grackle Documentation

Release 2.2

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Contents

Grackle is a chemistry and radiative cooling library for astrophysical simulations with interfaces for C, C++, and Fortran codes. It is a generalized and trimmed down version of the chemistry network of the Enzo simulation code. Grackle provides:

- two options for primordial chemistry and cooling:
    1. non-equilibrium primordial chemistry network for atomic H, D, and He as well as H_2 and HD, including H_2 formation on dust grains.
    2. tabulated H and He cooling rates calculated with the photo-ionization code, Cloudy.
- tabulated metal cooling rates calculated with Cloudy.
- photo-heating and photo-ionization from two UV backgrounds:
    1. Faucher-Giguere et al. (2009).
    2. Haardt & Madau (2012).

The Grackle provides functions to update chemistry species; solve radiative cooling and update internal energy; and calculate cooling time, temperature, pressure, and ratio of specific heats (gamma).

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CHAPTER 1

Installation

The compilation process for grackle is very similar to that for Enzo. For more details on the Enzo build system, see the Enzo build documentation.

Dependencies

In addition to C/C++ and Fortran compilers, the following dependency must also be installed:

- HDF5, the hierarchical data format. HDF5 also may require the szip and zlib libraries, which can be found at the HDF5 website. Compiling with HDF5 1.8 or greater requires that the compiler directive `H5_USE_16_API` be specified. This can be done with `-DH5_USE_16_API`, which is in the machine specific make files.

Downloading

Grackle is available in a mercurial repository here. The mercurial site is here and an excellent tutorial can be found here. With mercurial installed, grackle can be obtained with the following command:

```
~ $ hg clone https://bitbucket.org/grackle/grackle
```

Building

1. Initialize the build system.

```
~ $ cd grackle
~/grackle $ ./configure
```

2. Proceed to the source directory.

```
~/grackle $ cd src/clib
```

3. Configure the build system.

Note: As of version 2.1, Grackle uses `libtool` for building and installation. As such, both shared and static libraries will be built automatically and it is not necessary to add the -fPIC compiler flag.

Compile settings for different systems are stored in files starting with "Make.mach" in the source directory. Grackle comes with three sample make macros: `Make.mach.darwin` for Mac OSX, `Make.mach.linux-gnu` for Linux systems, and an unformatted `Make.mach.unknown`. If you have a make file prepared for an Enzo install, it cannot be used straight away, but is a very good place to start.

Once you have chosen the make file to be used, a few variables should be set:

- `MACH_LIBTOOL` - path to `libtool` executable. Note, on a Mac, this should point to `glibtool`, which can be installed with macports or homebrew.
- `LOCAL_HDF5_INSTALL` - path to your hdf5 installation.
- `LOCAL_FC_INSTALL` - path to Fortran compilers (not including the bin subdirectory).
- `MACH_INSTALL_PREFIX` - path where grackle header and library files will be installed.
- `MACH_INSTALL_LIB_DIR` - path where libgrackle will be installed (only set if different from MACH_INSTALL_PREFIX/lib).
- `MACH_INSTALL_INCLUDE_DIR` - path where grackle header files will be installed (only set if different from MACH_INSTALL_PREFIX/include).

Once the proper variables are set, they are loaded into the build system by doing the following:

```
~/grackle/src/clib $ make machine-<system>
```

Where system refers to the make file you have chosen. For example, if you chose `Make.mach.darwin`, type:

```
~/grackle/src/clib $ make machine-darwin
```

Custom make files can be saved and loaded from a **.grackle** directory in the home directory.

Compiler Settings

There are three compile options available for setting the precision of baryon fields, compiler optimization, and enabling OpenMP. To see them, type:

```
 ~/grackle/src/clib $ make show-config

MACHINE: Darwin (OSX)
MACHINE-NAME: darwin

CONFIG_PRECISION  [precision-{32,64}]                        : 64
CONFIG_OPT  [opt-{warn,debug,high,aggressive}]               : high
CONFIG_OMP  [omp-{on,off}]                                   : off
```

For example, to change the optimization to high, type:

```
~/grackle/src/clib $ make opt-high
```

Custom settings can be saved for later use by typing:

```
~/grackle/src/clib $ make save-config-<keyword>
```

They will be saved in the **.grackle** directory in your home directory. To reload them, type:

```
~/grackle/src/clib $ make load-config-<keyword>
```

For a list of all available make commands, type:

```
~/grackle/src/clib $ make help

========================================================================
   Grackle Makefile Help
========================================================================

   make                Compile and generate librackle
   make install        Copy the library somewhere
   make help           Display this help information
   make clean          Remove object files, executable, etc.
   make dep            Create make dependencies in DEPEND file

   make show-version   Display revision control system branch and revision
   make show-diff      Display local file modifications

   make help-config    Display detailed help on configuration make targets
   make show-config    Display the configuration settings
   make show-flags     Display specific compilation flags
   make default        Reset the configuration to the default values
```

4. Compile and Install

To build the code, type:

```
~/grackle/src/clib $ make
Updating DEPEND
Compiling calc_rates.F
Compiling cool1d_multi.F
....

Linking
Success!
```

Then, to install:

```
~/grackle/src/clib $ make install
```

5. Test your Installation

Once installed, you can test your installation with the provided example to assure it is functioning correctly. If something goes wrong in this process, check the `out.compile` file to see what went wrong during compilation, or use `ldd` (`otool -L` on Mac) on your executable to determine what went wrong during linking.

```
~/grackle/src/clib $ cd ../example
~/grackle/src/example $ make clean
~/grackle/src/example $ make

Compiling cxx_example.C
Linking
```

```
Success!

~/grackle/src/example $ ./cxx_example

The Grackle Version 2.2
Mercurial Branch   default
Mercurial Revision b4650914153d

Initializing grackle data.
with_radiative_cooling: 1.
primordial_chemistry: 3.
metal_cooling: 1.
UVbackground: 1.
Initializing Cloudy cooling: Metals.
cloudy_table_file: ../../input/CloudyData_UVB=HM2012.h5.
Cloudy cooling grid rank: 3.
Cloudy cooling grid dimensions: 29 26 161.
Parameter1: -10 to 4 (29 steps).
Parameter2: 0 to 14.849 (26 steps).
Temperature: 1 to 9 (161 steps).
Reading Cloudy Cooling dataset.
Reading Cloudy Heating dataset.
Initializing UV background.
Reading UV background data from ../../input/CloudyData_UVB=HM2012.h5.
UV background information:
Haardt & Madau (2012, ApJ, 746, 125) [Galaxies & Quasars]
z_min =  0.000
z_max = 15.130
Setting UVbackground_redshift_on to 15.130000.
Setting UVbackground_redshift_off to 0.000000.
Cooling time = -1.434987e+13 s.
Temperature = 4.637034e+02 K.
Pressure = 3.345738e+34.
gamma = 1.666645e+00.
```

In order to verify that Grackle is fully functional, try *running the test suite*.

