Final report

on the project

"Analysis of continuous and discrete mathematical models in biology, chemistry and genetics (SNN 125119)"

The main goal of the research was to design, extend and analyse continuous and discrete biological and chemical models. Particular attention has been paid to the study of epidemic spreading processes, including the understanding of the qualitative properties of continuous and discrete models and their mathematical verification. Thus, the results of our research can be divided into two parts: the direct mathematical and practical investigation of epidemic spread processes, and research, significant part of which has been (or may be) used as a tool to successfully investigate epidemic spread processes. We have structured our report to reflect this.

1. Mathematical modeling of epidemic spread

A significant part of our work has dealt with the very current topic of epidemic spread.

We investigated in more detail the different models describing SIR-type and so-called vector-born type propagations. As models we used ODE systems (in some versions containing delay and/or PDE), and focused on the preservation of qualitative properties when we use some numerical method to approximate the solution of the model. From the Roos model and its simple delayed version, we switched to more complex models. We constructed and analysed their discrete models by using the explicit and implicit Euler method.

We studied the effect of quarantine on the spread of Ebola. We compared the effectiveness of different control strategies during epidemic outbreaks. Furthermore, we have established new models for Zika transmission and for Varroa infestation among honeybees. (The results will be detailed on the next pages.)

We studied the effectiveness of different control strategies during epidemic outbreaks and determine the final epidemic size for the models describing the control strategies. We established a new, nonautonomous model for Zika transmission dynamics. We constructed a complete mathematical analysis of a simpler version of this model, as well as on mathematical models for describing the emergence of chemotherapy-resistant tumour cells. We also studied a scalar periodic delay equation which describes the population dynamics of a species with short reproduction period.

We proposed and analysed a mathematical model for infectious disease dynamics with a discontinuous control function, where the control is activated with some time lag after the density of the infected population reaches a threshold. The model is mathematically formulated as a delayed relay system, and the dynamics is determined by the switching between two vector fields (the so-called free and control systems) with a time delay with respect to a switching manifold. First we establish the usual threshold dynamics: when the basic reproduction number $R0 \leq 1$, then the disease will be eradicated, while for $R0>1$ the disease persists in the population. Then, for $R0>1$, we divide the parameter domain into three regions, and prove results about the global dynamics of the switching system for each case: we find conditions for the global convergence to the endemic equilibrium of the free system, for the global convergence to the endemic equilibrium of the control system, and for the existence of periodic solutions that oscillate between the two sides of the switching manifold. The proof of the latter result is based on the construction of a suitable return map on a subset of the infinite dimensional phase space. Our results provide insight into disease management, by exploring the effect of the interplay of the control efficacy, the triggering threshold and the delay in implementation.

Some members of our group intensively worked on modeling the spread of Covid-19 as members of the Hungarian Covid-19 Modelling and Analysis Response Team.

We have published a work on the evaluation of the risk of spread outside China, and a paper on the early phase of the outbreak in Hungary and on assessing post-lockdown scenarios. We have been working on mathematical models of the spread of various vector-borne diseases (Lassa fever, Zika fever, malaria) considering the seasonality of weather. We studied a scalar periodic delay equation which describes the population dynamics of a species with short reproduction period.

We studied a compartmental model for COVID-19, introducing a separate class for quarantined susceptibles, synonymous to isolation of individuals who have been exposed and are suspected of being infected. The current model assumes a perfect quarantine based on contact with infectious individuals. Numerical simulation is conducted to investigate the efficiency of disease control by segregating suspected individuals and other non-pharmaceutical interventions. In addition, we assort quantitatively the importance of parameters that influence the dynamics of the system. Fitting the system to the early phase of COVID-19 outbreaks in Bangladesh, by taking into account the cumulative number of cases with the data of the first 17-week period, the basic reproduction number is estimated as 1.69.

We established and studied a novel SIRS model to describe the dynamics of Nipah virus transmission, considering human-to-human as well as zoonotic transmission from bats and pigs as well as loss of immunity. We determined the basic reproduction number which can be obtained as the maximum of three threshold parameters corresponding to various ways of disease transmission and determining in which of the three species the disease becomes endemic. By constructing appropriate Lyapunov functions, we completely described the global dynamics of our model depending on these threshold parameters.

