

1 Remote Teaching of Programming in Mathematica: Lessons Learned

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Cite This: <https://dx.doi.org/10.1021/acs.jchemed.0c00684>

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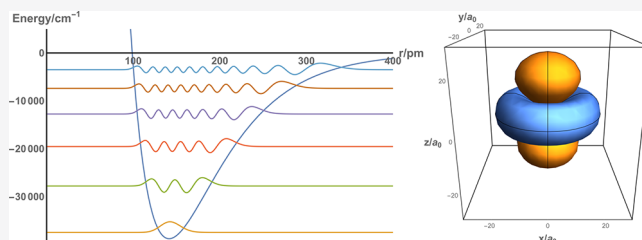
Article Recommendations



Supporting Information

3 **ABSTRACT:** The COVID-19 pandemic has resulted in a need for
 4 social distancing measures in public spaces and will have an
 5 important impact on university level teaching going forward.
 6 Remote methods to complete laboratory related activities are a
 7 potential means of students achieving practical credit while still
 8 isolating or social distancing. We outline the implementation of
 9 two novel remote exercises, based on coding in Mathematica, and
 10 the methods used to provide ongoing help to students. These
 11 exercises are used as a case study to identify potential problems
 12 with remote exercises based on student feedback. Suggestions for how these problems might be overcome in further iterations of
 13 these remote exercises are explored.

14 **KEYWORDS:** First-Year Undergraduate/General, Second-Year Undergraduate, Physical Chemistry, Computer-Based Learning,
 15 Distance Learning/Self Instruction, Thermodynamics, Kinetics, Quantum Chemistry



16 ■ INTRODUCTION

17 The 2020 COVID-19 global pandemic has had a dramatic and
 18 rapid effect on universities in the UK and across the globe.¹
 19 The Universities UK issued framework for a safe and successful
 20 emergence from lockdown includes the need for “changes to
 21 university...infrastructure” and “flexibility in place to...support
 22 students to achieve their learning outcomes in a safe manner”.²
 23 While some universities have already come forward with
 24 decisions to hold remote lectures to alleviate the spread of
 25 infection,³ there is a substantial responsibility for teaching
 26 laboratories to follow suit in reducing contact between
 27 students while still providing elements of practical teaching.⁴
 28 Because of its term structure, our department has been
 29 running a remote laboratory course from 26th April to present
 30 (15th June). While the teaching laboratory has been out of
 31 bounds, remote, computer-based, teaching has provided the
 32 opportunity to focus on other important and transferable skills
 33 such as data analysis and the introduction of coding
 34 languages.^{5,6} The introduction of exercises based around
 35 these topics has allowed students to continue to work toward
 36 their practical credit requirement (in the UK, a four year
 37 Masters’ course must contain a minimum of 400 h of practical
 38 work for accreditation by the Royal Society of Chemistry)⁷ but
 39 also broadened the scope of what practical exercises the
 40 laboratories may offer at the start of next academic year—with
 41 more advanced and applied coding activities being possible
 42 now that the students have a strong foundation.
 43 It should be noted that the likely need for social distancing
 44 in laboratories next academic year will reduce the number of
 45 students that can be working in the lab at any time. The
 46 continued use of computer-based exercises, alongside the
 47 reintroduction of practical laboratories, will let more students

undertake practical course work at the same time by moving
 some of this work outside of the lab. In this way the student
 throughput required for every student to meet their practical
 quota of lab hours can still be achieved, despite the change in
 circumstances.

In this communication we introduce two exercises, based in
 Mathematica, that were made available to our first and second
 year students. Our institution owns a site license for this
 software so that all students are able to download and install
 the application on their home computer and carry out these
 exercises while in isolation. The first exercise consists of a
 series of activities aimed at introducing syntax and useful
 applications of Mathematica, while the second seeks to build
 on this introduction through addressing some simple quantum
 mechanical problems. (All material relating to these two novel
 exercises are included as Supporting Information and are ready
 to be implemented by others. Further details of the topics
 covered can be found in Table 1.) To date, both of these
 exercises have been completed by 200 of our students, with a
 further 68 just completing the introductory exercise. We have
 used these exercises as a case study for lessons learned in
 rolling out remote exercises and to suggest ways in which we
 have, or other institutions might, learn from our initial trial.