CHAPTER 2

Running the Test Suite

Grackle contains a number of unit and answer tests to verify that everything is working properly. These will verify that:

- proper and comoving unit systems are consistent
- atomic, primordial collisional ionization equilibrium agrees with the analytical solution
- all code examples build and run
- all python examples run and give correct results
- all Python code conforms to PEP 8

Once you have installed *pygrackle*, the tests can be run from the **src** directory by typing `make test`:

```
~ $ cd grackle/src
~/grackle/src $ make test
```

or from the **src/python** directory by typing `py.test`:

```
~ $ cd grackle/src/python
~/grackle/src $ py.test

===================================== test session starts␣
↪======================================
platform darwin -- Python 2.7.11, pytest-2.8.1, py-1.4.30, pluggy-0.3.1
rootdir: /Users/britton/Documents/work/simulation/grackle/grackle/src/python, inifile:
collected 13 items

tests/test_chemistry.py ...
tests/test_examples.py ........
tests/test_flake8.py .
tests/test_primordial.py .

================================== 13 passed in 26.18 seconds␣
↪==================================
```

Now it’s time to *integrate grackle into your simulation code*.

CHAPTER 3

Adding Grackle to Your Simulation Code

This document follows the example files, **cxx_example.C** and **cxx_table_example.C**. For a list of all available functions, see the *API Reference*.

Example Executables

The grackle source code contains examples for C, C++, and Fortran codes. They are located in the **src/example** directory and detail different uses of the grackle library.

- **c_example.c** - full functionality C example that uses the units and chemistry data structures.
- **c_table_example.c** - tabulated cooling only (no chemistry) C example that uses the units and chemistry data structures.
- **c_example_nostruct.c** - full functionality C example that uses the `initialize_grackle_()` function instead of data structures.
- **c_table_example_nostruct.c** - tabulated cooling only (no chemistry) C example that uses the `initialize_grackle_()` function instead of data structures.
- **cxx_example.C** - full functionality C++ example that uses the units and chemistry data structures.
- **cxx_table_example.C** - tabulated cooling only (no chemistry) C++ example that uses the units and chemistry data structures.
- **cxx_omp_example.C** - C++ example using both the non-equilibrium and tabulated solvers wth OpenMP. Run the executable with the -h flag to see a full list of options.
- **fortran_example.F** - full functionality Fortran example that uses the `initialize_grackle_()` function.
- **fortran_table_example.F** - tabulated cooling only (no chemistry) Fortran example that uses the `initialize_grackle_()` function.

Once you have already installed the grackle library, you can build the examples by typing *make* and the name of the file without extension. For example, to build the C++ example, type:

```
$ make cxx_example
```

To run the example, make sure to add the path to the directory containing the installed **libgrackle.so** to your LD_LIBRARY_PATH (or DYLD_LIBRARY_PATH on Mac).

This document follows **cxx_example.C**, which details the use of the full-featured grackle functions. The table examples illustrate the use of the Grackle with fully tabulated cooling functions only. In this mode, a simplified set of functions are available. For information on these, see *Pure Tabulated Mode*.

Header Files

Six header files are installed with the grackle library. They are:

- **grackle.h** - the primary header file, containing declarations for all the available functions and data structures. This is the only header file that needs to be included for C and C++ codes.
- **grackle_types.h** - defines the variable type `gr_float` to be used for the baryon fields passed to the grackle functions. This can be either a 4 or 8 byte float, allowing the code to be easily configured for either single or double precision baryon fields.
- **grackle_fortran_types.def** - similar to **grackle_types.h**, but used with Fortran codes. This defines the variable type `R_PREC` as either real*4 or real*8.
- **grackle_macros.h** - contains some macros used internally.
- **chemistry_data.h** - defines the primary data structure which all run time parameters as well as the chemistry, cooling, and UV background data.
- **code_units.h** - defines the structure containing conversions from code units to CGS.

The only source file that needs to be included in your simulation code is **grackle.h**. Since this is a C++ example and the Grackle is pure C, we must surround the include with the 'extern "C"' directive.

```
extern "C" {
#include <grackle.h>
}
```

Data Types

The grackle library provides a configurable variable type to control the precision of the baryon fields passed to the grackle functions. For C and C++ codes, this is `gr_float`. For Fortran codes, this is `R_PREC`. The precision of these types can be configured with the *precision* compile option. Compile with *precision-32* to make `gr_float` and `R_PREC` a 4 byte float (*float* for C/C++ and *real*4* for Fortran). Compile with *precision-64* to make `gr_float` and `R_PREC` an 8 byte float (*double* for C/C++ and *real*8* for Fortran).

gr_float
Floating point type used for the baryon fields. This is of type *float* if compiled with *precision-32* and type double if compiled with *precision-64*.

R_PREC
The Fortran analog of `gr_float`. This is of type *real*4* if compiled with *precision-32* and type *real*8* if compiled with *precision-64*.

Enabling Output

By default, grackle will not print anything but error messages. However, a short summary of the running configuration can be printed by setting `grackle_verbose` to 1.

```
// Enable output
grackle_verbose = 1;
```

Code Units

It is strongly recommended to use comoving coordinates with any cosmological simulation. The *code_units* structure contains conversions from code units to CGS. If *comoving_coordinates* is set to 0, it is assumed that the fields passed into the solver are in the proper frame. All of the units (density, length, time, velocity, and expansion factor) must be set. When using the proper frame, *a_units* (units for the expansion factor) must be set to 1.0.

code_units
This structure contains the following members.

int **comoving_coordinates**
If set to 1, the incoming field data is assumed to be in the comoving frame. If set to 0, the incoming field data is assumed to be in the proper frame.

double **density_units**
Conversion factor to be multiplied by density fields to return densities in proper g/cm^3.

double **length_units**
Conversion factor to be multiplied by length variables to return lengths in proper cm.

double **time_units**
Conversion factor to be multiplied by time variables to return times in s.

double **velocity_units**
Conversion factor to be multiplied by velocities to return proper cm/s.

double **a_units**
Conversion factor to be multiplied by the expansion factor such that $a_{true} = a_{code} *$ *a_units*.

```
code_units my_units;
my_units.comoving_coordinates = 0; // 1 if cosmological sim, 0 if not
my_units.density_units = 1.67e-24; // 1 m_H/cc
my_units.length_units = 3.086e21;  // 1 kpc
my_units.time_units = 3.15569e13;  // 1 Myr
my_units.velocity_units = my_units.length_units / my_units.time_units;
my_units.a_units = 1.0;            // units for the expansion factor
```

If *comoving_coordinates* is set to 1, it is assumed that the fields being passed to the solver are in the comoving frame. Hence, the units must convert from code units in the **comoving** frame to CGS in the **proper** frame.

Note: With `comoving_coordinate` set to 1, velocity units need to be defined in the following way.

```
my_units.velocity_units = my_units.a_units *
  (my_units.length_units / a_value) / my_units.time_units; // since u = a * dx/dt
```

For an example of using comoving units, see the units system in the Enzo code. For cosmological simualations, a comoving unit system is preferred, though not required, since it allows the densities to stay close to 1.0.

