

Modelling and Simulation 2015/16

Grades, Practicals, Rules and Regulations

1. The final grade will take into account the grades for two practical reports and a written exam, averaged with equal weight 1/3 for each individual grade. However, both practicals and the exam have to be graded as sufficient (≥ 6), individually, in order to pass the course.

2. Example questions for the written exam will be provided in good time. An example report is available from Nestor.

3. There will be one practical assignment for each of the three main chapters of the course, but you have to do only two of these. The first one, assignment I, is obligatory, in addition you select either assignment II or III.

Typically, you will be asked to perform some computer experiments, which will include some – not too involved – programming. Occasionally, you will be asked to solve a simple subproblem analytically or to describe a potential modification of a model/ implementation in words. For the two selected projects, write up structured reports which contain a short description of the problem(s) you address, the methods that you use, and the results you obtained. Most importantly: discuss and interpret your results and observations and do include figures where appropriate. Program source code should not be included (only upon request) but if you have used special techniques or *tricks* please describe them or provide relevant bits of code (or pseudo-code).

4. Assignment sheets may include or point to additional materials which are not essential for the core assignment but provide information for the interested. Research in the literature or web is not required for the reports, but it may be helpful and makes sense anyway. If you make use of secondary literature, please cite properly!

5. Final reports are due at the end of the period. The **final deadline** for both of your reports is **Monday, October 26, 12:00 (noon)**.

You are strongly encouraged to hand in preliminary versions (please mark them as preliminary!) to obtain a first feedback. In order to allow enough time for feedback and improvements, submit **preliminary versions as early as possible** and no later than **September 28, 12:00 (noon)** for assignment I and **October 12, 12:00 (noon)** for II or III.

Details about how to submit (printed copies or e-mail) will be announced in good time.

6. Assignments will comprise so-called **core problems** which have to be solved in a satisfactory manner. On the basis of the core assignment, a grade on the scale of 1-10 will be determined for each report.

In addition, suggestions for further studies are provided, so-called **bonus problems**, which you may address and also include in the report. The same applies to interesting ideas of yourself which you are encouraged to discuss with the teacher or TAs, beforehand. The sections which relate to bonus problems should be clearly marked

For each report, a bonus of up to 1.0 points can be added to the grade, but only if the core assignment was marked as sufficient. Due to the bonus, individual grades for reports could be higher than 10. Obviously the final grade for the course is at most 10 :-)

7. You are **strongly encouraged to work in pairs** and hand in joint reports. When working in pairs, the following additional requirement and rules apply:

At the end of the report, a section has to be added in which you describe – as accurately as possible – who of you contributed how much to the project and report. Specify, for instance, the individual contribution to the programming, the write-up etc. in % of the total workload. Should you disagree within the team, you may include two individual evaluations or contact the teacher confidentially.

Individual grades (and bonus) may be adjusted based on your self-evaluation. If the self-evaluation is unclear or raises doubts, students may be interviewed separately about the workload.

Assignment I) The Chirikov map

In this project, you can use the programming language of your choice, but I would recommend Matlab or perhaps Mathematica. The Matlab routines used in the lectures for the one-dim. logistic map are available in Nestor.

Consider the following two-dimensional non-linear map, which iterates two real numbers $\{x_n, p_n\}$:

$$\begin{aligned} p_{n+1} &= p_n + K \sin[2\pi x_n]/(2\pi) \\ x_{n+1} &= x_n + p_{n+1} \end{aligned} \quad (1)$$

where $K \in \mathbb{R}$ is a control parameter.

This iteration is known as the *Chirikov map* or the *standard map* in the literature. An illustrating interpretation of (1) in terms of a physical system is presented in the Appendix, but it is not essential for the core problems.

