Projects for Modelling and Simulation

Michael Biehl and Michael H.F. Wilkinson

1 Simulating colliding galaxies

A galaxy is a large, self-contained mass of stars. A common shape of a galaxy is a bright center with spiral arms radiating outward. The sun belongs to the galaxy called the Milky Way. The universe contains billions of galaxies . With so many galaxies floating around it is clear that sometimes two galaxies collide, often resulting in two deformed galaxies. Prevalent shapes are a disk, bar, spiral or ring, for an overview see the Hubble telescope images: `http://hubblesite.org/gallery/album/galaxy`.

Project: simulate the collision of two disk-shaped galaxies in 3D. Experiment with various initial conditions, resulting in realistically shaped galaxies. Galaxies typically comprise 10^{11} stars. It is not feasible to do a simulation with that number of stars. Determine experimentally what is feasible. An important simplification/approximation is the use of the Barnes-Hut method. The essence of this method is that stars are grouped when they are close together. In this way the complexity of the algorithm is reduced from N 2 to N.log(N).

Literature:

1. J. Barnes and P. Hut (December 1986). ”A hierarchical O(N log N) force-calculation algorithm”. Nature 324 (4): 446449.

2 Simulation of Genetic Networks

Living cells contain many genes (between 3000 and 30000), each encoding for a protein. Genes can vary in their level of expression, i.e. the rate at which the protein they encode is produced. Some proteins are regulatory, which means they regulate the expression of genes (possibly even their own expression). They do this by attaching to so called *promotor* regions of genes, by binding to them. When bound they either stimulate (promote) or repress the expression of a gene.

The aim of bioinformatics is to understand the networks of regulation of genes (called genetic networks or circuits). Various models have been proposed to model such networks. The simplest are so called boolean networks, in which genes are switched either on or off. Other models model these reactions in a more continuous fashion. Finally, some people contend that stochastic processes should be included, due to the small number of regulatory molecules present at each point in time.

Your assignment is to compare these points of view, and implement at least one method. Think of a simulation to conduct to (i) verify claims made about the method (ii) test your own ideas about the strengths and weaknesses.

References:

1. H. H. McAdams and A. Arkin (1998) Simulation of prokaryotic genetic circuits. *Annual Reviews of Biophysics and Biomolecular Structure* **27**:199-224.

2. S. A. Kauffman (1969) Metabolic stability and epigenesis in randomly constructed genetic nets. *Journal of Theoretical Biology* **22**:437-467.

3. T. Mestl, E. Plahte and S. W. Omholt (1995) A mathematical framework for describing and analysing gene regulatory networks. *Journal of Theoretical Biology* **176**:291-300.

3 Game Theoretical Modelling

Game theory plays an important role in modelling in biology (evolution and ecology), economics, and artificial intelligence. In particular, game theoretical modelling of the evolution of behaviour is interesting, because provides a framework to explain such diverse things as the evolution of cooperation (through the famous prisoners' dilemma), the reason's why animals more often posture and threaten than fight (hawk-dove games), and the mate selection. In this project the aim is to select one (or perhaps more) topics which have been studied using game theory, to create a simulation programme, and to compare hypotheses (preferably your own). An idea could be to model the emergence of collaboration in predators, where one might lie in wait, while another drives the prey towards the trap. This behaviour could have started out by unintentional encounters between predators, leading to a modified hawk/dove game.
Reference:

1. J. Hofbauer and K. Sigmund (1998) *Evolutionary Games and Population Dynamics*. Cambridge University Press, Cambridge, UK.

2. B. Brembs (1996). Chaos, cheating and cooperation: potential solutions to the Prisoner s Dilemma. *Oikos* **76**: 14-24.

4 Simulation of Epidemics

The current situation has put epidemiological modelling into the spotlight. Numerous methods for modelling and simulation of epidemics exist, ranging from delay differential equations, which assume well-mixed populations, to models using discrete events in networks, which allow modelling of spatial extent, and social interconnections. Factors to be included are incubation times, speed of transmission, probability of death, and potential countermeasures such as quarantine, or vaccines. In this project you can either compare different modelling approaches, and study how their outcomes differ given similar input assumptions, or you could take one model, and study how different assumptions, and different factors influence the outcome.
Reference:

1. Duan, W., Fan, Z., Zhang, P., Guo, G., & Qiu, X. (2015). Mathematical and computational approaches to epidemic modeling: a comprehensive review. Frontiers of Computer Science, 9(5), 806-826.