Chemistry Data

The main Grackle header file contains a structure of type *chemistry_data* called `grackle_data`, which contains all of the parameters that control the behavior of the solver as well as all of the actual chemistry and cooling rate data. The routine, `set_default_chemistry_parameters()` is responsible for the initial setup of this structure and for setting of all the default parameter values. The parameters can then be set to their desired values. See *Parameters and Data Files* for a full list of the available parameters. The function will return an integer indicating success (1) or failure (0).

chemistry_data

This structure holds all grackle run time parameter and all chemistry and cooling data arrays.

```
if (set_default_chemistry_parameters() == 0) {
  fprintf(stderr, "Error in set_default_chemistry_parameters.\n");
}

// Set parameter values for chemistry.
grackle_data.use_grackle = 1;            // chemistry on
grackle_data.with_radiative_cooling = 1; // cooling on
grackle_data.primordial_chemistry = 3;   // molecular network with H, He, D
grackle_data.metal_cooling = 1;          // metal cooling on
grackle_data.UVbackground = 1;           // UV background on
grackle_data.grackle_data_file = "CloudyData_UVB=HM2012.h5"; // data file
```

Once the desired parameters have been set, the chemistry and cooling rates must be initialized with the `initialize_chemistry_data()`. This function also requires the initial value of the expansion factor for setting internal units. If the simulation is not cosmological, the expansion factor should be set to 1. The initializing function will return an integer indicating success (1) or failure (0).

```
// Set initial expansion factor (for internal units).
// Set expansion factor to 1 for non-cosmological simulation.
double initial_redshift = 100.;
double a_value = 1. / (1. + initial_redshift) / my_units.a_units;

// Finally, initialize the chemistry object.
if (initialize_chemistry_data(&my_units, a_value) == 0) {
  fprintf(stderr, "Error in initialize_chemistry_data.\n");
  return 0;
}
```

The Grackle is now ready to be used.

Running with OpenMP

As of version 2.2, Grackle can be run with OpenMP parallelism. To do this, the library must first be compiled with OpenMP support enabled by issuing the command, “make omp-on”, before compiling. See *Compiler Settings* for more information on how to change settings.

For an example of how to compile your code with OpenMP, see the **cxx_table_example.C** code example (*Example Executables*). Once your code has been compiled with OpenMP enabled, the number of threads used can be controlled by setting the *omp_nthreads* parameter, stored in the `grackle_data` struct.

```
// 8 threads per process
grackle_data.omp_nthreads = 8;
```

If not set, this parameter will be set to the maximum number of threads possible, as determined by the system or as configured by setting the OMP_NUM_THREADS environment variable.

Creating the Necessary Fields

With the *code_units* and *chemistry_data* structures ready, the only thing left is to create the arrays to carry the species densities. Pointers for all fields must be created, but the arrays only need to be allocated if the fields are going to be used by the chemistry network. Variables containing the dimensionality of the data, the active dimensions (not including the ghost zones), and the starting and ending indices for each dimensions must also be created.

```
// Allocate field arrays.
gr_float *density, *energy, *x_velocity, *y_velocity, *z_velocity,
  *HI_density, *HII_density, *HM_density,
  *HeI_density, *HeII_density, *HeIII_density,
  *H2I_density, *H2II_density,
  *DI_density, *DII_density, *HDI_density,
  *e_density, *metal_density;

// Set grid dimension and size.
// grid_start and grid_end are used to ignore ghost zones.
int field_size = 10;
int grid_rank = 3;
// If grid rank is less than 3, set the other dimensions to 1 and
// start indices and end indices to 0.
int grid_dimension[3], grid_start[3], grid_end[3];
for (int i = 0;i < 3;i++) {
  grid_dimension[i] = 1; // the active dimension not including ghost zones.
  grid_start[i] = 0;
  grid_end[i] = 0;
}
grid_dimension[0] = field_size;
grid_end[0] = field_size - 1;

density       = new gr_float[field_size];
energy        = new gr_float[field_size];
x_velocity    = new gr_float[field_size];
y_velocity    = new gr_float[field_size];
z_velocity    = new gr_float[field_size];
// for primordial_chemistry >= 1
HI_density    = new gr_float[field_size];
HII_density   = new gr_float[field_size];
HeI_density   = new gr_float[field_size];
HeII_density  = new gr_float[field_size];
HeIII_density = new gr_float[field_size];
e_density     = new gr_float[field_size];
// for primordial_chemistry >= 2
HM_density    = new gr_float[field_size];
H2I_density   = new gr_float[field_size];
H2II_density  = new gr_float[field_size];
// for primordial_chemistry >= 3
DI_density    = new gr_float[field_size];
DII_density   = new gr_float[field_size];
HDI_density   = new gr_float[field_size];
// for metal_cooling = 1
metal_density = new gr_float[field_size];
```

Note: The electron mass density should be scaled by the ratio of the proton mass to the electron mass such that the electron density in the code is the electron number density times the **proton** mass.

Calling the Available Functions

There are five functions available, one to solve the chemistry and cooling and four others to calculate the cooling time, temperature, pressure, and the ratio of the specific heats (gamma). The arguments required are the *code_units* structure, the value of the expansion factor, the field size and dimension variables, and the field arrays themselves. For the chemistry solving routine, a timestep must also be given. For the four field calculator routines, the array to be filled with the field values must be created and passed as an argument as well.

Solve the Chemistry and Cooling

```
// some timestep (one million years)
double dt = 3.15e7 * 1e6 / my_units.time_units;

if (solve_chemistry(&my_units, a_value, dt,
                    grid_rank, grid_dimension,
                    grid_start, grid_end,
                    density, energy,
                    x_velocity, y_velocity, z_velocity,
                    HI_density, HII_density, HM_density,
                    HeI_density, HeII_density, HeIII_density,
                    H2I_density, H2II_density,
                    DI_density, DII_density, HDI_density,
                    e_density, metal_density) == 0) {
  fprintf(stderr, "Error in solve_chemistry.\n");
  return 0;
}
```

Calculating the Cooling Time

```
gr_float *cooling_time;
cooling_time = new gr_float[field_size];
if (calculate_cooling_time(&my_units, a_value,
                           grid_rank, grid_dimension,
                           grid_start, grid_end,
                           density, energy,
                           x_velocity, y_velocity, z_velocity,
                           HI_density, HII_density, HM_density,
                           HeI_density, HeII_density, HeIII_density,
                           H2I_density, H2II_density,
                           DI_density, DII_density, HDI_density,
                           e_density, metal_density,
                           cooling_time) == 0) {
  fprintf(stderr, "Error in calculate_cooling_time.\n");
  return 0;
}
```

Calculating the Temperature Field

```
gr_float *temperature;
temperature = new gr_float[field_size];
if (calculate_temperature(&my_units, a_value,
                          grid_rank, grid_dimension,
                          grid_start, grid_end,
                          density, energy,
                          HI_density, HII_density, HM_density,
                          HeI_density, HeII_density, HeIII_density,
                          H2I_density, H2II_density,
                          DI_density, DII_density, HDI_density,
                          e_density, metal_density,
                          temperature) == 0) {
  fprintf(stderr, "Error in calculate_temperature.\n");
  return 0;
}
```

Calculating the Pressure Field

```
gr_float *pressure;
pressure = new gr_float[field_size];
if (calculate_pressure(&my_units, a_value,
                       grid_rank, grid_dimension,
                       grid_start, grid_end,
                       density, energy,
                       HI_density, HII_density, HM_density,
                       HeI_density, HeII_density, HeIII_density,
                       H2I_density, H2II_density,
                       DI_density, DII_density, HDI_density,
                       e_density, metal_density,
                       pressure) == 0) {
  fprintf(stderr, "Error in calculate_pressure.\n");
  return 0;
}
```

