Lily Ho

Astronomy 496 – Turk

Assignment 3 Writeup

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Note: Questions 1 and 2 were answered for n\_total = 2.00, safety factor = 10, and temperature = 1000K unless stated otherwise.

1. When was it slower or faster? When was it near equilibrium or far?
   1. We can tell that the reactions occur faster for some species when its number density rapidly increases or decreases. That is, the species has a steep slope when the species is being created (positive slope) or destroyed (negative slope) quickly. The steeper the slope, the faster the reaction. The flatter the slope, the slower the reaction. The reactions are at equilibrium when the number density for each species remains a flat line on the graph and the values on the left of the graph don’t change. When t\_final is under 3.00, there are no significant changes to the species number densities. When t\_final reaches 4.00, the number densities for Hm begins to slightly decrease while that of HII is clearly increasing. Right after t\_final passes 5.40 the lines of Hm and HII intersect and then Hm’s number density starts to decrease faster, indicating the destructive reaction is happening faster, while that of HII slowly reaches equilibrium. After t\_final hits 7.00, things get strange as Hm continues to decrease, though occasionally coming back up, and de and H2II begin to decrease as well. The other species’ number densities don’t change much during this time. Thus, they remain at equilibrium for the most part. This probably has to do with the initial number densities I assigned each species among other things…
2. Do you see any particularly interesting regions in phase space?
   1. Regardless of the initial values, Hm is the only species in my program that consistently shows changes in its number density over time. Specifically, it is always decreasing. Also, after t\_final hits 6.00 or 7.00, the number density of Hm seems to disappear from the graph at certain times. I don’t know if this is because the line just isn’t showing on the graph or because there are actually no values for Hm’s number density at that point… When n\_total gets larger, the number density for H2II changes quite noticeably as well, specifically from when t\_final is 10^2 to 10^3. Regardless of temperature, there were only one to three species that showed significant changes in their number densities.
3. What was easy or hard?
   1. Easy/Medium: Understanding what we were trying to achieve was probably the easiest part of the assignment, though I had some trouble with that in the beginning too. Specifically, I understood that were would be given some initial conditions for a gas cloud and that we’d have to simulate what would happen to the different elements in that gas cloud as they reacted with each other. Since I took chemistry last semester, the idea of reaction rates and chemical kinetic equations made some sense to me. However, when more details and numbers were introduced I got lost.
   2. Hard: Including the mu and energy equations and number densities completely threw me off. After asking a lot of questions I understood what they would be used for in our code, but I didn’t/still don’t completely understand the physics and chemistry behind their use when everything is put together. I actually believe that the reason I struggled so much with this assignment towards the end was because I didn’t understand what numbers I should be using. I came up with a good outline of what to do and what equations to use, but I don’t think my numbers ever worked out. I didn’t understand how to use the gas density and ionization fraction parameters in the equations we were told to use.
4. Steps I Took:
   1. Before the progress report I was still wrapping my head around how to approach the project and what components (equations and numbers) I needed. So, the first steps I took were to get down what I needed:
      1. I found and typed out the k functions (k1-k31) that I believed are going to be used.
      2. I created the sympy symbols for k1-k31
      3. I typed out reactions r1-r31
      4. I set up my state vectors with the initial number density of each species that were given in Turk’s sample code.
      5. I used get\_rhs() on each species (HI, HII, HeI, HeII, HeIII, H2I, H2II, Hm, de) and typed out the corresponding equations with the correct state vector values in rhs()
   2. After the previous steps, I ran into errors with my evolve function. So, for day or two before the progress report was due I went to some office hours to ask some questions about the equations we were supposed to use and how we were supposed to update everything. Afterwards I made this outline for how my evolve function should work:
      1. Calculate total num density for H, He, H2 where

n = rho \* massFraction/AtomicWeight

* + 1. Calculate individual number densities from ionization fractions and totalNumDensities from step i
    2. Sum all individual numDensities to get initial totalNumDensity
    3. Calculate initial mu (amu/atom) from rho and initial totalNumDensity
    4. Calculate initial e (constant) w/ initial T and mu
    5. Initialize state vector and timestep vector
    6. for i = 0; i < t\_final; i+=dt:
       1. Do the integration
       2. Find individual number densities -> from state\_vector\_values (integrator.y)
       3. Find totalNumDensity by summing values in integrator.y
       4. Calculate new mu
       5. Calculate new temperature, T, using e

1. Final Results: In the end, my code still didn’t work. I was unable to run the code or produce graphs when I tried implementing the above code scheme because I was missing some initial values such as the initial gas density and ionization fractions. I also wasn’t sure what to do with temperature. And I struggled with updating dt and with the safety factor because if I changed it from dt = t\_final/safety\_factor to dt = safety\_factor \* np.min(state\_vector\_values/integrator.y), my code would get stuck on the new dt line in the loop. I also recall Turk telling us the safety\_factor should be between 0 and 1 but if I do that nothing appears on my graph. I was also confused on how we were supposed to update the system since I was under the impression we weren’t supposed to…update the temperature?

Papers Used:

* http://articles.adsabs.harvard.edu/cgi-bin/nph-iarticle\_query?1991ApJS...76..759L&data\_type=PDF\_HIGH&whole\_paper=YES&type=PRINTER&filetype=.pdf
* <https://arxiv.org/pdf/astro-ph/0003212.pdf>
* <https://arxiv.org/abs/1610.09591>