5 Genetic Algorithms in Engineering

A modern trend in design is the use of different evolutionary methods, such as genetic algorithms (GA), genetic programming (GP), evolutionary strategies (ES), or evolutionary programming (EP). A large number of applications can be found in the book by Bentley (1999). In this book, various examples are given, and problems with different strategies are discussed. Certain problems stem from the fact that not all design problems are equally *evolvable*. However very often this boils down to problems in finding the right evolutionary design method or parameters to alter (or *genome design*).

In this assignment you must select some object to be designed. This could basically be anything you are interested in. You must then define quality criteria (or a *fitness function*) for your designs. Based on this fitness criterion, develop a computer aided evolutionary design approach, preferably using parallel algorithms. Try to evaluate whether any of the problems noted in the literature (such as evolvability and genome design).

References:

1. P. J. Bentley (1999) *Evolutionary Design by Computers*. Morgan Kaufmann, San Fransisco.

2. G. Winter, J. Périaux, M. Galán, and P. Cuesta (eds.) (1995) *Genetic Algorithms in Engineering and Computer Science*, John Wiley and Sons. Chichester, UK.

6 Simulation of Traffic Jams

Everyone in the western world is familiar with traffic jams, and much research has been done to try to find out what causes them, and how to control them. Many of you may have observed curious wave-like phenomena in traffic jams, in which traffic may alternate in flow speed. These wave (and indeed the traffic jam itself) may show a tendency to travel upstream (you may of course be to irritated to observe these phenomena when you are stuck in a jam, but next time try to watch out for them, it gives you something to do).

Traffic can be seen as the flow of many particles through some topology, with various speed restrictions and other limitations (number of lanes etc.). The particles themselves can be modeled in different levels of detail, but even the simplest models involve an apparent repulsive “force” due to the fact that people tend to keep a certain distance from each other. Also, if a car in front suddenly breaks, the car behind will tend to slow down even more. Other factor which can be included in the model are driver discipline (or lack of it) in sticking to speed restrictions.

Your assignment is to find different modelling methods in the literature, and compare them (at least in theory). Select one or two methods (or make your own) and demonstrate the strengths and weaknesses. Do they show any of the phenomena discussed above?

References:

1. D. Helbing (1995) Improved fluid-dynamic model for vehicular traffic. *Physical Review E* **51**:3164-3169.

2. T. Nagatani (1996) Effect of car acceleration on traffic flow in 1D stochastic CA model *Physica A* **223**:137-148.

3. T. Nagatani (1999) Jamming transitions and the modified Korteweg-de Vries equation in two lane traffic flow. *Physica A* **265**:297-310.

7 Optimizing Traffic Lights in Urban Street Grids

Controlling traffic lights in city streets can be done in a number of ways. The simplest is just switching the lights according to a fixed schedule, using a clock. Even here, there are various parameters to control: e.g. which lights stay green for longer (based e.g. on traffic statistics)? Other methods use either magnetic loops in the road or radar to assess current traffic load, and use some form of intelligent system to select an optimal strategy. These are still local strategies. It should in theory be possible to let traffic lights communicate, so they can optimize their behaviour globally. The aim of this project is to create a simulation which explores the different ways in which a traffic light might be programmed.

8 The Lattice-Boltzmann Method

The Lattice Boltzmann (LB) method is an efficient way to simulate fluid dynamics in complex geometries, especially when multiple phases (liquid/gas, oil/water) are mixed. It can also take reactions between components into account. This means you can use the method for reaction-diffusion systems. Because it deals with local interactions, it can easily be parallelized. This makes it a particularly suitable method for massively parallel computers.

Your assignment is to find out more about the LB method, create an example simulation, and study the strengths and weaknesses of this method. There are several types of problems you could try to apply this method to. One might be nutrient uptake at the intestinal wall (think of the "fractal" nature of that wall!) or coral colony (has been done already). Reaction-diffusion systems are also well worth investigating, because of the intricate patters they can generate.

References to get you started:

1. X. Shan and H. Chen (1993) Lattice Boltzmann model for simulating flows with multiple phases and components. *Physical Review E* **47**:1815-1819

2. N.S. Martys and H. Chen (1996) Simulation of multicomponent fluids in complex three-dimensional geometries by the lattice Boltzmann method. *Physical Review E* **53**:743-750.