Calculating the Gamma Field

```
gr_float *gamma;
gamma = new gr_float[field_size];
if (calculate_gamma(&my_units, a_value,
                    grid_rank, grid_dimension,
                    grid_start, grid_end,
                    density, energy,
                    HI_density, HII_density, HM_density,
                    HeI_density, HeII_density, HeIII_density,
                    H2I_density, H2II_density,
                    DI_density, DII_density, HDI_density,
                    e_density, metal_density,
                    gamma) == 0) {
  fprintf(stderr, "Error in calculate_gamma.\n");
  return 0;
}
```

Pure Tabulated Mode

If you only intend to run simulations using the fully tabulated cooling (*primordial_chemistry* set to 0), then a simplified set of functions are available. These functions do not require pointers to be given for the field arrays for the chemistry species densities. See the **cxx_table_example.C**, **c_table_example.c**, **c_table_example_nostruct.c**, and **fortran_table_example.F** files in the **src/example** directory for examples.

Note: No simplified function is available for the calculation of the gamma field since gamma is only altered in Grackle by the presence of H_2.

Solve the Cooling

```
// some timestep (one million years)
double dt = 3.15e7 * 1e6 / my_units.time_units;

if (solve_chemistry_table(&my_units, a_value, dt,
                          grid_rank, grid_dimension,
                          grid_start, grid_end,
                          density, energy,
                          x_velocity, y_velocity, z_velocity,
                          metal_density) == 0) {
  fprintf(stderr, "Error in solve_chemistry.\n");
  return 0;
}
```

Calculating the Cooling Time

```
gr_float *cooling_time;
cooling_time = new gr_float[field_size];
if (calculate_cooling_time_table(&my_units, a_value,
                                 grid_rank, grid_dimension,
                                 grid_start, grid_end,
                                 density, energy,
                                 x_velocity, y_velocity, z_velocity,
                                 metal_density,
                                 cooling_time) == 0) {
  fprintf(stderr, "Error in calculate_cooling_time.\n");
  return 0;
}
```

Calculating the Temperature Field

```
gr_float *temperature;
temperature = new gr_float[field_size];
if (calculate_temperature_table(&my_units, a_value,
                                grid_rank, grid_dimension,
                                grid_start, grid_end,
                                density, energy,
                                metal_density,
                                temperature) == 0) {
```

```
  fprintf(stderr, "Error in calculate_temperature.\n");
  return 0;
}
```

Calculating the Pressure Field

```
gr_float *pressure;
pressure = new gr_float[field_size];
if (calculate_pressure_table(&my_units, a_value,
                             grid_rank, grid_dimension,
                             grid_start, grid_end,
                             density, energy,
                             pressure) == 0) {
  fprintf(stderr, "Error in calculate_pressure.\n");
  return 0;
}
```

CHAPTER 4

Parameters and Data Files

Parameters

For all on/off integer flags, 0 is off and 1 is on.

int **`use_grackle`**

Flag to activate the grackle machinery. Default: 0.

int **`with_radiative_cooling`**

Flag to include radiative cooling and actually update the thermal energy during the chemistry solver. If off, the chemistry species will still be updated. The most common reason to set this to off is to iterate the chemistry network to an equilibrium state. Default: 1.

int **`primordial_chemistry`**

Flag to control which primordial chemistry network is used. Default: 0.

- 0: no chemistry network. Radiative cooling for primordial species is solved by interpolating from lookup tables calculated with Cloudy. A simplified set of functions are available (though not required) for use in this mode. For more information, see *Pure Tabulated Mode*.
- 1: 6-species atomic H and He. Active species: H, H^+, He, He^+, $^{++}$, e^-.
- 2: 9-species network including atomic species above and species for molecular hydrogen formation. This network includes formation from the H^- and H_2^+ channels, three-body formation (H+H+H and H+H+H_2), H_2 rotational transitions, chemical heating, and collision-induced emission (optional). Active species: above + H^-, H_2, H_2^+.
- 3: 12-species network include all above plus HD rotation cooling. Active species: above + D, D^+, HD.

Note: In order to make use of the non-equilibrium chemistry network (*`primordial_chemistry`* options 1-3), you must add and advect baryon fields for each of the species used by that particular option.

int **`h2_on_dust`**

Flag to enable H_2 formation on dust grains, dust cooling, and dust-gas heat transfer follow Omukai (2000). This assumes that the dust to gas ratio scales with the metallicity. Default: 0.

int **metal_cooling**
Flag to enable metal cooling using the Cloudy tables. If enabled, the cooling table to be used must be specified with the *grackle_data_file* parameter. Default: 0.

Note: In order to use the metal cooling, you must add and advect a metal density field.

int **cmb_temperature_floor**
Flag to enable an effective CMB temperature floor. This is implemented by subtracting the value of the cooling rate at T_{CMB} from the total cooling rate. Default: 1.

int **UVbackground**
Flag to enable a UV background. If enabled, the cooling table to be used must be specified with the *grackle_data_file* parameter. Default: 0.

char* **grackle_data_file**
Path to the data file containing the metal cooling and UV background tables. Default: "".

float **Gamma**
The ratio of specific heats for an ideal gas. A direct calculation for the molecular component is used if *primordial_chemistry* > 1. Default: 5/3.

int **three_body_rate**
Flag to control which three-body H_2 formation rate is used.

- 0: Abel, Bryan & Norman (2002)
- 1: Palla, Salpeter & Stahler (1983)
- 2: Cohen & Westberg (1983)
- 3: Flower & Harris (2007)
- 4: Glover (2008)
- 5: Forrey (2013).

The first five options are discussed in Turk et. al. (2011). Default: 0.

int **cie_cooling**
Flag to enable H_2 collision-induced emission cooling from Ripamonti & Abel (2004). Default: 0.

int **h2_optical_depth_approximation**
Flag to enable H_2 cooling attenuation from Ripamonti & Abel (2004). Default: 0.

int **photoelectric_heating**
Flag to enable a spatially uniform heating term approximating photo-electric heating from dust from Tasker & Bryan (2008). Default: 0.

int **photoelectric_heating_rate**
If *photoelectric_heating* enabled, the heating rate in units of erg cm^{-3} s^{-1}. Default: 8.5e-26.

int **Compton_xray_heating**
Flag to enable Compton heating from an X-ray background following Madau & Efstathiou (1999). Default: 0.

float **LWbackground_intensity**
Intensity of a constant Lyman-Werner H_2 photo-dissociating radiation field in units of 10^{-21} erg s^{-1} cm^{-2} Hz^{-1} sr^{-1}. Default: 0.

int **LWbackground_sawtooth_suppression**
Flag to enable suppression of Lyman-Werner flux due to Lyman-series absorption (giving a sawtooth pattern), taken from Haiman & Abel, & Rees (2000). Default: 0.

int **`omp_nthreads`**

Sets the number of OpenMP threads. If not set, this will be set to the maximum number of threads possible, as determined by the system or as configured by setting the `OMP_NUM_THREADS` environment variable. Note, Grackle must be compiled with OpenMP support enabled. See *Running with OpenMP*.

