Integration of chemistry in math courses

Kenneth Eriksson, Niklas Ericsson and Stig Larsson

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Background

The reformed math program

A basic idea of the reformed math program, delivered by the Department of Computational Mathematics at Chalmers, is a *full integration* of the "body" and "soul" aspects of mathematics, that is of the *concrete/computational/numerical* parts representing the "body", including programming, and the *abstract/analytical/symbolic* aspects representing the "soul".

In our view, the traditional separation of the "body" and "soul" parts of mathematics, with typically the abstract/analytical/symbolic math presented in first year courses, and the concrete/computational/numerical math in a later course, does not have a rational motivation, and in fact is inadequate. We think that the conceptually simple and generally applicable computational/numerical math, with an obvious rational motivation from applications, where problems in general are nonlinear and fairly complex, should be presented from start, along with basic analytical math focusing on important related conceps such as convergence, limit, linearization and derivative.

The outcome of this is a fully integrated math course where the development of efficient computational tools for mathematical modelling is the central theme that in turn requires a thorough theoretical analysis to be succesful and fully understood.

The ambition of the program is to present to the students a mathematics curricula that is *modern*, *understandable* and *useful*.

We strongly believe that the integration of numerical and analytical mathematics offers important pedagogical advantageous. For example, the concept of a *function* is an important programming construct, and implementing and using concrete (matlab, say) functions on a computer makes it easier to understand the mathematical aspects of the function concept, and vice versa. Similarly, *sequences*, *convergence* and *limit* are mathematical concepts that are best introduced, analysed and understood in connection with implementing and using simple iterative equation solvers on the computer.

Integration of numerical and analytical math also solves the problem of motivating the student for the subject. Computational/numerical math has an *obvious motivation* from the applications, and the development and performance analysis of computational methods and tools naturally leads into and motivates posing many abstract "soul-type" mathematical questions.

Modern computer-oriented math thus offers both generally applicable and powerful tools for all sorts of computation and visualisation, but also many challanging intellectual "analytical math" type problems. A proper and succesful handling of the new tools requires both quite a bit of deep mathematical insight, but also quite of bit of time and experience.

The reformed math program was first presented in -99/00 to the 30+30 first year students of the Kb and Kf programs, then extended in -00/01 to incorporate the second year students and the extended number of first year Kb students, and from -01/02 the program also included the 70 K (mainstream chemistry) first year students. From -02/03 all of the 340 first and second year K, Kb and Kf students will be enrolled in the program.

Integration of chemistry into math courses

Application projects

Integration of chemistry and math can be implemented in many different ways. What is considered here is to bring more examples of applications from chemistry into the math courses, for motivation and better understanding, and to incorporate more math into the chemistry courses to reach a higher level. A "full" integration of math and chemistry courses would probably be to push things too far.

In the mathematics courses we consider very general types of problems in abstract form, with applicas then important to meet particular concretizations of such problems and to investigate the performance of solvers in a concrete setting, to get the perspective and a better understanding. In the first matematics course where the focus is on general algebraic equations of the form $f(x) = 0$, and methods for solving such equations, a project for the students has been to i) implement solvers for such equations, ii) to choose/find a concrete such equation of interest related to chemistry or some other engineering or real life application, iii) to apply the solvers to the particular problem under consideration, and iv) to present the results in written and oral form.

On several levels

More or less the same concept was used in one of the final math courses for the second year students focusing on systems of partial differential equations modelling e.g. fluid flow and convection-diffusion-reaction processes in such flows. In this case the project has a more dominating role and was also the basis of the examination of the course.

Other examples

The molecule project

This project uses molecule geometry and conformation analysis of molecules as a framework for applying and visualising basic geometry concepts and operations such as computing distances (between atoms in the molecule), angles (between bonds), and translations, rotations and reflections (of the molecule or part thereof). From next fall this project will also be part of the new integrated chemistry course as a lab project.

The tank reactor project

The mixed tank reactor is a simple model taken from chemical reaction engineering. We have developed a sequence of exercises that can be used as the starting point for a project involving all of, or some of, the following:

1. Modelling, starting with a very simplified model, including one more aspect after the other: mass balance, heat balance, cooling system.
2. Writing the equations in non-dimensional form.
3. Viewing the model as a dynamical system, identifying state variables, observable variables, and control variables.
4. Computing model parameters from measured reaction rates by means of the least squares method.
5. Numerical simulation.
6. Stability analysis by linearization and computation of eigenvalues, parameter study of eigenvalues as functions of a design parameter.
7. Finding stationary points by means of Newton's method.
8. Final design of the reactor for stable operation.

