

24.07.2016

1 Dynamic systems modeling

System: a potential source of data

- boundary
- inputs / outputs

Experiments: Extracting data from a system

- apply condition to input and observe outputs (Observability / Controllability)

Model: of a system and an experiment is anything to which exp can be applied. This results in an experimental frame of the model. A model in the general case doesn't need to be mathematical or computational. No model is valid for all experiments but the system itself. The purpose of modeling is to simplify. "All models are wrong but some of them are useful"

Simulation: Perform the experiment on the model.

Continuity:

- Discrete and Deterministic (Molecular Dynamics)
- Continuous and Deterministic (Partial differential equations)
- Discrete and Stochastic (Agent based models)
- Continuous and Stochastic (Stochastic differential equations)

The continuum limit assumes the changes of a single molecule does not matter for the overall concentration in the region of the length scale λ . The length scale L field gradients are established

$$Kn := \frac{\lambda}{L} \quad (1.1)$$

If $Kn \ll 1$ the continuum assumption is justified.

Extensive quantities: depend on the system size. (Mass, Volume, molecules ...)

Intensive quantities: do not depend on the system size (Temperature, concentration ...).

Differential equations are always expressed in terms of intensive quantities in simulation needs to use extensive quantities. This is not necessary but helpful to design the simulation experiment properly.

24.07.2016

Dimensional Analysis:

- dependence of variables (Which are the important variables?)
- orders of magnitude
- Model - System similitude (Where show model and system same dynamics?)

Dim: Mass, length, time, force, ...

Units: kg, lb ...

Theorem:

All dimensions are power series of 6 basic dimensions.

- mass M
- length L
- time T
- temperature θ
- charge C
- resistance R

Example: $force = M^1 L^1 T^{-1}$

Buckingham Theorem:

If n is the number of basic dimensions and p variables of a system. The system is completely described by $p-n$ dimensionless groupings.

Example:

A force acting on a point mass in vacuum:

$$n = 3(M, L, T)$$

$$p = 4(m, F, t, v)$$

Therefore, the system is described by a single dimensionless quantity.

All physical equations are dimensionally homogeneous: $A + B = C$. The dimensions of A , B and C needs to be the same.

Taylor (1979) proposed an algorithm to find the dimensionless groupings of a system.

Example:

Shear stress on red blood cell traveling with a velocity u through an artery. If the shear stress τ is too high the blood cell would be destroyed. The shear stress then depends on the distance from the wall h , the viscosity η , the density ρ and the velocity u .

$$n = 3(M, L, T)$$

$$p = 4(\eta, \rho, h, \tau, u)$$

$$\begin{array}{cccc}
\begin{array}{c} M \\ h \\ u \\ \eta \\ \rho \\ \tau \end{array} & \begin{array}{c} L \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{array} & \begin{array}{c} T \\ 1 \\ 1 \\ -1 \\ -3 \\ -1 \end{array} & \begin{array}{c} 0 \\ 0 \\ -1 \\ 0 \\ -2 \end{array} \\
\begin{array}{c} M \\ h \\ u \\ \eta \\ \rho \\ \tau \end{array} & \begin{array}{c} L \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{array} & \begin{array}{c} T \\ 1 \\ 1 \\ 2 \\ -3 \\ 2 \end{array} & \begin{array}{c} 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ -2 \end{array} \\
\begin{array}{c} L \\ h \\ u \\ \eta/\rho u \\ \tau/\rho u^2 \end{array} & \begin{array}{c} T \\ 1 \\ -1 \\ 1 \\ 0 \end{array} & \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{array} & \begin{array}{c} L \\ 0 \\ 0 \\ 0 \\ 0 \end{array}
\end{array} \rightarrow \begin{array}{c} L \\ h \\ u \\ \eta/\rho u \\ \tau/\rho u^2 \end{array} \rightarrow \begin{array}{c} L \\ 0 \\ 0 \\ 0 \\ 0 \end{array} \quad (1.2)$$

The dimensionless numbers are then $\Pi_1 = \frac{\eta}{\rho u h}$ and $\Pi_2 = \frac{\tau}{\rho u^2}$.

