DOCTORAL PROGRAM IN ASTRONOMY

PROGRESS REPORT

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Towards Exoplanetary Atmospheres: new data reduction methods for the nIR

Author:
Jason James Neal

Supervisors:
Pedro Figueira (IA)
Claudio Melo (ESO, Chile)

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Departamento de Física e Astronomia

Instituto de Astrofísica e Ciências do Espaço

Faculdade de Ciências da Universidade do Porto

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Overview

Exo-atmospheres, one of the forefronts of exoplanetary science, has shaped science and scientific instrumentation for the last decade. Over the past years we have been developing new methodologies and software tools for the extraction of minute signals from the NIR (near-Infrared) spectra of exoplanets.

The two main goals defined in the thesis proposal submitted were:

1. Development of tools for high spectral fidelity
2. Application to brown dwarf and exoplanet targets

The tools created last year were tidied up, and some were used to reduce CRIRES spectra for other researchers. Due to problems with the observations further tools for the spectral differential method were not produced. I also the improved the performance of tools that were used to calculate the RV information content of NIR spectra. This will be used to analyse the NIR information content of M-dwarfs from CARMENES observations. This extends our previous work the information content of synthetic spectra in Figueira et al. (2016). Unfortunately the completion of this analysis is dependent on the release of the CARMENES spectral catalogue which was expected in January 2017.

Problems occurred in the application to the brown dwarfs as we discovered the data was insufficient to perform the differential spectral recovery we were attempting. This has caused delays in the generation of the promised paper as we attempt other techniques to recover the companion spectra from the observations. This has caused some tools to be stopped, different tools to be created and others to be updated but these have yet to be used for any publication.

This report covers the activities performed and the tools developed during the academic year 2016-2017 in further detail and outlines the adjusted plan for the remainder of the PhD.

Brief Description of the Work Done

Spectral differential analysis

In the progress reported from last year I thought I was at the stage to recover the differential spectra, even showing a plot of the subtraction between the two observations. Unfortunately the result I showed did not take into account the relative star motion correctly and were incorrect. A corrected version is shown at the top of Figure 1 and was used in a poster and seminar I presented in July and September 2016. As the main features observed still coincide with the shaded stellar (yellow) and telluric (green) regions these are likely due to incorrect telluric removal. To attempt the identification of any signal present I synthesized the differential spectra from synthetic PHOENIX-ACES spectra. I use the synthetic spectra with the parameters closest to the estimated temperature of the companion (from the Baraffe et al. (2003) evolution models) with the logg and metalicity closest to the host star. The spectra of the companion were wavelength shifted to match the radial velocity (RV) predicted by the published orbital parameters at the time of each observation and then subtracted. To obtain the RV for the companion from the published K_1 semi-major velocity of the host we use the mass ratio q with the estimated companion mass value M_2, $q = M_1/M_2 = K_2/K_1$. Only the synthetic spectra of the companion was used which simulates a "perfect" host star subtraction.

At this point it was observed that there was a serious problem with this method as the synthetic differential spectrum was over an order magnitude smaller then the measured one. Upon studying the orbit of the target as in the bottom of Figure 1, it was observed that the observations marked were not well separated in RV. The largest RV separation between two observations is just over $2 km/s$. At $2.1 \mu m$ and the instrumental resolution of $R \sim 50000$ the $FWHM = \lambda/R$ of a single line is $\sim 6 km/s$. Therefore, the companion spectra are only shifted by $> 1/3$ the FWHM and mutually cancel out when subtracted, creating a signal well below the SNR level.

We simulated adding a fake companion with a spectra identical to the observed spectra and adding it to itself at the flux ratio of $\sim 1\%$ and the correct RV of each observation. When subtracting the two spectra the fake planet produced a signal that was significantly smaller then the difference spectra from the observations at the RV separation of the observations. Figure 1 (middle) shows the change in the differential signal when the fake planet is shifted to RV difference of K_2 ($19.8 km/s$) and $2 \times K_2$ ($39. km/s$, the maximum difference possible). With the noise level we have it is not possible to observe at the differential signal of the companion at the small RV separation between the observations.

There are two (interconnected) reasons for the short separation in time between the observations included in the program: the inability to set a minimum time separation constraint in service mode at the time, and the long orbital period of the companion, longer than an observing proposal semester (it was impossible to ask for time over several semester in a regular proposal). Some of the targets have very long orbital periods (e.g. > 2000 days) so that an optimal pair of observations would need to be obtained from separate observing periods and depending on the phase of these long period orbits even observations from each end of the observing period probably would not provide sufficient RV separation. In one case observations for the same target were performed back to back so that the RV difference between them the two observations is same as the RV variation during each observation.