In another work we presented a compartmental model for the spread of a disease with an imperfect vaccine available, also considering transmission from diseased infected in general, as during several epidemics, transmission from diseased people significantly contributed to disease spread. The global dynamics of the system was completely described by constructing appropriate Lyapunov functions. To support our analytical results, we performed numerical simulations to assess the importance of transmission from the diseased, considering the data collected from three infectious diseases, Ebola virus disease, COVID-19, and Nipah fever.

We formulated and studied mathematical models to investigate control strategies for the outbreak of the disease caused by SARS-CoV-2, considering the transmission between humans and minks. We proposed two novel models to incorporate human-to-human, human-to-mink, and mink-to-human transmission. For the definition of the reproduction number for both models we have used the next-generation matrix technique. We fitted our model to the daily number of COVID-19-infected cases among humans in Denmark as an example. Numerical simulations were conducted to investigate the impact of control measures, such as mink culling or vaccination strategies, on the number of infected cases in both humans and minks.

We established a compartmental model for Zika virus disease transmission, with particular attention paid to microcephaly, the main threat of the disease.

To this end, we considered separate microcephaly-related compartments for affected infants, as well as the role of asymptomatic carriers, the influence of seasonality and transmission through sexual contact. We determined the basic reproduction number of the corresponding time-dependent model and time-constant model and study the dependence of this value on the mosquito-related parameters. In addition, we demonstrated the global stability of the disease-free periodic solution if $\mathcal{R}0<1$, whereas the disease persists otherwise. We fitted our model to data from Colombia between 2015 and 2017 as a case study. The fitting was used to figure out how sexual transmission affects the number of cases among women as well as the number of microcephaly cases. Our sensitivity analyses concluded that the most effective ways to prevent Zika-related microcephaly cases are preventing mosquito bites and controlling mosquito populations, as well as providing protection during sexual contact.

SIRS models capture transmission dynamics of infectious diseases for which immunity is not lifelong. Extending these models by a W compartment for individuals with waning immunity, the boosting of the immune system upon repeated exposure may be incorporated. Previous analyses assumed identical waning rates from R to W and from W to S. This implicitly assumes equal length for the period of full immunity and of waned immunity. We relaxed this restriction, and allow an asymmetric partitioning of the total immune period in the SIRWS model to these two phases, characterized by a newly introduced bifurcation parameter. Other parameters were chosen to mimic pertussis. Stability switches of the endemic equilibrium are investigated with a combination of analytic and numerical tools. Then, continuation methods are applied to track bifurcations along the equilibrium branch. We found rich dynamics: Hopf bifurcations, endemic double bubbles, and regions of bistability. Our results highlight that the length of the period in which waning immunity can be boosted is a crucial parameter significantly influencing long term epidemiological dynamics.

In the joint research with our Slovenian partners we have investigated a space-dependent epidemic model equipped with a constant latency period. We constructed a delay partial integro-differential equation and showed that its solution possesses some biologically reasonable features. We propose some numerical schemes and show that by choosing the time step to be sufficiently small the schemes preserve the qualitative properties of the original continuous model. Also numerical experiments are presented that confirm the aforementioned theoretical results. Concerning the qualitative investigation of spatial epidemic models we introduced space dependency into the SIR models and give sufficient conditions for the mesh size and the time step that guarantee the nonnegativity, monotonicity and mass conservation properties even for higher spatial dimensional problems.

We also proposed a seasonal model for NiV disease transmission taking into account all human-to-host animal transmission as well as the loss of immunity in those who have recovered. We studied the existence and uniqueness of a disease-free ω-periodic solution and dealt with the basic reproduction number and stability analysis. Numerical examples were studied to assess the effect of parameter changes on disease dynamics, enabling us to understand how to avoid a yearly periodic recurrence of the disease.