Chemistry in the first math course

About the course

The first mathematics course Analysis and Linear Algebra part a, or ALA-a, runs in the first quarter of year one, and is followed by ALA-b and ALA-c in quarters 2 and 3. Unfortunately, the fairly traditional names of these courses do not much reflect the full integration of computational/numerical math, and programming, in the curriculum. The content of the first course is briefly as follows:

- fundamentals: numbers, algebra, variables, functions, equations

- solvers: bisection, fixed point iteration, sequences, convergence, limit
- linear algebra: vectors, matrices, geometry in 2d and 3d, complex numbers
- linearization: the derivative, partial derivatives, Newtons method

The course thus centers around general algebraic equations of the form $f(x) = 0$ and their solution using iterative computational tools, including arbitrary systems of nonlinear algebraic equations and Newtons method for such systems based on succesive linearisation and linear algebra.

Project $f(x) = 0$

Since the students for so long (12 years) have been exposed only to problems (designed to be) solvable in closed form using elementary pen and paper arithmetic or sometimes a pocket calculator, it is quite difficult to get them to understand that only very few equations can be solved this way, and that the normal procedure is to use iterative, "trial and error" type methods to solve equations. To help the student realize this (unfortunate) fact and get into the new and more general approach to equation solving, they are given a project assignment in the middle of the course with the task to derive/find particular equations of the form $f(x) = 0$, to implement bisection and fixed point iteration solvers for this type of equation, and to apply these to the problem under consideration, and finally to report their findings in oral and written form.

The purpose of the project is to help the student appreciate the new more general computational methodology considered in the course, by discovering its indispensibility in real life problems, and to get to know the technique by considering some particular application.

The project also aims to train the students in working in group in project form and practising oral and written communication.

Implementation

The project work was carried out in groups of 2-3 during weeks 3-4 of the course, and the task was to i) implement the bisection and fixed point iteration solvers, as matlab functions, ii) find an application of interest involving an a (non-trivial) equation of the form $f(x) = 0$, iii) apply your solvers to the equation obtained, and iv) present your work in oral and written form.

To help the student find a problem of interest leading to a (nontrivial) equation of the general form under consideration, a list of possible problem areas was presented from a broad variety of fields, to suit many different tastes. In addition, three different lecturers from the School of Chemistry and Biotech were invited to present problems from different fields of chemistry that naturally leads to equations of the considered form. These presentations were delivered in the third week as parts of three regular math lectures.

The results of the projects were presented in oral form to a small audience of fellow students and some teachers, and in a written report.

An example written report was provided, and some feedback on both the oral and written reports.

Evaluation

In order to evaluate how the students experienced the application projects in general, and the integration of chemistry application projects, in particular, an e-mail inquiry was put together and submitted to all the first year K/Kb/Kf students just before the Easter holliday of the Spring semester. At that time they had also met the ALA-b and ALA-c courses, and their first chemistry courses, and thus got some perspective of their first year studies.

On the other hand, the details of the project $f(x) = 0$ some five months earlier probably had faded somewhat from memory at that time.

The questions posed to the students was as follows:

1. Which was the subject of your project?
2. Descibe briefly what it was all about.
3. Which was the main reason for you choosing that particular subject?
4. Which was the strength/weaknesses of the chemistry projects suggested?
5. Why did/didn't you choose one of these?
6. How would you describe your outcome of the project?
7. Is the idea of coupling the equation solving focus of the course to concrete applications/equations a good idea?
8. Is it important to find convincing applications from chemistry?
9. Would a closer integration of math and chemistry help you better understand the math content do you think?
10. How relevant did you find the material of ala-a for your later studies and work?
11. Engineering program?
12. Sex?

Results

Out of some 75 ("mainstream") K students, 60 Kb students and 30 Kf students, only 20 students answered the inquiry. The rather poor response is probably due to a combination of the subject of the inquiry being somewhat out of date, and a general feeling of being fed up with evaluations; also the regular course inquiries are very difficult to get back.

The 20 students who did respond come in equal numbers from the three programs, and the male/female sex.

Choice of application

Many students seem to have a rather clear picture of the project they worked on, although quite some time had passed at the time of the inquiry.

It turned out that one particular project proposal was far more popular than the others. Although there were quite a few project proposals to choose from, approximately one out of four picked a particular problem about a water reservoir.

The reason for this particular project proposal (not involving any chemistry) to come out so popular is probably a combination of 1) the project was presented first in the list 2) the problem was easy to get into involving simple volume computations, introduced by an illuminating figure.

