sudo aptitude install python-matplotlib
sudo aptitude install python-netcdf
sudo aptitude install python-scientific
sudo aptitude install python-scipy
sudo aptitude install texlive
```

Installing python-scipy will also install NumPy and f2py, so you don't have to install the python-numpy package separately.

Early-on as I debugged my qtcm install on Ubuntu, I encountered errors that I thought came from an old version of NumPy⁴⁸, and thus I replaced Ubuntu's packaged NumPy with NumPy 1.1.0 built directly from source.⁴⁹ (Note, you shouldn't install your new NumPy in the default location, which may cause problems later-on with Ubuntu's package manager.) Later on, I concluded the errors I had encountered were not because of the NumPy version, but by then I didn't want to try to reinstall NumPy again. So strictly speaking, the version

⁴⁸http://cens.ioc.ee/pipermail/f2py-users/2008-June/001617.html

⁴⁹http://sourceforge.net/project/showfiles.php?group_id=1369&package_id=175103

of Numpy I used is not the one bundled with python-scipy, but that shouldn't be a problem.

- 3. Manually install netCDF 3.6.2 from source (see Section 2.8.3).
- 4. Manually install the **basemap** package of **matplotlib**. The source for the **basemap** toolkit is available from Sourceforge⁵⁰ I obtained version 0.9.9.1 using the following **curl** command:

```
curl -o basemap.tar.gz \
http://voxel.dl.sourceforge.net/sourceforge/matplotlib/basemap-0.9.9.1.tar.gz
```

The *README* file in the *basemap-0.9.9.1* directory has detailed installation instructions. Note that you have to install the GEOS library first (*README* has detailed directions on how to do that too). To be on the safe-side, I would set the FC environment variable to the G95 compiler (e.g., with export FC=g95 in Bash).

5. From this point on, you can follow the general instructions given in Section 2.1, starting with step 3. Please do not ignore, however, Section 2.8's Ubuntu-specific details.

 $^{^{50}} http://sourceforge.net/project/showfiles.php?group_id=80706$

Chapter 3 Getting Started With qtcm

3.1 Your First Model Run

Figure 3.1 shows an example of a script to make a 30 day seasonal, aquaplanet model run, with run name "test", starting from November 1, Year 1.

```
from qtcm import Qtcm
inputs = {}
inputs['runname'] = 'test'
inputs['landon'] = 0
inputs['yearO'] = 1
inputs['monthO'] = 11
inputs['dayO'] = 1
inputs['lastday'] = 30
inputs['mrestart'] = 0
inputs['compiled_form'] = 'parts'
model = Qtcm(**inputs)
model.run_session()
```

Figure 3.1: An example of a simple qtcm run.

The class describing the QTCM1 model is Qtcm. An instance of Qtcm, in this example model, is created the same way you create an instance of any class. When instantiating an instance of Qtcm, keyword parameters can be used to override any default settings. In the example above, the dictionary inputs specifying all keyword parameters is passed in on the instantiation of model.

The keyword parameter settings in Figure 3.1 have the following meanings:

• runname: This string ("test") is used in the output filename. QTCM1 writes mean and instantaneous output files to the directory given in model.outdir.value,

with filenames $qm_runname.nc$ for mean output and $qi_runname.nc$ for instantaneous output.

- landon: When set to "0", the land is turned off and the run is an aquaplanet run. When set to "1", the land model is turned on.
- year0: The year the run starts on.
- month0: The month the run starts on (11 = November).
- day0: The day of the month the run starts on.
- lastday: The model runs from day 1 to lastday.
- mrestart: When set to "0", the run starts from default initial conditions (see Section 4.7.2 for a table of those values). When set to "1", the run starts from a restart file.
- compiled_form: This keyword sets what form the compiled QTCM1 model has, and its value is saved to the instance's compiled_form attribute. It is a string and can be set either to "parts" or "full". Most of the time, you will want to set it to 'parts'. This keyword is the only one that must be specified on instantiation; the model instance will at least instantiate using only the default settings for all the other keyword parameters (given in Appendix A). See Section 4.4 for details about what the compiled_form attribute controls.

By default, the **SSTmode** attribute, which controls whether the model will use climatological sea-surface temperatures (SST) or real SSTs, is set to the **value** "seasonal", thus giving a run with seasonal forcing at the lower-boundary over the ocean.

This example assumes that the boundary condition files, sea surface temperature files, and the model output directories are as specified in submodule defaults. Those values are described in Section A.1.

3.2 Managing Directories

Most of the time, your boundary condition files and output files will not be in the locations specified in Section A.1, or in the directory your Python script resides. The easiest way to tell your Qtcm instance where your input/output files are is to pass them in as keyword parameters on instantiation.

Figure 3.2 shows an example run where those directories are explicitly specified; in all other aspects, the run is identical to the one in Figure 3.1. In Figure 3.2, output from the model is directed to the directory described by string variable dirbasepath. dirbasepath is created by joining the current working directory

```
from qtcm import Qtcm
rundirname = 'test'
dirbasepath = os.path.join(os.getcwd(), rundirname)
inputs = {}
inputs['bnddir'] = os.path.join( os.getcwd(), 'bnddir',
                                 'r64x42')
inputs['SSTdir'] = os.path.join( os.getcwd(), 'bnddir',
                                 'r64x42', 'SST_Reynolds' )
inputs['outdir'] = dirbasepath
inputs['runname'] = rundirname
inputs['landon'] = 0
inputs['year0'] = 1
inputs['month0'] = 11
inputs['day0'] = 1
inputs['lastday'] = 30
inputs['mrestart'] = 0
inputs['compiled_form'] = 'parts'
model = Qtcm(**inputs)
model.run_session()
```

Figure 3.2: An example qtcm run showing detailed description of input and output directories.

with the run name given in string variable rundirname.¹ Setting keyword parameter outdir to dirbasepath sends output to dirbasepath. Keywords bnddir and SSTdir specify the directories where non-SST and SST boundary condition files, respectively, are found.

Interestingly, the default version of QTCM1 does *not* send all output from the model to **outdir**. The restart file *qtcm_yyyymmdd.restart* (where *yyyymmdd* is the year, month, and day of the model date when the restart file was written) is written into the current working directory, not the output directory. Thus, if you do multiple runs, you'll have to manually deal with the restart files that will proliferate.

Neither the QTCM1 model nor the Qtcm object create the directories specified in bnddir, SSTdir, and outdir. Failure to do so will create an error. I use Python's file management tools to make sure the output directory is created, and any old output files are deleted. Here's an example that does that, using the dirbasepath and rundirname variables from Figure 3.2:

```
if not os.path.exists(dirbasepath): os.makedirs(dirbasepath)
qi_file = os.path.join( dirbasepath, 'qi_'+rundirname+'.nc' )
qm_file = os.path.join( dirbasepath, 'qm_'+rundirname+'.nc' )
if os.path.exists(qi_file): os.remove(qi_file)
if os.path.exists(qm_file): os.remove(qm_file)
```

3.3 Model Field Variables

The term "field" variable refers to QTCM1 model variables that are accessible at both the compiled Fortran QTCM1 model-level as well as the Python Qtcm instance-level. Field variables are all instances of the Field class, and are stored as attributes of the Qtcm instance.²

Field class instances have the following attributes:

- id: A string naming the field (e.g., "Qc", "mrestart"). This string should contain no whitespace.
- value: The value of the field. Can be of any type, though typically is either a string or numeric scalar or a numeric array.
- units: A string giving the units of the field.
- long_name: A string giving a description of the field.

¹The Python os module enables platform-independent handling of files and directories. The os.path.join function resolves paths without the programmer needing to know all the possible directory separation characters; the function chooses the correct separation character at runtime. The os.getcwd function returns the current working directory.

²Note non-field variables can also be instances of Field, and that Qtcm instances have other attributes that are not equal to Field instances.

Field instances also have methods to return the rank and typecode of value.

Remember, if you want to access the value of a Field object, make sure you access that object's value attribute. Thus, for example, to assign a variable foo to the lastday value for a given Qtcm instance model, type the following:

```
foo = model.lastday.value
```

For scalars, this assignment sets foo by value (i.e., a copy of the value of attribute model.lastday is set to foo). In general, however, Python assigns variables by reference. Use the copy module if you truly want a copy of a field variable's value (such as an array), rather than an alias. For more details about field variables, see Section 4.7.

3.4 Run Sessions

3.4.1 What is a Run Session?

A run session is a unit of simulation where the model is run from day 1 of simulation to the day specified by the lastday attribute of a Qtcm instance. A run session is a "complete" model run, at the beginning of which all compiled QTCM1 model variables are set to the values given at the Python-level, and at the end of which restart files are written, the values at the Python-level are overwritten by the values in the Fortran model, and a Python-accessible snapshot is taken of the model variables that were written to the restart file.

3.4.2 Changing Variables

Between run sessions, changing any field variable is as easy as a Python assignment. For instance, to change the atmosphere mixed layer depth to 100 m, just type:

```
model.ziml.value = 100.0
```

When changing arrays, be careful to try to match the shape of the array.³ You can use the NumPy shape function on a NumPy array to check its shape.

3.4.3 Continuing a Model Run

Figure 3.3 shows an example of two run sessions, where the second run session is a continuation of the first.

³At the very least, match the rank of the array, which is required for the routines in **setbypy** to properly choose which Fortran subroutine to use in reading the Python value. I haven't tested if only the rank is needed, however, for the passing to work, for a continuation run (my hunch is it won't).

```
inputs['year0'] = 1
inputs['month0'] = 11
inputs['day0'] = 1
inputs['lastday'] = 10
inputs['mrestart'] = 0
inputs['compiled_form'] = 'parts'
model = Qtcm(**inputs)
model.run_session()
model.u1.value = model.u1.value * 2.0
model.init_with_instance_state = True
model.run_session(cont=30)
```

Figure 3.3: An example of two qtcm run sessions where the second run session is a continuation of the first. Assume inputs is a dictionary, and that earlier in the script the run name and all input and output directory names were added to the dictionary.

The first run session runs from day 1 to day 10. The second run session runs the model for another 30 days. Setting the init_with_instance_state of model to True tells the model to use the the values of the instance attributes (for prognostic variables, right-hand sides, and start date) are currently stored model as the initial values for the run_session.⁴ The cont keyword in the second run_session call specifies a continuation run, and the value gives the number of additional days to run the model.

The set of runs described above would produce the exact same results as if you had gone into the Fortran model after 10 days, doubled the first baroclinic mode zonal velocity, and continued the run for another 30 days. With the Python example above, however, you didn't need to know you were going to do that ahead of starting the model run (which is what a compiled model requires you to do). Section 4.5 describes continuation runs in detail.

3.4.4 Passing Restart Snapshots Between Run Sessions

The pure-Fortran QTCM1 uses a restart file to enable continuation runs. A Qtcm instance can also make use of that option, through setting the mrestart attribute value (see Section 4.5 and Neelin et al. [4] for details). It's easier, however, instead of using a restart file, to pass along a "snapshot" dictionary.

The Qtcm instance method make_snapshot copies the variables that would be written out to a restart file into a dictionary that is saves as the instance attribute

⁴Unless overridden, by default, init_with_instance_state is set to True on Qtcm instance instantiation.

snapshot. This snapshot can be saved separately, for later recall. Note that snapshots are automatically made at the end of a run session.

The following example shows a model run_session call, following which the snapshot is saved to the variable snapshot:⁵

```
model.run_session()
mysnapshot = model.snapshot
```

After taking the snapshot, you might continue the run a while, and then decide to return to the snapshot you saved. To do so, use the sync_set_py_values_to_snapshot method to reset the model instance values to mysnapshot before your next run session:

```
model.sync_set_py_values_to_snapshot(snapshot=mysnapshot)
model.init_with_instance_state = True
model.run_session()
```

See Section 4.5.5 for details regarding the use of snapshots, as well as for a list of what variables are saved in a snapshot.

3.5 Creating Multiple Models

3.5.1 Model Instances

Creating a new QTCM1 model is as simple as creating another Qtcm instance. For instance, to instantiate two QTCM1 models, model1 and model2, type the following:

```
from qtcm import Qtcm
model1 = Qtcm(compiled_form='parts')
model2 = Qtcm(compiled_form='parts')
```

model1 and model2 do *not* share any variables in common, including the extension modules holding the Fortran code. In creating the instances, a copy of the extension modules are saved in temporary directories.

3.5.2 Passing Snapshots To Other Models

The snapshots described in Section 3.4.4 can also be passed around to other model instances, enabling you to easily branch a model run:

⁵Remember Python assignment defaults to assignment by reference, so in this example the variable mysnapshot is a pointer to the model.snapshot attribute. (However, note that model.snapshot itself is not a reference, but a distinct copy of those variables; to do otherwise would result in a non-static snapshot.) If the model.snapshot attribute is dereferenced, then mysnapshot will become the sole pointer to the dictionary.