We assessed the potential consequences of the SARS-CoV-2 waves caused by the Omicron variant. Our results suggested that even with the Delta variant controlled by a combination of non-pharmaceutical interventions and population immunity, a significant Omicron wave was to be expected. We stratified the population according to prior immunity status, and characterized the possible outbreaks depending on the population level of pre-existing immunity and the immune evasion capability of Omicron. We pointed out that two countries having similar effective reproduction numbers for the Delta variant can experience very different Omicron waves in terms of peak time, peak size and total number of infections among the population at risk. We also developed a compartmental model to study the applicability of pooling (testing a compound of several samples with one single test) and compared different pooling strategies. The model includes isolated compartments as well, from where individuals rejoin the active population after some time delay. We developed a method to optimize Dorfman pooling depending on disease prevalence and established an adaptive strategy to select variable pool sizes during the course of the epidemic. We showed that optimizing the pool size can avert a significant number of infections. The adaptive strategy is shown to be much more efficient, and may prevent an epidemic outbreak even in situations where a fixed pool size strategy cannot. Extending our previous model by including infected forager bees and considering model parameters as time-periodic functions, we established and studied a novel mathematical model for a honeybee colony infected with Varroa mites. The model describes the parallel phenomena of the spread of both the mites and the virus transmitted by them. We studied the autonomous version of the model and showed stability of equilibria, depending on the reproduction numbers. We presented two simulation scenarios to study the impact of seasonality on the spread of Varroa mites and the disease they carry. We performed numerical studies to show how the parameter changes might lead to the colony's failure.

We investigated the qualitative performance of different numerical methods applied to the Ross-MacDonald malaria model. It is known that for this model a certain set is positively invariant. We considered a method qualitatively correct if the resulting discrete system inherits this property. We investigated the explicit and implicit Euler methods, as a sub-procedure, moreover a semi-implicit method and finally, we combined them with non-local discretization. In another work we applied the nonstandard finite difference scheme to obtain reliable models, particularly to ensure the positivity preservation property. We suggest a step-size function for the system to preserve the positively invariant property for the total population. The suggested step-size function improves the accuracy and absolute stability of the explicit Euler scheme, while for the semi-implicit schemes the nonlocal discretization of the standard θ-method with the step-size function $\Phi(\Delta t) = \Delta t$ generates more precise results.

In some works we examined the properties of different epidemic models. After the properties of the continuous models were proven, an appropriate numerical scheme was constructed to approximate the continuous solution of the original equation. It was proven that for a sufficiently small timestep, the Runge-Kutta method (written in the Shu-Osher form) preserves not only the positivity of the continuous solution but conservation of mass and the asymptotic properties also hold. Later non-standard methods were also constructed, which also preserve the aforementioned properties for any step size. The theoretical results were also confirmed by numerical experiments.

We analysed numerical methods with operator splitting procedures, and applied them to an epidemic model, which takes into account the space dependence of the infection and the role of the vaccination. We showed the advantage of splitting by proving that its application leads to a wider interval of the time step where the methods preserve the non-negativity and monotonicity properties of the exact solution. Our results were illustrated by numerical experiments.

The generalized space dependent epidemic SIR models contain an integral term where the densitiy funtion of the infected members are integrated with a weight function. This results in a system of integro-differential equations. We have analyzed the uniqueness and the qualitative properties of the continuous model. We have revealed the step-size restrictions that guarantee the population conservation, positivity, and monotonicity preservation of the discrete model for higher order numerical schemes. The results were verified with computational experiments.

We also derived a numerical method based on the Magnus series expansion, and showed its second-order convergence when applied to a system of quasilinear delay equations. As an application, we considered the delayed epidemic model and illustrated our results with numerical experiments. We introduced and analysed numerical methods with operator splitting procedures, applied to an epidemic model which takes into account the space-dependence of the infection. We gave conditions on the time step, under which the numerical methods preserve the non-negativity and monotonicity properties of the exact solution. Our results were illustrated by numerical experiments. We also investigated an epidemic model with spatial dependence and analysed its stability and numerical approximation. It turned out that under biologically reasonable assumptions, a unique and qualitatively well-behaving solution to the problem exists, whose properties are also preserved by the high-order numerical solution using a well-chosen timestep.