We also know that: $\Pi_1 = f(\Pi_2)$ this helps us to design an experiment because only the dimensionless numbers need to be varied to understand the function that relates Π_1 and Π_2

Modeling Dynamics:

- 1) Define the system boundaries and the input and outputs
- 2) Identify reservoirs (for any quantity) of relevant time scales
- 3) Formulate equations for the flows to the reservoirs.
All flows have the form $flow = f(activatinglevel - inhibitinglevel)$.
- 4) Formulate the balance equations for the reservoirs. $\frac{d}{dt}level = \sum inflows - \sum outflows$
- 5) Simplify the system of equations
- 6) Solving the systems will give $level(t)$
- 7) Identify unknown parameters based on the given data
- 8) **Validate the model**. Prove that the model can predict another experiment!

2 Recap of vector calculus

3 Spatiotemporal models

Control volumes:

Discretization of space into finite small volumes. Considering that the control volumes can vary with time the rate of change of the intensive variable f . For being the density $f = m/V$:

$$\frac{df}{dt} = \frac{1}{V} \frac{dm}{dt} + \frac{m}{V} \frac{1}{V} \left(-\frac{dV}{dt} \right) \quad (3.1)$$

Fixes control volumes / Eulerian :

When using fixed control volumes the flow between the control volumes V_i is defined by the field derivative:

$$\frac{\partial f(x, t)}{\partial t} \Big|_{x=const} = D \nabla^2 f - \nabla \cdot (f \cdot \mathbf{v}(\mathbf{r}, t)) + k(f) \quad (3.2)$$

Co-moving control volume / Lagrangian:

When considering moving volumes the flow of the intensive quantity is given by the material

24.07.2016

derivative:

$$\frac{df}{dt} = \frac{\partial}{\partial t} [f(\mathbf{r}(r), t)] = \nabla f \cdot \frac{\partial \mathbf{r}(t)}{\partial t} + \frac{\partial f}{\partial t} \quad (3.3)$$

For considering mass conservation:

$$m = \int f dV \quad (3.4)$$

$$\frac{dm}{dt} = 0 \quad (3.5)$$

Inserting the derivative above leads to the Reynolds transport theorem:

$$\frac{dm}{dt} = \int_V \frac{\partial f}{\partial t} dV + \int_V f \mathbf{v} \cdot \mathbf{n} dS \quad (3.6)$$

Infinitesimal control volumes: For $V \rightarrow 0$ the Conservation:

$$\frac{dm}{dt} = 0 \quad (3.7)$$

translate Lagrange to Eulerian:

$$\frac{dm}{dt} = \int_V \frac{\partial f}{\partial t} dV + \int_V f \mathbf{v} \cdot \mathbf{n} dS \quad (3.8)$$

With the field \mathbf{v} Fick's law is defined as:

$$f \cdot \mathbf{v} = -D \nabla f \quad (3.9)$$

Where D is Diffusion tensor with the elements $D_{ij}, [i, j] \{x, y, z\}$ Insertion of the the relations derived above gives:

$$\frac{dm}{dt} = \int_V \left[\frac{\partial f}{\partial t} - \nabla(D \nabla f) \right] dV = 0 \quad (3.10)$$

This relation recovers Fick's second law:

$$\frac{\partial f}{\partial t} = D \Delta f \quad (3.11)$$

Conclusion:

In an Eulerian description the formulation of the advective transport needs to be addressed with the term $-\nabla \cdot (f \cdot \mathbf{v}(\mathbf{r}, t))$. This can be avoided using a Lagrangian formalism as the convective transport is described by the movement of the control volumes

24.07.2016

1 Cellular Automata

Simple model of complex systems: Simple rules between the finite control volumes can reproduce the complex behavior exhibited by the differential equations. The complex behavior emerges of the population of interacting control volumes. The emerging behavior is lost when isolating the components.

Example: Self organization of heart cells.

Definition of the CA:

- Discrete space, lattice or cells (nodes and sites)
- States: a discrete - typically small set of states that characterize the cells
- Neighborhood: cells that interact with the i th cell
- Update rules

Types of update rules:

- Deterministic (Eularian)
- Stochastic: Execution of the rule has a probability
- Lattice Gas CA for moving cells
- Solidification CA with absorbing state for architectural models e.g. branching morphogenesis

Example: John Conway's Game of Life

2D System with two states and three rules: Birth, Survival and Death.