Data Files

All data files are located in the **input** directory in the source.

The first three files contain the heating and cooling rates for both primordial and metal species as well as the UV background photo-heating and photo-ionization rates. For all three files, the valid density and temperature range is given below. Extrapolation is performed when outside of the data range. The metal cooling rates are stored for solar metallicity and scaled linearly with the metallicity of the gas.

Valid range:

- number density: $-10 < \log_{10} (n_H / cm^{-3}) < 4$
- temperature: the temperature range is $1 < \log_{10} (T / K) < 9$.

Data files:

- **CloudyData_noUVB.h5** - cooling rates for collisional ionization equilibrium.
- **CloudyData_UVB=FG2011.h5** - heating and cooling rates and UV background rates from the work of Faucher-Giguere et. al. (2009), updated in 2011. The maxmimum redshift is 10.6. Above that, collisional ionization equilibrium is assumed.
- **CloudyData_UVB=HM2012.h5** - heating and cooling rates and UV background rates from the work of Haardt & Madau (2012). The maximum redshift is 15.13. Above that, collisional ionization equilibrium is assumed.

The final file includes only metal cooling rates under collisional ionization equilibrium, i.e., no incident radiation field. This table extends to higher densities and also varies in metallicity rather than scaling proportional to the solar value. This captures the thermalization of metal coolants occuring at high densities, making this table more appropriate for simulations of collapsing gas-clouds.

Valid range:

- number density: $-6 < \log_{10} (n_H / cm^{-3}) < 12$
- metallicity: $-6 < \log_{10} (Z / Z_{sun}) < 1$
- temperature: the temperature range is $1 < \log_{10} (T / K) < 8$.

Data file:

- **cloudy_metals_2008_3D.h5** - collisional ionization equilibrium, metal cooling rates only.

CHAPTER 5

API Reference

The Grackle has a few different versions of the various functions for solving the chemistry and cooling and calculating related fields. One set of functions requires the user to work with C structs, while the other does not. The set that does not use structs is simpler to implement in Fortran codes. Both of these rely internally on a *chemistry_data* type struct called `grackle_data`, which exists in the grackle namespace. A third set of functions also exists that requires the user to hold and pass their own *chemistry_data* struct.

Functions using structs (best for C and C++)

These functions require the user to directly access the `grackle_data` data structure to set parameters and to creata a `code_units` struct to control the unit system. These functions are used in the examples, **c_example.c**, **c_table_example.c**, **cxx_example.C**, and **cxx_table_example.C**.

`int set_default_chemistry_parameters();`

Initializes the `grackle_data` data structure. This must be called before run time parameters can be set.

Return type int

Returns 1 (success) or 0 (failure)

`int initialize_chemistry_data(code_units *my_units, double a_value);`

Loads all chemistry and cooling data, given the set run time parameters. This can only be called after `set_default_chemistry_parameters()`.

Parameters

- **`my_units`** (`code_units*`) – code units conversions
- **`a_value`** (*`double`*) – the expansion factor in code units (a_code = a / a_units)

Return type int

Returns 1 (success) or 0 (failure)

`int solve_chemistry(code_units *my_units, double a_value, double dt_value, int grid_rank,`

Evolves the species densities and internal energies over a given timestep by solving the chemistry and cooling rate equations.

Parameters

- **my_units** (code_units*) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **dt_value** (*double*) – the integration timestep in code units
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int**) – array holding the size of the baryon field in each dimension
- **grid_start** (*int**) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int**) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (gr_float*) – array containing the density values in code units
- **internal_energy** (gr_float*) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **x_velocity** (gr_float*) – array containing the x velocity values in code units
- **y_velocity** (gr_float*) – array containing the y velocity values in code units
- **z_velocity** (gr_float*) – array containing the z velocity values in code units
- **HI_density** (gr_float*) – array containing the HI densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 1.
- **HII_density** (gr_float*) – array containing the HII densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 1.
- **HM_density** (gr_float*) – array containing the H^- densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 2.
- **HeI_density** (gr_float*) – array containing the HeI densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 1.
- **HeII_density** (gr_float*) – array containing the HeII densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 1.
- **HeIII_density** (gr_float*) – array containing the HeIII densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 1.
- **H2I_density** (gr_float*) – array containing the H_2: densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 2.
- **H2II_density** (gr_float*) – array containing the H_2^+densities in code units equivalent those of the density array. Used with *primordial_chemistry* >= 2.
- **DI_density** (gr_float*) – array containing the DI (deuterium) densities in code units equivalent those of the density array. Used with *primordial_chemistry* = 3.
- **DII_density** (gr_float*) – array containing the DII densities in code units equivalent those of the density array. Used with *primordial_chemistry* = 3.
- **HDI_density** (gr_float*) – array containing the HD densities in code units equivalent those of the density array. Used with *primordial_chemistry* = 3.
- **e_density** (gr_float*) – array containing the e^- densities in code units equivalent those of the density array but normalized to the ratio of the proton to electron mass. Used with *primordial_chemistry* >= 1.

- **metal_density** (`gr_float*`) – array containing the metal densities in code units equivalent those of the density array. Used with *metal_cooling* = 1.

Return type int

Returns 1 (success) or 0 (failure)

`int calculate_cooling_time(code_units *my_units, double a_value, int grid_rank, int *grid_d`

Calculates the instantaneous cooling time.

Parameters

- **my_units** (`code_units*`) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int **) – array holding the size of the baryon field in each dimension
- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (`gr_float*`) – array containing the density values in code units
- **internal_energy** (`gr_float*`) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **x_velocity, y_velocity, z_velocity** (`gr_float*`) – arrays containing the x, y, and z velocity values in code units
- **HI_density, HII_density, HM_density, HeI_density, HeII_density, HeIII_density, H2I_density, H2II_density, DI_density, DII_density, HDI_density, e_density, metal_density** (`gr_float*`) – arrays containing the species densities in code units equivalent those of the density array
- **cooling_time** (`gr_float*`) – array which will be filled with the calculated cooling time values

Return type int

Returns 1 (success) or 0 (failure)

`int calculate_gamma(code_units *my_units, double a_value, int grid_rank, int *grid_dimensio`

Calculates the effective adiabatic index. This is only useful with *primordial_chemistry* >= 2 as the only thing that alters gamma from the single value is H_2.

Parameters

- **my_units** (`code_units*`) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int **) – array holding the size of the baryon field in each dimension
- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.

- **density** (gr_float*) – array containing the density values in code units
- **internal_energy** (gr_float*) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **HI_density, HII_density, HM_density, HeI_density, HeII_density, HeIII_density, H2I_density, H2II_density, DI_density, DII_density, HDI_density, e_density, metal_density** (gr_float*) – arrays containing the species densities in code units equivalent those of the density array
- **my_gamma** (gr_float*) – array which will be filled with the calculated gamma values

Return type int

Returns 1 (success) or 0 (failure)

int calculate_pressure(code_units *my_units, double a_value, int grid_rank, int *grid_dimer

Calculates the gas pressure.