This has revealed that care needs to be taken when trying to perform this spectral differntial approach in the future. I have created some tools that are not quite finished to try help avoid this issue in the future. These plot the RV curve for the target (given the known parameters), allow you to mark previous observations and indicate the times to observe any new spectra to achieve the desired RV separation. I have also heard that the newer scheduling systems allow for tighter constrains on observations which would have been necessary for this approach.

Synthetic Spectral Recovery (Ongoing)

Even though we cannot use a differential approach each observation still contains a combined spectrum of the host and companion. We are now trying to recover the mass of the companions using a "faint companion spectral recovery" technique. We match our observed spectra to a synthetic combination spectra in a brute force χ^2 approach. The spectra is composed of a host and companion spectrum combined in relation to a flux ratio and the relative RV. We vary the spectral model by $Teff$, as well as the flux ratio and the RV of the companion. This approach was extremely simple to apply to a generated combination spectra with added noise added (see Figure 2), but has proved difficult when dealing with actual observations.

A test was initially done with a synthetic observation to test the χ^2 approach, varying with different resolution, flux ratio and SNR. This revealed the expected relations that the "detection" improves with a higher SNR, resolution and flux ratio (brighter companion). For actual observations it has been more challenging to implement the analysis with the things outstanding that need to be addressed detailed in § .

My current task is to write up what I have done so far in a paper, detail how we plan to finish this work off and then finish the coding and analysis for this.

Corrections to IRAF reductions

Over the course of this year I have continued to improve upon the reduction tools/methods for CRIRES data. While working with the reduced CRIRES spectra I noticed artifacts in some of the results, which took multiple attempts to work out a solution. Some of these artifacts are shown in Figure 3 where the individual nod spectra of a ABBAABBA nod cycle are shown. Most of the spectra reduce well but one or two do not, visually identified by the different spectral shape seen in the top two panels.

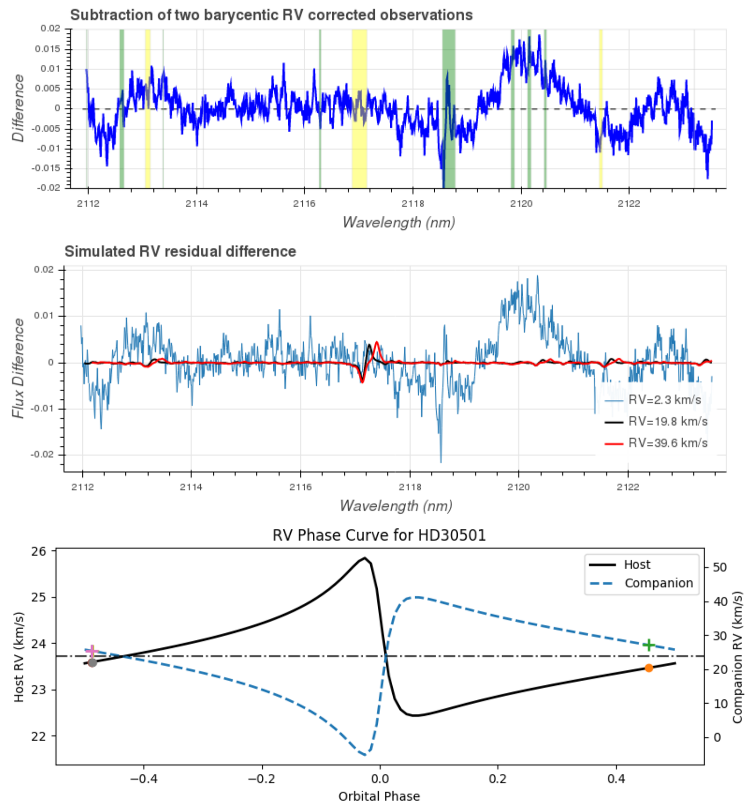

Figure 1: (top) Spectral difference between two observations. Regions where large ($> 5\%$) stellar (yellow) and telluric (green) lines were present in the original spectra are highlighted. (middle) Difference between the spectral difference when including a fake planet. The blue line is the spectral difference at the observation radial velocity. The red and black lines indicate the deviation from the blue line when the fake planet is shifted to a RV separation of $19.8 km/s$ and $39.6 km/s$, respectively, corresponding to 50% and 100% the maximum RV difference possible for this target. (bottom) The orbital RV phase curve for HD30501 with the points indicating the 4 observations taken. The solid black line is the RV of the host star while the blue dashed line is the RV of the companion.