Special Issue: Insights Gained While Teaching Chemistry in the Time of COVID-19

Received: June 16, 2020

Revised: July 14, 2020

Table 1. Topics Covered in the Two Mathematica Exercises

Practical Title	Topics
S217: Introduction to Mathematica	<ul style="list-style-type: none"> Defining variables and expressions. Implementing text strings. Manipulating lists. Employing in-built functions and defining novel functions. Plotting data and functions. Solving algebraic and differential equations. Integrating and differentiating functions. Linear regression and nonlinear curve fitting.
C214: Quantum Mechanics in Mathematica	<ul style="list-style-type: none"> Plotting wave functions and probability distributions for particle-in-a-box, harmonic and Morse oscillator, and hydrogen orbital problems. Exploring different visualizations of 2D probability distributions. Evaluating expectation values and uncertainties.

INTRODUCING EXERCISES AND IMPLEMENTING HELP FOR STUDENTS

The two exercises, along with introductions detailing instructions, credit hours, and methods for downloading, installing, and running Mathematica (see Supporting Information) were made available to students via our university's virtual learning environment.

Given the potential for increased cognitive load when working from home, the introductory practical (known as S217) was constructed in a scaffolded manner with worked examples throughout to help guide students comfortably through the activity.^{8–10} The introduction of each new aspect of code was accompanied by one or more exercises and revisited in later activities through progressively more complex tasks. The follow up quantum mechanics exercise (known as C214) was written with reduced scaffolding and was designed to allow students to put aspects of what they had learned from the introduction into practice—there were potentially multiple methods of achieving the correct answer and all methods would be treated equally during assessment.

As was made clear in the introduction to both exercises, a help system was implemented so that students could make enquiries in the event that they had difficulties while working through the exercises. Students were invited to send enquiries via e-mail to a dedicated address to which all teaching staff had access. Students were requested to title their e-mails with the

practical code, for ease of administration, and to briefly describe the nature of the problem, if possible. Students were also instructed that short conversations via video conferencing would be available if they felt that e-mail contact would not prove sufficient to solve their problem. With our university having a substantial number of international students in its chemistry cohort, we took the decision not to timetable exercises and to do our best to provide round-the-clock help to facilitate those students working in other time zones or difficult work environments.

FEEDBACK RESULTS

An anonymous survey was issued to students via our virtual learning environment (see the Supporting Information for a full list of questions). The main goal of our survey was to ascertain how long students were taking to complete each exercise and how they were finding the help available. Out of 268 students, 71 provided information about introductory exercise, S217, while 53 of 200 provided feedback for C214 (due to anonymity of each survey, it is not possible to determine the extent of overlap between the two sets of respondents).

Time Taken to Complete Exercises

Our initial credit allocations for the two exercises were 12 h for the introduction and 6 h for the follow up quantum mechanics exercise. These allowances were based on feedback from teaching assistants who had little, or no, experience in coding. A distribution of hours taken for each exercise is provided in Figure 1.

The feedback showed that 50% of the total student respondents completed S217 within our estimated time (12 ± 3 h), with 6% taking below 9 h and the remaining 44% of students taking greater than 15 h to complete the exercise. The results were more dramatic for the follow up exercise C214, where only 32% of the students completed the exercise within the estimated time (6 ± 3 h) and the other 68% took greater than 9 h.

These results show that a sizable number of students were taking longer than expected to complete the two exercises, too many in the case of C214 (we would anticipate 50–60% of the cohort to fall within a ± 3 h range). These results may be due to difficulties completing the exercise and a lack of immediate help from teaching assistants due to the remote learning