An important observation is that only some ten percent of the students were attracted by any of the suggested chemistry projects, specially presented in the lectures of the course by chemistry lecurers. It is quite clear from the comments that the main reason for this is that all of these projects appeared to be “too difficult”. Almost everyone claimed this to be one of the main weaknesses with these projects. Another reason mentioned by several students is that they didn’t find any of these projects “interesting enough” and in some case even “boring”. Of course, this can be a natural consequence of the problems being too difficult to grasp, but evidently something that looks difficult and not interesting enough is not attractive! The students then rather choose something that seems easier to get into.

Personal outcome

Concerning the personal outcome of the projects, one can find the following comments: I learned bisection and fixed point iteration, a nice “break” from a rather abstract course so far, nice to see applications and how math can contribute in practice, useful to practice working in groups, useful practice of oral presentation to a smaller group with feedback, fun

Applications of interest?

One questions was: Is it a good idea to couple the equation solving focus of the course to applications.
Not too surprisingly, the majority of the students find this a very good idea. But they also point out that the applications should be kept as simple as possible so that its complexity doesn’t hide the performance of the solver, which the application is supposed to illustrate.

Chemistry applications important?

Many of the students express that they think its important to see applications from chemistry. However, the Kf students would as well see applications from physics or mechanics. Also some of the other students claim that applications from chemistry is not that important at this early stage. Here are two such

answers:
"Yes, but when we have learned more chemistry."
"No, I dont quite see that relevance ... the thing is that many of us dont have control of what we do in the math course in the beginning, so to then also include chemistry, I think, is not a good idea. To get something out of this one must understand the math well first."

Can integration of chemistry help you understand the math?

Here one finds many different answers. Very few seems to think this should generally be the case; again only if the applications are very simple som that they dont hide basic principles. Some say it may be good for motivation but not necessarily for understanding. Several students say it is important to keep math a separate subject, and that it is more important that math be used in the chemistry courses that that chemistry be introduced in the math courses. Several students clearly claim that chemistry may be a disturbing element in the math course. Here are a few answers:
"It is good with concrete examples, but to practice these subjects together already from start, I think, can be more confusing than positive. I think it was good as it was in the couse now."
"First we study math, then how to use math in applications. This is what I think is best. Not include unnecessary and complicated material in an already complicated course."
"Perhaps .. but not too much since later in life one may not work with chemistry. After all, math is math."
"As long as one doesn't have to know a lot of chemistry, which we don't do then, it is ok with chemistry problems. The problems of this year were appropriate."
"Now when I have been here for a while I understand that everything is connected, from math to chemistry. Unfortunately this was not the case in the gymnasium and therefore this was not obvious from the beginning..."
"The integration of the subjects should not be exaggerated."
"Difficult to say, of course its nice to see .. but math must also be math, that is, a tool useful not only in chemistry."
"I think it can be good, as long as one sticks to basic principles and not complicate things to much, so that it gets the opposite effect."

Material of first course relevant for future courses and work?

Most students express that they found the first course give a very adequate basis for their following math courses, but do not much refer to usefulness in chemistry courses except "fysikalkemi".

Discussion

General opinion

The general opinion of the 20 responding students seems to be that they *appreciate integration* of chemistry and applications in the math course, in the present form, for motivation and some concrete experience of the methods they meet and study in the course.

Not too much integration

Several students express that the integration aspirations should not be carried too far. Some express that with too much integration and application there is a risk that the role and performance of the mathematical tools becomes less transparent. Some student may also have got the impression that the question concerned a "full integration" of the math and chemistry courses which has not been the idea so far.

Simple

A common view seems to be that the application problems should be *as simple as possible*, not to put focus on irrelevant details and hide basic ideas. The main reason the students were not much attracted by the suggested chemistry problems, quite clearly, was that they appeared too difficult, or at least not interesting enough to motivate the anticipated hard work to get into the problem.

The Kf students

Many of the Kf (Chemistry with Physics) students point out that they missed a contribution from physics among the special project proposals presented, and to them it is not too important to see applications from chemistry.

Freedom

Many students indicate that they appreaciated to have a wide collection of application problems to choose from for their project work. In fact, this seems quite reasonable at the very early stage in the education with the chemistry knowledge base being very limited. To have a rich diversity of project subjects is also an advantage when it comes to the oral presentations of the projects of course.

Conclusion

Same approach

The advise of the students seem to be to keep the integration project basically in its present form.

Very simple examples

The students seem to appreciate the inclusion of applications from chemistry, but evidently these application must be simpler and easier to get into to be competitive

Freedom of choice

The students want to keep the freedom to choose applications from other areas than chemistry, like physics, mechanics, electrical engineering etc.