Final report on the research project K 112157

The work of our group has produced the expected results in the research period. The proposed ideas and approaches, including operator methods, have been used in several different situations for various nonlinear problems. Both numerical efficiency and qualitative properties have been studied, general and extended models have been involved, and several applications have been considered. Our work has resulted in 46 refereed publications.
Compared to the research plan, an important portion of new work has been added involving applications to biological models, motivated by our collaborations.
Partial change in participants and its effects. PhD student G. Csörgő left the group after his PhD studies and started work at a company. In spite of his missing part of work in subdiffusive problems, this subtopic has been completed essentially as expected. B. Kovács moved abroad after getting a postdoc position and was involved in other research there, but he could still contribute to our planned work and papers, including two in Q1 journals.

I. Detailed description of the research results

1. Numerical methods for elliptic problems using operator-based iterations

We have elaborated and analysed iterative methods for the finite element (FEM) solution of various elliptic problems, motivated by real-life models. These problems include both linear and nonlinear ones. The linear cases may serve as subproblems in an outer nonlinear iteration, moreover, studied on their own for linear models, the phenomenon of superlinear convergence of Krylov iterations has been proved in several situations.

Variable preconditioning, Sobolev gradients. We have extended the variable preconditioning approach in quasi-Newton context from uniformly elliptic nonlinear PDEs to problems with stronger nonlinearities, allowing power order growth, using an extension of our previous Hilbert space theory to suitable Banach space background. Numerical experiments have fully reinforced the theoretical convergence estimates.
We have also proved the convergence of the method for problems with lower non-uniformities, allowing its application to power-law type PDEs such as stationary quasi-Newton fluids or minimal surfaces.
We have developed Sobolev gradient preconditioning for nonlinear elliptic reaction–diffusion problems with nonsmooth nonlinearities, where a quasi-Newton approach is not applicable.

Robustness w.r.t parameters. We have considered convection-dominated problems using the streamline diffusion FEM stabilization and proper CG iteration. Thereby we have extended the operator preconditioning approach and have derived robust estimates and parameter independence of the convergence.
We have also investigated preconditioners for regularized saddle point problems, and obtained convergence rates independently of material parameters for heterogeneous Darcy flow problems.

Superlinear convergence. We have studied solvers for interior Helmholtz equations, which arise as an important model in acoustic wave propagation. Using shifted Laplace preconditioning operators, we have proved superlinear convergence of Krylov iterations for the preconditioned problem and its mesh-independence under FEM discretizations. This work is carried out in collaboration with Owe Axelsson (Ostrava, AS CR) and Frederic Magoules (Université Paris-Saclay): during visits in Paris, we have numerically investigated acoustic

problems in the compartment of a car and in the interior of an auditorium, respectively. We then extended these ideas to a proper saddle-point formulation using block preconditioning.
We have also investigated iterative methods for PDE-constrained optimal control problems. The constraint described by a PDE leads to a special block form, similar to a saddle-point system, in the FEM approximation. The applications range from distributed elliptic control problems to time-harmonic parabolic equations. We have proved mesh-independence superlinear convergence under various types of constraints.

Finite differences. We have also studied error estimates for finite difference matrices arising from discretized elliptic problems. We have shown that the bounds in maximum norm can be extended to convergent operator splittings of the difference matrix. Here also the discretized Helmholtz equation was used to test the error bounds.

2. Numerical methods for nonlinear parabolic problems

(a) Construction of numerical methods

We have constructed a general numerical method for a class of nonlinear transport type problems. We have extended our earlier method to problems with mixed boundary conditions and localized interface conditions. Our approach involves implicit time discretization and FEM space discretization, and then the crucial part is the introduction of uncoupled linear preconditioning operators on the elliptic levels. An important type of such problems arises for systems modelling air pollution, which may involve a huge number of coupled equations: in contrast, our preconditioning steps include uncoupled single equations.

(b) Qualitative properties of continuous and discrete models

We have established new results on the qualitative properties of PDEs and, motivated by these, on their analogues for the numerical solutions. The preservation of certain properties, such as nonnegativity and maximum principles, represent an important measure of the qualitative reliability of both the studied model and the numerical method.