2. Other related results

In this section, we present our results that are indirectly related to the main topic of our project and can be used mostly as a tool for mathematical investigation of epidemic spreading processes. At the same time, we emphasize that these results reflect a general approach and are therefore important in their own right in a number of other areas.

For the qualitative properties of ODEs and their numerical solutions we analysed certain systems of ODEs for some characteristic properties, like conservation of the energy, the phase space volume and the symplectic structure. We investigated Lotka—Volterra systems and were also interested in the analysis of the effect of operator splitting techniques to the symplecticness of the numerical methods. We gave conditions which guarantee that the combination of the Euler method and the symplectic Euler method forms a symplectic numerical method again. For the PDEs our goal was to extend our previous investigations from linear to nonlinear problems.

We have investigated certain important qualitative properties of the numerical solutions of nonlinear parabolic PDEs. We have extended our earlier work in this topic. We have characterized various types of maximum-minimum principles on the discrete level, where we have clarified a general case of mesh operators and then proper finite element discretizations. Under suitable conditions, if the spatial mesh is non-degenerate and the time-step is chosen from an appropriate interval, then the nonnegativity preservation is satisfied, and this implies the validity of some other maximum principles. We applied our general result to the finite element solution of a special nonlinear parabolic problem.

In the investigation of the qualitative properties of one-dimensional nonlinear parabolic problems, we have turned to the more complicated case, namely to the general case of the theta-method. Here, using the theory of totally nonnegative matrices, we have given such consitions for the time step of finite different methods that guarantee the decrease of the number of the local extrimizers when time passes.

One of our research topics is the mathematical investigation of neural field models. In the early 1970s, Wilson and Cowan modelled the dynamics of two populations of excitatory and inhibitory neurons using a nonlinear system of integro-differential equations. Amari in 1977 used mathematical tools to show how these equations could be combined into one, describing the interaction dynamics of a mixed population of excitatory and inhibitory neurons.
Inspired by our earlier numerical results, we first considered the Amari model and investigated the role of delays in the spatial and temporal dynamics of the system. This single (mixed) population of neurons is distributed over a bounded, connected region whose state is described by its membrane potential. These potentials are assumed to evolve according to an integro-differential equation with space-dependent (distributed) delays. Delayed neural field models can be viewed as a dynamical system in an appropriate functional analytic setting. Therefore, we study the neural field model in the framework of an abstract delay differential equation, where the theory of dual semigroups provides a natural framework for its analysis, and we use it to study the stability and bifurcation of steady states.

On two-dimensional rectangular space domains, and for a special class of connectivity and delay functions, we describe the spectral properties of the linearized equation. We transform the characteristic integral equation for the delay differential equation (DDE) into a linear partial differential equation (PDE) with boundary conditions. We demonstrate that finding eigenvalues and eigenvectors of the DDE is equivalent to obtaining nontrivial solutions of this boundary value problem (BVP). When the connectivity kernel consists of a single exponential, we construct a basis of the solutions of this BVP that forms a complete set in L^2. This gives a complete characterization of the spectrum and is used to construct a solution to the resolvent problem. As an application, we give an example of a Hopf bifurcation and compute the first Lyapunov coefficient.

In a number of biological models, delay differential equations are more suitable to describe real-life phenomena than systems of classical differential equations. We have formulated the numerical solution with Elsgolts's method and with the Runge-Kutta method, and proved that if the time step is sufficiently small, then the solution satisfies some inherent qualitative properties of the disease propagation: such as nonnegativity, the preservation of the mass, and monotonicity in the number of the susceptible and recovered members. The results were numerically verified with test problems.

We have considered a specific scalar delay differential equation depending on a parameter, and we have verified that a saddle-node bifurcation of periodic orbits takes place as the parameter varies. These periodic solutions are of large amplitude in the sense that they oscillate about both unstable fixed points of the dynamical system.