Birth: if cell is empty and has exactly three living neighbors

Survival: if cell is living and has two or three living neighbors

Death: else ? ...

2 Particle Methods

Discretization:

Physical quantities are usually present as continuous fields. In computer simulation the fields needs to be sampled at "representative points". The required resolution is determined by the field limit L and the continuous limit λ .

$$\lambda < \Delta x < L \rightarrow \Delta x < \frac{2}{a} \quad (2.1)$$

where $a = \max(Eig.val.)$. The discretization method can be structured or unstructured. Possible methods are:

- Finite Differences, 1D Grid
- Finite Elements, 2D Triangles
- Finite Volumes, 3D Volumes
- Particle Methods, 0D Points

Particles as reservoirs: Every particle is a reservoir and interchange its interchanging flows with it surrounding particles.

Particle methods:

In terms of discretization particle methods are very suited for the simulation of biological system because its easy to from complex geometry.

A Particle is a set $(\mathbf{r}, \{w_1, w_1 \dots\})$ where \mathbf{r} is the position and w_i are arbitrary variables.

$$\frac{d\mathbf{r}}{dt} = \sum_{q=1}^N K(\mathbf{r}, \{w_1, w_1 \dots\}) \quad (2.2)$$

$$\frac{d\mathbf{w}}{dt} = \sum_{q=1}^N F(\mathbf{r}, \{w_1, w_1 \dots\}) \quad (2.3)$$

In General the implementation of particle methods is always the same only the functions K and F need to be provided.

Libraries: PPM, Puma .. .

Solve a differential equation:

$$\frac{du}{dt} = f \quad (2.4)$$

First possibility to compute the solution is discretization of the equation and then numerical integration. Therefore, the consistency is crucial for discretization and numerical stability for the actual computation. This methods is called intensive solution.

$$\frac{u_n - u_{n-1}}{\delta t} = f_{n-1} \rightarrow u_n = u_{n-1} + \delta t f_{n-1} \quad (2.5)$$

Second possibility express the differential equation as an integral and then compute this integral numerically. In contrast to the first possibility the expression of the integral is exact numerical error is only exhibited by computation of the integral (stability is not an issue). This method is called is intensive.

$$u = \int f(t)dt \rightarrow u = \sum w_i f(x_i) \quad (2.6)$$

Numerical stability can be derived for a simple first order equation solved with the Euler scheme as :

$$\frac{x_n - x_{n-1}}{\delta t} = -\lambda x_{n-1} \quad (2.7)$$

is stable for

$$|1 - \lambda t| < 1 \rightarrow 0 < \delta t < \frac{2}{\lambda} \quad (2.8)$$

Particle Function Approximation:

$$u(x) = \int_{\Omega} u(y)\delta(x - y)dy = \int_{\Omega} u(y)\xi(x - y)dy + \mathcal{O}(\epsilon^r) \quad (2.9)$$

where ξ is a smoothing function the is similar to delta

$$\xi_{\epsilon} = \frac{1}{\epsilon} \xi\left(\frac{x}{\epsilon}\right) \quad (2.10)$$

If we consider the space discretized with the particle positions x_p

$$u(x) \approx \sum_{\Omega} u(x_p)\xi(x - x_p)V_p = \sum_{p=1}^N \omega_p \xi(x - x_p) + \mathcal{O}\left(\frac{h}{\epsilon}\right)^S \quad (2.11)$$

Choosing ξ will determine $\mathcal{O}(\epsilon^r)$ where r is the r th moment that differs from the delta function. Thus for a Gaussian function $r = 2$. The error $\mathcal{O}\left(\frac{h}{\epsilon}\right)^S$ where S is the smoothness of the function defined be the n th defined derivative. For a Gaussian function this l leads to $S \rightarrow \infty$ therefore the discretization length h of the particles is required to be smaller than ϵ . This leads to an overlap of particles. This leads to smoothed particle methods.

Remeshig:

Use a gird with the a grid size $a < \epsilon$. If the the overlap condition is violated: Interpolate the values to the mesh nodes. Delete the particles. Reinitialize particles at the mesh points. Therefore, the discretization is adaptive.