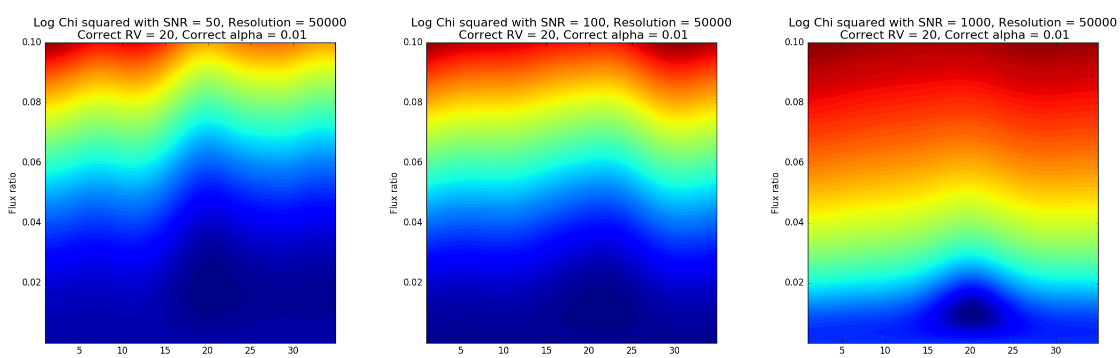

Figure 2: Simulated χ^2 recovery of a synthetic "observation". A minimum χ^2 (blue) is observed around the parameters chosen for the simulation. From left to right these figures are for SNR level of 50, 100, 1000 respectively. The other parameters held constant, a companion flux ratio of 1%, RV difference $20km/s$ and $R = 50000$.

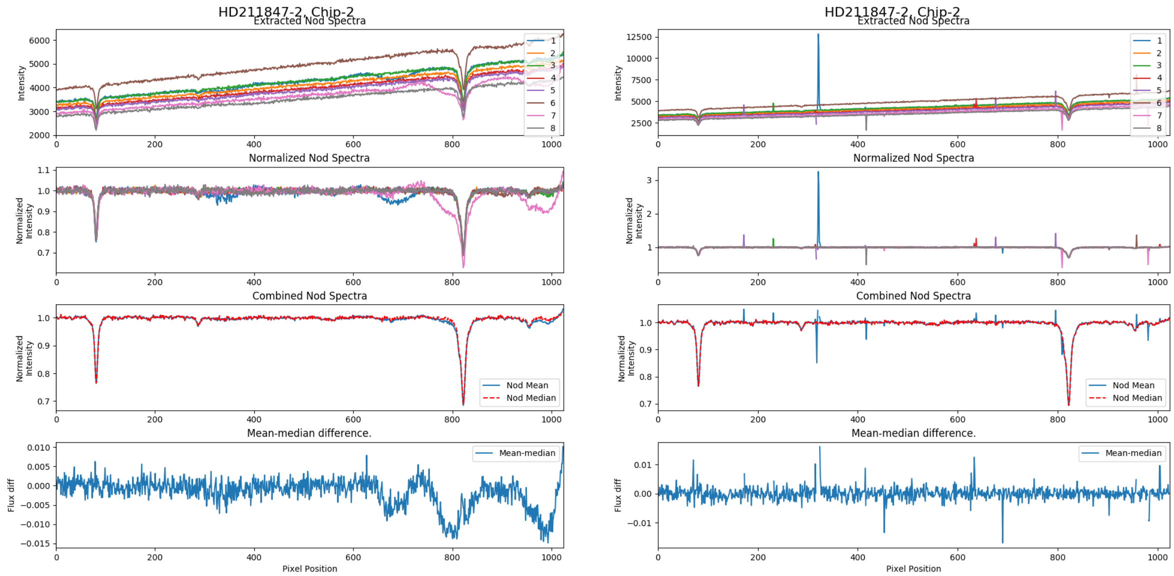

Figure 3: The individual ABBAABBA nod spectra quick-look plots to used visually identify artifacts in the extracted spectra. (top) The 8 unnormalized nod spectra. (second) The same spectra normalized to the continuum. Here it is clearly seen that something is wrong with the pink and blue spectra. (third) The mean and median of the 8 nod spectra. (bottom) The difference between the mean and median, again clearly showing there is an artifact (outliers) in the optimal spectra. The left plot shows the non-optimally extracted spectra while the right plot shows the optiamally extracted spectra (variance weighted). The artifacts in the optimal spectra clearly match with the locations of "bad pixel" spikes in the non-optimal case.