Parameters

- **my_units** (code_units*) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int**) – array holding the size of the baryon field in each dimension
- **grid_start** (*int**) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int**) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (gr_float*) – array containing the density values in code units
- **internal_energy** (gr_float*) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **HI_density, HII_density, HM_density, HeI_density, HeII_density, HeIII_density, H2I_density, H2II_density, DI_density, DII_density, HDI_density, e_density, metal_density** (gr_float*) – arrays containing the species densities in code units equivalent those of the density array
- **pressure** (gr_float*) – array which will be filled with the calculated pressure values

Return type int

Returns 1 (success) or 0 (failure)

int calculate_temperature(code_units *my_units, double a_value, int grid_rank, int *grid_di

Calculates the gas temperature.

Parameters

- **my_units** (code_units*) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int**) – array holding the size of the baryon field in each dimension

- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (gr_float *) – array containing the density values in code units
- **internal_energy** (gr_float *) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **HI_density, HII_density, HM_density, HeI_density, HeII_density, HeIII_density, H2I_density, H2II_density, DI_density, DII_density, HDI_density, e_density, metal_density** (gr_float *) – arrays containing the species densities in code units equivalent those of the density array
- **temperature** (gr_float *) – array which will be filled with the calculated temperature values

Return type int

Returns 1 (success) or 0 (failure)

Tabular-Only Functions

These are slimmed down functions that require *primordial_chemistry* = 0 and use only the tabulated cooling rates (no chemistry).

int solve_chemistry_table(code_units *my_units, double a_value, double dt_value, int grid_

Evolves the internal energies over a given timestep by solving the cooling rate equations. This version allows only for the use of the tabulated cooling functions.

Parameters

- **my_units** (code_units *) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **dt_value** (*double*) – the integration timestep in code units
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int **) – array holding the size of the baryon field in each dimension
- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (gr_float *) – array containing the density values in code units
- **internal_energy** (gr_float *) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **x_velocity** (gr_float *) – array containing the x velocity values in code units
- **y_velocity** (gr_float *) – array containing the y velocity values in code units
- **z_velocity** (gr_float *) – array containing the z velocity values in code units
- **metal_density** (gr_float *) – array containing the metal densities in code units equivalent those of the density array. Used with *metal_cooling* = 1.

Return type int

Returns 1 (success) or 0 (failure)

int calculate_cooling_time_table(code_units *my_units, double a_value, int grid_rank, int *

Calculates the instantaneous cooling time. This version allows only for the use of the tabulated cooling functions.

Parameters

- **my_units** (code_units*) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int **) – array holding the size of the baryon field in each dimension
- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (gr_float*) – array containing the density values in code units
- **internal_energy** (gr_float*) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **x_velocity, y_velocity, z_velocity** (gr_float*) – arrays containing the x, y, and z velocity values in code units
- **metal_density** (gr_float*) – array containing the metal densities in code units equivalent those of the density array. Used with *metal_cooling* = 1.
- **cooling_time** (gr_float*) – array which will be filled with the calculated cooling time values

Return type int

Returns 1 (success) or 0 (failure)

int calculate_pressure_table(code_units *my_units, double a_value, int grid_rank, int *gri

Calculates the gas pressure. This version allows only for the use of the tabulated cooling functions.

Parameters

- **my_units** (code_units*) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int **) – array holding the size of the baryon field in each dimension
- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (gr_float*) – array containing the density values in code units
- **internal_energy** (gr_float*) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **pressure** (gr_float*) – array which will be filled with the calculated pressure values

Return type int

Returns 1 (success) or 0 (failure)

`int calculate_temperature_table(code_units *my_units, double a_value, int grid_rank, int *g`

Calculates the gas temperature. This version allows only for the use of the tabulated cooling functions.

Parameters

- **my_units** (*code_units**) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)
- **grid_rank** (*int*) – the dimensionality of the grid
- **grid_dimension** (*int **) – array holding the size of the baryon field in each dimension
- **grid_start** (*int **) – array holding the starting indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones
- **grid_end** (*int **) – array holding the ending indices in each dimension of the active portion of the baryon fields. This is used to ignore ghost zones.
- **density** (*gr_float **) – array containing the density values in code units
- **internal_energy** (*gr_float **) – array containing the specific internal energy values in code units corresponding to *erg/g*
- **pressure** (*gr_float **) – array which will be filled with the calculated pressure values

Return type int

Returns 1 (success) or 0 (failure)

Functions without structs (best for Fortran)

These functions do not use any structs and are therefore much simpler to implement in Fortran codes. These are used in the example files, **c_example_nostruct.c**, **c_table_example_nostruct.c**, **fortran_example.F**, and **fortran_table_example.F**.

Note: In Fortran codes, these should be called without the trailing underscore. The variable types can be mapped to Fortran as: int* becomes integer, double* becomes real*8, and *gr_float ** becomes *R_PREC*.

`int initialize_grackle_(int *comoving_coordinates, double *density_units, double *length_u`

Initializes the grackle data structures and associated chemistry and cooling data. This performs the operations of both `set_default_chemistry_parameters()` and `initialize_chemistry_data()`.

Parameters

- **comoving_coordinates** (*int **) – *comoving_coordinates* parameter
- **density_units** (*double **) – *density_units* conversion factor
- **length_units** (*double **) – *length_units* conversion factor
- **time_units** (*double **) – *time_units* conversion factor
- **velocity_units** (*double **) – *velocity_units* conversion factor
- **a_units** (*double **) – *a_units* conversion factor
- **a_value** (*double **) – expansion factor in code units (a_code = a / *a_units*)
- **use_grackle** (*int **) – *use_grackle* parameter

- **with_radiative_cooling** (*int **) – *with_radiative_cooling* parameter
- **grackle_file** (*char **) – *grackle_data_file* parameter
- **primordial_chemistry** (*int **) – *primordial_chemistry* parameter
- **metal_cooling** (*int **) – *metal_cooling* parameter
- **UVbackground** (*int **) – *UVbackground* parameter
- **h2_on_dust** (*int **) – *h2_on_dust* parameter
- **cmb_temperature_floor** (*int **) – *cmb_temperature_floor* parameter
- **gamma** (*double **) – *Gamma* parameter

Note: The last argument should omitted.

int solve_chemistry_(int *comoving_coordinates, double *density_units, double *length_units
Evolves the species densities and internal energies over a given timestep by solving the chemistry and cooling rate equations.

int calculate_cooling_time_(int *comoving_coordinates, double *density_units, double *lengt
Calculates the instantaneous cooling time.

int calculate_gamma_(int *comoving_coordinates, double *density_units, double *length_units
Calculates the effective adiabatic index. This is only useful with *primordial_chemistry* >= 2 as the only thing that alters gamma from the single value is H_2.

int calculate_pressure_(int *comoving_coordinates, double *density_units, double *length_u
Calculates the gas pressure.

int calculate_temperature_(int *comoving_coordinates, double *density_units, double *lengt
Calculates the gas temperature.

Tabular-Only Functions

These are slimmed down functions that require *primordial_chemistry* = 0 and use only the tabulated cooling rates (no chemistry).

int solve_chemistry_table_(int *comoving_coordinates, double *density_units, double *lengt
Evolves the internal energies over a given timestep by solving the cooling rate equations. This version allows only for the use of the tabulated cooling functions.

int calculate_cooling_time_table_(int *comoving_coordinates, double *density_units, double
Calculates the instantaneous cooling time. This version allows only for the use of the tabulated cooling functions.

int calculate_pressure_table_(int *comoving_coordinates, double *density_units, double *le
Calculates the gas pressure. This version allows only for the use of the tabulated cooling functions.

int calculate_temperature_table_(int *comoving_coordinates, double *density_units, double
Calculates the gas temperature. This version allows only for the use of the tabulated cooling functions.