For some delay differential equation suggested by Nazarenko we proved that under some condition the positive periodic solution oscillating slowly about the positive equilibrium is unique, and the corresponding periodic orbit is asymptotically stable. We could also determine the asymptotic shape of the periodic solution. For the limit equation of the famous Mackey-Glass equation were able to construct a homoclinic orbit, too.

We presented a new space-time discontinuous Galerkin finite element method for the approximation of the solutions of delayed integro-differential equations originating from neural field models, in particular when the delay in the system is space dependent. We provided a theoretical analysis of the stability and order of accuracy of the numerical discretization. We investigated the neural field model in the framework of an abstract delay differential equation, where the theory of dual semigroups provides a natural framework for their analysis. One of our goals was to use it for the investigation of stability and bifurcation of steady states. The main idea is to transform the integral (characteristic) equation to an equivalent boundary value problem and solve it using partial differential equation tools.

We have also investigated in detail a neural field model with transmission delays on a rectangular domain, with a connectivity kernel that is a single exponential. This PDE can be separated into two differential equations of Sturm-Liouville type. We constructed a basis of solutions to these differential equations that is complete in L^2. These basis functions allowed us to determine whether a point in the complex plane belongs to the spectrum.

In one of our works we extended the results on neural fields with transmission delays on spherical domains in several directions: we considered two distinct populations of excitatory and inhibitory neurons, similar to the models of Wilson and Cowan, in contrast to the effective single population model of Amari and we added a diffusion term to model gap junctions. We also extended the analysis of Hopf bifurcations with spherical symmetry, in particular by studying the equivariant normal forms. In addition, this work extends the methods for numerical simulations of delay neural fields on the sphere to include two populations and diffusion.

We investigated the local bifurcations leading to oscillatory behaviour in a distributed dynamical system with local and non-local interactions, caused by intrinsic dynamics, diffusion, and propagation delays. While the general strategy to study such phenomena is well-known and is based on the center manifold reduction and the computation of the normal forms, its actual implementation in the presence of spherical symmetry proved to be rather involved and non-trivial.

We considered weak solutions of boundary value problems for quasilinear elliptic equations, containing non-local terms (e.g., integrals of the unknown function). Several type of such equations were shown which have several solutions. Then we constructed similar nonlinear parabolic equations (with zero initial and boundary condition) and systems of nonlinear elliptic equations (with zero boundary condition).

We have established new results on the qualitative properties of the numerical solutions of parabolic PDEs. The preservation of certain properties, such as nonnegativity and maximum principles, represents an important measure of the qualitative reliability of both the studied model and the numerical method. We have extended the characterization from parabolic PDEs to the discrete level. First we revealed the relations and gave sufficient conditions for the main qualitative properties of general and two-level discrete mesh operators, then we applied this to the FEM solution of nonlinear parabolic problems. The results cover various reaction-diffusion models.

Neural field equations are also models that describe the spatio-temporal evolution of (spatially) coarse grained variables such as synaptic o rfiring rate activity in populations of neurons. We considered a single population of neurons, distributed over some bounded, connected region, whose state is described by their membrane potential. These potentials are assumed to evolve according to the integro-differential equation with space-dependent delay. The spectrum can then be characterized by the non-trivial solutions of this boundary value problem. The solution is, however, nontrivial in the most general case. The main result is that we could give a complete description of the spectrum and resolvent when there is a single exponential in the connectivity, modeling a population with only inhibitory neurons.

Neural fields serve as useful models for understanding the macroscopic spatio-temporal behaviour of the brain, which can be measured by an electroencephalogram (EEG). Synchronised waves of neural activity observed in patients with Parkinson's disease have been linked with an increase in gap junctions, electrical connections in the brain. Neural fields offer a natural way to study this link. Earlier works considered neural fields on an interval and a rectangle. However, on finite domains, boundary conditions play a critical role in pattern formation in neural fields, therefore a spherical domain is a more natural topology when considering activity in the brain.

Weak solutions of initial-boundary value problems for semilinear and nonlinear parabolic differential equations with certain nonlocal terms were considered.