After varying many extraction settings I finally discovered that it was a problem with the optimal exactaction which employs a variance weighting to reduce the noise. When comparing optimal and non-optimal extractions side by side it is clear that they occur around spikes in the extracted spectra that do not seem to be identified and removed properly. I developed a spectral combination method that replaces the optimally extracted nods with artifacts with the non-optimal extractions. As these have the spikes still present a 4σ bad pixel identification method was applied using all 8 nod spectra with the bad pixels linearly interpolated over before the spectra are combined together. The artifacts found in the optimally reduced nods affected the flux of the normalized combined spectra by around order ~ 0.005 as seen in the bottom panel of Figure 3 which is significant when searching for companion spectra with an expected flux ratio around $> 1\%$. In hindsight I probably would not have had this issue if I had used the ESO pipeline, but I would still have needed to make the bad pixel rejection algorithm for the ESO pipeline, only earlier.

NIR radial velocity information content

With the inability to use the differential spectral method we turned to other options to explore. It was understood that a catalogue of CAMENES NIR spectra for M-dwarf stars was going to be a release in early 2017. I had previously reviewed the python code used in the paper "Radial velocity information content of M dwarf spectra in the near-infrared" (Figueira et al. 2016), of which I was a part of. It was seen as a good opportunity to use the same technique to measure the RV information content of real observations.

I took the code from the previous work and made several modifications to improve it. I improved the performance by $> 250\times$ and simplified the codebase making it easier to read and understand. I extended the range of synthetic spectra possible, to analyse the effect of logg and metalicity on the RV information content in the future. I added *automated testing* principles to this project to insure that the code is correct and that my modifications still reproduce the published results. This care led to the discovery of errors in the published paper results. The telluric line masking was incorrect which affected 1/3 set of results but not the overall conclusions in the published paper. We will make a note of this in the future paper. Unfortunately there has been a delay in its release with no news when this release will happen. I spent about 1.5 months on this upgrade and stopped when it was clear that the CARMENES release was not happening soon. A small amount of work will still be required to interface to code with the CARMENES data. I have also turned this code into a public repository and will point to this in the future paper.

Collaborations

In March 2017 I reduced some CRIRES spectra for *Janis Hagelberg*. The target eta tel is a fast rotating brown dwarf and Janis plans to measure with the broadening of strong K I doublet lines. I only performed the extraction spectra and then passed it to Solène, another doctoral student, to perform wavelength calibration and telluric correction with the Molecfit software (Smette et al. 2015). This will hopefully lead to a publication but it is out of my hands now.

I also was invovled in the collaboration on K2 follow up with HARPS, a large observing program which received time. So far, I have only reviewed some upcoming papers (two submitted) and it is expected that I will perform observations with the HARPS instrument in Chile in the upcoming year.

Complementary activities

This year I have attended one advanced school and presented a talk at a national conference. I was fortunate to perform 3 nights of astronomical observing alone on HARPS-N at the TNG, which was a great experience. The details of these activities are listed below.

- IVth Azores International Advanced School in Space Sciences, 2016, Horta, Faial, Azores Islands, Portugal
- HARPS-N Observations at the TNG, 6-8 Feburary 2017, La Palma, Spain
- XXVI Encontro Nacional de Astronomia e Astrofísica (ENAA), 9 Sept. 2016, Aveiro, Portugal
- Monitoring the, 12^{th} Escola de Verao de Fisica, 28 Aug. - 2 Sept. 2016, Porto, Portugal
- Completed and submitted the report for the AST732 PDA unit.

Codes Developed

I recently moved most of my work into public github repositories. Over the last year I have made $> 1,860$ contributions which are publicly available on my GitHub. The newer tools completed or in development this year are listed below.

- companion_simulations - Brute force χ^2 analysis between observations and a mixed synthetic spectra - Still a work in progress.
- barraffe_tables - A tool which uses the Baraffe 2003/2015 evolution models to simply transform between a estimated companion mass and a companion-host flux ratio.
- enric - The code for the updated NIR information content analysis. A $> 250\times$ speed up with extensions to analyse logg, metalicity and alpha. I am currently waiting for CRAMENES data to finish this code and use it.
- iastro - Observation-tools - Contributed to the “IA's ” iastro github repository. Contributing a tool to calculate the RV difference between observations.
- nod_combination - Combine nods in a way to avoid the artifacts observed in the “optimal” CRIRES reduction.