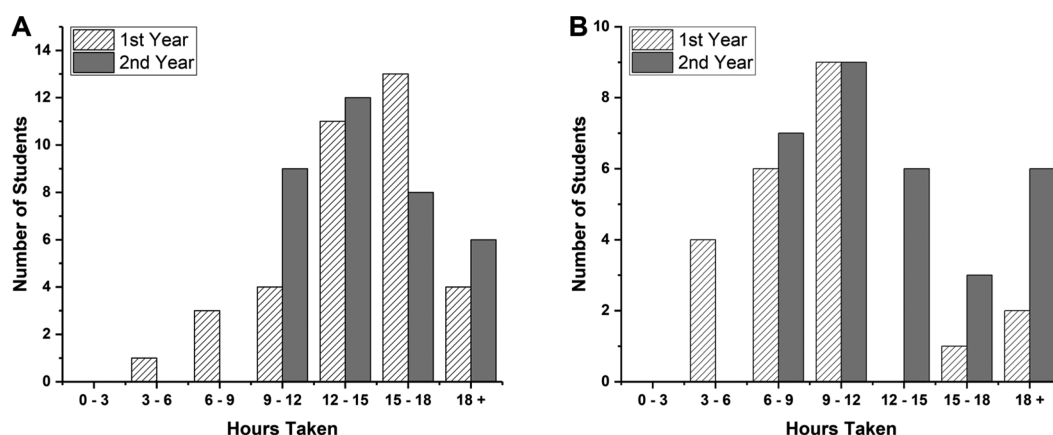


Figure 1. Distribution of hours taken to complete the Mathematica exercises. (A) Reported hours taken to complete the introductory exercise S217. (B) Reported hours taken to complete the quantum mechanics exercise C214.

environment (see below), or an increased cognitive load due to the nonideal working environment.^{11,12}

Student Enquiries

As stated above, remote help was provided to students completing this exercise via email and video call (the latter on request). Our team worked hard to ensure that waiting times for responses to e-mail queries were kept to a minimum so as to minimize any disruption to flow that the students might experience. Of the students that responded to our survey, 38% contacted staff with help enquiries about S217 and 63% contacted with enquiries about C214. An outline of the topics of these enquiries is provided in Figure 2. Enquiries ranged

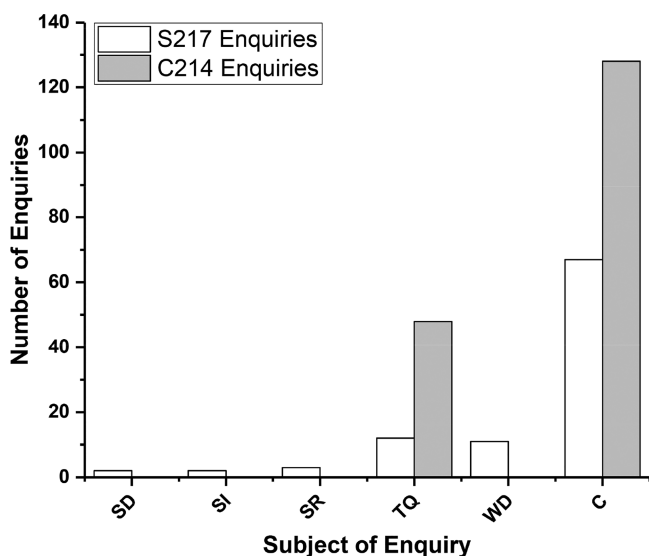


Figure 2. A summary of enquiries received via e-mail during the course of the term. Enquiries are categorized according to the particular problems encountered by the students: SD, software download; SI, software installation; SR, software registration; TQ, theory or understanding of question; WD, setting a working directory; C, code syntax or implementation.

from technical difficulties such as software issues to theory associated with chemical questions (3% and 22%, respectively), but most enquiries were specifically about aspects of coding or use of the Mathematica software package (note that, due to its

nature as a followup exercise, there were no download and installation enquiries relating to C214).

Other than general errors in syntax, the most common coding problem in S217 was students not being able to set a working directory (11% of all enquiries relating to S217)—a number of students seemed to have difficulty navigating through general file structure or typing out folder addresses. Errors in coding were spread across the five notebooks, with no particular clustering of problems. For C214 there was a greater portion of enquiries relating to theory (27% of total C214 enquiries), with the most common being students forgetting how to normalize wave functions or calculate probabilities through integration. The greatest number of coding issues related to typing out the full hydrogenic wave functions in the third notebook; students were much more error prone in this exercise and often struggled to debug what they had written—perhaps a little surprising since students are simply required to convert a mathematical formula to code (albeit a long one) rather than implement any novel features.

We initially suspected that those students who sent e-mail enquiries would complete the two exercises at a faster pace since they would not get stuck troubleshooting their code when it was passed to a teaching staff member. Figure 3 shows that this is not really the case—the percentage of students taking greater than 15 h to complete S217 was 44% and 43% for those sending enquiries and those not sending enquiries, respectively. For C214 the numbers were the opposite of our initial guess with 42% of students taking greater than 12 h to complete the task when sending enquiries versus 16% of nonenquiring students.