We are only interested in the non-integer parts of x and p . Note that (1) yields the same values (modulo 1), if we add an arbitrary integer to x_n and/or p_n . Thus, we restrict ourselves to the following, modified map:

$$\begin{aligned} p_{n+1} &= \{p_n + K \sin[2\pi x_n]/(2\pi)\} \bmod 1 \\ x_{n+1} &= \{x_n + p_{n+1}\} \bmod 1 \end{aligned} \quad (2)$$

a) 'Orbits' in the x - p plane for fixed K

(core problem)

Implement the iteration (2), for instance as a Matlab function. Write a program or procedure which, for given K and initial values $\{x_o, p_o\} \in [0, 1] \times [0, 1]$, performs n iteration steps (e.g. $n = 1000$). Display the sequence $\{x_i, p_i\}_{i=1}^n$ in the x - p -plane. If you vary the initial values for fixed K (use $K = 1$ here), you should find three types of sequences: sets of discrete points (zero-dim.), sets of closed curves (one-dim.) and orbits which fill two-dimensional areas in the plot. Produce example plots for each of these scenarios and observe and describe the corresponding behavior of the iteration in words. Address questions like: Are the single points or curves visited in a fixed order? What happens in the filled areas?

By plotting the orbits for many different (e.g. random) initial conditions you should be able to produce decorative images like the one shown in Figure 1.

b) Explore the behavior for different K

(core problem)

Plot orbits in the x - p -plane for different K . For the case $K = 0$, determine the orbits analytically (trivial). Observe and describe how orbits change with increasing K . Do you find, for instance, scenarios that are similar to *period doubling*? Discuss in words the similarities and differences of the observed behavior and that of the logistic map.

Some one-dimensional orbits (lines) traverse the entire picture horizontally, i.e. they contain all x -values in $[0, 1]$. Such orbits are named KAM-orbits after Kolmogorow, Arnold and Moser. The extension of chaotic behavior is limited by the KAM orbits, i.e. chaotic orbits cannot cross these lines. Obviously there are KAM orbits for small K , but they cannot be found for arbitrary large K . From your computer experiments, obtain a rough estimate of the value K_c where the KAM orbits disappear. Alternatively you can find the precise K_c in the literature and try to confirm that KAM orbits exist just below but not above K_c .

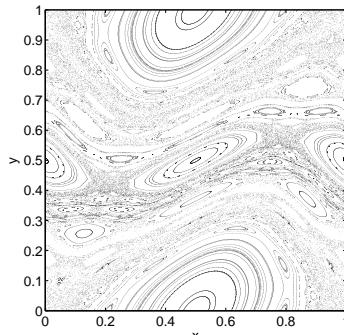


Figure 1: Orbits of the Frenkel-Kontorova model

Appendix: Further aspects and bonus problem suggestions

The Frenkel–Kontorova Model

Consider a chain of equal particles in a periodic potential energy landscape $V(x)$, you can think of a corrugated iron sheet, for instance (see Fig. 2). We will set the period to 1, i.e. $V(x+1) = V(x)$, which defines the dimensionless unit length in the following. We will consider the specific example

$$V(x) = \frac{K}{(2\pi)^2} (1 - \cos[2\pi x]).$$

The positions of the particles are denoted as x_i and neighbor pairs of particles contribute an additional $W(x_i - x_{i-1})$ to the total potential energy. This corresponds to linking neighboring particles by horizontal springs, for instance. Here, we set

$$W = 1/2 ((x_i - x_{i+1}) - \sigma)^2$$

where σ is the length of the springs in absence of the external potential V .

Note: V and W are considered to be dimensionless here, so we can omit (set to "1") physical quantities like the mass of the particles and the spring constant, which would only define the energy scale.

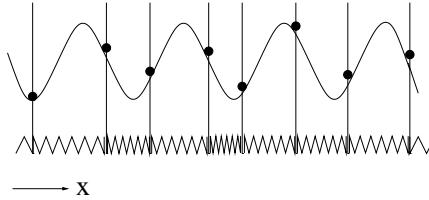


Figure 2: Illustration of the Frenkel–Kontorova Model

This can be interpreted as a very simple model of atoms of chemical element B placed upon the surface of a perfect crystal made from another element A . The regular crystal surface provides essentially a periodic potential $V(x)$, whereas the interactions between neighboring B atoms can be very roughly approximated by the quadratic potential W . Interesting effects arise when the natural spacing σ of the B atoms differs from the spacing in the A-crystal which we have set to 1. The total potential energy of a long segment of the chain (particles M to N) is given by