Theorems on the number of solutions were proved; further, some qualitative properties of the solutions at infinity were shown. The proofs are based on fixed points of real functions and operators, respectively, and on existence-uniqueness theorems on partial differential equations, without functional terms.

We considered general first and second order evolution equations in $(0,\infty)$ with functional (nonlocal) terms, based on the theory of monotone operators. In the case where the nonlocal terms are operators of Volterra type, existence and uniqueness of the solution was proved; with terms without the Volterra property, existence of multiple solutions was shown.

We have carried out a study of iterative methods for elliptic PDE-constrained optimization problems in optimal control. These methods use the special block form of the finite element system. We have given a summary of suitable preconditioners including block diagonal and more general forms, with applications to distributed elliptic control problems, box constraints and also time-harmonic parabolic equations.

We intensively worked on iterative methods for the finite element (FEM) solution of elliptic PDE problems. We have studied Krylov type improvements of the Uzawa method for Stokes-type operator matrices, and in particular, we have derived superlinear convergence of the iteration in Sobolev space in the case of smooth domains. We achieved new results for the preconditioned iterative solution of variable-coefficient Helmholtz equations, motivated by acoustic problems. We have extended earlier theoretical results on superlinear convergence and started to run computer tests in a collaboration.

We have considered the analysis of superlinear convergence for elliptic PDEs in order to find the magnitude of the superlinearity as a power order function of the integrability of the coefficients. These result were first proved for the case of scalar equations and underlined with numerical tests. Then we extended our estimates for Newton-Krylov methods for nonlinear elliptic problems, where the superlinear convergence of the inner iterations has been studied in the solution process for the inner iterations.

We have studied iterative methods for nonlinear elliptic problems, too. We have extended variable preconditioning from uniformly elliptic PDE problems with stronger nonlinearities, allowing power order growth. These are methods of quasi-Newton type. Numerical tests underline the theoretical estimates. We have continued our work on iterative methods for the finite element (FEM) solution of nonlinear elliptic problems. We have extended the variable preconditioning approach in quasi-Newton context from uniformly elliptic nonlinear PDEs to problems with stronger nonlinearities, using an extension of our previous Hilbert space theory to suitable Banach space background. We have proved the convergence of the method for problems allowing power order growth and with lower non-uniformities, allowing its application to power-law type PDEs such as stationary quasi-Newton fluids or minimal surfaces. Numerical experiments have fully reinforced the theoretical convergence estimates. We have also developed Sobolev gradient preconditioning for nonlinear elliptic reaction–diffusion problems with nonsmooth nonlinearities, where a quasi-Newton approach is not applicable. We have constructed a linearly implicit scheme, and we have shown that it satisfies the maximum principle under generally mild restrictions on the time-step. In particular, it preserves nonnegativity of the solution, which is relevant in problems arising in physical or chemical models such as reaction-diffusion processes.

We have developed a variable-coefficient shifted Laplace preconditioner for the iterative solution of heterogeneous wave propagation problems, modeled by Helmholtz equations with nonconstant coefficients. Based on the compactness of the arising operator, we have derived robust superlinear convergence and estimated its speed. Computer realization is under development in a collaboration. Further, we have investigated numerically the phenomenon of dead cores with free boundaries arising in nonlinear stationary reaction–diffusion problems with non-Lipschitz nonlinearities. We have developed a theoretical background for the finite element discretization and iterative solution of such problems, and we have run numerical experiments for various situations in order to explore the existence and the possible shape and other geometric properties of the dead cores. We have also studied 3-dimensional nonlinear stationary heat conduction problems arising in cooling processes via radiation. In this case a nonlinearity occurs on the boundary. We have constructed a quasi-Newton method in the proper function space, in which one can spare computational cost by applying variable preconditioners from precomputable parts. We have carried out numerical experiments using trilinear FEM, and the reduced computational cost has been reinforced.

As an important application, the Gao type beam models involving a geometrical type of nonlinearity with respect to the Euler–Bernoulli hypothesis was considered. We have constructed a quasi-Newton iteration and compared its performance to the gradient iteration and full Newton's method. Further, we described this approach for a wide class of nonlinear nonuniformly monotone elliptic problems imposed in Banach spaces, allowing more general nonlinearities. Finally, we extended the above results to fourth order problems arising in the deformation theory of elastic plates, and ran numerical experiments with coupling this approach to the Fourier solution of the linearized problems.