```
model.run_session()
mysnapshot = model.snapshot
model1.sync_set_py_values_to_snapshot(snapshot=mysnapshot)
model2.sync_set_py_values_to_snapshot(snapshot=mysnapshot)
model1.run_session()
model2.run_session()
```

The state of model after its run session is used to start model1 and model2. This is an easy way to save time in spinning-up multiple models.

3.6 Run Lists

This feature of Qtcm objects is what really gives Qtcm model instances their flexibility. A run list is a list of strings and dictionaries that specify what routines to run in order to execute a particular part of the model. Each element of the run list specifies the method or subroutine to execute, and the order of the elements specifies their execution order.

For instance, the standard run list for initializing the the atmospheric portion of the model is named "qtcminit", and equals the following list:

```
['__qtcm.wrapcall.wparinit',
'__qtcm.wrapcall.wbndinit',
'varinit',
{'__qtcm.wrapcall.wtimemanager': [1]},
'atm_physics1']
```

This list is stored as an entry in the runlists dictionary (with key 'qtcminit'). runlists is an attribute of a Qtcm instance. Table 4.3 lists all standard run lists.

When the run list element in the list is a string, the string gives the name of the routine to execute. The routine has no parameter list. The routine can be a compiled QTCM1 model subroutine for which an interface has been written (e.g., __qtcm.wrapcall.wparinit), a method of the of the Python model instance (e.g., varinit), or another run list (e.g., atm_physics1).

When the run list element is a 1-element dictionary, the key of the dictionary element is the name of the routine, and the value of the dictionary element is a list specifying input parameters to be passed to the routine on call. Thus, the element:

```
{'__qtcm.wrapcall.wtimemanager': [1]}
```

calls the <u>__qtcm.wrapcall.wtimemanager</u> routine, passing in one input parameter, which in this case is the value 1.

If you want to change the order of the run list, just change the order of the list. To add or remove routines to be executed, just add and remove their names from the

Qtcm Attribute Name	NetCDF Output Name
'Qc '	'Prec'
'FLWut'	'OLR'
'STYPE'	'stype'

Table 3.1: NetCDF output names for Qtcm field variables that are different from the Qtcm and compiled QTCM1 model variable names. The netCDF names are case-sensitive.

run list. Python provides a number of methods to manipulate lists (e.g., append). Since lists are dynamic data types in Python, you do not have to do any recompiling to implement the change.

The compiled_form attribute must be set to 'parts' in the Qtcm instance in order to take advantage of the run lists feature of the class. Run lists are not available for compiled_form = 'full', because subroutine calls are hardwired in the compiled QTCM1 model Fortran code in that case.

3.7 Model Output

3.7.1 NetCDF Output

Model output is written to netCDF files in the directory specified by the Qtcm instance attribute outdir. Mean values are written to an output file beginning with qm_{-} , and instantaneous values are written to an output file beginning with qi_{-} .

The frequency of mean output is controlled by ntout, and the frequency of instantaneous output is controlled by ntouti. ntout.value gives the number of days over which to average (and if equals -30, monthly means are calculated). ntouti.value gives the frequency in days that instantaneous values are output (monthly if it equals -30). (See Section 4.7.2 for a description of other output-control variables, and see the QTCM1 manual [4] for a detailed description of how these variables control output.)

Figure 3.4 gives an example of a block of code to read netCDF output, where datafn is the netCDF filename, and id is the string name of the field variable (e.g., 'u1', 'T1', etc.). (Note that the netCDF identifier for field variables is the same as the name in Qtcm, except for the variables given in Table 3.1.)

In the code in Figure 3.4, the array value is read into data, and the longitude values, latitude values, and time values are read into variables lon, lat, and time, respectively. As netCDF files also hold metadata, a description and the units of the variable given by id, and each dimension, are read into variables ending in _name and _units, respectively.

NB: All netCDF array output is dimensioned (time, latitude, longitude) when read into Python using the **Scientific** package. This differs from the way **Qtcm**

```
import numpy as N
import Scientific as S
fileobj = S.NetCDFFile(datafn, mode='r')
data = N.array(fileobj.variables[id].getValue())
data_name = fileobj.variables[id].long_name
data_units = fileobj.variables[id].units
lat = N.array(fileobj.variables['lat'].getValue())
lat_name = fileobj.variables['lat'].long_name
lat_units = fileobj.variables['lat'].units
lon = N.array(fileobj.variables['lon'].getValue())
lon_name = fileobj.variables['lon'].long_name
lon_units = fileobj.variables['lon'].units
time = N.array(fileobj.variables['time'].getValue())
time_name = fileobj.variables['time'].long_name
time_units = fileobj.variables['time'].units
fileobj.close()
```

Figure 3.4: Example of Python code to read netCDF output. See text for description.

saves field variables, which follows Fortran convention (longitude, latitude). Please be careful when relating the two types of arrays. Section 4.7.4 for a discussion of why there is this discrepancy.

3.7.2 Visualization

The plotm method of Qtcm instances creates line plots or contour plots, as appropriate, of model output of average fields of run session(s) associated with the instance. Some examples, assuming model is an instance of Qtcm and has already executed a run session:

- model.plotm('Qc', lat=1.875): A time vs. longitude contour plot is made for the full range of time and longitude, at the latitude 1.875 deg N, for mean precipitation.
- model.plotm('Qc', time=10): A latitude vs. longitude contour plot of precipitation is made for the full spatial domain at day 10 of the model run.
- model.plotm('Evap', lat=1.875, lon=[100,200]): A contour plot of time vs. longitude of evaporation is made for the longitude points between 100 and 200 degrees E, at the latitude 1.875 deg N.
- model.plotm('cl1', lat=1.875, lon=[100,200], time=20): A deep cloud amount vs. longitude line plot is made for the longitude points between 100 and 200 degrees east, at the latitude 1.875 deg N, at day 20 of the model run.

In these examples, the number of days over which the mean is taken equals model.ntout.value. Also, the plotm method automatically takes into account the Qtcm/netCDF variable differences described in Table 3.1.

3.8 Documentation

Section 1.4 gives the online locations of the transparent copies of this manual. Model formulation is fully described in Neelin & Zeng [3] and model results are described in Zeng et al. [5] ([3] is based upon v2.0 of QTCM1 and [5] is based on QTCM1 v2.1). Additional documentation you'll find useful include:

- The qtcm Package API Documentation⁶
- The Pure-Fortran QTCM1 Manual⁷ [4]

⁶http://www.johnny-lin.com/py_pkgs/qtcm/doc/html-api/

⁷http://www.atmos.ucla.edu/~csi/qtcm_man/v2.3/qtcm_manv2.3.pdf

Chapter 4

Using qtcm

4.1 Introduction

Now that you've successfully run your first model instances, in this chapter I provide detailed explanations regarding the features of qtcm. I present these explanations in a documentary rather than didactic fashion; my goal is to document how the features work. More details are given in the code docstrings. At the end of the chapter, in Section 4.10, I provide a few cookbook ideas/examples of ways to use the model.

4.2 Model Instances

An instance of a Qtcm model is created in qtcm the same way you create an instance of any class. For instance, to instantiate two Qtcm models, model1 and model2, I type the following:

```
from qtcm import Qtcm
model1 = Qtcm(compiled_form='full')
model2 = Qtcm(compiled_form='parts')
```

In the above example, model1 uses the compiled QTCM1 model that runs the model (essentially) using the Fortran driver, while model2 uses the compiled QTCM1 model where execution order and content all the way down to the atmospheric timestep level is controlled by Python run lists. (Section 4.4 has more details about the difference between compiled forms.)

For each instance of Qtcm, copies of all needed extension modules (e.g., .so files) are copied to a temporary directory that is automatically created by Python. The full path name of that directory is saved in the instance attribute sodir. These extension modules are then associated with the specific instance through private instance attributes, and thus every instance of Qtcm has its own separate variable and name

space on both the Fortran and Python sides.¹ The temporary directory and all of its contents are deleted when the model instance is deleted.

On instantiation, Qtcm instances set all scalar field variables to their default values as given in the submodule defaults (and listed in Section A.1), and assign the fields as instance attributes. The instance attribute init_with_instance_state is set to True by default, unless overridden on instantiation.

4.3 Initializing a Model Run

In the pure-Fortran QTCM1, there are three broad classes of initialized variables:

- 1. Those that are read-in using a namelist,
- 2. Those that the are read-in from a restart file, and
- 3. Those that are set by assignment in the Fortran code.

These variables are a combination of scalars and arrays.

For qtcm, interfaces were built so that all classes of initialized variables that could be user-controlled are accessible and changeable at the Python-level. For qtcm, the set of variables that could be changed is also expanded, to include not just the first and second classes of pure-Fortran QTCM1 initialized variables. This was done to make qtcm more flexible. All variables that can be passed between the compiled QTCM1 model and Python model levels are called field variables, and are described in detail in Section sec:field.variables.

As it happens, all the namelist-set variables are scalars. In the pure-Fortran QTCM1, those variables are given default values prior to reading in of the namelist. To duplicate this functionality, on model instantiation, all scalar fields are set to their default values as given in the submodule defaults and listed in Section A.1. Most of the default values in defaults are the same as in the pure-Fortran QTCM1, but there are a few differences.² This setting of scalar defaults is the same for both compiled_form = 'full' and compiled_form = 'parts' instances. Of course, all qtcm fields are user-controllable, both via keyword input parameters at model instantiation as well as through direct manipulation of the instance attribute that stores the field variable.

The pure-Fortran QTCM1 initialized prognostic variables and right-hand sides are set in the Fortran subroutine varinit. Their they are read-in from a restart file or, as default, set by assignment. In qtcm, the same variables are initialized by a Qtcm instance method of the same name, varinit, for the case when compiled_form = 'parts'.

¹The private instance attribute is <u>__qtcm</u>. See Section 6.7.3 for details about private Qtcm instance attributes.

²One difference being mrestart, which in qtcm will have the value of 0 in contrast to the pure-Fortran QTCM1 where the default is the 1.

For the case of compiled_form = 'full', the compiled QTCM1 subroutine that is the same as in the pure-Fortran case is used, and that routine is inaccessible at the Python level. See Section 4.5.5's listing of snapshot variables, which also includes the prognostic variables and right-hand sides that are set in varinit (both Fortran and Python).

4.4 The compiled_form Keyword

The qtcm package is a Python wrap of the Fortran routines that make up QTCM1. The wrapping layer adds flexibility and functionality, but at the cost of speed. Thus, I created two types of extension modules from the Fortran QTCM1 code, one which permits very little control over the compiled Fortran *routines* at the Python level, and one that allows the Python-level to control model execution in the compiled QTCM1 model all the way down to the atmospheric timestep level.³ The former extension module corresponds to compiled_form='full' and the latter extension module to compiled_form='full'.

For compiled_form='full', the compiled portion of the model encompasses (nearly) the entire QTCM1 model as a whole. Thus, the only compiled QTCM1 model modules or subroutines that Python should interact with is the driver routine (which executes the entire model) and the setbypy module (which enables communication between the compiled model and the Python-level of model fields.⁴

For compiled_form = 'parts', the compiled portion of the model does not encompasses the model as a whole, but rather is broken up into separate units (as appropriate) all the way down to an atmosphere timestep. Thus, compiled QTCM1 model modules/subroutines that are accessible at the Python-level include those that are executed within an atmosphere timestep on up.

Because the difference in compiled forms fundamentally affects how the Qtcm instance facilitates Python-Fortran communication, this attribute must be set on instantiation via a keyword input parameter.

In the rest of this section, to avoid being verbose, when I write 'full', I mean the situation where compiled_form='full'. Likewise, when I write 'parts', I mean the situation where compiled_form='parts'.

4.4.1 Initialization for compiled_form = 'full'

For a model run of this case, the Qtcm instance will initialize the model using the Fortran varinit subroutine in the compiled QTCM1 model. This subroutine does the following:

³That control is via run lists, which are described in Section 4.6.

⁴The setbypy Python module is the wrap of the Fortran QTCM1 SetByPy module.

- If mrestart = 1, the restart file is used to initialize all prognostic variables. In terms of start date, the following rules are used:
 - 1. Variable dateofmodel is read from the restart file.
 - 2. If day0, month0, and year0 are negative, or otherwise invalid (e.g., month0 greater than 12), the invalid value is replaced with the day, month, and/or year of the day *after* that given by dateofmodel. If the value of day0, month0, or year0 is not invalid in this sense, it is not replaced.

Thus, if the restart file gives dateofmodel equal to 101102 (year 10, month 11, day 2), and day0 = -1, month0 = -1, year0 = -1, and mrestart = 1, the model will start running from year 10, month 11, day 3. If dateofmodel equals to 101102, and day0 = -1, month0 = 3, year0 = -1, the model will start running from year 10, month 3, day 3.

• If mrestart = 0, all prognostic variables and right-hand sides are set to an initial value (which for most of those variables is zero). In terms of start date, day0 is set to 1 (and thus the value of day0 previously input is ignored), and both month0 and year0 are set to 1 if their previously input values are invalid (where invalid means less than 1, or, for month0, greater than 12). Otherwise, month0 and year0 are left unchanged. Variable dateofmodel has the value it had when the variable was declared (which is determined by the compiler and usually is zero; dateofmodel will not be properly set until subroutine TimeManager is called.

Thus, if day0 = -1, month0 = -1, year0 = -1 is input into the model (say from a namelist) and mrestart = 0, the model will start running from year 1, month 1, day 1, and dateofmodel at the exit of subroutine varinit will equal its compiler-set default. If day0 = 14, month0 = 3, year0 = 11, and mrestart = 0 on input into the model, the model will start running from year 11, month 3, day 1, and dateofmodel at the exit of subroutine varinit will equal its compiler-set default.

Note that dateofmodel can thus be inconsistent with month0 and year0 at the exit of subroutine varinit.

This behavior with respect to initializing the start date is different than in QTCM1 versions 1.0 and 2.1. Please see the source code from those earlier QTCM1 versions for details.

4.4.2 Initialization for compiled_form = 'parts'

For 'parts' model, the methodology of how initialized prognostic variables, righthand sides, and start date related variables are set is controlled by the Qtcm instance attribute/flag init_with_instance_state. The initialization is (mostly) executed in the Python variant method in the following way:

- If init_with_instance_state is False: The method as described for initialization for the 'full' case is generally followed, with the exception that dateof-model is set to match day0, month0, year0, prior to exit of varinit.
- If init_with_instance_state is True: the model object will initialize the model based on the current state of the model instance. This enables you to set a model run session's initial conditions based upon the state of the prognostic variables and parameters stored at the Python level, which is accessible at runtime.

Since the init_with_instance_state = False case is mainly described by the initialization method for the 'full' case, I refer the reader to Section 4.4.1. For the case of init_with_instance_state is True, however, the task is more complicated. Specifically, for that case, initialization includes the following:

- 1. If not currently defined, variable dateofmodel is set to a default value of 0, which is specified in the module defaults.
- 2. The **mrestart** flag is ignored for variable initialization.
- 3. All prognostic variables and right-hand sides are set to an initial value (which for most of those variables is zero), unless the variable is defined at the Python level, in which case the initial value is set to the Python level defined value.
- 4. If dateofmodel is greater than 0, day0, month0, and year0 are overwritten with values derived from dateofmodel in order to set the run to start the day *after* dateofmodel.
- 5. If dateofmodel is less than or equal to 0, day0, month0, and year0 are set to their respective instance attribute values, if valid. For invalid instance attribute values, the invalid day0, month0, and/or year0 is set to 1.
- Variable dateofmodel is recalculated and overwritten to match day0, month0, year0, prior to exit of varinit.

As a result, for init_with_instance_state is True, the way you indicate to the model that a run session is a brand-new run is by setting, before the run_session method call, dateofmodel to a value less than or equal to 0, and day0, model0, and year0 to the day you want the model to begin the run session. To indicate to the model you wish to continue a run, set dateofmodel to the day *before* you want the model to start running from.

Examples:

- If day0=-1, month0=-1, year0=-1, and dateofmodel=0 is input into the model the model will start running from year 1, month 1, day 1, and variable dateofmodel at the exit of subroutine variant will equal 10101.
- If day0=14, month0=3, year0=11, and dateofmodel=0 is input into the model, the model will start running from year 11, month 3, day 14, and variable dateofmodel at the exit of subroutine variant will equal 110314.
- If day0 = 14, month0 = 3, year0 = 11, and dateofmodel = 341023 is input into the model, the model will start running from year 34, month 10, day 24, and at the exit of subroutine varinit, dateofmodel will equal 341024, with day0 = 24, month0 = 10, and year0 = 34.

4.4.3 Communication Between Python and Fortran-Levels

After initialization, the second major difference between a 'full' and 'parts' model is how and when communication between the Python and Fortran levels can occur. For the 'full' case, except for the passing in and out of variables before and after a run session, all variable passing and subroutine calling happens in the compiled QTCM1 model, with no control at the Python level. For the 'parts' case, variables can be passed between the Python and Fortran-levels at all levels down to the atmospheric timestep, and many Fortran QTCM1 subroutines can be called from the Python-level.

Passing Variables

For all compiled_form cases, variables are passed back and forth between the Python Qtcm instance level and the compiled QTCM1 model Fortran-level using the Qtcm instance methods get_qtcm1_item and set_qtcm1_item:⁵

- get_qtcm1_item(key): Returns the value of the field variable given by the string key. If the compiled QTCM1 model variable given by key is unreadable, the custom exception FieldNotReadableFromCompiledModel is thrown. The value returned is a copy of the value on the Fortran side, not a reference to the variable in memory.
- set_qtcm1_item: Sets the value of a field variable in the compiled QTCM1 model and at the Python-level, automatically overriding any previous value at both levels. Thus, calling this method will change/create the Qtcm instance

⁵All Fortran routines used to pass variables back and forth are defined in the **setbypy** module of the .so extension module stored in the Qtcm instance variable __qtcm. All Fortran wrappers that enable Python to call compiled QTCM1 model subroutines are defined in the wrapcall module stored in the Qtcm instance variable __qtcm. These modules are described in detail in Sections 6.3.1 and 6.3.2, respectively.

4.4. THE COMPILED_FORM KEYWORD

attribute corresponding to the field variable. When the compiled QTCM1 model variable is set, a copy of the Python value is passed to the Fortran model; the variable is *not passed by reference*. This value comes from the set_qtcm1_item calling parameter list, *not* from the Qtcm instance attribute corresponding to the field variable.

The **set_qtcm1_item** method has two calling forms, one with one argument and the other with two arguments:

- One argument: The method is called as set_qtcm1_item(arg), where arg is either a string giving the name of the field variable or a Field instance.
- Two arguments: The method is called as set_qtcm1_item(key, value), where key is the string giving the name of the field variable and value is the value to set the model field variable to (note value can be a Field instance).

In either calling form, if no value given, the default value as defined in module **defaults** is used.

Some compiled QTCM1 model variables are not in a state where they can be set. An example is a compiled QTCM1 model pointer variable, prior to the pointer being associated with a target (an attempt to set would yield a bus error). In such cases, the set_qtcm1_item method will throw a FieldNotReadableFromCompiledModel exception, nothing will be set in the compiled QTCM1 model, and the Python counterpart field variable (if it previously existed) would be left unchanged.⁶

Examples, typed in at a Python prompt, and assuming that model is a Qtcm instance:

- dtvalue=model.get_qtcm1_item('dt'): Retrieves the value of field variable dt (timestep) from the compiled QTCM1 Fortran model and sets it to the Python variable dtvalue.
- model.set_qtcm1_item('dt'): Sets the value of field variable dt in the compiled QTCM1 Fortran model to the default value (as given in defaults), and sets the value of Python attribute model.dt also to that default value. Remember that model.dt is a Field instance.
- model.set_qtcm1_item('dt', 2000.): Sets the value of field variable dt in the compiled QTCM1 Fortran model to 2000 (as a real), and sets the value of Python attribute model.dt also to 2000.

⁶We handle this situation in this way to enable the Qtcm instance to store variables even if the compiled model is not yet ready to accept them.

Calling Compiled QTCM1 Model Subroutines

All compiled QTCM1 model subroutines that can be called (except driver and varptrinit) are in the setbypy or wrapcall modules of the Qtcm instance private attribute __qtcm. (On Qtcm instance instantiation, __qtcm is set to the .so extension module that is the compiled QTCM1 Fortran model.) Thus, to call wmconvct in wrapcall at the Python-level, just type model.__qtcm.wrapcall.wmconvct() (where model is a Qtcm instance). For driver and varptrinit, these subroutines are not contained in a __qtcm module, and thus can be called directly (e.g., just type model.__qtcm.driver()). See Sections 6.3.1 and 6.3.2 for more information on the setbypy and wrapcall modules.

For the 'full' case, the only compiled QTCM1 model subroutine you can usefully call during a run session is driver. For the 'parts' case, while you can essentially call any subroutine given in a run list, you usually will not directly call a compiled QTCM1 model subroutine but will instead call it through including it in a run list. For example, if you have the following run list in a 'parts' model:

