CHEG 831 CHEMICAL ENGINEERING PRINCIPLES I
FALL 2020
COMPUTER PROJECT

Due: Thursday, December 10

The overall objective of this project is to demonstrate the utility of some of the methods of solution discussed in this class in modeling an engineering or science problem of your choice. Of particular interest are non-linear differential equations (ordinary or partial) that give rise to multiple solutions and bifurcations as a function of key parameters in the problem. An extensive but necessarily incomplete list of published articles that describe potential problems of interest is included later, and you are asked to reproduce and expand on the analysis presented in such an article or articles. The analysis and solution methods that you should use include solution of linear and nonlinear systems of algebraic and differential equations, eigenvalue problems, as well as any other methods that you feel may be informative.

There are **two specific goals** of this project. First, you should show that you can **reproduce at least one set of key results** reported in the relevant article pertaining to the model system discussed in that paper and provide additional information on the computational aspects of these results. The paper may also include additional data; you are welcome to use them in trying to interpret the results and in presenting your own results and putting them in perspective. However, in the second specific goal of the project, using the best method and suitable parameter values as determined in the first goal, **you should explore the model further to produce new results** beyond those presented in the paper (e.g., selecting new values or ranges of model parameters, new initial conditions, etc.). Are there new types of dynamic behavior that you can show? Can you offer a rational analysis of the results (possibly using a **local eigenvalue analysis**)? Can you expand further the parameter space of the problem explored in the published work? Can you apply the model to describe and fit experimental data?

Therefore, you should select a suitable model, modify it if you feel that that is necessary, and use it to find steady-state and dynamic solutions using numerical calculations, e.g., in MATLAB, for a selection of different model parameters, initial and boundary conditions. You should select a representative set of parameter values and initial guesses to show the characteristic dynamic behavior discussed in the paper and you should focus on the dependence of the results on the numerical approach used, and its associated numerical parameter values. Of particular interest is to **estimate the error involved** (by comparison with the published results or with the most accurate techniques that you used) as a function of the computational workload involved, which can be roughly approximated by the total computational time required. Based on those results and consideration of the accuracy and stability of the numerical scheme involved, as well as the particular characteristics of the system that you are simulating, can you justify the numerical method of your choice and the proposed numerical parameters to use for this task? Supporting analysis, e.g., of the eigenvalues of the linearized system at the conditions of the simulation, may be invoked as well.

A list of articles that may be suitable reference points for the project is included in the last section of this document. These fall generally in two categories:

- Problems that are representative of chemical engineering systems that include chemical reaction, diffusion, fluid flow, etc., and where the published analyses employ familiar conservation and constitutive relations to demonstrate the existence of such phenomena as multiple steady states, bifurcations, and oscillatory dynamics.
- Generic models of transport, reaction, etc., or conceptual dynamic systems that give rise to chaotic dynamics.

The problems in these categories vary in different respects but it is useful to recognize that there is not necessarily a simple relation between how complicated the equations appear or how difficult it is to solve them and how complex the full portfolio of solutions may be.

Good luck!

Procedures and schedule

1. Please form a working group of up to three people, hopefully with similar research interests. Anyone not yet confirmed as a member of a group by **Friday, October 23** will be assigned to a group randomly.

2. Each group should submit a project proposal by **Friday, October 30**. This should include, at a minimum, identification of the published work that is your reference, but you may also include a provisional identification of which results you plan to reproduce and what form your new results may take. You should also include at least one other reference as a backup in case of conflicts. Although it is acceptable for more than one group to work on the same system, the scope of the two projects should be sufficiently different to avoid any overlap. Confirmation of topic selection will be confirmed during the weekend (trick or treat!).

3. Each group should meet with one of the instructors during the week of November 16 and submit an interim report by **Friday, November 20**.

4. A final report is due by **Thursday, December 10**; an outline of the scope and organization is provided below.

Groups are also encouraged to interact with the instructors and the TA and to ask for help when needed.