We have carried out an extensive study of quasi-Newton methods for nonlinear 3D problems arising in elasto-plasticity. We have constructed proper variable preconditioners and proved the convergence of the arising iteration. Then we have shown that the overall runtime of the quasi-Newton iteration can be smaller than that of the full Newton linearization for various possible values of the problem and mesh parameters.

We have investigated two special qualitative properties of the finite difference solutions of one-dimensional nonlinear parabolic initial boundary value problems. We have generated the numerical solution of this problem with the implicit Euler finite difference method and have shown that the obtained numerical solution satisfies the discrete versions of the above properties without any requirements on the mesh parameters.

We investigated a new type of convergence (the discrete C1 convergence) of linear multistep methods (LMM) and we proved that strongly stable LMMs converge wrt. to the discrete C1-norm, moreover the order of convergence is the same as their order of convergence wrt. the max-norm, under some assumptions about the initial values. We also investigated weakly stable LMMs and the importance of the assumption about the initial values.

Strongly and weakly stable linear multistep methods (LMMs) are usually compared from a qualitative point of view, namely, weakly stable LMMs may (spuriously) oscillate in some situations, while strongly stable LMMs behave correctly. We showed that weakly stable LMMs may lose (depending on the choice of the starting values) one order if we measure the converge in the discrete C1-norm, while strongly stable methods are unaffected.

In the investigation of the qualitative properties of one-dimensional nonlinear parabolic problems, we have considered the general theta-method. We have given sufficient conditions that guarantee the decrease of the number of the local extremizers and the number of the sign-changes of the solution on the parabolic boundary. We have extended the investigations to finite element methods.

We conducted research on the Richardson extrapolation, which is a powerful tool to enhance the accuracy of time integration methods. The classical Richardson extrapolation consists in a linear combination of the numerical solutions obtained by two different time-step sizes. This procedure can be generalized by combining more than two numerical solutions by suitable weights, which leads to the method of repeated Richardson extrapolation. We investigated the accuracy and absolute stability of the several-times Repeated Richardson Extrapolation for explicit and implicit Runge-Kutta methods as underlying numerical methods. We applied the Richardson extrapolation both in time and space to enhance the accuracy of the Crank-Nicolson method when applied to the advection equation. We investigated two possible generalizations of the classical Richardson extrapolation (RE), the repeated and multiple Richardson extrapolation methods for the solution of ordinary differential systems. We developed an algorithm for applying the repeated Richardson extrapolation (RRE) in an adaptive way during the time integration of ordinary differential equations. This algorithm chooses the version of the RRE and the time-step size in each time-step on the basis of an inner error estimation. The proposed variable stepsize-variable formula method was tested on a three-parameter test example as well as on the chemical submodule of the Danish Eulerian Model. A thorough consistency analysis was given for the classical Richardson extrapolation when the underlying method is a first, second or third order Runge-Kutta method. We applied the classical Richardson extrapolation

(RE) technique to accelerate the convergence of sequences resulting from linear multistep methods (LMMs). The advantage of the LMM-RE approach is that the combined method possesses higher order and favorable linear stability properties in terms of A- or A(α)-stability, and existing LMM codes can be used without any modification. This research can be useful in neural network approach for epidemic modeling since one may use parallel methods like LMM-RE.

We also considered the heat transfer problem in a solid body with temperature-dependent thermal conductivity that is in contact with a tank filled with liquid. We proposed a one-dimensional mathematical model that consists of a nonlinear PDE for the temperature along the solid body, coupled to a linear ODE for the temperature in the tank, the boundary and the initial conditions. To solve the transient problem, a nontrivial numerical approach is proposed whereby the differential equations are first discretized in time. This reduces the problem to a sequence of nonlinear two-point boundary value problems (TPBVP) . This problem was succesfully solved by our new method (Fourier-Legendre).