Internal Functions

These functions are mostly for internal use, but can also be used to call the various functions with different parameter values within a single code.

chemistry_data _set_default_chemistry_parameters();

Initializes and returns *chemistry_data* data structure. This must be called before run time parameters can be set.

Returns data structure containing all run time parameters and all chemistry and cooling data arrays

Return type *chemistry_data*

int _initialize_chemistry_data(chemistry_data *my_chemistry, code_units *my_units, double a

Loads all chemistry and cooling data, given the set run time parameters. This can only be called after `_set_default_chemistry_parameters()`.

Parameters

- **my_chemistry** (chemistry_data*) – the structure returned by `_set_default_chemistry_parameters()`
- **my_units** (code_units*) – code units conversions
- **a_value** (*double*) – the expansion factor in code units (a_code = a / a_units)

Return type int

Returns 1 (success) or 0 (failure)

int _solve_chemistry(chemistry_data *my_chemistry, code_units *my_units, double a_value, do

Evolves the species densities and internal energies over a given timestep by solving the chemistry and cooling rate equations.

int _calculate_cooling_time(chemistry_data *my_chemistry, code_units *my_units, double a_va

Calculates the instantaneous cooling time.

int _calculate_gamma(chemistry_data *my_chemistry, code_units *my_units, double a_value, in

Calculates the effective adiabatic index. This is only useful with *primordial_chemistry* >= 2 as the only thing that alters gamma from the single value is H_2.

int _calculate_pressure(chemistry_data *my_chemistry, code_units *my_units, double a_value,

Calculates the gas pressure.

int _calculate_temperature(chemistry_data *my_chemistry, code_units *my_units, double a_val

Calculates the gas temperature.

Tabular-Only Functions

These are slimmed down functions that require *primordial_chemistry* = 0 and use only the tabulated cooling rates (no chemistry).

int _solve_chemistry_table(chemistry_data *my_chemistry, code_units *my_units, double a_val

Evolves the internal energies over a given timestep by solving the cooling rate equations. This version allows only for the use of the tabulated cooling functions.

int _calculate_cooling_time_table(chemistry_data *my_chemistry, code_units *my_units, doubl

Calculates the instantaneous cooling time. This version allows only for the use of the tabulated cooling functions.

int _calculate_pressure_table(chemistry_data *my_chemistry, code_units *my_units, double a_

Calculates the gas pressure. This version allows only for the use of the tabulated cooling functions.

int _calculate_temperature_table(chemistry_data *my_chemistry, code_units *my_units, double

Calculates the gas temperature. This version allows only for the use of the tabulated cooling functions.

CHAPTER 6

Pygrackle: Running Grackle in Python

Grackle comes with a Python interface, called Pygrackle, which provides access to all of Grackle's functionality. Pygrackle requires the following Python packages:

- Cython
- flake8 (only required for the test suite)
- matplotlib
- NumPy
- py.test (only required for the test suite)
- yt

The easiest thing to do is follow the instructions for installing yt, which will provide you with Cython, matplotlib, and NumPy. Flake8 and py.test can then be installed via pip.

Installing Pygrackle

Once the Grackle library has been built and the above dependencies have been installed, Pygrackle can be installed by moving into the **src/python** directory and running `python setup.py install`.

```
~/grackle $ cd src/python
~/grackle/src/python $ python setup.py install
```

Note: Pygrackle can only be run when Grackle is compiled without OpenMP. See *Running with OpenMP*.

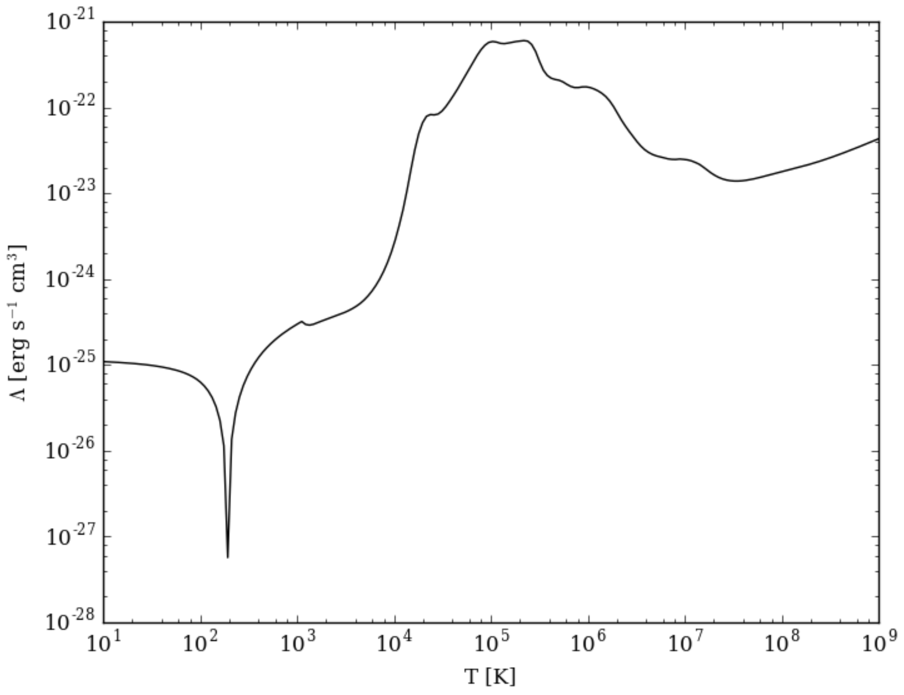
Running the Example Scripts

A number of example scripts are available in the **src/python/examples** directory. These scripts provide examples of ways that Grackle can be used in simplified models, such as solving the temperature evolution of a parcel of gas at constant density or in a free-fall model. Each example will produce a figure as well as a dataset that can be loaded and analyzed with yt.