```
[ 'qtcminit', '__qtcm.wrapcall.woutpinit' ]
```

Running this list using the Qtcm instance method run_list will result in Qtcm instance method qtcminit first being run, then the compiled QTCM1 Fortran model subroutine woutpinit in Fortran module wrapcall being run. See Section 4.6 and Table 4.3 for a discussion and list of the standard run lists that control routine execution content and order in the 'parts' case.

4.5 Restart and Continuation Run Sessions

4.5.1 Restart Runs In the Pure-Fortran QTCM1

To enable restart of a model run, the pure-Fortran QTCM1 model writes out a restart file with the state of the prognostic variables and select right-hand sides at that point in the run (for a list of the variables, see Section 4.5.5). This binary file can then be read in by later model runs. The Fortran mrestart flag is passed in via a namelist; if mrestart is 1, the run uses the restart file (named *qtcm.restart*).

One of the problems with using the restart file to do a continuation run is that the continuation run will not be perfect. In other words, a 15 day run followed by a 25 day run based on the restart file generated at the end of the 15 day run will *not* give the exact same output as a continuous 40 day run.

4.5.2 Overview of Restart/Continuation Options In qtcm

For a Qtcm instance, in contrast to the pure-Fortran QTCM1, more than one method of continuation is available. Thus, for a continuation run, you need to tell the model

"continue from what?" The Qtcm class provides three choices for restart/continuing a run:

- 1. From a restart file: Move/rename a QTCM1 restart file to the current working directory to *qtcm.restart*.
- 2. From a snapshot from another run session (see Sections 3.4.4 and 4.5.5).
- 3. From the values of the Qtcm instance you will be calling run_session from.

Restart/continuation methods 1 and 2 both suffer from the same problem as the pure-Fortran QTCM1 restart process: They do not produce perfect restarts (see Section sec:puref90.restart for details). In this section, I discuss the restart/continuation options for each compiled_form option.

Methods 1 and 2 are best used when making a run session from a newly instantiated Qtcm instance. Method 3 is best used when executing a run session using a Qtcm instance that has already gone through at least one run session. Regardless of which method you use, however, please note that anytime you execute a run session using a Qtcm instance that already has made a previous run session, some variables *cannot be updated* between run sessions. This feature is most noticeable with the output filename, and occurs because the name persists in the compiled QTCM model, and is stored in the extension module (.so files in sodir) associated with the instance. If you wish to control all variables possible from the Python level (including output filename), you need do the run session from a new model instance.

4.5.3 Restart/Continuation for compiled_form='full' Model Instances

The only option for restart when using compiled_form = 'full' model instances is method 1, to use a QTCM1 restart file.⁷ To use this option, the value of the mrestart attribute must equal 1, the restart file must be named *qtcm.restart*, and the restart file must be in the current working directory. As with the pure-Fortran QTCM1 restart process, this method does not produce perfect restarts.

4.5.4 Restart/Continuation for compiled_form = 'parts' Model Instances

For the compiled_form = 'parts' case, all three restart/continuation methods described in Section 4.5.2 are available.

⁷The cont keyword parameter in run_session and the value of the init_with_instance_state attribute have no effect if compiled_form='full'. With 'full', the call to initialize variables all happens at the Fortran level (via the Fortran varinit, not the Python varinit), with no reference to the Python field states (or even existing Fortran field states, if present).

Method 1: From a QTCM1 Restart File

To use the QTCM1 restart file mechanism, not only must the **mrestart** attribute have a value to 1, but the **init_with_instance_state** flag also has to be **False**, otherwise the **mrestart** attribute value will be ignored. As with the pure-Fortran QTCM1 restart process, this method does not produce perfect restarts.

Method 2: From a Qtcm Instance Snapshot

You can take snapshots of the model state of a Qtcm instance by the make_snapshot instance method. This snapshot saves a copy of all the variables saved to a QTCM1 restart file (see Section 4.5.5 for the full list of fields), which then can be passed to other Qtcm instances for use in other run sessions.

The key difference between this method and method 3 (described below) is that run_session calls using the snapshot are done *without* the cont keyword input parameter (by default, cont is False). If the cont keyword is not False, it says the run session is a continuation run that uses the state of the compiled QTCM1 model for all variables that are not specified at, and read-in from, the Python level. If the cont keyword is False, the run session initializes as if it were a new run.

See Section 3.4.4 for details and an example of using snapshots to initialize a run session. Note that as with the pure-Fortran QTCM1 restart process, this method does not produce perfect restarts.

Method 3: From the Calling Qtcm Instance

This method is used when you want to make a run session that is a "true" continuation run, i.e., one that uses the current state of the compiled QTCM1 model for all variables that are not read-in from the Python level (remember that Qtcm instances hold a subset of the variables defined at the Fortran level). The key reason to use this method for a continuation run session is that the continuation is byte-for-byte the same (if no fields are changed) as if the run just went straight on through. Thus, the continuation would be perfect: A 15 day run followed by a 25 day run using the same Qtcm instance with the cont keyword will give the exact same output as a continuous 40 day run. This is not the case when making a new instance and passing a restart file or a snapshot, because a separate extension module is used for those new instances.

Control of this method is accomplished through the cont keyword input parameter to the run_session method and the init_with_instance_state attribute of a Qtcm instance:

• cont: If set to False, the run session is not a continuation of the previous run, but a new run session. If set to True, the run session is a continuation of the previous run session. If set to an integer greater than zero, the run session is a continuation just like cont = True, but the value cont is set to is used for lastday and replaces lastday.value in the Qtcm instance.

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• init_with_instance_state: If True, for a run_session call using the cont keyword, whatever the field values are in the Python instance are used in the run session. If False, model variables are set and initialized as described in Section 4.4.2. In that case, previous compiled QTCM1 model values will likely be overwritten. Thus, if you want a continuation run that uses the state of all field variables except for those you explicitly change at the Python-level, make sure init_with_instance_state is True.

(Note that the cont keyword has no effect if compiled_form is 'full'. The default value of cont in a run_session call is False. The value of keyword cont is stored as private instance attribute _cont, in case you really need to access it elsewhere; see Section 6.7.3 for more details).

The example described in Section 3.4.3 is an example of method 3 in the list above: The second run session is continued from the state of model, with the values of model's instance variables overriding any values in the compiled QTCM1 model in initializing the second run session.

This method has a few caveats worthy of note:

- The init_with_instance_state attribute value will have no effect unless the instance prognostic variables are set, i.e., unless a previous run session has been done. Another way to put it is for an initial run session right after a Qtcm instance is created, varinit will use the same initial values for prognostic variables (defined in defaults module variable init_prognostic_dict)⁸ as it would with for both init_with_instance_state set to True or False).
- Continuation run sessions using this method have to continue with the next day from wherever the last run session left off, contiguously.⁹ If you want to do a non-contiguous run, create a new Qtcm instance initialized with a snapshot instead of the continuation method describe in this section. will use restart rules to run a new model.
- When making a continuation run session using this method, you cannot change some variables, for instance, **outdir** and any of the date related variables. In fact, the only thing you should change for your continuation run session are the prognostic and diagnostic variables and **lastday**. This is because some variables cannot be updated between run sessions. As noted in Section 4.5.2, if you wish to control all variables possible from the Python level (including output filename), you need to execute the run session from a new model instance.

⁸init_prognostic_dict is the dictionary giving the default initial values of each prognostic variable and right-hand side (as defined by the restart file specification).

 $^{^{9}}$ For continuation run sessions, you keep the same extension module (the compiled .50 library), and all the values that define the state where it left off.

4.5.5 Snapshots of a Qtcm Instance

The snapshot dictionary (briefly described in Section 3.4.4), saved as the Qtcm instance attribute snapshot, and generated by the method make_snapshot, saves the current state of the following instance field variables:

Field	Shape	Units	Description
T1	(64, 44)	Κ	
Ts	(64, 42)	Κ	Surface temperature
WD	(64, 42)		
dateofmodel			Date of model coded as an integer
			as yyyymmdd
psi0	(64, 43)		
q1	(64, 44)	Κ	
rhsu0bar	(3,)		
rhsvort0	(64, 42, 3)		
title			A descriptive title
u 0	(64, 44)	m/s	Barotropic zonal wind
u0bar			
u1	(64, 44)	m/s	Current time step baroclinic zonal
			wind
v0	(64, 43)	m/s	Barotropic meridional wind
v1	(64, 43)	m/s	
vort0	(64, 42)		

These are the same variables saved to a QTCM1 restart file, and so a snapshot duplicates the restart functionality in the Python environment, but with more flexibility. Since the **snapshot** dictionary is a Python variable like any other, you can manipulate it and alter it to fit any condition you wish.

4.6 Creating and Using Run Lists

Section 3.6 provides an introduction to the role and use of run lists. A run list is a list of methods, Fortran subroutines, and other run lists that can be executed by the Qtcm instance run_list method. Run lists are stored in the Qtcm instance attribute runlists, which is a dictionary of run lists. The names of run lists should not be preceeded by two underscores (though elements of a run list may be very private variables), nor should names of run lists be the same as any instance attribute. Run lists are not available for compiled_form='full'.

4.6. CREATING AND USING RUN LISTS

The **run_list** method takes a single input parameter, a list, and runs through that list of elements that specify other run lists or instance method names to execute. Methods with private attribute names are automatically mangled as needed to become executable by the method. Note that if an item in the input run list is an instance method, it should be the entire name (not including the instance name) of the callable method, separated by periods as appropriate.

Elements in a run list are either strings or 1-element dictionaries. Consider the following example, where model is a Qtcm instance, and run_list is called using mylist as input:

The first element in mylist refers to a method that requires no positional input parameters be passed in (as shown by the None). The second and third elements in mylist also refers to methods that require no positional input parameters be passed in. The last element in mylist refers to a method with two input parameters. Note that while I use the term "method" to describe the elements, the strings/keys do not have to be only Python instance methods. The second element, for instance, refers to another run list, and the third element refers to a compiled QTCM1 model subroutine (note the __qtcm attribute).

When the run_list method is called, the items in the input run list are called in the order given in the list. For each element, the run_list method first checks if the string or dictionary key name corresponds to the key of an entry in the Qtcm instance attribute runlists. If so, run_list is called using that run list (i.e., it is a "recursive" call). If the string or dictionary key name does not refer to another run list, the run_list method checks if the string or dictionary key name is a method of the Qtcm instance, and if so the method is called. Any other value throws an exception.

If input parameters for a method are of class Field, the run_list method first tries to pass the parameters into the method as is, i.e., as Field object(s). If that fails, the run_list method passes its parameters in as the value attribute of the Field object.

If you want a variable that is being passed into a run list to be continuously updated, you have to set the parameter in the run list to a Field instance that is a Qtcm instance attribute, not just to the value of the field variable (or to a non-Field object). Otherwise, subsequent calls to that run list element will not use the updated values as input parameters.

For instance, if you had a run list element:

```
{'__qtcm.timemanager': [model.coupling_day,]}
```

and model.coupling_day were an integer (it's not by default, but pretend it was), then run_list calling __qtcm.timemanager will pass in a scalar integer rather than a binding to the variable model.coupling_day. In such a situation, if the variable model.coupling_day were updated in time, the run_list call of __qtcm.timemanager would not be updated in time. This happens because when the dictionary that is the run list element is created, the value of list element(s) attached to the dictionary element is set to the scalar value of model.coupling_day at that instant.

You can get around this feature by setting Qtcm instance attributes that will change with model execution to Field instances, and then referring to those attributes in the parameter list in the run list element. In that case:

{'__qtcm.timemanager':[model.coupling_day,]}

will use the current value of model.coupling_day anytime __qtcm.timemanager is called by run_list, if model.coupling_day is a Field object.

When **run_list**, encounters a calling input parameter that is a **Field** object, it will first try to pass the entire **Field** object to the method/routine being called. If that raises an exception, it will then try to pass just the value of the entire **Field** object. This is done to enable **run_list** to be used for both pure-Python and compiled QTCM Fortran model routines. Fortran cannot handle **Field** objects as input parameters, only values.

Table 4.3 shows all standard run lists stored in the **runlists** attribute upon instantiation of a Qtcm instance.

Of course, feel free to change the contents of any of the run lists after instantiation, or to add additional run lists to the **runlists** attribute dictionary. The ability to alter run lists at runtime gives the **qtcm** package much of its flexibility.

4.7 Field Variables and the Field Class

The term "field" variable refers to QTCM1 model variables that are accessible at both the compiled Fortran QTCM1 model-level as well as the Python Qtcm instance-level. Field variables are all instances of the Field class (though non-field variables can also be instances of Field).

Section 3.3 gives a brief introduction to the attributes and methods in a Field instance. A nitty gritty description of the class is found in its docstrings.

4.7.1 Creating Field Variables

To create a **Field** instance whose value is set to the default, instantiate with the field id as the only positional input argument. Thus:

Run List Name/Description	List Element(s) Name(s)	$\# \operatorname{Arg}(s)$
atm_bartr_mode (calculate the at-	$_{}$ qtcm.wrapcall.wsavebartr	None
mospheric barotropic mode at the	qtcm.wrapcall.wbartr	None
barotropic timestep)	$_{-}$ qtcm.wrapcall.wgradphis	None
	_first_method_at_atm_oc_step	None
atm_oc_step (calculate the atmo-	qtcm.wrapcall.wtimemanager	1
sphere and ocean models at a cou-	qtcm.wrapcall.wocean	2
pling timestep)	qtcm	None
	$_{-qtcm.wrapcall.woutpall}$	None
	qtcm.wrapcall.wmconvct	None
atm_physics1 (calculate atmo-	qtcm.wrapcall.wcloud	None
1 5	qtcm.wrapcall.wradsw	None
spheric physics at one instant)	qtcm.wrapcall.wradlw	None
	qtcm.wrapcall.wsflux	None
atm_step (calculate the entire atmosphere at one atmosphere	atm_physics1	None
	qtcm.wrapcall.wsland1	None
	qtcm.wrapcall.wadvctuv	None
	qtcm.wrapcall.wadvcttq	None
	qtcm.wrapcall.wdffus	None
timestep)	qtcm.wrapcall.wbarcl	None
	_bartropic_mode_at_atm_step	None
	$_{-}$ qtcm.wrapcall.wvarmean	None
init_model (initialize the entire	qtcminit	None
model, i.e., the atmosphere and	$_{-qtcm.wrapcall.woceaninit}$	None
ocean components and output)	$_{-}$ qtcm.wrapcall.woutpinit	None
	qtcm.wrapcall.wparinit	None
qtcminit (initialize the atmo-	$_{-qtcm.wrapcall.wbndinit}$	None
sphere portion of the entire	varinit	None
model)	qtcm.wrapcall.wtimemanager	1
	atm_physics1	None

Table 4.3: Standard run lists stored in the **runlists** attribute upon instantiation of a Qtcm instance. The run list and list element names are stored as strings.

