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A Web Teaching Module for Stochastic Modelling in Chemical Engineering

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Abstract

We describe a web-module designed for the use in conjunction with the course on SStochastic Modelling in Chemical Engineeringtaught in the fourth year in the Department of Chemical Engineering at the University of Cambridge. The central aim of the web-module is to enable students without knowledge of a programming language to gain hands on experience testing a Monte Carlo algorithm. For this purpose two sets of reactions in a batch reactor are studied, one of which is the Belousov-Zhabotinski reaction system, which shows oscillating behaviour.

1 Motivation

Computational modelling in chemical engineering is becoming more and more a field in its own right, mainly due to the rapidly increasing power of computers but also because of the progress being made in developing numerical algorithms necessary to solve sophisticated models. Moreover, industry is highly interested because of the significantly lower costs of computer simulations compared to experimental studies. Important ingredients for the field include accurate physical and chemical models in mathematical form, numerical values for the parameters that occur in these models either taken from carefully selected experiments or from first principle calculations, fast computers, efficient and powerful numerical methods and, most importantly, competent engineers who are aware of the limitations of the models, parameters and numerical methods.

Needless to say, the whole field of computational engineering is far too rich to be taught in a single course. Here, we focus on teaching stochastic (or Monte Carlo) methods to students of chemical engineering. Monte Carlo methods have been shown to be highly efficient in many applications and can be found in various areas in the process and chemical industry, such as polymer synthesis, crystallisation, liquid-liquid extraction, etc. They are also useful when it comes to simulating turbulent flames and their emissions and aerosol transport in the atmosphere. More general, it has been demonstrated in some cases that stochastic models can account for effects that the corresponding deterministic model cannot. This is because fluctuations can sometimes significantly change the overall behaviour of non-linear physical models.

Another important aspect of Monte Carlo methods is, in our opinion, the connection to mathematics, which provides an appropriate language by means of the theory of stochastic processes. In the last decades a number of important mathematical results have been achieved that shift Monte Carlo methods from an intuitive naive modelling level to the rigorous mathematical discipline of interacting stochastic particle systems and their corresponding limit equations. A class of stochastic processes, which are relevant for chemical engineering, are Markov processes and in particular jump and Wiener processes (Brownian motion). To the best knowledge of the authors, so far in chemical engineering the subject has been taught from an intuitive point of view, focusing mainly on the physical motivation of the model; see for instance reference[6] and the course CH 235 (JAN) 3:0 in the Master programme taught at the IISc-Bangalore (http://www.iisc.ernet.in/soi/ch.htm), which is based in parts on the book by D. M. Himmelblau and K. B. Bischoff " Process Analysis and Simulation" first published by John Wiley in 1967; just two name two examples.

With this in mind the authors felt a need to design a course to bridge the gap between the physical, say direct simulation methods, and the more rigorous mathematical approach. Firstly, we aim to enable students to understand current Monte Carlo methods on a more fundamental level and also to help them improve a given Monte Carlo method in terms of its numerical efficiency. Secondly, we teach students the connections between deterministic models and their stochastic counterparts given

