Lecture 1

A general scheme of Mathematical Modelling

No new specific mathematic is included into this scheme.

Still it is based on advanced chapters of classical and recent mathematical theories.

It is important to say that recent advances in computer science, including Machine learning, Artificial Neural Networks and AI, programming languages are important member of this family

In various textbooks this mathematical modelling scheme can be presented in different forms. Even titles can be different:

- computational experiments
- virtual reality
- digital world (digital twins)

In this course we will use the following scheme:

1. <u>Physical</u> (technological) model.

We select all important information on the given procedure, process, event. It can be formulated as technological, engineering, medical, economic, finance problems.

2. Make (~~develops~~) mathematical models of simpler subtasks

In most cases it is sufficient ~~to~~ select an existing, well tested models.

Only in exceptional cases we should develop new models of some subtask (a recursive stage with respect ~~to~~ general mathematical model we are interested in).

3. We link all selected models of subtasks into one common system (mathematical model).

Required initial and boundary conditions are added.

Next we test if a solution of the formulated problem exists, investigate if this solution depends continuously on given parameters, boundary and initial conditions.

Remark 1. Such models can be nonlinear, multidimensional, then the analysis described above is done for simplified equations (we consider linear approximations in smooth domains, one-dimensional, constant coefficients)

4. We construct a tool-box (collection, suite) with approximations of the full mathematical model.

Then the given problem can be solved faster, but the accuracy of the solution is degraded.

We are looking for a compromise between these two requirements.

This point is very important when the aim is ~~to~~ control complicated dynamic processes in a specified time limits (automatic car control), also in solution of optimization problems.

5. Solution of obtained mathematical problems. It is clear that only in most simple case we can find an analytic solution.

A typical situation when the given problems are solved numerically, i.e. we apply numerical solvers.

5.1. Mathematical models are approximated by ~~disrete~~ nonlinear (discrete) systems

a) estimates of approximation accuracy orders, usage of high-order numerical algorithms

b) the schemes and algorithms should be $\boxed{\text{stable.}}$

c) solution costs should of polynomial order $O(N^{\alpha})$, where N is the number of unknows.

5.2. Here we state one very important property of this general scheme of mathematical modelling

- all steps of this scheme are interconnected.

Let us consider some examples

If we can't construct an efficient and robust numerical algorithm (i.e. we can't solve such problems in time with our computational resources) then we return back to the stage of selection of subproblems / submodels and try to fix more simple models.

(as simple as possible but not simpler)

6. Selection of parameters/coefficients in equations of the model

The accuracy of the developed mathematical model depends on the selected parameters.

- we find these values in special literature or scientific textbooks/papers
- new experiments are done to determine missing information
- the number of such additional experiments can be reduced/limited sinse such measurements can be costly or dangerous and not friendly (e.g. we want to protect patients in hospitals).

In general we are interested to select parameters and coefficients in order to guarantee that results of virtual simulation and real world experiments agree well.

If this aim is not achieved we return back to the step of model specification.

Some times it is sufficient to take a more complex mathematical model from our box of models developed in Step. 4.

When the full mathematical model is constructed, parameters are selected and the accuracy is tested, we can use it for different applications:

- Prediction

By changing the values of coefficients and parameters we can simulate different scenarios and make important predictions (i.e. weather prediction, selection of a patient's optimal treatment plan, the analysis of the quality of new products and technologies).

The developed solvers become the basis for managing and control of complex technological processes

- Optimization

We have a possibility to find optimal constructions of complicated technologies, processes or new products skipping a big part (sometimes even all) of physical experiments (take examples from aviation and car industry)

- Visualization / animation of computer experiments and results

Virtual reality is not only based on big amount of data but it also generate huge amounts of new data. It is very important to have efficient tools to analyse them.

Usage of AI

The technology of Mathematical Modelling and Virtual (digital) simulations can be extended to many new areas due to the possibility to solve big parts of such projects by applying Machine Learning, Artificial Inteligence and Artificial Neural Networks. A big part of coding (programming) task also can be done by such tools as Gemini and ChatGPT.