Dengo Documentation

Release 0.1

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January 17, 2014

| Contents |
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| 1 | Tutorial: A Chemistry Solver from Scratch | | | |
|---|---|---------------------------------------|---|--|
| | 1.1 | Defining a Species | 3 | |
| | 1.2 | Creating Reactions | 4 | |
| | 1.3 | Specifying Reaction Rate Coefficients | 4 | |
| | 1.4 | Cooling Functions | 4 | |
| | 1.5 | Creating a Network | 4 | |
| | | | | |
| 2 | Indices and tables | | | |

Hi there! Welcome to Dengo. Dengo is a Python system for symbolically describing a system of chemical species, chemical kinetic rate equations, cooling functions, and then producing from these a set of numerical kernels to calculate the "right hand side" and Jacobian of this system. These two numerical kernels can then be linked into one of several ODE solvers.

Dengo is best thought of as a way to create a chemistry and cooling solver that you can stick into a codebase. Rather than trying to tie together the four separate parts – species, reactions, rate coefficients and the solver itself – into a single whole, Dengo allows you to construct each item individually and join them at the final step before inserting them into a simulation code.

Contents:

Tutorial: A Chemistry Solver from Scratch

This tutorial walks you through the steps to create a new chemical kinetic rate equation solver. These solvers all utilize very similar structures for calculating the right and side and the Jacobian, and will export a standardized API to those functions.

While Dengo provides a number of pre-packaged rate equations, species, rate coefficients and cooling functions, here we provide the necessary steps in order to create new species and rates from scratch.

1.1 Defining a Species

We start by defining individual species. This can be done inside a python module of your choosing, which we will run at the end to output our new network. Species are defined by a small number of attributes:

- Name (which will be used in cooling functions and internally to the solver)
- Number: Mostly unused except when handling ions.
- Atomic weight (in integer AMU)
- Number of free electrons that is contributes

This information is used when calculating things like the contribution of a species to the number density.

Warning: At the present time, Dengo does not support variable gammas for species. This is a planned future incorporation.

To create a new species, you can both create the species object and register it in the global dictionary like so:

from dengo.reaction_classes import Species

```
HI = Species('HI', 1.0, 1.0, 0.0)
HII = Species("HII", 1.0, 1.0, 1.0)
de = Species("de", 1.0, 1.0, 0.0)
```

We now have three symbolic "species" objects for hydrogen, ionized hydrogen, and electrons. Note that Dengo will happily create ions for species defined in the CHIANTI database.

- **1.2 Creating Reactions**
- **1.3 Specifying Reaction Rate Coefficients**
- **1.4 Cooling Functions**
- **1.5 Creating a Network**

CHAPTER 2

Indices and tables

- genindex
- modindex
- search