9 Simulation of an inverted pendulum in 2D

Consider a rod that can, at one end, rotate freely around a horizontal axis. Obviously, in the stable state the rod hangs with its center of mass below the axis. Now we start oscillating the axis in the vertical direction. Then there is, quite counter-intuitively, also a stable state with the rod standing upright. Project: model the rod with particles and springs and impose a vertical oscillatory motion to the axis. Show that there are stable and unstable frequencies. Visualize the system. Does the frequency of the stable situation correspond with the literature? Google: Inverted pendulum with a vertically oscillated pivot.

Literature:

1. J. P. Ryckaert, G. Giccotti, H. J. C. Berendsen. Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n- alkanes. Journal of computational physics 23, 327-341, 1977.

2. B. Hess, H. Bekker, H. J. C. Berendsen, J. G. E. M. Fraaije. LINCS: A Linear Constraint Solver for Molecular Simulations. Journal of Computational Chemistry, Vol. 18, No. 12, pages 1463-1472, 1997 (http://www.cs.rug.nl/ bekker/publications/lincs.pdf)

10 Simulated demolition

Demolition by imploding (rather than blowing up) a building is very difficult to get right. It is important that the structure collapses neatly onto a given area, with minimal use of explosive, and minimal blow-out of debris. The aim of this project is to select a simple structure (such as a radio mast), and simulate the behaviour of it as it collapses when certain structural elements are suddenly removed or weakened.

Two references available in the library:

1. B.M. Luccioni, R.D. Ambrosini, and R.F. Danesi (2004) Analysis of building collapse under blast loads *Engineering Structures* **26**: 63-71.
2. J.M. Loiseaux and D.K. Loiseaux (1995) Demolition by implosion. *Scientific American***55(1)**: 52-59.

11 Computing asteroid orbits

Asteroids are small bodies which are largely found in the asteroid belt between Mars and Jupiter. However, some are in "Earth-crossing" orbits and could collide with Earth with disasterous effects (incidentally "disaster" = "bad star"). Another group of asteroids, called the Trojans, can be found in the same orbit as Jupiter, but at angles of $\pm 60^\circ$ with respect to the direction from the Sun to Jupiter. Try to simulate the behaviour of small objects within a simplified solar system, and find out why the Trojans are in this peculiar position. Also, if time allows, try to compute the uncertanties in orbits of Near-Earth Asteroids (NEAs).

Reference found in digital library:

1. A. Milani (1993) The Trojan asteroid belt: Proper elements, stability, chaos and families. *Celestial Mechanics and Dynamical Astronomy* **57(1-2)**: 59-94.

12 Moons of Pluto

Data from the Hubble Space Telescope and the New Horizons probe has shown several interesting features in the orbits and rotational motion of the moons of Pluto. Not only are Pluto and Charon tidally locked (same hemisphere of each object faces the other at all times), but the moons of Pluto also show chaotic orbits and rotation, in part due to their excentric shapes. In a variant of the previous assignment, try to simulate these kinds of behaviour. Unlike the previous assignment, you must not assume the objects are point masses or uniform spheres, adding to the complexity of the simulation.

1. M.R. Showalter, and D. P. Hamilton (2015) Resonant interactions and chaotic rotation of Pluto's small moons. *Nature* **522.7554**: 45-49.

13 Simulating the cracking of a clay layer

After an area has been flooded by a river a thin layer of clay is left behind. When this layer dries the clay crackles in a typical pattern. The same kind of pattern can be seen on old paintings and pottery. In this project you are asked to generate this kind of pattern by modelling the clay as a set of particles and springs. Springs will break when a maximum force is exceeded. Simulate how the cracking proceeds over time. Also, experiment with various types of springs and particle placement strategies in order to generate different types of patterns. Don't hesitate to use huge numbers of particles.

Literature:

1. Studies of crack dynamics in clay soil II. A physically based model for crack formation. H.J. Vogel, H. Hoffmann, A. Leopold, K. Roth

14 Diffusion Limited Aggregation: Off-lattice simulations

For the growth of DLA clusters in absence of an underlying lattice structure several modifications of the code/model presented in class are necessary. Implement off-lattice cluster growth, aiming at large cluster sizes and perform an analysis of their fractal properties, growth dynamics etc. along the lines of and extending the discussion of lattice-based DLA in class.

Literature will be provided through Nestor together with the lecture notes on DLA.