$$H_{MN} = \sum_{n=M+1}^N [V(x_n) + W(x_n - x_{n-1})].$$

In any rest position of the chain, the forces on each particle add up to zero and the system satisfies the condition (for all n)

$$\frac{\partial H_{MN}}{\partial x_n} = 0 = V'(x_n) + W'(x_n - x_{n-1}) - W'(x_{n+1} - x_n).$$

For our example potentials we have

$$\begin{aligned} V'(x_n) &= \frac{K}{2\pi} \sin[2\pi x_n] \quad \text{and} \quad W'(x_n - x_{n-1}) = x_n - x_{n-1} - \sigma, \\ \text{hence: } 0 &= \frac{K \sin[2\pi x_n]}{2\pi} + (x_n - x_{n-1}) - (x_{n+1} - x_n) \end{aligned} \tag{3}$$

Now we define $p_n = x_n - x_{n-1}$, and together with the condition (3) this yields the recursion relation for the x_n and p_n :

$$\begin{aligned} p_{n+1} &= p_n + \frac{K}{2\pi} \sin[2\pi x_n] \\ x_{n+1} &= p_{n+1} + x_n \end{aligned}$$

Here, we have obtained the lower equation directly from the definition of p_n and the upper one from solving (3) for p_{n+1} .

In terms of our chain of particles this means: if we fix two neighboring positions x_o and x_{-1} , or x_o and p_o respectively, we have uniquely determined the position of all other particles! The corresponding sequence of positions is given by the Chirikov map (1)! Remember that here x and p correspond to the actual physical quantities, whereas in the problems a) and b) they were reduced to their non-integer parts.

For the physical system we are interested in the energy of a given rest configuration

$$H_{MN} = K \sum_{n=M+1}^N \frac{1}{(2\pi)^2} (1 - \cos[2\pi x_n]) + \sum_{n=M+1}^N \frac{1}{2} (p_n - \sigma)^2.$$

The energy per particle $h = \frac{1}{N-M} H_{MN}$, correspondingly. By means of the above recursion, it is a function of $\{x_o, p_o\}$. Note that σ appears in the energy, whereas it does not in the iteration.

An important quantity in this context is the so-called *winding number*. It is defined via the average distance between neighboring particles in a very long (infinite) chain

$$w = \lim_{(N-M) \rightarrow \infty} \frac{x_N - x_M}{N - M} \quad (4)$$

The winding number characterizes the Chirikov orbits and indicates whether a chain configuration is *commensurate* or *incommensurate* with the periodicity of $V(x)$.

Suggested further problems (bonus)

- Write a program that, for given K and initial x_o, p_o
 - displays the corresponding position of the particles in our chain model together with the periodic potential. Obviously we omit the modulo operation here, because we are interested in the true coordinates x , not just the non-integer part.
 - evaluates the winding number
- Characterize the different types of orbits with respect to their winding numbers. Which role do, for instance, rational or irrational winding numbers play?
- (Difficult) For, say, $K = 1$ and $\sigma = 2/5$, try to find the configuration with minimal energy $h(x_o, p_o)$ by varying the initial conditions. The winding number w^* that corresponds to the minimal energy is a highly complicated function of σ , which has an infinite number of steps at all rational w^* (a so-called *devil's staircase*).

Suggested further reading

1. W. Kinzel and G. Reents, *Physics by Computer*, Springer (1998)
2. E. Ott, *Chaos in Dynamical Systems*, Cambridge University Press (1993)
3. H.G. Schuster, *Deterministic Chaos: An Introduction*, VCH (1995)
4. R.B. Griffiths, *Frenkel-Kontorova Models of Commensurate-Incommensurate Phase Transitions*, in: H. van Beijeren (ed.), *Fundamental Problems in Statistical Physics VII*, Elsevier (1990), pgs. 69–11-.