- spectrum_overload - Python class for easily operating on spectra, e.g. subtract two spectra for the spectral differential method.

Updated Work Plan

CRIRES brown dwarfs companions

The most urgent and pressing task is completing the paper on the work done on the brown dwarfs companions. The first part of the paper is mostly written and presents the extraction, calibration, telluric correction steps and the spectral differential method we have attempted and why these observations were insufficient. In the second part of the paper we are attempting the spectral recovery using a combination of synthetic spectra with the aim of estimating an upper-limit on the mass of the companions. This second part is incomplete and is without successful results yet.

We are developing this method using our two largest companions. One of which was recently discovered to actually be a low-mass star of 155_{M_J} (estimated flux ratio $\sim 32\%$) and the other has a mass around 90_{M_J} (flux ratio $\sim 1\%$). Even with this favourable result we can not yet get a result that is consistent with what we expect. There are a still couple of things that still need to be investigated before the results can be trusted. These are:

- Continuum normalization

  It has recently been identified that the continuum normalization level of the observed spectra effects the recovered flux ratio. For example a continuum that is consistently high (above 1) will favor the spectral component that has less (or shallower) absorption lines as it will be closer in a χ^2 sense. We will try and fit a continuum offset as a free parameter to see if that solves this issue.

- Other Spectral models

  Currently I have only focused on the PHOENIX-ACES models but there are other models specifically for low-mass-stars and brown dwarfs such as BT-SETTL Allard et al. (2012), or BT-DUSTY (Allard et al. 2001). Currently there are spectral mismatches between the observations and the models, with lines present or missing in each other which may be solved by moving to these other models. These other models also extend down beyond the lower temperature limit of $\sim 2300K$ for the PHOENIX-ACES models which covers the two largest companions only so the cooler models will likely be necessary for the lower mass companions.

  Once the recovery technique is properly working then it should be relatively simple to swap out one set of synthetic models for another, it may even be necessary to use separate models from the different libraries for the host and companion.

- Inherent synthetic flux ratio

  Currently the model we use to combine the synthetic spectra varies the flux ratio. Another idea that has not been tested yet is to use the inherent flux ratio in the synthetic spectra (accounting for the host and companion surface area). This will reduce the problem by one parameter so it may be easier to identify the spectral components and the radial velocity offset of the companion.

NIR information content

The work on the CARMENES NIR information content is currently stalled until the release of the spectral catalogue. There are a couple of CARMENES spectra in the exoplanet team which could be used to finish off the software and test it to enable a quicker analysis when the catalogue release happens. The analysis of information content with different logg and metalicity and the paper for this work can also be started without the CARMENES release.

Changed Plans

Last year it was proposed that we may try reanalyze the results of Snellen et al. (2010) using our analysis tools. As with our data the Snellen et. al. dataset would not be sutiable for the spectral differential method. The observations are taken in a small window during the transit, therefore, the RV difference would be too small. If we did repeat their work it would only be a test of the extraction, wavelength calibration and telluric correction tools developed. We have not investigated this any further due to this and the time constraints faced.

I also indicated last year report that was the opportunity to contribute on the *SOAP-Opera* programming project. There was no work done on this project during this year.

Other tasks

There are a couple of other tasks that are expected this year.

- As part of the ESO-K2 collaboration it is expected that I will perform observations with HARPS in Chile in the upcoming year.
- Reveiwing any papers that result from the ESO-K2 collaboration.
- Thesis writing should begin in early 2018.

Expected Publications

Major contributions:

- Brown dwarfs companion - spectral differential and synthetic spectral recovery. (My work so far)
- NIR RV information content of the CARMENES M-dwarf catalogue.

Minor contributions:

- ESO-K2 collaboration papers. Two submitted, so far.
- Rapidly rotating Brown Dwarf. I reduced the data and it is now out of my hands.

Time-line

Again there have been adjustments to the proposal time-line shown in Figure 4. This is to reflect the progress made and change in direction.