These results have led us to believe that students having difficulties have only been contacting us for help as a last resort, rather than at any time that they encounter an issue—this result is backed up by students' written feedback (see below), but stands in contrast to the information given alongside these exercises as well as further e-mails sent from the department emphasizing that students should get in touch whenever they have any problems with computational exercises. Another possibility is that students have a different perception of the requirement for completion of the exercise: in the lab, a student must leave at closing time regardless of whether they have completed their practical or not, but there is no cutoff time in these remote exercise unless the student imposes it themselves.

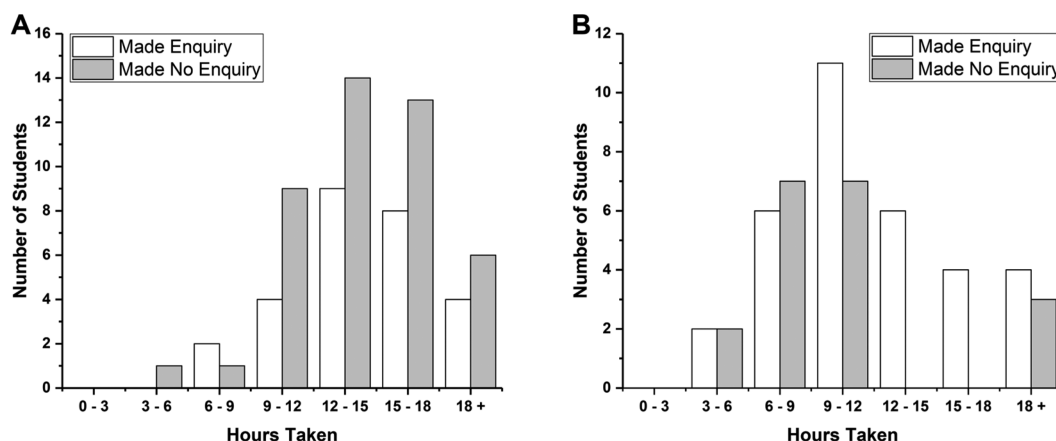


Figure 3. Distribution of hours taken to complete the Mathematica exercises separated by students who did or did not send e-mail enquiries. (A) Reported hours taken to complete S217. (B) Reported hours taken to complete C214.

Other Sources of Information

The students who had not contacted us for assistance were polled on other sources of information they had employed when they had encountered problems. This information is summarized in Figure 4. As seen, 29% of responses indicated

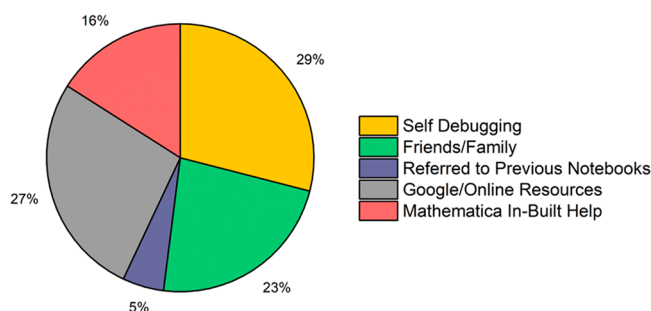


Figure 4. Other types of help students reported as methods to solve problems during the two exercises. Percentage of total responses that mentioned each of five major methods of troubleshooting.

that students were simply able to fix their problems through taking the time to debug the code themselves with a further 5% of responses citing the previous introductory notebooks as a useful reference. Further, 16% of responses indicated that Mathematica's in-built documentation was a useful guide, while online searches and help from friends or family were the most popular sources of information at 27% and 23% of responses, respectively.

We believe that all of these sources of information are valid: students are actively encouraged to browse the Mathematica documentation in a couple of the exercises, and the ability to search online for a solution to a coding problem is a regular source of information for active programmers. One potential concern is those students citing friends and family as a source of help, while peer-based learning and collaboration are important and useful methods in scientific teaching,¹³ there is a fine line between collaboration and copying—something that is particularly difficult to root out when scanning through programming code.¹⁴

Reasons for Not Making Contact When Needing Assistance

Some reasons for students not making enquiries are grouped thematically in Table 2. Three common themes were that students found e-mail communication difficult or were unable to explain their problem in text, students thought that e-mail responses would be too slow, and students felt unable to contact with what they viewed as problems that were too small about which to bother staff.