15 Diffusion Limited Aggregation: Growth site probilities

For a given DLA cluster, the probability for the next particle to attach to one of the potential growth sites can be determined by solving (numerically) a Laplace equation with appropriate boundary conditions. In particular, estimating very small probabilities in the "inner fjords" of the cluster is difficult. In this project you are to determine the growth site probability density and investigate its mathematical properties.

Literature will be provided through Nestor together with the lecture notes on DLA.

16 Invasion Percolation

The so-called percolation model can be interpreted in many different ways. The name originally relates to a liquid percolating through a porous medium. Percolation can also be understood as an extremely simple randomized growth model, which does not include particle diffusion (in contrast to DLA). In this project a variant will be considered: the so-called *Invasion Percolation* which is very interesting in the context of *self-organized criticality* in models of *avalanches* or *forest fires*.

In the project you will study, for instance, fractal properties of the growing percolation clusters and aspects of *criticality*.

A more detailed description of the project and literature will be provided through Nestor.

17 Integrate-and-fire neural networks

In class, Integrate-and-fire neural networks will be discussed under the simplifying assumption of inhibitory synapses only. In the project, you are supposed to include exitatory synapses as well, which requires several modifications of the model and the simulations.

With this more realistic model, some of the aspects discussed in class can be studied in greater detail and other questions can be addressed.

Ultimately, you should also incorporate a form of *Hebbian Learning* in the system, which changes the synaptic strengths in order to stabilize particular activity patterns in the network.

Literature will be provided through Nestor together with the lecture notes on Neural Networks.

18 On-line Gradient Descent in layered neural networks

Stochastic or on-line gradient descent techniques play a key role in the training of layered neural networks. Theoretical analyses as well as empirical observations show that the success of training can be hindered by so-called plateau states. In these extended, quasi-stationary phases of training, almost no progress is made and the network is *stuck* in sub-optimal configurations. Plateaus have to be broken by the process of *hidden-unit-specialization.*

The problem has been studied extensively in *shallow* neural networks, but surfaced again, recently, in the context of *deep learning*. In the project you should simulate and investigate plateaus in Monte Carlo simulations of on-line gradient descent, i.e. with randomized training data in student/teacher scenarios. In particular, potential methods to shorten plateaus should be studied.

The topic can be addressed in several separate projects. Examples:

a) Effects due to unlearnable targets or noise in the training data

b) Over-fitting effects in too powerful student networks

c) The influence of *momentum* or *learning rate schedules* on the properties of plateau states

References:

1. Saad, D.; Solla, S.A. On-line learning in soft committee machines *Phys. Rev. E* **1995**, 52, 4225-4243.

2. Biehl, M.; Riegler, P.; Wöhler, C. Transient dynamics of on-line learning in two-layered neural networks. *J. Phys. A: Math. Gen.* **1996**, 29, 4769-4780.

3. Vicente, R.; Caticha, N. Functional optimization of online algorithms in multilayer neural networks. *J. Phys. A: Math. Gen.* **1997**, 30, L599-L605.

4. Y.N. Dauphin et al. Identifying and attacking the saddle point problem in high-dimensional non-convex optimization. https://arxiv.org/pdf/1406.2572.pdf

19 Cluster algorithms in Monte Carlo simulations of Ising systems

An efficient speed-up over the conventional *single spin flip* algorithms in Monte Carlo simualations of Ising systems can be achieved by the identification of appropriate clusters of spins that are then flipped simultaneously.

In the project, you will implement the Wolff algorithm and study the two-dimensional Ising Ferromagnet in greater detail. For instance, you can investigate scaling laws near criticality.

Reference (starting point)

1. Wolff, U. Collective Monte Carlo Updating for Spin Systems", Physical Review Letters, 62 (4): 361 (1989). doi:10.1103/PhysRevLett.62.361

20 Frenkel-Kontorova-Model

The so-called *Chirikov* or *Standard Map* is a basic example for a non-linear iteration it two dimensions which displays non-trivial chaotic behavior. In the project, you implement the Chirikov Map and investigate in detail its behavior and the influence of the control parameter along the lines of the discussion of the one-dimensional Logistic Map in class.

Moreover, the Chirikov Map can be interpreted in the context of the so-called Frenkel-Kontorova model, which describes interacting particles in a periodic potential. In the model, the so-called *winding number* is of central interest and displays highly non-trivial mathematical properties.

References

1. H.-J. Jodl, H.-J. Korsch, *Chaos: A Program Collection for the PC*, Springer (1994)

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 Bejeren (ed.), *Fundamental Problems in Statistical Physics VII*, Elsevier (1990), pg. 96.