```
foo = Field('lastday')
```

will return foo as a Field instance with foo.value set to the value listed in Section A.1. The value of all Field instances upon creation are specified in the defaults submodule of package qtcm, and listed in Sections A.1 and A.2.

To create Field instances whose attributes are set different from their defaults, you can specify the different settings in the instantiation parameter list, or change the attributes once the instance is created. See the Field docstring for details.

4.7.2 Initial Field Variables

Field variables include both model parameters that do not change for a Qtcm instance as well as prognostic variables that do change during model integration. As a result, many field variables have values different from the default values listed in Sections A.1 and A.2. In this section, I list the *initial* values of all field variables. The "initial" values are the settings for Qtcm field variables execution of the run_session method, but prior to cycling through an atmosphere-ocean coupling timestep. This is in contrast to "default" values, which the field variables are given on instantiation, if no other value is specified. Numerical values are rounded as per the conventions of Python's %g format code.

Scalars

Field	Value	Units	Description
SSTdir	value varies		Where SST files are
SSTmode	seasonal		Decide what kind of SST to use
VVsmin	4.5	m/s	Minimum wind speed for fluxes
bnddir	value varies		Boundary data other than SST
dateofmodel	10101		Date of model coded as an integer
			as yyyymmdd
day0	1	dy	Starting day; if < 0 use day in
		-	restart
dt	1200	s	Time step
eps_c	0.000138889	1/s	$1/tau_c NZ (5.7)$
interval	1	dy	Atmosphere-ocean coupling interval
it	1	-	Time of day in time steps
landon	1		If not 1: $land = ocean with fake SST$
lastday	0	dy	Last day of integration
month0	1	mo	Starting month; if < 0 use mo in
			restart

For the fields that give the input/output directory names, and the run name, the entry "value varies" is provided in the "Value" column.

4.7. FIELD VARIABLES AND THE FIELD CLASS

Field	Value	Units	Description
mrestart	0		=1: restart using qtcm.restart
mt0	1		Barotropic timestep every mt0
			timesteps
nastep	1		Number of atmosphere time steps
			within one air-sea coupling interval
noout	0	dy	No output for the first noout days
nooutr	0	dy	No restart file for the first nooutr
			days
ntout	-30	dy	Monthly mean output
ntouti	0	dy	Monthly instantaneous data output
ntoutr	0	dy	Restart file only at end of model run
outdir	value varies		Where output goes to
runname	value varies		String for an output filename
title	value varies		A descriptive title
u0bar	0		
visc4x	700000	m^2/s	Del 4 viscocity parameter in x
visc4y	700000	m^2/s	Del 4 viscocity parameter in y
viscxT	1.2e + 06	m^2/s	Temperature diffusion parameter in
			х
viscxq	1.2e + 06	m^2/s	Humidity diffusion parameter in x
viscxu0	700000	m^2/s	Viscocity parameter for u0 in x
viscxu1	700000	m^2/s	Viscocity parameter for u1 in x
viscyT	1.2e + 06	m^2/s	Temperature diffusion parameter in
			У
viscyq	1.2e + 06	m^2/s	Humidity diffusion parameter in y
viscyu0	700000	m^2/s	Viscocity parameter for u0 in y
viscyu1	700000	m^2/s	Viscocity parameter for u1 in y
weml	0.01	m/s	Mixed layer entrainment velocity
year0	1	yr	Starting year; if < 0 use year in
			restart
ziml	500	m	Atmosphere mixed layer depth \sim
			cloud base

Arrays

Field	Shape	Max	Min	Units	Description
Evap	(64, 42)	1502.56	223.552		
FLW	(64, 42)	74.5136	74.5136		
FLWds	(64, 42)	206.424	206.424		
FLWus	(64, 42)	429.708	429.708		
FLWut	(64, 42)	148.771	148.771		

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Field	Shape	Max	Min	Units	Description
FSW	(64, 42)	147.767	0		
FSWds	(64, 42)	410.895	-6.99713		
FSWus	(64, 42)	356.831	-4.49983		
FSWut	(64, 42)	332.431	0		
FTs	(64, 42)	930.115	138.383		
Qc	(64, 42)	0	0	K	Precipitation
S 0	(64, 42)	534.264	0		
STYPE	(64, 42)	3	0		Surface type; ocean or
					vegetation type over land
T1	(64, 44)	-100	-100	K	
Ts	(64, 42)	295	295	K	Surface temperature
WD	(64, 42)	350	0		
WDO	(4,)	500	0		Field capacity SIB2/CSU
					(approximately)
arr1	(64, 42)	0	0		Auxiliary optional output
					array 1
arr2	(64, 42)	0	0		Auxiliary optional output
		-	-		array 2
arr3	(64, 42)	0.138699	0.138699		Auxiliary optional output
	(01, 1-)	0.1000000	0.1000000		array 3
arr4	(64, 42)	0	0		Auxiliary optional output
	(01, 1-)	Ŭ	, in the second se		array 4
arr5	(64, 42)	0	0		Auxiliary optional output
arro	(01, 12)	Ŭ	, v		array 5
arr6	(64, 42)	0	0		Auxiliary optional output
urro	(01, 12)	0			array 6
arr7	(64, 42)	0	0		Auxiliary optional output
arr	(01, 12)	0	0		array 7
arr8	(64, 42)	0	0		Auxiliary optional output
diio	(04, 42)	0	0		array 8
psi0	(64, 43)	0	0		allay 0
q1	(64, 44)	-50	-50	K	
y⊥ rhsu0bar	(04, 44) (3,)	-50	0	11	
rhsvort0	(64, 42, 3)	0	0		
taux	(64, 42, 3) (64, 42)	0	0		
	(64, 42) (64, 42)	0	0		
tauy u0	(64, 42) (64, 44)	0	0	m/s	Barotropic zonal wind
		0		m/s	_
u1	(64, 44)	U	U	m/s	Current time step baro- clinic zonal wind
	(61 12)	0	0	m	
v0	(64, 43)	0	0	m/s	Barotropic meridional
					wind

Field	Shape	Max	Min	Units	Description
v1	(64, 43)	0	0	m/s	
vort0	(64, 42)	0	0		

4.7.3 Passing Fields Between the Python and Fortran-Levels

Section 4.4.3 discusses the differences between how the 'full' and 'parts' compiled forms pass field variables between the Python and Fortran-levels. That discussion gives a detailed description of the methods used for passing fields to and from the Python and Fortran-levels (i.e., the get_qtcm1_item and set_qtcm1_item methods).

Please note the following regarding field variables as you pass them back and forth between the Python and Fortran-levels:

- Field variables with ghost latitudes, such as u1, on the Python end are always the full variables (i.e., including the ghost latitudes). On the Fortran end, variables like u1 also always have the ghost latitudes while in the model, but when stored as restart files, do not have the ghost latitudes; the end points are not saved in restart files or written to the netCDF output files. See the QTCM1 manual¹⁰ [4] for details about ghost latitudes.
- You should assume there is only a full synchronizing between compiled QTCM1 model and Python model field variables at the beginning and end of a run session.
- If you have a variable at the Python-level, but at the compiled QTCM1 Fortran model-level the variable is not readable, if you try to call set_qtcm1_item on the variable, nothing is done, and the Python-level value is left alone. If you have a compiled QTCM1 model variable, but no Python-level equivalent, if you call set_qtcm1_item on the variable, the Python-level variable (as an attribute) is created.
- To be precise, only compiled QTCM1 model variables can be passed pass back and forth between the Python and Fortran-levels; there are many Qtcm instance attributes that do not have any counterparts at the Fortran-level.¹¹
- Although dayofmodel is described in module setbypy as an option for the get_qtcm1_item and set_qtcm1_item methods to operate on, in reality those methods cannot operate on dayofmodel, but dayofmodel is not defined in defaults.¹²

 $^{^{10}} http://www.atmos.ucla.edu/\sim csi/qtcm_man/v2.3/qtcm_manv2.3.pdf$

¹¹I use the term "field variables" to refer to compiled QTCM1 model variables that can be passed back and forth to the Python level.

¹²All field variables must be defined in **defaults** in order for the proper Fortran routine to be called according to the variable's type.

4.7.4 Field Variable Shape

Normally, Python arrays have a different dimension order than Fortran arrays. While Fortran arrays are dimensioned (col, row, slice), with adjacent columns being contiguous, then rows, and then slices, Python arrays are dimensioned (slice, row, col), with adjacent columns being contiguous, then rows, and then slices. Based on this, you would think that everytime you passed an array between the Python and Fortranlevels you would need to transpose the array.

Thankfully, we don't have to do this because f2py handles array dimension order transparently so we can refer to each element the same way whether we're in Python or Fortran. Thus, the array Qc in Fortran is dimensioned (longitude, latitude), (64,42) by default, and the Python Qtcm instance attribute Qc has a value attribute also dimensioned (longitude, latitude), (64,42) by default. And at both the Fortran and Python-levels, the first longtude, second latitude element is referred to as Qc(1,2).

In contrast, however, netCDF output saved by the compiled QTCM1 model and read into Python (using the Scientific package) is *not* in Fortran array order. Arrays read from netCDF output into Python are in Python array order, and are dimensioned (latitude, longitude) or (time, latitude, longitude). The Qtcm routines that manipulate netCDF data (e.g., plotm), however, automatically adjust for this, so you only need to be aware of this when reading in output for your own analysis (see Section 4.8).

4.8 Model Output

Section 3.7 gives an overview of how to use qtcm model output to netCDF files.

All netCDF array output is dimensioned (time, latitude, longitude) when read into Python using the Scientific package. This differs from the way Qtcm saves field variables, which follows Fortran convention (longitude, latitude). Thus, the shapes in Section 4.7.2, Appendix A, etc., are not the shapes of arrays read from the netCDF output. See Section 4.7.4 for a discussion of why there is this discrepancy.

Because netCDF files allow you to specify an "unlimited" dimension, it is possible to close a netCDF file, reopen it, and add more slices of data to the file. Thus, continuous Qtcm run sessions (i.e., those that use the cont keyword input parameter in the run_session method) will automatically append output to the netCDF output files.

Field variables with ghost latitudes, such as u1, on the Python and Fortran ends are always the full variables (i.e., including the ghost latitudes). The ghost latitudes are not written to the netCDF output files, however. See the QTCM1 manual¹³ [4] for details about ghost latitude structure.

Qtcm instances have a few built-in tools to visualization model output. These are briefly described in Section 3.7.2. Note that the plotm method is linked to a specific

¹³http://www.atmos.ucla.edu/~csi/qtcm_man/v2.3/qtcm_manv2.3.pdf

4.9. MISCELLANEOUS

```
inputs = {}
inputs['runname'] = 'test'
inputs['landon'] = 0
inputs['year0'] = 1
inputs['month0'] = 11
inputs['day0'] = 1
inputs['lastday'] = 30
inputs['mrestart'] = 0
inputs['init_with_instance_state'] = True
inputs['compiled_form'] = 'parts'
```

Figure 4.1: The initial definition of the **inputs** dictionary for examples given in Section 4.10. These settings imply that a run session will start on November 1, Year 1, last for 30 days, and will be an aquaplanet run.

Qtcm instance. Do not use plotm outside of the instance it is linked to. It must also be used only after a successful run session (i.e., not in the middle of a run session).

4.9 Miscellaneous

A few miscellaneous items/issues about the model:

- The land model runs at same timestep as the atmosphere.
- If the land model runs less often than sflux in physics1, the calculation of evaporation over the land needs to be fixed in sflux.
- The units of some field variables are not what you would expect. For instance, Qc is in energy units, i.e., K, and not mm/day. See the QTCM1 manual¹⁴ [4] for details.

4.10 Cookbook of Ways the Model Can Be Used

This cookbook of a few ways to use the model is arranged by science tasks, i.e., certain types of runs we want to do. For some of the examples below, I assume that the dictionary **inputs** is initially defined as given in Figure 4.1. All examples assume that **from qtcm import Qtcm** has already been executed.

Plain model run: Here I just want to make a single model run. Tasks: Instantiate a fresh model and execute a run session. The code to run the model is just:

¹⁴http://www.atmos.ucla.edu/~csi/qtcm_man/v2.3/qtcm_manv2.3.pdf

```
inputs['init_with_instance_state'] = False
model = Qtcm(**inputs)
model.run_session()
```

where **inputs** is initialized with the code in Figure 4.1.

Explore parameter space with a set of models: Here I want to create an entire suite of separate models, in order to determine the sensitivity of the model to changing a parameter. To do this, I instantiate multiple fresh models, and execute a run session for each instance, all within a **for** loop:

```
import os
inputs['init_with_instance_state'] = False
for i in xrange(0,1002,10):
    iname = 'ziml-' + str(i) + 'm'
    ipath = os.path.join('proc', iname)
    os.makedirs(ipath)
    model = Qtcm(**inputs)
    model.ziml.value = float(i)
    model.runname.value = iname
    model.outdir.value = ipath
    model.run_session()
    del model
```

The loop explores mixed-layer depth ziml from 0 m to 1000 m, in 10 m intervals. I create the **outdir** directory before every model call, since the compiled QTCM1 model requires the output directory exist, specifying the run name and output directory as the string **iname**. The output directories are assumed to all be in the *proc* sub-directory of the current working directory. **inputs** is initialized with the code in Figure 4.1.

- Conditionally explore parameter space: Here I want to conditionally explore the parameter space, on the basis of some mathematical criteria. To do this, I instantiate a model, evaluate results using that criteria, and run another fresh model depending on the results (passing the previous model state via a snapshot), all within a while loop. Note that this type of investigation is very difficult to automate if all you can use are shell scripts and Fortran. See Figure 4.2 for a detailed example.
- With interactive adjustments at run time: The example in Figure 3.4.3 illustrates this type of run. In this example, I instantiate a fresh model, execute a run session, analyze the output, change variables in the model instance, and then execute a continuation run session.

4.10. COOKBOOK OF WAYS THE MODEL CAN BE USED

Test alternative parameterizations: I've already described how we can use run lists to arbitrarily change model execution order and content at run time. We can take advantage of Python's inheritance abilities, along with run lists, to simplify this. Figure 4.3 provides an example of this use.

Of course, you can use pre-processor directives and shell scripts to accomplish the same functionality seen in Figure 4.3 using just Fortran. The Python solution, however, shortcuts the compile/linking step, and enables you to easily do run time swapping between subroutine choices based upon run time calculated tests (see Figure 4.2 for an example of such tests).

```
import os
import numpy as N
maxu1 = 0.0
while maxu1 < 10.0:
    iziml = 0.1 * maxu1
    iname = 'ziml-' + str(iziml) + 'm'
    ipath = os.path.join('proc', iname)
    os.makedirs(ipath)
    model = Qtcm(**inputs)
    try:
        model.sync_set_py_values_to_snapshot(snapshot=mysnapshot)
        model.init_with_instance_state = True
    except:
        model.init_with_instance_state = False
    model.ziml.value = iziml
    model.runname.value = iname
    model.outdir.value = ipath
    model.run_session()
    maxu1 = N.max(N.abs(model.u1.value))
    mysnapshot = model.snapshot
    del model
```

Figure 4.2: This code explores different values of mixed-layer depth ziml for 30 day runs, as a function of maximum u1 magnitude, until it finds a case where the maximum u1 is greater than 10 m/s. (The relationship between ziml and the maximum of the speed of u1, where ziml = 0.1 * maxu1, is made up.) With each iteration, the new run uses the snapshot from a previous run to initialize (as well as the new value of ziml); the try statement is used to ensure the model works even if mysnapshot is not defined (which is the case the first time around). The inputs dictionary is initialized with the code in Figure 4.1.