These responses are interesting given the information that was provided to students about accessing help. Multiple students said that e-mail was not a preferred method of communication, but we thought we had made clear that video calls were another option for seeking help. We have also worked very hard to provide rapid responses to all e-mail enquiries throughout the term (subject to time zone differences), with response times of 5–10 min during working hours and 30–60 min during evenings and weekends. Evidently these times are not rapid enough for students, or (if they are suitably fast) students are assuming that responses will be slow and so have decided not to make an enquiry.

Table 2. Reasons for Students Not Contacting for Help via Email

Theme	Quotes
Difficulty with contact via e-mail	<ul style="list-style-type: none"> “talking to someone one on one about a problem is obviously much more useful than an email” “At times I wasn't sure what the problem was, so it is difficult to ask for help when you don't know what is wrong” “I didn't think I could explain my issues in an email” “it feels difficult to explain the problem I am facing via e-mail”
Email too slow	<ul style="list-style-type: none"> “by the time I had emailed and received a reply in that time I could probably do a google and find out” “emailing about every small question I had...would have made the lab take a lot longer” “Tried to sort problems out myself and thought this might be quicker than emailing” “wanted to get the practical done in a reasonable time, rather than start-stopping and waiting for a response”
Felt issue too simple/ viewed contact as a last resort	<ul style="list-style-type: none"> “I found myself stuck most because of errors that seemed too uncomplicated to ask someone about them” “I did not want to email the CTL until I'd exhausted all other options”

We find the last category of reasons more troubling. In a laboratory setting, teaching assistants are able to look over the shoulder of students, actively providing help when they are having difficulties, and keeping the weaker students in step with the cohort so that they complete their exercise in a sensible time.¹⁵ With remote exercises, this is not possible and the onus is solely on students to ask for help. Should students decide that their problems are not sufficient to bother teaching staff, it is near impossible to provide help in a remote teaching context and students will likely take a lot longer to complete exercises.

DISCUSSION

We have successfully implemented two remote exercises using Mathematica which, at the time of writing, have been completed by more than 200 students across the first and second year cohort. While the majority of students have successfully completed all of the outlined tasks with a good quality of work, we have found that the time taken for students to complete these exercises has substantially exceeded expectations. In the case of our second exercise, C214, we have re-evaluated the credit allowance for this exercise from 6 to 12 h, based on student feedback.

We believe that the time taken by students to complete these exercises has been increased due to a greater cognitive load generated by the need to work from home, but is also the product of a lack of active feedback from teaching staff, which comes as a consequence of remote working. While we have manned an enquiry email address and fielded video calls to help many students when they have had difficulty, this is reliant on students actively seeking help. Our concern is that those students who need the most help to complete exercises in a timely manner may not be the ones to seek help themselves. In a teaching lab environment these students would typically be identified and assisted throughout a session to make sure that they complete an exercise on time. Reasons for students not making contact include difficulties with communication by e-mail, an assumption that responses to e-mail enquiries are, or will be, too slow, or that their problems are too small to warrant bothering teaching staff.

To try to increase our help for struggling students, and students in general, if further remote laboratory teaching needs to be implemented in the future we propose the following modifications to the help provided this term:

- We will construct a written FAQ for each exercise, using what we have learned from answering queries to these implemented exercises to provide a list of common problems and solutions that students may reference at any time and independent of having to write an enquiry. This may, for example, include further information on how to set a working directory, or provide additional theory-based hints on how to complete exercises, alongside additional coding instruction.
- We will propose having video call drop-in sessions in which one or multiple teaching staff members are available for all or part of a day and which students can dial into to ask for help without the need for typing out an e-mail. This is a much more intensive method of providing help and feedback and so will likely require more staff and teaching assistants to avoid fatigue.

We hope that, by making these changes, students who find writing emails formal and impersonal will be more likely to contact us for help and with any problem they might have. In this way we would aim to increase the help available to all students, increase their productivity, and bring the time taken for exercise completion more in line with our expectation. By aligning our proposed credit hours more with the time that students take to complete each exercise we should maintain a greater student focus and, hence, make these activities greater teaching aids through improved student engagement.^{16,17}

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00684>.

- Introduction to Mathematica, complete notes (PDF)
- Introduction to Mathematica, student notebooks (ZIP)
- Quantum Mechanics in Mathematica, complete notes (PDF)
- Quantum Mechanics in Mathematica, student notebooks (ZIP)
- Survey questions (PDF)

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Notes

The authors declare no competing financial interest.

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