Cooling Rate Figure Example

This sets up a one-dimensional grid at a constant density with logarithmically spaced temperatures from 10 K to 10^9 K. Radiative cooling is disabled and the chemistry solver is iterated until the species fractions have converged. The cooling time is then calculated and used to compute the cooling rate.

```
python cooling_rate.py
```



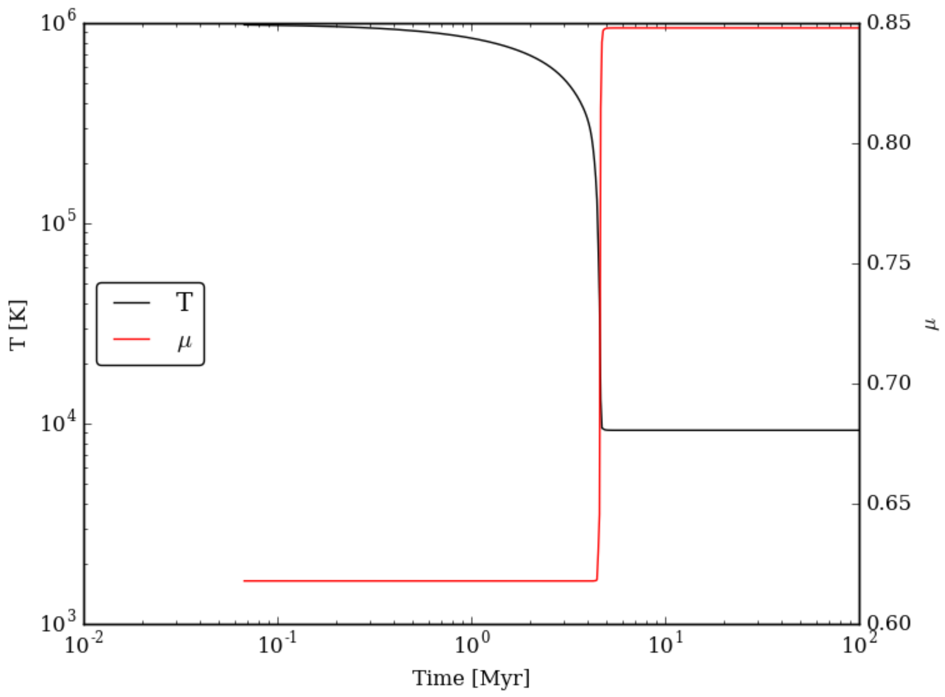
After the script runs, and hdf5 file will be created with a similar name. This can be loaded in with yt.

```
>>> import yt
>>> ds = yt.load("cooling_rate.h5")
>>> print ds.data["temperature"]
[  1.00000000e+01   1.09698580e+01   1.20337784e+01   1.32008840e+01, ...,
   7.57525026e+08   8.30994195e+08   9.11588830e+08   1.00000000e+09] K
>>> print ds.data["cooling_rate"]
[  1.09233398e-25   1.08692516e-25   1.08117583e-25   1.07505345e-25, ...,
   3.77902570e-23   3.94523273e-23   4.12003667e-23   4.30376998e-23] cm**3*erg/s
```

Cooling Cell Example

This sets up a single grid cell with an initial density and temperature and solves the chemistry and cooling for a given amount of time. The resulting dataset gives the values of the densities, temperatures, and mean molecular weights for all times.

```
python cooling_cell.py
```

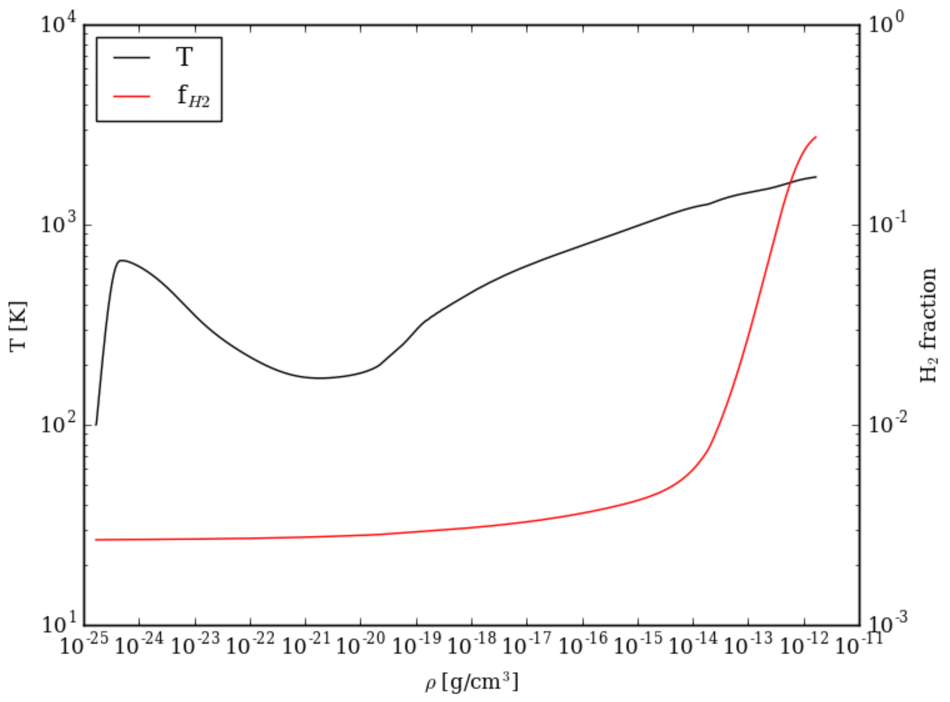


```
>>> import yt
>>> ds = yt.load("cooling_cell.h5")
>>> print ds.data["time"].to("Myr")
YTArray([  0.00000000e+00,   6.74660169e-02,   1.34932034e-01, ...,
         9.98497051e+01,   9.99171711e+01,   9.99846371e+01]) Myr
>>> print ds.data["temperature"]
YTArray([ 990014.56406726,  980007.32720091,  969992.99066987, ...,
           9263.81515866,     9263.81515824,     9263.81515865]) K
```

Free-Fall Collapse Example

This sets up a single grid cell with an initial number density of 1 cm^{-3}. The density increases with time following a free-fall collapse model. As the density increases, thermal energy is added to model heating via adiabatic compression. This can be useful for testing chemistry networks over a large range in density.

```
python freefall.py
```



The resulting dataset can be analyzed similarly as above.

```
>>> import yt
>>> ds = yt.load("freefall.h5")
>>> print ds.data["time"].to("Myr")
[   0.             0.45900816    0.91572127 ...,  219.90360841  219.90360855
  219.9036087 ] Myr
>>> print ds.data["density"]
[  1.67373522e-25   1.69059895e-25   1.70763258e-25 ...,   1.65068531e-12
   1.66121253e-12   1.67178981e-12] g/cm**3
>>> print ds.data["temperature"]
[   99.94958248   100.61345564   101.28160228 ...,  1728.89321898
  1729.32604568  1729.75744287] K
```

Simulation Dataset Example

This provides an example of using the grackle library for calculating chemistry and cooling quantities for a pre-existing simulation dataset. To run this example, you must also download the *IsolatedGalaxy* dataset from the yt sample data page.

```
python run_from_yt.py
```

CHAPTER 7

Help

If you have any questions, please join the Grackle Users Google Group. Feel free to post any questions or ideas for development.

CHAPTER 8

Citing grackle

The Grackle library was born out of the chemistry and cooling routines of the Enzo simulation code. As such, all of those who have contributed to Enzo development, and especially to the chemistry and cooling, have contributed to the Grackle. There is currently no paper that specifically presents the Grackle library on its own, but the functionality was fully described in the Enzo method paper. The Grackle was originally designed for the AGORA Project and first referred to by name in the AGORA method paper.

If you used the Grackle library in your work, please cite it as "the Grackle chemistry and cooling library (The Enzo Collaboration et al. 2014; Kim, J. et al. 2014)." Also, please add a footnote to https://grackle.readthedocs.org/.

The Enzo Collaboration, Bryan, G. L., Norman, M. L., et al. 2014, ApJS, 211, 19

Kim, J.-h., Abel, T., Agertz, O., et al. 2014, ApJS, 210, 14

CHAPTER 9

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