```
import os
class NewQtcm(Qtcm):
    def cloud0(self):
        [...]
    def cloud1(self):
        [...]
    def cloud2(self):
        [...]
    [...]
inputs['init_with_instance_state'] = False
for i in xrange(10):
    iname = 'cloudroutine-' + str(i)
    ipath = os.path.join('proc', iname)
    os.makedirs(ipath)
    model = NewQtcm(**inputs)
    model.runlists['atm_physics1'][1] = 'cloud' + str(i)
    model.runname.value = iname
    model.outdir.value = ipath
    model.run_session()
    del model
```

Figure 4.3: Let's say we have 9 different cloud physics schemes we wish to try out in 9 different runs. The easiest way to do this is to create a new class NewQtcm that inherits everything from Qtcm, and to which we'll add the additional cloud schemes (cloud0, cloud1, etc.). In the for loop, I change the cloud model run list entry in the run list that governs atmospheric physics at one instant to whatever the cloud model is at this point in the loop. The inputs dictionary is initialized with the code in Figure 4.1. Of course, we could do the same thing by running the 9 models separately, but this set-up makes it easy to do hypothesis testing with these 9 models. For instance, we can create a test by which we will choose which of the 9 models to use: Within this framework, the selection of those models can be altered by changing a string.

Chapter 5

Troubleshooting

5.1 Error Messages Produced by qtcm

- Error-Value too long in SetbyPy module getitem_str for *key*: This message is produced by the Fortran subroutine getitem_str in the module SetbyPy in the compiled QTCM1 Fortran code. The code is in the file *setbypy.F90*. This error occurs when the Fortran variable whose name is given by the string *key* has a value that is greater than the local parameter maxitemlen in getitem_str. To fix this, you have to go into *setbypy.F90* and change the value of maxitemlen.
- Error-real_rank1_array should be deallocated: Fortran module SetByPy's subroutine getitem_real_array generates this message (or a similar message for other ranks) if the Fortran variable for the input *key* are allocated on entry to the routine. This may indicate the user has written another Fortran routine to access the real_rank1_array variable outside of the standard interfaces..
- Error-Bad call to SetbyPy module ...: Often times, this error occurs because a get or set routine in SetByPy tried to act on a variable for which the corresponding input *key* is not defined. The solution is to add that case in the if/then construct for the get and set routines in SetByPy and rebuild the extension modules.

5.2 Other Errors

Python cannot find some packages: This error often happens when the version of Python in which you have installed all your packages is not the version that is called at the Unix command line by typing in python. To get around this, define a Unix alias that maps python2.4 (or whichever version of Python has all your packages installed) to python. If you have multiple Python's installed on your system, you might have to use a more specific name for the Python executable. As a result, you may have to change the test scripts in *test* in the qtcm distribution directory.

- get_qtcm1_item and compiled QTCM1 model pointer variables: If you try to use the get_qtcm1_item method on a compiled QTCM1 model pointer variable (i.e., u1, v1, q1, T1), before the compiled model variant subroutine is run, you'll get a bus error with no additional message.
- Mismatch between Python and Fortran array field variables: You change an array field variable on the Python side, but it seems like the wrong elements are changed on the Fortran side. Or you type in the same index address for accessing a qtcm netCDF output array as well as its Qtcm instance attribute counterpart, and find you get different answers. Some possible reasons and fixes:
 - This will occur if you haven't accounted for the difference in how field variables are saved at the Python-level, Fortran-level, and in a netCDF file. All netCDF array output is dimensioned (time, latitude, longitude) when read into Python using the Scientific package. This differs from the way Qtcm saves field variables, *both* at the Python- and Fortran-levels, which follows Fortran convention (longitude, latitude).

Note that the way Qtcm saves field variables at the Python- and Fortranlevels is different than the default way Python and Fortran save arrays. Section 4.7.4 for more information.

- You may have forgotten that array indices in Python start at 0, while indices in Fortran (generally) start at 1. Also, ranges in Python are exclusive at the upper-bound, while ranges in Fortran are inclusive at the upper-bound. (Both Python and Fortran array indice ranges are inclusive at the lower-bound.)
- You may have forgotten some field variables have ghost latitudes, and thus there are extra latitude bands when the array is stored as a Python or Fortran field variable, but there are *no* extra latitude bands when the array is stored as netCDF output (the QTCM1 output routines strip off the ghost latitudes when writing those field variables out). See the QTCM1 manual¹ [4] for details about ghost latitudes.

The safest and easiest way to tell whether the variable has a ghost latitudes is to look at its shape. A call to the Qtcm instance method get_qtcm1_item will give you the array, and the use of NumPy's shape function will give you the shape.

 $^{^{1}}http://www.atmos.ucla.edu/\sim\!csi/qtcm_man/v2.3/qtcm_manv2.3.pdf$

Chapter 6

Developer Notes

6.1 Introduction

This section describes programming practices and issues related to the qtcm package that might be of interest to users wishing to add/change code in the package. Please see the package API documentation,¹ which includes the source code, for details.

6.2 Changes to QTCM1 Fortran Files

The source code used to generate the shared object files used in this Python package is unchanged from the pure-Fortran QTCM1 model source code, except in the following ways:

- The suffix of all source code files has been changed from .*f90* to .*F90*, in order to ensure the compiler preprocesses the source code. Some compilers use the capitalization to tell whether or not to run the code through a preprocessor.
- In all .F90 files, occurrences of:

```
Character(len=130)
```

are changed to:

```
Character(len=305)
```

This enables the model to properly deal with longer filenames. The number "305" is chosen to make search and replace easier.

• In *qtcmpar.F90*, the **eps_c** variable is changed from an unchangable parameter to a changeable real, so that it can be changed in the model at runtime.

¹http://www.johnny-lin.com/py_pkgs/qtcm/doc/html-api/

- All occurrences of an underscore ("_") character in a subroutine or function name are removed. The presence of the underscore messes up the dynamic lookup mechanism for the f2py generated extension module. The following names are changed, both in subroutine definitions and calls:
 - out_restart to outrestart,
 - save_bartr to savebartr,
 - grad_phis to gradphis.
- *driver.F90* is changed so that program *driver* becomes a subroutine, and subroutine *driverinit* is deleted (along with all calls to it) because basic model initialization is handled at the Python level.
- In *clrad.F90*, subroutine cloud, the first COUNTCAP preprocessor macro, a comment line for that ifdef is moved to prevent a warning message during building with f2py.
- The order of subroutine qtcminit is changed. The original pure-Fortran QTCM1 qtcminit code has the following calling sequence:

```
Call parinit !Initialize model parameters
Call varinit !Initialize variables
Call TimeManager(1) !mm set model time
Call bndinit !input boundary datasets
Call physics1 !diagnostic fields for initial condition
```

For the qtcm package, I've altered this order so bndinit comes after parinit but before varinit:

> Call parinit !Initialize model parameters Call bndinit !input boundary datasets Call varinit !Initialize variables Call TimeManager(1) !mm set model time Call physics1 !diagnostic fields for initial condition

This is done because STYPE is not read in for the landon True case until bndinit, but in varinit STYPE is used to calculate the original values of WD for the non-restart case. This also corrects the conflicting order found in the pure-Fortran QTCM1 manual (compare pp. 29 and 32). As far as I can tell, bndinit has no dependencies that require it to come after timemanager or varinit.

In addition, the Fortran files *setbypy.F90*, *wrapcall.F90*, and *varptrinit.F90* are added. The routines in these files, however, just add more flexibility and functionality to the model; they do not automatically affect any model computations. See Section 6.3 for details.

6.3 New Interfaces and Fortran Functionality

As described in Section 6.2, the Fortran files *setbypy.F90*, *wrapcall.F90*, and *varp-trinit.F90* are added to the QTCM1 source directory. The first two files define the Fortran 90 modules (SetbyPy and WrapCall) needed to interface the Python and Fortran levels. The last file defines a new Fortran subroutine varptrinit that associates QTCM1 model pointer variables at the Fortran level. In a pure-Fortran run of QTCM1, this occurs in subroutine varinit; for a compiled_form='parts' run, since the functionality of the Fortran varinit is now in the Python varinit method, a separate Fortran pointer association subroutine needed to be defined. The Fortran subroutine varptrinit is called as the varptrinit function of the compiled_form='parts'.so extension module.

6.3.1 Fortran Module SetbyPy

Design Description

This module defines functions and subroutines used to read variables from the Fortranlevel to the Python-level, and in setting Fortran-level variables using the Python-level values. These routines are used by Qtcm methods get_qtcm1_item and set_qtcm1_item (and dependencies thereof) to "get" and "set" the Fortran-level variables. Note that the Fortran module SetbyPy is referred to in lowercase at the Python level, i.e., as the attribute __.qtcm.setbypy of a Qtcm instance.

Because Fortran variables are not dynamically typed, separate Fortran functions and subroutines need to be defined to get and set variables of different types.² The Qtcm methods get_qtcm1_item and set_qtcm1_item know which one of the Fortran routines to call on the basis of the type and rank of the value for the field variable in the defaults submodule. This is why all field variables need to have defaults defined in defaults. For array variables, the field variable defaults also provide the rank of the Fortran-level variable being gotten or set. However, the array default values do *not* have to have the same shape as the Fortran-level variables; on the Python-side, variable shape adjusts to what is declared on the Fortran-side. Thus, if you change the resolution of the compiled QTCM1 model, you do not have to change the dimensions of the field variable values in defaults.

The Qtcm method get_qtcm1_item directly calls the SetByPy routines. The Qtcm method set_qtcm1_item makes use of private instance methods that make the calls

²The interface construct in Fortran 90 is supposed to provide a way to create a single interface to multiple routines, e.g.:

Interface setitem
Module Procedure setitem_real, setitem_int, setitem_str
End Interface

This construct, however, causes a bus error (Mac OS X 10.4, Intel). Thus, I put the same functionality in the Python code.

to the **SetByPy** routines.

For scalar field variables, SetByPy provides functions and subroutines that provide the value of the variable on output. For array field variables, SetByPy dynamic *module* arrays are used to pass array variables in and out; I could not get the SetByPy Fortran routines to set locally defined dynamic arrays (that is, locally within a function or subroutine).³ In the SetByPy module, these dynamic arrays are defined as follows:

```
Real, allocatable, dimension(:) :: real_rank1_array
Real, allocatable, dimension(:,:) :: real_rank2_array
Real, allocatable, dimension(:,:,:) :: real_rank3_array
```

For all field variables, scalar or array, the SetByPy module has a fourth module variable defined, is_readable, that the Fortran get and set routines will set to .TRUE. if the variable is readable and .FALSE. if not (it's declared as a logical variable). This Fortran variable can be used to prevent Python from accessing pointer variables that aren't yet associated to targets.

In general, SetByPy routines make use of Fortran constructs to enable them to accomodate all possible variables of a given type and shape. However, for string scalars, the SetByPy function getitem_str has to have a return value of a predefined length, in order to work properly. That length is given by the parameter maxitemlen and is set to 505 (the value is chosen to be larger than all filename variables described in Section 6.2 and to be easily found in the *.F90* files).

Module Structure

If you're a Fortran programmer, you can probably get all the information in this section from just reading the *setbypy.F90* file directly. This description of the module structure, however, permits me to highlight what you need to do if you want to make additional compiled QTCM1 variables accessible to Python Qtcm objects.

- All Use statements are given in the beginning of the SetByPy module. These statements cover nearly all of the QTCM1 Fortran modules that contain variables of interest. If the QTCM1 variable you're interested in isn't in a module listed here, you'll have to add your own Use statement of that module here.
- Next comes the definitions for the real_rank1_array, real_rank2_array, and real_rank3_array dynamic array variables, and the is_readable boolean variable.
- The Contains block of the module defines the module routines called by the Qtcm instance methods to set and get the compiled QTCM1 model variables. The routines are:

³I tried to implement Fortran subroutine getitem_real_array using traditional array dimension passing (e.g., subroutine foo(nx, ny, a)) as well as declaring the allocatable array inside the subroutine, but neither option worked on my f2py (version 2.3816) and Python (version 2.4.3).

- Function getitem_real
- Subroutine getitem_real_array
- Function getitem_int
- Function getitem_str
- Subroutine setitem_real
- Subroutine setitem_real_array
- Subroutine setitem_int
- Subroutine setitem_str

Each of the routines in the module Contains block is essentially a list of if/elseif statements. The list tests for the name of the variable of interest (a string), and gets or sets the compiled QTCM1 model variable corresponding to that name. For pointer array variables, a test is also made as to whether or not the variable has been associated. If not, the variable is not readable and is_readable is set to .FALSE. accordingly.

If you wish to add another compiled QTCM1 model variable to be accessible to Qtcm instance methods get_qtcm1_item and set_qtcm1_item, just add another if/elseif, like the other if/elseif blocks, in the Fortran set and get routines corresponding to the QTCM1 variable type (scalar vs. array, and real, integer, or string). On the Python side, add an entry in defaults corresponding to the new field variable you've created access to. I would strongly recommend making the Python name of your new field variable (given in defaults) be the same as the compiled QTCM1 model variable name.

6.3.2 Fortran Module WrapCall

Most of the time, if you want to call a compiled QTCM1 model subroutine from the Python level, you will use the version of the subroutine that is found in this Fortran module. Note that the Fortran module WrapCall is referred to in lowercase at the Python level, i.e., as the attribute __.gtcm.wrapcall of a Qtcm instance.

All the routines in this module do is wrap one of the compiled QTCM1 model routines. For instance, WrapCall subroutine wadvcttq is defined as just:

Subroutine wadvcttq Call advcttq End Subroutine wadvcttq

All subroutines in this module begin with "w", with the rest of the name being the Fortran QTCM1 subroutine name. The calling interface for the "w" version is the same as the Fortran QTCM1 original version. There are no subroutines in this module that do not have an exact counterpart in the Fortran QTCM1 code, and thus this module's subroutines sole purpose is to call other subroutines in the compiled QTCM1 model.

These wrapper routines are needed because f2py, for some reason I can't figure out, will not properly wrap Fortran routines (that are then callable at the Python level) that create local arrays using parameters obtained through a Fortran use statment. Thus, as an example, a Fortran subroutine foo with the following definition:

subroutine foo
 use dimensions
 real a(nx,ny)
 [...]
end subroutine foo

where **nx** and **ny** are defined in the module varsdimensions, will return an error, with the result that the extension module will not be created, or an extension modules that yields output that is different from running the pure-Fortran version of QTCM1.

By wrapping these calls into this file, I also avoid having to separate out the Fortran QTCM1 subroutines into separate *.F90* files. For Fortran subroutines that you want callable from the Python level, f2py seems to require each Fortran subroutine to be in its own file of the same name (e.g., the version of *driver.F90* for this package). If several Fortran subroutines are all found in a single *.F90* files, f2py seems unable to create wrappers for those subroutines.

6.4 Python qtcm and Pure-Fortran QTCM1 Differences

This section describes differences between how the qtcm package and the pure-Fortran QTCM1 assign some varables. A list of changes to the QTCM1 Fortran Files for use in the qtcm package is found in Section 6.2.

6.4.1 QTCM1 driverinit

In the pure-Fortran version of QTCM1, by default, the following variables are set by reference (as given below), not by value, in the **driverinit** routine:⁴

⁴In the pure-Fortran version of QTCM1, this routine is found in *driver.F90*.

```
lastday = daysperyear
viscxu0 = viscU
viscyu0 = viscU
visc4x = viscU
visc4y = viscU
viscxu1 = viscU
viscyu1 = viscU
viscyT = viscT
viscyT = viscT
viscyq = viscQ
viscyq = viscQ
```

Thus, in pure-Fortran QTCM1, if you change daysperyear, viscU, etc. and recompile (as needed), you will automatically change lastday, viscxu0, etc. (Though, in the pure-Fortran QTCM1, the default values may be overwritten by namelist input values.)

The driverinit routine is eliminated in the Python qtcm package. Instead, inital values of field variables are specified in the defaults submodule and set by value to attributes of the Qtcm instance. Thus, for instance, in a Qtcm instance, lastday is set to 365 by default, not to some variable daysperyear. For the diffusion and viscosity terms, the Qtcm instance attributes corresponding to those terms are set to literals.⁵

In contrast, in the pure-Fortran QTCM1, driverinit declares local variables viscU, viscT, and viscQ, and reads values into those variables via the input namelist. Those values are then used to set viscxu0, viscyu0, etc., as described above. In pure-Fortran QTCM1, viscU, viscT, and viscQ are not directly accessed anywhere else in the model. Thus, viscU, viscT, and viscQ are not defined as field variables in the qtcm package, and Qtcm instances do not have attributes corresponding to those names. Additionally, if you wish to change a viscosity parameter visc* (given above), the parameter for each direction must be set one-by-one even if the flow is isotropic.

6.4.2 The variant Routine

One of the functions of the pure-Fortran QTCM1 varinit subroutine is to associate the pointer variables u1, v1, q1, and T1. For the extension modules in the qtcm package, a Fortran subroutine varptrinit is added that can also do this association. This subroutine is called in the Qtcm instance method varinit⁶ (which duplicates and extends the function of its pure-Fortran counterpart, enabling alternative ways of handling restart).

The varptrinit is not accessed via wrapcall. Remember that wrapcall contains only those routines that were in the original pure-Fortran QTCM1 code, and that we want to have access to at the Python level.

⁵Those literals are defined by **defaults** private module variables **__viscT**, **__viscQ**, and **__viscU**. ⁶http://www.johnny-lin.com/py_docs/qtcm/doc/html-api/qtcm.qtcm.Qtcm-class.html#varinit

6.4.3 The qtcm Method of Qtcm

The Qtcm method qtcm duplicates the functionality of the qtcm subroutine in the pure-Fortran QTCM1 model. There are a few differences, however. First, the qtcm method for Qtcm instances does not include a call to cplmean, which uses mean surface flux for air-sea coupling. This state is consistent with the pure-Fortran QTCM1 pre-processor macro CPLMEAN being off. Thus, if you wish to use mean surface flux for air-sea coupling, you will have to revise the qtcm method of Qtcm to call cplmean. You'll also have to check for any other code additions needed that are associated with the CPLMEAN macro.

Second, the qtcm method for Qtcm instances does not include the option of not using the atmospheric boundary layer model. This is consistent with macro NO_ABL being off. If you wish to have no atmospheric boundary layer model, change the run list atm_bartr_mode so that the wsavebartr and wgradphis routines are not called. You'll also have to check for any other code additions needed that are associated with the NO_ABL macro.

6.4.4 Miscellaneous Differences

- In Python Qtcm instances, dateofmodel is set to 0 by default. In contrast, in the compiled QTCM1 model, the default (i.e., initial value) is calculated from day0, month0, and year0. See Section 4.4.1 for details.
- The Qtcm instance attribute __qtcm is not copyable using copy.deepcopy.
- In general, when executing a Qtcm instance method, if you change a Qtcm instance attribute that has a counterpart in the compiled QTCM1 model, the compiled QTCM1 counterpart is not changed until the end of the method. Likewise, if you call a compiled QTCM1 model subroutine and change a compiled QTCM1 model variable with a Qtcm instance counterpart, the Qtcm instance counterpart is not changed until the end of the subroutine.
- In general, even though some of the compiled QTCM1 model Fortran subroutines/functions have counterparts in Qtcm that duplicate the former's functionality, the Fortran versions are kept intact so that the compiled_form = 'full' case will work.

6.5 Considerations When Adding Fortran Code

In this section I describe issues to consider if you wish to add your own compiled code to the package as separate extension modules. (This is different from creating new standard extension modules, which is described in Section 6.6.):

- The Qtcm class assumes that the directory path to the original shared object file is the same as for the package_version module.
- If you want to be able to pass other Fortran variables in and out to/from Python, please see the Section 6.3.1 discussion of the Fotran SetByPy module.
- Fortran and Python routines to get and set compiled QTCM1 model arrays are currently written only for floating point array.
- If you ever change Qtcm instance method <u>_set_qtcm_array_item_in_model</u> to work with non-floating point values, you will also have to change the array handling section in <u>set_qtcm1_item</u>.
- The restart mechanism in the pure-Fortran QTCM1 model is *not* bit-for-bit correct. Thus, if you compare the final output from a 40 day run with a 30 day run restarted from a 10 day run, the output will not be the same. This behavior has been duplicated in Qtcm instances when the mrestart flag is used and applicable.
- When creating new extension modules using the *src* makefile, be sure you first use the make clean command to clean-up any old files.

6.6 Creating New Standard Extension Modules

The steps involved in creating the standard extension modules (e.g., _qtcm_full_365.so, etc.) on installation are given in Section 2.4. The makefile provided in /buildpath/src uses a Fortran compiler to create the object code, runs f2py to create the shared object file in src, and moves the shared object files into .../lib, overwriting any pre-existing files of the same name. In this section, I describe the makefile and f2py in a little more detail, in case you wish to create standard extension modules with additions from the ones the default makefile creates.

6.6.1 Makefile Rules

This section describes the rules of the makefile found in the *src* directory of the qtcm distribution. This makefile is used by the Python package to create the extension module (*.so* files) imported and used by qtcm objects (as described in Section 2.4). The makefile will, in general, be used only during qtcm installation, but if you wish to recompile the QTCM1 libraries and make changes in the Python extension module, you'll want to use/change this makefile.

clean Removes old files in preparation for compiling new extension modules.

- libqtcm.a Creates library *libqtcm.a* that contains all QTCM1 object files in the directory *src*, except *setbypy.o*, *wrapcall.o*, *varptrinit.o*, and *driver.o*. This archive is compiled with the netCDF libraries. Previous versions of *libqtcm.a* are overwritten.
- _qtcm_full_365.so Creates the extension module _qtcm_full_365.so. f2py is run on applicable code in *src*, and the extension module is moved to ../*lib*. Any previous versions of ../*lib*/_qtcm_full_365.so are overwritten.
- _qtcm_parts_365.so Creates the extension module _qtcm_parts_365.so. f2py is run on applicable code in *src*, and the extension module is moved to ../*lib*. Any previous versions of ../*lib/_qtcm_parts_365.so* are overwritten.

6.6.2 Using f2py

This section briefly describes how f2py is used in the makefile during the creation of the extension modules. F2py is a program that generates shared object libraries that allow you to call Fortran routines in Python. F2py comes with Python's NumPy array handling package, so you do not need to install anything extra if you have NumPy already installed.

To create the extension modules in qtcm using the makefile described in Section 6.6.1, I use a method similar to the "Quick and Smart Way,"⁷ described in the f2py manual. For the _qtcm_full_365.so extension module, the f2py call is:

```
f2py --fcompiler=$(FC) -c -m _qtcm_full_365 driver.F90 \
    setbypy.F90 libqtcm.a $(NCLIB)
```

and for the _qtcm_parts_365.so extension module, the call is:

```
f2py --fcompiler=$(FC) -c -m _qtcm_parts_365 \
            varptrinit.F90 wrapcall.F90 setbypy.F90 \
            libqtcm.a $(NCLIB)
```

For both calls, FC and NCLIB are the environment variables in the makefile specifying the Fortran compiler and netCDF libraries, respectively. The -m flag specifies the extension module name (without the .so suffix). The .F90 files specify the files that have modules and routines that will be accessible at the extension module level, and the rest of the Fortran files in QTCM1 are compiled and archived in a library *libqtcm.a.* For f2py to work properly, the .F90 files may define *only one* module or routine.

If you add Fortran files containing new modules, and you wish those modules to be accessible at the Python level, compile your new code with f2py. If we have a file of such new code, *newcode.F90*, the f2py call to create the _*qtcm_parts_365.so* extension module will become:

⁷http://cens.ioc.ee/projects/f2py2e/usersguide/index.html#the-quick-and-smart-way