As the smoothing function was designed to conserve the first two moments, an interpolation methods is desired the conserve this moments. A interpolation scheme of an arbitrary order convolved with itself will give the interpolation scheme of the next higher order. This a methods conserving moments to the order of 3 is given by:

$$M'(s) = \begin{cases} 1 - \frac{1}{2}(5s^2 - 3s^3) & 0 \leq s \leq 1 \\ \frac{1}{2}(2 - s)^2(-s) & 1 \leq s \leq 2 \\ 0 & s > 2 \end{cases} \text{ where } s = \frac{|x_p - x_m|}{h} \quad (2.12)$$

24.07.2016

To compute the interactions in between N particle pairs has a complexity of $\nu(N^2)$. But if the function F only changes the particle locally the complexity reduces to $\nu(N)$. If F is global a method 1984 Barnes & Hut can compute all interaction with a complexity $\nu(N \log(N))$. The idea is to cluster particles into cells and compute the interaction of the particles with its nearby particle and the interaction with the clusters. Another method proposed by Greengard & Roklin 1989 reduces this further $\nu(N)$. The Greengard & Roklin let only representative cluster interact with each other.

Cell List:

Create a grid with the grid size of the cutoff radius r_c . You loop over every particle and you get the index of the cell $i = \text{Int}(x_p/r_c)$. In a next step the particle is added to the list of this cells. To read out the nearest neighbors of the particle all particles in the particles cell and the cells neighbors.

Verlet list:

Every particle carries a list of interacting particles. Therefore, the Verlet list uses a slightly larger cutoff radius than the cell list it is created from. As long as no particle moves in this skin the same Verlet list can be used for the particle and the list doesn't need to be constructed.

3 Simulation of Diffusion

Mesoscopic picture: Consider microscopic phenomena on a macroscopic length scale. We consider the probability of a particle to change its position with in the time interval δt . The probability density function of the particle to be at the position x is then:

$$P(x, t + \delta t) = q_+ P(x - \delta x, t) + q_- P(x + \delta x, t) + P(x, t)[1 - (q_- + q_+)] \quad (3.1)$$

where q is the transition property and P is a probability density function. Using the second order Taylor expansion:

$$P(x, t) + \delta t \frac{\partial P}{\partial t} + \frac{\delta t^2}{2!} \frac{\partial^2 P}{\partial t^2} + \mathcal{O}(\delta t^3) = q_+ \left[P(x, t) - \delta x \frac{\partial P}{\partial x} \right] + q_- P(x + \delta x, t) + P(x, t)[1 - (q_- + q_+)] \quad (3.2)$$

For $\delta t \rightarrow 0$

$$\frac{\partial P}{\partial t} = \frac{\partial P}{\partial x} \left[\frac{q_- \delta x - q_+ \delta x}{\delta t} \right] + \frac{\partial^2 P}{\partial x^2} \left[\frac{\delta x^2}{2} \frac{q_- + q_+}{\delta t} \right] + \mathcal{O}(\delta t^3) \quad (3.3)$$

Partial stochastic equation:

$$\frac{\partial P}{\partial t} = V \frac{\partial P}{\partial x} + D \frac{\partial^2 P}{\partial x^2} \quad (3.4)$$

A solution for the probability density is :

$$P(x|x_0, \delta t) = \frac{1}{\sqrt{4\pi D \delta t}} e^{-\frac{(x-x_0)^2}{4D \delta t}} \quad (3.5)$$

With the mean squared displacement of a particles can then be described as:

$$\langle x^2(t) \rangle = 2Dt \quad (3.6)$$

The results can also be recovered for the random walk:

$$x(t + \delta t) = x(t) + r\sqrt{\delta t}; r \sim N(0, 2dD) \quad (3.7)$$

Random walk Particle method:

Consider a particle with its position x_p and the number of molecules on the particle $w_p = u^0(x_p)V_p$

$$x_p(t_i + \Delta t) \leftarrow x_p(t_i) + \mathbf{r}\sqrt{\Delta t} \quad (3.8)$$

Using the random walk the diffusion equation is sufficiently described therefore:

$$\frac{dw_p}{dt} = 0 \quad (3.9)$$

Continuum:

In a continuous description diffusion is described using the densities $u(x, t) \rightarrow$ Density or Concentration. The development in time can be recovered from Fick's law:

$$\frac{\partial u}{\partial t} = D\nabla^2 u \quad (3.10)$$

Where D is not a function of space and time, and the fluid is isotropic and homogeneous.