by a Monte Carlo algorithm. A first result of the authors' activity is the 16-lecture course taught in the Department of Chemical Engineering at the University of Cambridge. The course, named "Stochastic Modelling in Chemical Engineering", is given to students who are at an advanced undergraduate/beginning postgraduate level in the last (fourth) year of the undergraduate education. At that stage students have already been exposed to some computational techniques in process engineering and they have a solid knowledge of models used in chemical engineering. The stochastic modelling course comprises the following. It starts with examples in chemical engineering that lend themselves to a stochastic approach. After the introduction we discuss how random numbers can be obtained using numerical algorithms. Then the notion of a Markov process is introduced and the particular example of a jump process (death process) is examined. Using this we then develop a jump process that can be used to model a perfectly mixed gas in a tank reactor. For this system a Direct Simulation Monte Carlo (DSMC) method is introduced that simulates how the physical quantities of interest change with time. The DSMC algorithm is based on the work of Gillespie and Ramkrishna published in the 70's. We demonstrate, looking at a particular example, how a stochastic process can be obtained from its Master equation and discuss how a Monte Carlo algorithm should be implemented on a computer. For this algorithm we present techniques for investigating numerical properties of Monte Carlo algorithms in general. We then generalise the DSMC algorithm to arbitrary systems of ordinary differential equations (ODEs) and study coagulation of particles as described by the Smoluchowski equation. Finally, we introduce stochastic reactor models, which account for non-ideally mixed chemical reactors. These models are based on the joint scalar probability density function transport equation, which is also frequently used for modelling turbulent reacting flow. For all examples we state a DSMC algorithm that can be easily implemented on a computer. The lectures are accompanied by example papers, which are discussed in small group supervisions. These example papers are pencil and paper problems in a classical fashion. They do not contain any programming exercises, which would have to be carried out on a computer. This is partly because the students have not been taught a high-level computer language such as FORTRAN or C and the implementation of algorithms as part of computer science does not provide any insight from the modelling perspective. The overall assessment of the students learning progress is at the end of the academic year where the have to take four papers that cover all the courses taught in this academic year. To introduce an element of continuous assessment and to give the students the possibility to get some working experience with stochastic algorithms the Stochastic Modelling course is complemented by a Web-Module, which is the subject of this paper. The purpose of this Web-Module is to let the students gain some experience on how to perform and investigate a Monte Carlo simulation algorithm without assuming any knowledge in a programming language. The Web-Module can be accessed via the World Wide Web from every computer that runs Microsoft Internet Explorer or a similar Java-enabled browser. All students who participated in Cambridge and a large proportion of students worldwide have access to such computers either through their personal computer at home or computers made available in their Departments

or Colleges. The Web-Module, as it has been set up, also introduces an element of continuous assessment. As described in more detail below it contains a set of tasks and exercises, which students have to complete either in small groups or on their own. They are asked to summarise their results and send a short report by mail to the research assistant or the lecturer who accompanied the student's progress. Some students did in fact complete their report during the vacation period at home and kept in touch via email. The content and design of the Web-Module is described in detail in the next section. It refers to one particular part of the Stochastic Modelling course, which deals with the direct simulation of chemical reactions in a perfectly stirred batch reactor. Two reactions are studied: a simple chemical reaction for efficiency and convergence analysis and the Belousov-Zhabotinsky (BZ) reaction as an example of a chaotic chemical system. The well-known BZ system has been chosen to study the influence of fluctuations on chemical reactions. Furthermore, it presents an example of an oscillating reaction and aims to illuminate how such a system can be studied analytically using local stability analysis. In various exercises involving a number of numerical experiments with the Java applet students have the opportunity to develop an understanding of the chemical reactions and see how the theoretical analysis is related to the actual behaviour of the system.

Finally, we hope that by making this teaching resource available on the Internet we can encourage other university teachers to use it as an addition to their lecture courses. In our opinion the module is not limited to chemical engineering courses but might be also useful in all physics, chemistry or mathematics courses that contain elements of stochastic processes and/or non-linear ordinary differential equations.

2 Description of the website

The Web-Module can be accessed through the homepage of the course Stochastic Modelling in Chemical Engineering, with the following address:

www.cheng.cam.ac.uk/∼mkraft/pages/teaching/CETIIB-StoMo/StoMo.htm

or directly via:

www.cheng.cam.ac.uk/∼mkraft/pages/teaching/CETIIB-StoMo/WebModule/bz/index.html

The site is structured as follows: On the title page, the table of contents is shown in the form of links to all subsequent pages. Furthermore, on top of every page, there are navigation buttons, so that the user is led through the whole site step by step. The following pages can be found:

- Introduction
- Theory

  Some theory for a simple example

  Some theory for the Belousov-Zhabotinsky system

- Algorithms

  Algorithm for the simple example

  Algorithm for the Belousov-Zhabotinsky system

- Numerical experiments
- Videos of actual experiments
- Questionnaire
- Web-based teaching – a survey
- Bibliography

On the introductory page we explain the subjects and the aims of the web module and its connections to other teaching units. We focus on three areas: reaction engineering, Monte Carlo methods, and dynamical systems and chaos and discuss how the Web-Module is related to these areas. We also specifically state the aims we want to achieve. These are:

1. to provide a numerical tool based on a Monte Carlo method to simulate chemical reactions and understand the numerical properties of Monte Carlo methods for chemical reactions,
2. to study a chemical reaction system analytically using linear stability analysis and,
3. to present an example for oscillating reactions and chemical feedback.