Scope of project and final report

All projects should include:

A. A computer program (in MATLAB) to perform the numerical simulation, allowing selection of numerical parameters, initial guesses, etc., and calls to MATLAB solvers. The program should be appended to the report and an electronic copy should be submitted; comments should be included to make the key steps in the code, including input/output steps, comprehensible to a reader. Procedures for validating the results, such as testing for any possible dependence of the results on the numerical method and numerical parameters, should also be devised.
B. A procedure for error and/or eigenvalue analysis.
C. Graphs should be supplied to show the dependence of the results on key model and numerical parameters.
D. The main text should encompass no fewer than 5 and no more than 15 pages (excluding figures, references and appendices) and should contain the following sections:
    a. Title/Names/Abstract (1 page maximum)
    b. Introduction – an executive summary of the problem studied (2 pages maximum)
    c. Methodology for the numerical simulation (How was the simulation carried out? How were the solvers selected? Procedure followed for error estimation. How were the parameter values chosen?)
    d. Methodology for analysis of the results. Distinguish between local behavior and global behavior (based on local eigenvalue analysis and some limited phase plots or statistics of the phase space if a complex behavior is predicted). Try to correlate it to the system's conditions (through eigenvalue analysis of the locally linearized system.)
    e. Results and discussion/interpretation of the data. In this section you should relate your results and conclusions to the discussion in the paper. It is also useful here to summarize qualitatively the behavior that you see in the simulations, within the context of the analysis presented in the paper.
    f. Conclusions
    g. References
    h. Appendix (where the programs and any secondary calculations/data plots may be placed)

Possible topical areas

Chaos: Generic or transport/reaction models leading to chaotic dynamics

(Principal references are indicated here; those and additional ones (recommended reading) are to be found in CANVAS files in the folder for the project in the subfolder with the corresponding name).

A1. The Lorenz model (this is the paper that started the study of chaos in deterministic systems)
E.N. Lorenz, "Deterministic nonperiodic flow" J. Atmos. Sci. 20 (1963) 130-141.
(MANY additional resources available on the INTERNET can be found through GOOGLE).

A2. The Willamowski-Rössler model
P. Geysermans and G. Nicolis, "Thermodynamic fluctuations and chemical chaos in a well-stirred reactor: A master equation analysis" J. Chem. Phys. 99 (1993) 8964-8969.

A3. The ABCDE model
R. Friedrich and H. Haken, "Nonequilibrium Phase Transition in a System with Chaotic Dynamics. The ABCDE Model" Phys. Let. A 164 (1992) 299-304

A4. The hematopoiesis model
M.C. Mackey, "Unified Hypothesis for the Origin of Aplastic Anemia and Periodic Hematopoiesis" Blood 51 (1978) 941-956
(investigate the model described in Appendix 2; check results shown in Fig. 8 and explore the parameter region such that $\omega\tau > \cos^{-1}\left(-A/B\right)$)
Also, look to reproduce results shown in Figure 6 of:
L. Glass and M.C. Mackey, "Pathological Conditions Resulting from Instabilities in Physiological Control Systems" Annals New York Academy of Sciences 316 (1979) 214-235.
In that reference you can find other models from human physiology---of usefulness for comparison purposes and general information.

A5. Rössler's attractor
Information can be found in many sources, starting from the Wikipedia and Scholarpedia references (Rössler attractor), the notes of Barry McQuarrie on Chaos and Fractals, and references therein.
(Of interest is to investigate parametrically how the results of the integration depend on the values of the three parameters (a, b, c) appearing in the set of 3 ODES defining this attractor. It is recommended to first try to reproduce some of the presented in the literature results and then try to evaluate some new ones. Of special interest are (study a from 0.2 to 0.38 and higher (if possible!) when b=0.2 and c=5.7).) Try also to perform a Liapunov analysis as discussed in McQuarrie's notes, chapter 13.

A6. Extended Rössler attractors
O.E. Rössler, "Chaotic Behavior in Simple Reaction Systems" Z. Naturforsch. 31a (1976) 259-264.
O.E. Rössler, "Chaos in Abstract Kinetics: Two Prototypes" Bulletin of Mathematical Biology 39 (1977) 275-289.
O.E. Rössler, "Continuous Chaos-Four Prototype Equations" Annals New York Academy of Sciences 316 (1979) 376-392.
(Here you should work on the models beyond the standard Rössler Attractor---Eq. (2))

A7. Chaos in a bienzymatic cyclic model
H. Berry, "Chaos in a bienzymatic cyclic model with two autocatalytic loops" Chaos, Solitons and Fractals 18 (2003) 1001-1014.