For the 1D diffusion the particle method for a continuous particle method (Particle Strength Exchange) is recovered from the PDE:

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \quad (3.11)$$

Expanding $u(x)$ with the Taylor expansion:

$$u(y) = u(x) + \frac{y-x}{1!} \frac{\partial u}{\partial x} + \frac{(y-x)^2}{2!} \frac{\partial^2 u}{\partial x^2} + \dots \quad (3.12)$$

$$\int_{\Omega} [u(y) - u(x)] \eta(y-x) dy = \int_{\Omega} \frac{y-x}{1!} \frac{\partial u}{\partial x} \eta(y-x) dy + \int_{\Omega} \frac{(y-x)^2}{2!} \frac{\partial^2 u}{\partial x^2} \eta(y-x) dy + \dots \quad (3.13)$$

The Kernel $\eta_{\epsilon}(\xi) = \frac{1}{\epsilon} \eta\left(\frac{\xi}{\epsilon}\right)$ shall be the delta function for $\epsilon \rightarrow 0$

$$\int_{\Omega} [u(y) - u(x)] \eta(\xi) d\xi = \int_{\Omega} \frac{\xi}{\epsilon} \frac{\partial u}{\partial x} \eta(\xi) d\xi + \int_{\Omega} \frac{\xi^2}{2\epsilon} \frac{\partial^2 u}{\partial x^2} \eta(\xi) d\xi + \dots \quad (3.14)$$

For the construction of the Kernel we choose:

$$\int \xi \eta(\xi) d\xi = 0 \quad (3.15)$$

$$\int \xi^2 \eta(\xi) d\xi = 2 \quad (3.16)$$

$$\int \xi^s \eta(\xi) d\xi = 0; 3 \leq s \leq r+1 \quad (3.17)$$

24.07.2016

The gradient of $u(x)$ is then:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{1}{\epsilon} \int_{\omega} [u(y) - u(x)] \eta_{\epsilon}(y - x) dy + \mathcal{O}(\epsilon^r) \quad (3.18)$$

In terms of particles this is written as a sum:

$$\frac{\partial^2 u_p}{\partial x^2} = \frac{1}{\epsilon^2} \sum_{q=1}^N V_q [u_q - u_p] \eta_{\epsilon}(y - x) \quad (3.19)$$

In general the derivative of the order β is given by:

$$\frac{\partial^{\beta} u_p}{\partial x^{\beta}} = \frac{1}{\epsilon^{\beta}} \sum_{q=1}^N V_q [u_q \pm u_p] \eta_{\epsilon}^{\beta}(y - x) \quad (3.20)$$

A solution for the second derivative the one dimensional Kernel is

$$\eta(\xi) = \frac{1}{2\sqrt{\pi}} e^{-\frac{\xi^2}{4}} \quad (3.21)$$

A solution for the second derivative the three dimensional Kernel is

$$\eta(\xi = \{x, y, z\}) = \frac{1}{(2\pi)^{3/2}} e^{-\frac{\xi^2}{2}} \quad (3.22)$$

Diffusion and Advection:

The general equation considering advective and diffusive transport is:

$$\frac{\partial u}{\partial t} + \nabla \cdot (uV) = D \nabla^2 u \quad (3.23)$$

For incompressible fluids $\nabla \cdot V = 0$ holds. Thus the equation simplifies to

$$\frac{\partial u}{\partial t} + V \cdot (\nabla u) = D \nabla^2 u - u(\nabla \cdot V) \quad (3.24)$$

To derive the particle method it is required to express it in an Lagrangian framework:

$$\frac{dx_p}{dt} = V_p(x_p, t) \quad (3.25)$$

$$\frac{du_p}{dt} = D \nabla^2 u_p - u_p(\nabla \cdot V) \quad (3.26)$$

$$\frac{du_p}{dt} \approx \frac{D}{\epsilon^2} \sum_{q=1}^N V_p (u_q - u_p) \eta_{\epsilon}(x_q - x_p) - u_p(\nabla \cdot V)_p \quad (3.27)$$