The connection to other teaching units are specific to the chemical engineering course in Cambridge but are taught in similar fashion in other chemical engineering departments all over the world. The following teaching units contain materials that provide the basis for the successful use of the module and completion of the problems. The courses are: Computer-Aided Process Engineering, Statistics, Mathematical Modelling of Chemical Reactors, Combustion, Bioprocess engineering, Thermodynamics, Kinetic Theory.

In the theory section we introduce two example systems that are to be considered. The first consists of two very simple chemical reactions such that students can focus on investigating numerical properties of the algorithm rather than struggling with the complexity of the system itself. Secondly, students are familiarised with the BZ reaction in some detail, but in order to avoid impenetrable confusion we restrict ourselves to a simplified oregonator mechanism due to Field, Körös and Noyes. By making further simplifications we derive a system of three dimensionless ordinary differential equations from which we subsequently deduce several elementary facts about its qualitative behaviour. Specifically, students are lead through the calculation of the steady state and the so-called nullclines, which, using a number of graphs,

provide an intuitive understanding of the time evolution in the phase space. Finally, we demonstrate how to perform a local stability analysis by means of linearisation at the point of steady state including a classification of the eigenvalues of the Jacobi matrix.

On the algorithm pages, we write down explicitly the stochastic algorithms for both systems of chemical reactions. This is simply a specialisation of the general method presented in the lectures, using the same notation. As mentioned above, instead of referring to a particular programming language, we describe in words and formulae every step of the algorithm.

The description of the Java applet as well as the list of exercises are the central part of the website. The corresponding page explains first the purpose of the applet, its elements and parameters, how to run a simulation and how to obtain measurement data. The applet can be started by clicking on a link which opens a new window containing just the applet such that students can run simulations and browse the website at the same time. **Figure 2** shows the program with a typical output of the time evolution of the species, the phase space diagram and numerical measurement data. It might be necessary to download the Java 2 Runtime Environment plug-in first (The page has been tested using version 1.3.1_03).