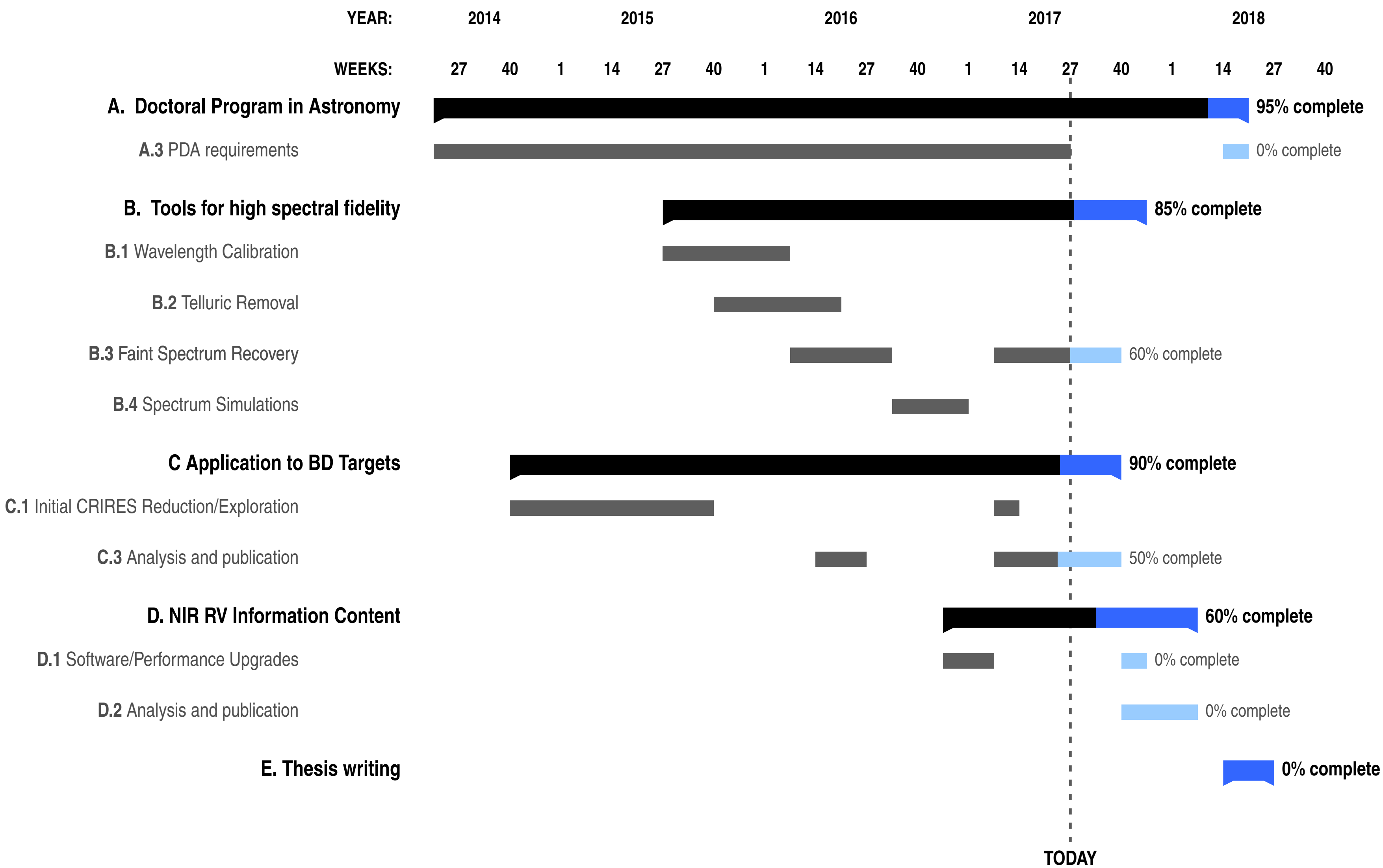

Figure 4: Updated time-line showing the current progress.

Conclusion

This year has been difficult with a few setbacks. Discovering that the observations were insufficient to apply the differential spectral method was frustrating. I have however explored why they are insufficient and have built a tool which could be useful to plan future observations for this method. I have had a hard time staying focusing on writing the paper about this unfinished work, while also trying to salvage some results with the companion spectral recovery approach. The paper I had planned is behind schedule, and currently my primary focus.

I have discovered that I much prefer the software development side of my work compared to the reading/writing academic articles. This was shown with the performance improvements I added to the RV information content code. This work is waiting on CARMENES catalogue data and will hopefully be released by the time I finish the brown dwarf companion paper. I am really looking forward to the day that this Ph. D is finished, within in the coming year.

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