For a two dimensions the system writes:

$$(\nabla \cdot V)_p = \frac{1}{\epsilon} \sum_{q=1}^N \Omega_q (V_{xq} + V_{xp}) \eta^{(1,0)}(x_p - x_q) + \frac{1}{\epsilon} \sum_{q=1}^N \Omega_q (V_{yq} + V_{yp}) \eta^{(0,1)}(y_p - y_q) + \mathcal{O}(\epsilon^3) \quad (3.28)$$

With the kernels:

$$\eta_\epsilon^{(1,0)}(x, y) = \frac{-2x}{\epsilon^2\pi} e^{\frac{x^2+y^2}{\epsilon^2}} \quad (3.29)$$

$$\eta_\epsilon^{(0,1)}(x, y) = \frac{-2y}{\epsilon^2\pi} e^{\frac{x^2+y^2}{\epsilon^2}} \quad (3.30)$$

$$\frac{dx_p}{dt} = V_p(x_p, t) \quad (3.31)$$

To solve the equations in time a first order explicit Euler scheme can be implemented according to:

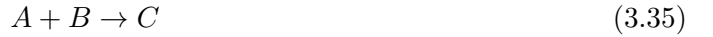
$$x_p(t + \delta t) = x_p(t) + \delta t V_p(x_p, t) + \mathcal{O}(\delta t^2) \quad (3.32)$$

$$u_p(t + \delta t) = u_p(t) + \delta t(\dots) + \mathcal{O}(\delta t^2) \quad (3.33)$$

The maximal timestep $\delta t < c \|\nabla \mathbf{V}\|_\infty^{-1}$ or also $\delta t < c \delta x / V$

Chemical Reactions:

Consider the reaction Network:



With the rate constants R_1 , R_2 and R_3 the reaction kinetics are described by:

$$\frac{d[A]}{dt} = R_1 - R_2[A][B] \quad (3.37)$$

$$\frac{d[B]}{dt} = -R_2[A][B] \quad (3.38)$$

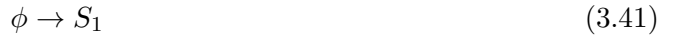
$$\frac{d[C]}{dt} = R_2[A][B] - R_3[C] \quad (3.39)$$

Using the explicit Euler scheme the evolution of the concentration of the concentration is given by:

$$[A](t + \delta t) = [A](t) + (k_1 - k_2[A](t)[B](t))\delta t \quad (3.40)$$

Diffusion - Advection - Reaction Equation :

Assume three chemical species S_1 , S_2 , S_3 , the system also exhibits a flow field V , the species have the diffusion constants D_1 , D_2 and D_3 . Assume the reaction network of



The general system is described by:

$$\frac{du_1}{dt} + \nabla \cdot (u_1 V) = D_1 \nabla^2 u_1 + k_1 - k_2 u_1 u_2 \quad (3.44)$$

24.07.2016

$$\frac{du_2}{dt} + \nabla \cdot (u_2 V) = D_2 \nabla^2 u_2 - k_2 u_1 u_2 \quad (3.45)$$

$$\frac{du_2}{dt} + \nabla \cdot (u_3 V) = D_3 \nabla^2 u_2 + k_2 u_1 u_2 - k_3 u_3 \quad (3.46)$$

A particle is now by described by its position x_p and the three concentrations u_1 , u_2 and u_3 . In the lagrangian framework the equations read then:

$$\frac{dx_p}{dt} = V_p \quad (3.47)$$

$$\frac{du_{1p}}{dt} = D_1 \nabla^2 u_{1p} - u_{1p}(\nabla \cdot V_p) + k_1 - k_2 u_{1p} u_{2p} \quad (3.48)$$

$$\frac{du_{2p}}{dt} = D_2 \nabla^2 u_{2p} - u_{2p}(\nabla \cdot V_p) - k_2 u_{1p} u_{2p} \quad (3.49)$$

$$\frac{du_{3p}}{dt} = D_3 \nabla^2 u_{3p} - u_{3p}(\nabla \cdot V_p) + k_2 u_{1p} u_{2p} - k_3 u_{3p} \quad (3.50)$$

26.07.2016

1 Stability analysis

1. Temporal (ODE) models

$$\frac{d}{dt}\mathbf{u}(t) = \mathbf{f}(\mathbf{u}(t), k_i) \quad (1.1)$$

Nullclines also called stationary states. Stable steady state with an unstable environment leads to oscillations. A stationary state is found by setting all the fluxes to zero:

$$\frac{d}{dt}u^*(t) = 0 = \mathbf{f}(u^*(t), k_i) \quad (1.2)$$

With that we can construct the functions f_1 and f_2 in the form that $u_1^* = f_1(u_2^*)$. The steady states at a given u_i is then given by the intersections of the functions f_1 and f_2 . The steady states for u_2 are found for a given parameter set. If the number of steady state changes on the choice of parameters this is called bifurcation.