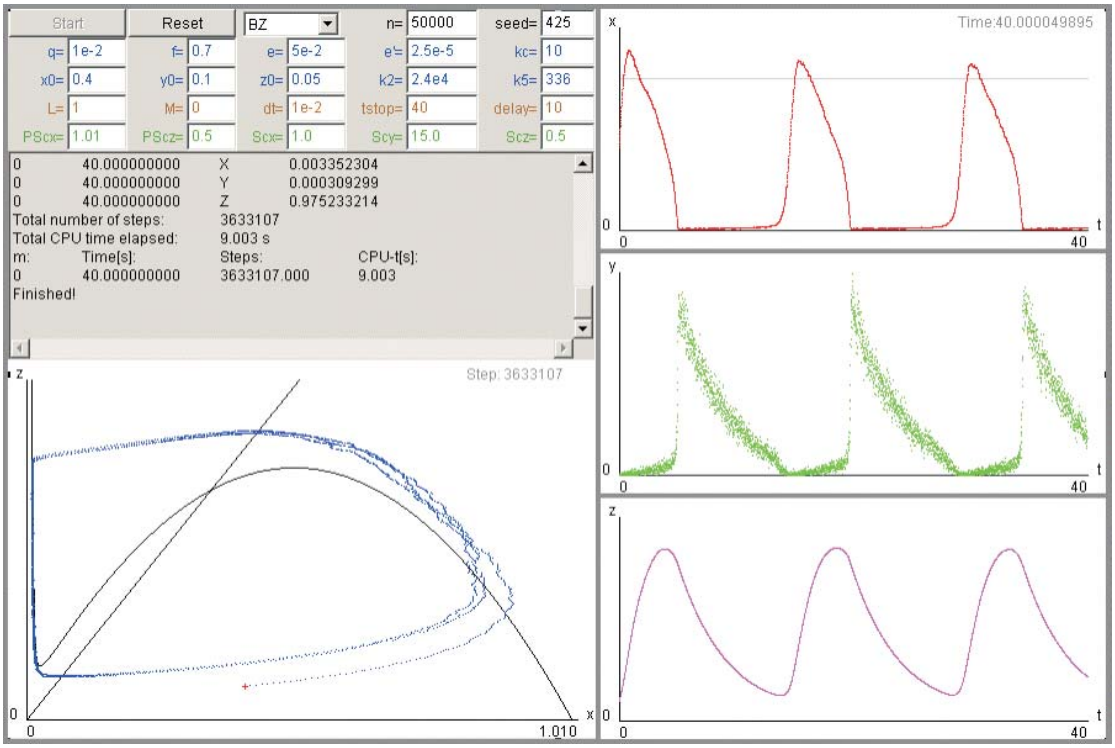

Figure 1: *Screenshot of the Java applet in action*

Apart from 'playing' with the applet in a rather unsystematic way we expect students to complete a number of problems and exercises. The students who participated in

the lecture course were asked to include the answers of the problem in an essay, which had to be handed in for marking. The exercises focus on three areas, the numerical properties of the stochastic algorithm, the physical properties of the BZ system and the characteristic features of dynamical systems. On the numerical side, students are asked to study systematic and statistical errors, their convergence and some efficiency related issues using the simple system of chemical reactions as a test case. Then, by investigating the BZ system, the theoretical knowledge on dynamical systems developed earlier is to be consolidated. Feedback on the reports was given in supervisions. In some cases students did get in contact with research assistants through email to ask specific questions.

We include for motivation purposes an extra page with links to videos of BZ reaction experiments. These videos were not produced by the authors but they do complement the Web-Module as running the Java applet can nicely reproduce the qualitative behaviour of the experiments.

Finally, the students can give some feedback by filling in an online evaluation form. We compiled a number of questions of which we thought would provide us some information on how to improve the Web-Module for use in the next academic year. We offer two types of feedback. The students can answer a question by choosing a number between 1 and 5 to indicate a specific answer or by making more general comments in text fields. Different criteria are evaluated, including technical usability, organisation of content and quality of the problems and exercises. We also ask for the time required to complete the problems to get an estimate how to alter or add exercises in future. In text boxes we offer the opportunity to give a more detailed feedback. Users can identify strengths and weaknesses of Web-Module and comment on the Internet based teaching approach in general.

On the page "Web-based teaching – a survey" we list a number of websites also attempting to supplement conventional courses. We do this mainly because during the design phase of this Web-Module we came across so many nice examples, which we thought, deserve some advertising. We distinguish between different classes of teaching material and give short descriptions of a selection of web pages. More details on various aspects of the material presented can be found in references [1] - [8] which are all included in the Web-Module.

3 Concluding remarks

In this paper we presented a Web-Module complementing the fourth year course "Stochastic Modelling in Chemical Engineering". With this Web-Module students can practise concepts that have been taught in the lectures. Two chemical reactions in a perfectly mixed batch reactor can be studied using a DSMC algorithm implemented in the Java-applet. By working through the Web-Module the users are supposed to write an essay that includes the answers to a set of problems given in the module. To obtain these answers students need to make extensive use of

the Java-applet. The Web-Module also contains some additional material on the chemical and physical background of the reactions being studied. It also provides some basic material on linear stability analysis. Some videos and a survey on web-based teaching complete the Web-Module. An online questionnaire gives users the opportunity to comment on various aspects and suggest improvements. We view this course as a first step into web-based teaching. We are planning to increase the number of Web-Modules for this particular course but also plan taking some steps in direction of a virtual laboratory. Funding for this activity has already been made available by the Cambridge MIT Institute (CMI) and first results will be published in due course.

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