```
f2py --fcompiler=$(FC) -c -m _qtcm_parts_365 \
    varptrinit.F90 wrapcall.F90 setbypy.F90 \
    newcode.F90 \
    libqtcm.a $(NCLIB)
```

If you write new Fortran code for the compiled QTCM1 model that will *not* be accessed from the Python-level, just add the object code filename to the variable QTCMOBJS in the makefile; you don't have to do anything else. If you are adding Fortran code to existing Fortran modules, it's even easier: You don't need change the makefile. Note that for 64 bit processor machines, you may have to use f2py with the -fPIC flag; see Section 2.8.4 for details on how the lines above will change.

6.6.3 Two Examples

A Function: Let's say you have written a piece of Fortran code called *myfunction.F90* that contains one function called *myfunction*, and you want to have this function callable from the Python level through the Qtcm instance method __qtcm.myfunction. Do the following:

- 1. Move myfunction.F90 to src in the qtcm distribution directory /buildpath.
- 2. Add myfunction.o to the end of the object file list lines after the target names _qtcm_full_365.so and _qtcm_parts_365.so.
- 3. In the _qtcm_full_365.so and _qtcm_parts_365.so target descriptions, add myfunction.F90 to the beginning of the list of .F90 names in the f2py lines.

A Module: Let's say you have written a piece of Fortran code called *mymod-ule.F90* that contains the Fortran module MyModule containing multiple routines and variables. You want to have those routines and variables callable from the Python level through the Qtcm instance attribute __qtcm.mymodule. The steps to add MyModule to the extension modules are exactly the same as for a single function, with mymodule being substituted in the makefile everywhere you have myfunction.

6.7 Attributes and Methods in Qtcm Instances

In this section I describe some attributes, particularly private ones, that may be of interest to developers. As is the convention in Python, private attributes and methods are prepended by one or two underscores, with two underscores being the "more" private attribute. Please see the package API documentation⁸ for details about all variables, including private variables.

⁸http://www.johnny-lin.com/py_pkgs/qtcm/doc/html-api/

6.7.1 Public num_settings Submodule Attributes/Methods

- **typecode**: This module function returns the type code of the data array passed in as its argument.
- typecodes: This dictionary is the same as the NumPy (or Numeric and numarray) dictionary typecodes, except that the character 'S' and 'c' are added to the typecodes['Character'] entry, if absent. This functionality is added because I found typecodes['Character'] had different values in Mac OS X and Ubuntu GNU/Linux.

6.7.2 Private qtcm Submodule Attributes

This submodule of the package qtcm is the module that defines the Qtcm class.

- _init_prog_dict: This dictionary contains the default values of all prognostic variables and right-hand sides that can be initialized. In the submodule qtcm, it is set to the init_prognostic_dict module variable in submodule defaults.
- _init_vars_keys: List of all keys in _init_prog_dict, plus 'dateofmodel' and 'title'. These names correspond to the field variables that are usually written out into a restart file.
- _test_field: Field object instance used in type tests.

6.7.3 Private Qtcm Attributes

- _cont: A boolean attribute that is True if the run session is a continuation run session and False if not. Set the value passed in by the keyword cont when the run_session method is executed.
- _monlen: Integer array of the number of days in each month, assuming a 365 day year.
- __qtcm: The extension module that is the compiled QTCM1 Fortran model for this instance. This attribute is unique for every instance: The extension module .so file is first copied to a temporary directory (given by the sodir instance attribute) and then imported to the Qtcm instance. This private attribute is set on instantiation.
- _qtcm_fields_ids: Field ids for all default field variables, set on instantiation.
- <u>runlists_long_names</u>: Dictionary holding the descriptions of the standard run lists. The keys of the dictionary are the names of the standard run lists.

6.8 Creating Documentation

I use the *make_docs* shell script in *doc* creates all these documents. Briefly, that script does the following:

- In the *doc/latex* directory, uses python to run *code_to_latex.py*, which generates the LATEX files describing the current qtcm package settings, including text in the manual which gives all uses of the current version number.
- LATEX is run on the LATEX files in the *doc/latex* directory. The PDF generated by the run is moved from *doc/latex* to *doc*.
- LATEX2HTML is run on the LATEX files in *doc/latex*. The HTML files generated by the run are moved to *doc/html*.
- epydoc is run on the qtcm package libraries. This is run in *doc*, to make use of the *epydoc* configuration file present there. The syntax from the command line is:

epydoc -v --config epydocrc [name]

[name] is either qtcm, if the qtcm package is installed in a directory listed in sys.path, or [name] is the name of the directory the qtcm package is located in (e.g., /usr/lib/python2.4/site-packages/qtcm).

The *make_docs* script cannot be used without customizing it to your system, so please **DO NOT USE IT** if you do not know what you are doing. You could easily wipe out all your documentation by mistake.

CHAPTER 6. DEVELOPER NOTES

Chapter 7 Future Work

This section describes the features and fixes I plan to work on in this package. The most urgent items are listed closer to the beginning of the lists.

- Automate the installation using Python's **distutils**¹ utilities.
- Describe a way of using job control (either via the operating system or IPython's jobctrl module) to do a quick-and-dirty parallelization of multiple Qtcm instance run sessions. Or use some sort of threading to fire up two simulataneously running models. Check that the simultaneously running models have different memory space.
- Add capability for *create_benchmark.py* to overwrite existing benchmark files.
- Make compiled_form set to 'parts' as the default instantiation. Change documentation accordingly.
- Currently, the Qtcm plotm method works only on 3-D output (time, latitude, longitude). Some of the fields in the netCDF output files are 2-D. Add the capability to plot_netcdf_output in the plot submodule to handle 2-D fields.
- Add documentation about removing temporary files. Add documentation in Section 4.2 of details of what occurs during instantiation of a Qtcm instance.
- Add the units and long names for all field variables in the **defaults** module.
- Create a keyword to automatically change precipitation and evaporation units to mm/day (or similar).
- Add ability to calculate and plot fields at different pressure levels. Create another module like defaults that specifies the vertical fields and gives the equation to use to calculate those fields; call the module "derivfields" or something similar.

¹http://docs.python.org/dist/dist.html

- Throughout the qtcm package I use the condition N.rank(arg) = 0 to test whether arg is a scalar. This works fine for numpy objects, but it does not work properly for Numeric and numarray arrays. In those array packages, rank('abc') returns the value 1. This is not a problem, as long as everyone has numpy, but in order to make the package interoperable, I need to find a better way of testing for scalars. The definitions of isscalar need to be changed in num_settings.
- num_settings needs to be changed to truly enable me to test whether qtcm works for numarray and Numeric arrays. The tests do not do this right now, because num_settings defaults to numpy, if it exists.
- Create makefiles for other platforms.
- A few fields (e.g., u1) have data for extra latitude bands, due to the use of "ghost latitudes" as part of the implementation of the numerics. Details are found in the QTCM1 manual² [4].

Though adjusting to this idiosyncracy is not that difficult, in the future I hope to implement a method of handing fields with ghost latitudes so that they have the same dimensions as the other gridded output variables. In order to do this, I plan to write a Python method to read the Fortran generated binary restart file.

- Change the **set_qtcm_item** method so that it can automatically accomodate setting Fortran real variables if integer values are input.
- Currently, the get_item_qtcm and set_item_qtcm methods will not work on integer and character arrays, only scalars and real arrays. Add that missing functionality to those methods.
- Currently, the make_snapshot method duplicates the functionality of the pure-Fortran QTCM1 restart file mechanism. However, the restart file mechanism itself does not do a true restart. A continuous run does not provide the same results as two runs over the same period, joined by the restart file.

To see whether saving more variables would do the trick, I altered make_snapshot to store all Python level variables (i.e., self._qtcm_fields_ids). However, the restart failing described above still continued. In the future, I hope to figure out exactly how many variables are needed in order to make the restart feature do a true restart.

• Add a test of using the **mrestart = 1** restart option. Does the *qtcm.restart* file need to be in the current working directory or another?

²http://www.atmos.ucla.edu/~csi/qtcm_man/v2.3/qtcm_manv2.3.pdf

- Add a test in the unit test scripts to confirm that the init_with_instance_state attribute setting only has an effect if compiled_form = 'parts'.
- Document tmppreview keyword in plot.plot_ncdf_output.
- Confirm and document that for netCDF output, time is model time since dd-mm-yyyy.
- Add to the **plotm** method the ability to plot as text onto the figure the runname string and the calling line for the plotm method.
- Couple with the CliMT³ climate modeling toolkit.
- Enable Python to set arr1name, etc., which are string variables at the Python level. I haven't really thought through how arr1 variables work with the Python Qtcm instance.
- Possible: In the Qtcm method __setattr__, add a test to raise an exception if the instance tries to set viscU, viscT, or viscQ as attributes. Also create a method isotropic_visc that will set all viscosity parameters non-dependent on direction. See Section 6.4.1 for details.
- Go through the manual and create HTML-only versions of tables that have table numbers (use a similar construct as in figure environments).
- Go through documentation to check that output variable names are capitalized consistently.
- Create way to redirect stdout.
- Create a step method to run an arbitrary number of timesteps at the atmosphere level.

⁸⁹

³http://maths.ucd.ie/~rca/climt/

CHAPTER 7. FUTURE WORK

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Appendix A Field Settings in defaults

A.1 Scalar Field Variables

This table lists the default settings for scalar qtcm fields as set by the defaults submodule. All fields are of class Field. Numerical values are rounded as per the conventions of Python's %g format code. To create a Field instance whose value is set to the default, instantiate with the field id as the argument

Field	Value	Units	Description
SSTdir	/bnddata/SST_Reynolds		Where SST files are
SSTmode	seasonal		Decide what kind of SST
			to use
VVsmin	4.5	m/s	Minimum wind speed for
			fluxes
bnddir	/bnddata		Boundary data other
			than SST
dateofmodel	0		Date of model coded as
			an integer as yyyymmdd
day0	-1	dy	Starting day; if < 0 use
			day in restart
dt	1200	s	Time step
eps_c	0.000138889	1/s	$1/tau_c NZ (5.7)$
interval	1	1 dy	
			pling interval
it	1		Time of day in time steps
landon	1		If not 1: land $=$ ocean
			with fake SST
lastday	365	dy	Last day of integration
month0	-1	mo	Starting month; if < 0 use
			mo in restart

APPENDIX A. FIELD SETTINGS IN DEFAULTS

Field	Value	Units	Description	
mrestart	0		=1: restart using	
			qtcm.restart	
mt0	1		Barotropic timestep ev-	
			ery mt0 timesteps	
nastep	1		Number of atmosphere	
-			time steps within one air	
			sea coupling interval	
noout	0	dy	No output for the firs	
			noout days	
nooutr	0	dy	No restart file for the firs	
			nooutr days	
ntout	-30	dy	Monthly mean output	
ntouti	0	dy	Monthly instantaneous	
			data output	
ntoutr	0	dy	Restart file only at end o	
			model run	
outdir	/proc/qtcm_output		Where output goes to	
runname	runname		String for an output file	
			name	
title	QTCM default title		A descriptive title	
u0bar	0			
visc4x	700000	$ m^2/s$	Del 4 viscocity paramete	
			in x	
visc4y	700000	m^2/s	Del 4 viscocity paramete	
		2	in y	
viscxT	1.2e + 06	m^2/s	Temperature diffusion	
		2	parameter in x	
viscxq	1.2e + 06	m^2/s	Humidity diffusion pa	
			rameter in x	
viscxu0	700000	m^2/s	Viscocity parameter for	
		2.4	u0 in x	
viscxu1	700000	m^2/s	Viscocity parameter for	
	1.000	27	u1 in x	
viscyT	1.2e + 06	m^2/s	Temperature diffusion	
	1.0	27	parameter in y	
viscyq	1.2e + 06	m^2/s	Humidity diffusion pa	
	700000	2.1	rameter in y	
viscyu0	700000	m^2/s	Viscocity parameter for	
	700000	2.1	u0 in y	
viscyu1	700000	m^2/s	Viscocity parameter for	
			u1 in y	

A.2. ARRAY FIELD VARIABLES

Field	Value	Units	Description
weml	0.01	m/s	Mixed layer entrainment
			velocity
year0	0	yr	Starting year; if < 0 use
			year in restart
ziml	500	m	Atmosphere mixed layer
			depth \sim cloud base

A.2 Array Field Variables

This table lists the default settings for array qtcm fields as set by the defaults submodule. All fields are of class Field. Numerical values are rounded as per the conventions of Python's %g format code.

Field	Shape	Max	Min	Units	Description
Evap	(1, 1)	0	0		
FLW	(1, 1)	0	0		
FLWds	(1, 1)	0	0		
FLWus	(1, 1)	0	0		
FLWut	(1, 1)	0	0		
FSW	(1, 1)	0	0		
FSWds	(1, 1)	0	0		
FSWus	(1, 1)	0	0		
FSWut	(1, 1)	0	0		
FTs	(1, 1)	0	0		
Qc	(1, 1)	0	0	Κ	Precipitation
S0	(1, 1)	0	0		-
STYPE	(1, 1)	0	0		Surface type; ocean or vegeta-
					tion type over land
T1	(1, 1)	0	0	Κ	
Ts	(1, 1)	0	0	Κ	Surface temperature
WD	(1, 1)	0	0		_
WDO	(1,)	0	0		Field capacity SIB2/CSU (ap-
					proximately)
arr1	(1, 1)	0	0		Auxiliary optional output array
					1
arr2	(1, 1)	0	0		Auxiliary optional output array
					2
arr3	(1, 1)	0	0		Auxiliary optional output array
					3
arr4	(1, 1)	0	0		Auxiliary optional output array
					4

Field	Shape	Max	Min	Units	Description
arr5	(1, 1)	0	0		Auxiliary optional output array
					5
arr6	(1, 1)	0	0		Auxiliary optional output array
					6
arr7	(1, 1)	0	0		Auxiliary optional output array
					7
arr8	(1, 1)	0	0		Auxiliary optional output array
					8
psi0	(1, 1)	0	0		
q1	(1, 1)	0	0	K	
rhsu0bar	(1,)	0	0		
rhsvort0	(1, 1, 1)	0	0		
taux	(1, 1)	0	0		
tauy	(1, 1)	0	0		
u0	(1, 1)	0	0	m/s	Barotropic zonal wind
u1	(1, 1)	0	0	m/s	Current time step baroclinic
					zonal wind
v0	(1, 1)	0	0	m/s	Barotropic meridional wind
v1	(1, 1)	0	0	m/s	
vort0	(1, 1)	0	0		