Reaction, diffusion, transport, etc., problems leading to multiple solutions, bifurcations, oscillatory dynamics

B1. The Oregonator
R.J. Field and R.M. Noyes, "Oscillations in chemical systems. IV. Limit cycle behavior in a model of a real chemical reaction. J. Chem. Phys. 60 (1974) 1877-1884.

B2. The Brusselator
RenC Lefever, Grdgoire Nicolis" and Pierre Borckmans, "The Brusselator: It does Oscillate all the same" J. Chern. Soc., Faraday Trans. I , 84 (1988) 1013-1023.

B3. The Allen model
P.M. Allen, "Darwinian evolution and a predator-prey ecology" Bull. Math. Biology 37 (1975) 389-405.

B4. The Belousov-Zhabotinski reaction
J.J. Tyson "Analytic representation of oscillations, excitability, and traveling waves in a realistic model of the Belousov-Zhabotinski Reaction" J. Chem. Phys. 66 (1977) 905-915.
J.J. Tyson "Oscillations, bistability, and echo waves in models of the Belousov-Zhabotinski Reaction" Annals New York Academy of Sciences 316 (1979) 279-295.
I.R. Epstein and K. Showalter "Nonlinear Chamical Dynamics: Oscillations, Patterns and Chaos" J. Phys. Chem. 100 (1996) 13132-13147.

B5. Modeling chemical reactions in biological systems
J.E. Haag, A. Vande Wouwer and M. Remy "A General Model of Reaction Kinetics in Biological Systems" Bioprocess Biosyst. Eng. 27 (2005) 303-309.
D.J. Higham "Modeling and Simulating Chemical Reactions" SIAM Review 50 (2008) 347-368.

B6. Reaction-diffusion pattern formation
J. Elezgaray and A. Arneodo "Modeling reaction-diffusion pattern formation in the Couette flow reactor" J. Chem. Phys. 95 (1991) 323-350.

B7. Biological pattern formation
A.A. Tsonis, J.B. Elsner and P.A. Tsonis "On the Dynamics of a Forced Reaction-Diffusion Model for Biological Pattern Formation" Proceedings of the National Academy of Sciences of the United States of America 86 (1989) 4938-4942.

Reactor engineering

C1. A. Uppal, W. H. Ray and A. B. Poore, "On the dynamic behavior of continuous stirred tank reactors", Chemical Engineering Science 29 (1974) 967-985; DOI: 10.1016/0009-2509(74)80089-8

C2. A. Uppal, W. H. Ray and A. B. Poore, "The classification of the dynamic behavior of continuous stirred tank reactors—influence of reactor residence time", Chemical Engineering Science 31 (1976) 205-214; DOI: 10.1016/0009-2509(76)85058-0

C3. K. F. Jensen and W. H. Ray, "The bifurcation behavior of tubular reactors", Chemical Engineering Science 37 (1982) 199-222; DOI: 10.1016/0009-2509(82)80155-3

Heterogeneous catalysis

D1. K. Krischer, M. Eiswirth and G. Ertl, "Bifurcation analysis of an oscillating surface reaction model", Surface Science 251-252 (1991) 900-904; DOI: 10.1016/0039-6028(91)91121-D

D2. R. Imbihl and G. Ertl, "Oscillatory Kinetics in Heterogeneous Catalysis", Chem. Rev. 95 (1995) 697–733; DOI: 10.1021/cr00035a012

Bioreactor analysis

E1. Y. Zhang and M. A. Henson, "Bifurcation Analysis of Continuous Biochemical Reactor Models", Biotechnol. Progr. 17 (2001) 647-660.

Metabolic dynamics

F1. M. Markus and B. Hess, "Transitions between oscillatory modes in a glycolytic model system", Proc. Natl. Acad. Sci. USA 81 (1984) 4394-4398.

Circadian rhythms

G1. A. Goldbeter, "A model for circadian oscillations in the *Drosophila* period protein (PER)", Proc. Roy. Soc. B 261 (1995) 319-324; DOI: 10.1098/rspb.1995.0153

G2. J.-C. Leloup and A. Goldbeter, "Toward a detailed computational model for the mammalian circadian clock", Proceedings of the National Academy of Sciences 100 (2003) 7051-7056; DOI: 10.1073/pnas.1132112100