In the study of the population dynamics of the Easter Island we turned to spatially continuous models from the discrete ones. We investigated spatially two-dimensional models given in the form of systems of partial differential equations with homogeneous Neumann boundaries. Besides the usual dynamics between the people, rats and trees, we also added diffusion terms to the equations that account for the motion of the individuals. We showed that only one nontrivial stationary point exists. We proved that the diffusion of the trees stabilizes the system. The theoretical results were verified on numerical test problems.

We investigated inverse problems for Schrödinger operators on connected equilateral graphs. On each edge there is a Schrödinger equation with an unknown integrable potential; these equations are linked in the vertices with standard matching conditions. The graph G consists of at least two odd cycles glued together at a common vertex. We proved an Ambarzumian type result, i.e., if a specific part of the spectrum is the same as in the case of zero potential, then the potential has to be zero.

In the joint research with our Slovenian partners we worked in a slightly different directions, too. We considered the nonlinear Schrödinger equations solved on the hyperbolic space. This investigation was motivated by the large number of applications of the eigenvalue problem for the Laplace-Beltrami operator in the hyperbolic framework. In our general equation with the Laplace-Beltrami operator, we assumed that a nonnegative nontrivial radially symmetric potential is present and that the nonlinear term on the right-hand side satisfies a special growth condition and an asymptotic condition. By the use of the Palais principle of symmetric criticality, and suitable group theoretical arguments, we have established the existence of a nontrivial (weak) solution.

In other work we considered some nonlinear problems with unbalanced growth. We were interested in the mathematical analysis of standing wave solutions of some classes of Dirichlet boundary value problems driven by nonhomogeneous differential operators. This potential produces the (p, q)-Laplace operator, which generates a “double-phase energy” and lack of compactness. We established existence and non-existence results and related properties of the solutions. Our analysis combined variational methods with the generalized Pucci–Serrin maximum principle.

We compared the stability preserving properties of the Lie–Trotter, Strang–Marchuk, and symmetrically weighted sequential splitting schemes for a simple 2-dimensional linear system. We found that the stability region has a fingered structure. We provided estimates for the thickness of the stability fingers as well as the gaps between them. Counterintuitively, both the thickness and the size of gaps grow with decreasing the splitting time step.

We analysed the operator splitting procedures from a theoretical point of view. We showed that the abstract operator theoretic (general) Trotter-Kato formulae yield the convergence of numerical methods used for solving differential equations. These methods combine operator splitting procedures with certain time discretisation schemes which should be consistent, strongly A-stable, positive rational approximations of the exponential function. We also showed that it is possible to apply more numerical steps in one splitting time step and the convergence results remain true.

We studied operator splitting procedures for a certain class of coupled linear abstract Cauchy problems, where the coupling is such that one of the sub-problems prescribes a "boundary type" extra condition for the other one. We proved the convergence of splittings along with error bounds under fairly general assumptions. Numerical examples showed that the obtained theoretical bounds can be computationally realised. As a continuation, we derived a numerical method based on sequential splitting to abstract parabolic semilinear boundary coupled systems. The method decouples the linear components that describe the coupling and the dynamics in the abstract bulk- and surface-spaces, and treats the nonlinear terms similarly to an exponential integrator. We derived a precise error analysis, and showed the novel method's convergence rate. We also presented numerical experiments reporting on convergence rates, which included problems with dynamic boundary conditions, too.

We applied a Magnus integrator to quasilinear Cauchy problems with time delay first defined on finite dimensional space, then on a general Banach space. In both cases, we showed the appropriate conditions under which the method introduced is convergent of second order. Moreover, we showed the existence of invariant sets, especially, the positivity preservation of the method. As an example, we treated the space-dependent epidemic model which takes into account the random movement of individuals, the effect of the vaccination, and the latent period as time delay. We proved that this model satisfies the condition of the second-order convergence, moreover, preserves the positivity and the total population. Besides the results concerning the approximate solution, we also gave sufficient conditions to the existence, uniqueness, and regularity of the analytical solution to the quasilinear delay equation.

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