To find the steady state the Jakobi-Matrix J is derived for the function $\mathbf{f}(\mathbf{u}(t), k_i)$. In a first order approximation the function \mathbf{f} can then be expressed as:

$$\mathbf{f}(\mathbf{u}(t), k_i) = \mathbf{f}(\mathbf{u}^*) + J \cdot (\mathbf{u}(t) - \mathbf{u}^*) + \mathcal{O}((\mathbf{u}(t) - \mathbf{u}^*)^2) \quad (1.3)$$

$$\frac{d}{dt}(\mathbf{u}(t) - \mathbf{u}^*) = \mathbf{f}(\mathbf{u}^*) + J \cdot (\mathbf{u}(t) - \mathbf{u}^*) + \quad (1.4)$$

With this we can use the general Ansatz for a linear equation with the eigenvalues $\lambda_i(k_i)$ of Jacobian J .

$$\mathbf{u}(t) - \mathbf{u}^* = \sum_i A_i e^{\lambda_i t} \quad (1.5)$$

Stability of \mathbf{u}^* is given if all $\text{Re}[\lambda_i] < 0$. The bifurcation points are given for $\text{Re}[\lambda_j] = 0$ for one j .

2. Spatiotemporal (PDE) models

Consider a one dimensional system with a constant velocity $\mathbf{v}(\mathbf{x}, t) = v = \text{const.}$ the transport equations read then:

$$\frac{\partial u(x, t)}{\partial t} = f(u) + D \frac{\partial^2 u(x, t)}{\partial x^2} - v \frac{\partial u(x, t)}{\partial x} \quad (1.6)$$

The steady steady state u^* is assumed to be uniform $\partial u / \partial t = 0$ and $\partial u / \partial x = 0$. In terms of the Taylor expansion $f(u)$ is expressed as:

$$f(u) = f(u^*) + f_u|_{u^*} \cdot (u - u^*) + \mathcal{O}((u - u^*)^2) \quad (1.7)$$

26.07.2016

Thus a gain the rate of change near u^* is given by:

$$\frac{\partial(u - u^*)}{\partial t} = f_u(u - u^*) + D \frac{\partial^2(u - u^*)}{\partial x^2} - v \frac{\partial(u - u^*)}{\partial x} \quad (1.8)$$

Using a Fourier transform and an the trivial ansatz $u - u^*$ reads

$$u - u^* = \int_{-\infty}^{\infty} dk a_k e^{ikx} e^{\lambda_k t} \quad (1.9)$$

Insertion into the PDE leads to:

$$\lambda_k \int dk a_k e^{ikx} e^{\lambda_k t} = f_u \cdot \int dk a_k e^{ikx} e^{\lambda_k t} + D(ik)^2 \int dk a_k e^{ikx} e^{\lambda_k t} - V(ik) \int dk a_k e^{ikx} e^{\lambda_k t} \quad (1.10)$$

Integration of $\int \dots dx e^{ik'x}$ leads to $\delta(k - k')$ therefore

$$a_k \lambda_k e^{\lambda_k t} = f_u a_k e^{\lambda_k t} + D(-k^2) a_k e^{\lambda_k t} - V(ik) a_k e^{\lambda_k t} \quad (1.11)$$

$$\lambda_k = f_u + D(-k^2) - V(ik) \quad (1.12)$$

For the linearized equations we obtain then the solution:

$$u(x, t) = u^* + \int a_k e^{ik(x-vt)} e^{(f_u - Dk^2)t} \quad (1.13)$$

From the solution we can conclude that spatial patterns induced travel in space with the flow speed $x - vt$ and depending on the function f_u and the diffusion these patterns decay of $f_u - Dk^2 < 0$