Qualitative properties of PDEs. Our main interest has been to give a characterization of the connection of various qualitative properties of parabolic problems, including discrete nonnegativity, various discrete maximum principles, contractivity properties for second order nonlinear problems with general boundary conditions.
First we studied single equations. The achieved characterization is an extension of earlier results on linear parabolic operators with Dirichlet boundary conditions. We also gave sufficient conditions that guarantee the qualitative properties. This research was carried out in collaboration with S. Korotov (Bilbao-Bergen).
Then we extended the characterization from a single equation to cooperative systems with diagonally dominant coupling. We have also included the case of mixed boundary conditions. The nonnegativity preservation property, motivated by the reliable description of the underlying physical processes, has been derived e.g. for cross-catalytic stationary reaction-diffusion systems in chemistry.

Qualitative properties of numerical solutions. First, we extended the parabolic discrete maximum principle for problems with non-monotone coupling in the lower order terms. We also derived a discrete maximum principle for a class of nonlinear elliptic problems, allowing

possible degeneracy motivated by various applications. This was a starting point for the nonstationary (parabolic) case.
Then we proved the analogues of the previously mentioned 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.

3. Numerical solution of extended models

(a) Fractional diffusion problems

We have investigated the numerical solution of space-fractional elliptic diffusion problem. First, for the case of no-flux boundary conditions in one space dimension, we established the convergence of a corresponding discretization using a reflection principle. Later, as a major result, we developed a convergence theory for the finite element discretization for the fractional Dirichlet Laplacian. Also, the finite difference discretization was investigated for space-fractional diffusion and again a quasi-optimal convergence order was established, which was expected by many practitioners. The corresponding technical method uses of results on the approximation of Laplace eigenvalues. Having these results and studying the recent achievements of this hot topic and the existing vast literature on fractional differentiation, we compared the corresponding mathematical equations from the modeling point of view. Here we pointed out the favor of using fractional Laplacian operators compared to other approaches.

In all discretizations, we made use of the so-called matrix transformation technique, i.e., we applied the power of the (finite element or finite difference) discretization of the Dirichlet Laplace or Neumann Laplace operator. We established a method to compute matrix power-vector products efficiently with a high precision. On this solid background, the results were extended to arbitrary time discretizations (rather than Crank—Nicolson and implicit Euler).

Realizing the popularity and the practical aspects of this research area, we organized a minisymposium on this topic at the 20th ECMI conference, where a number of recent results and research directions could be discussed. An interesting application for stabilization of fluid dynamical simulations was also presented.

(b) PDEs on surfaces

Motivated by the connection of our group to the work on surface PDEs in Tübingen, we have studied the validity of the discrete maximum principle for nonlinear elliptic PDEs on surfaces with boundary. We have verified for a wide class of such problems that the acute angle condition, arising in Euclidean problems, is also able to ensure the validity of the DMP for the surface PDE.

4. Applications in biology

We have also achieved several results in numerical population dynamics. This research, due to its special topics, attracted a lot of interest at conferences, moreover, we have got several e-mail requests. We collaborated with Michael Radin (Rochester Institute of Technology, New

York, USA) and we had contact with e.g. Ivan Cheltsov (University of Edinburgh, UK) and Ashok Krishnamurthy (Mount Royal University, Canada).

(a) Spatial epidemic models in disease propagation

Most of the models of epidemic propagation are so-called compartmental models: they do not consider the spatial distribution of the individuals, but only give the temporal value of the number of the infected (I), susceptible (S) and recovered (R) members. Of course, the knowledge of the spatial dependence can be highly important, it can facilitate the intervention into the processes. We have recently investigated the possible spatial extensions of the classical SIR models and their qualitative properties.

Main extension directions. The first possible extension uses Kendall's method by forming a system of integro-partial differential equations (shortly IPDE model, where we assume that the infection is localized and comes from a certain neighborhood of the susceptible individual), and the other one introduces some diffusion terms (shortly DPDE model, where the individuals assumed to move according to some diffusion rules). The investigated properties were the nonnegativity, the monotonicity and the local mass conservation properties, moreover, we also studied the condition of an epidemic wave solution.

One spatial dimension. We started the investigation on 1D discrete one-step IPDE models (that can be considered also as full discretizations of continuous models.) We gave conditions for the time-step parameter and the mesh size that guarantee the above qualitative properties a priori. We have found that if the wave front of the infectives has a strictly concave decreasing part in the direction of the motion, the time-step is sufficiently small and the density of the susceptibles is sufficiently large (we have exact expressions for the bounds) then the wave of the infectives (the epidemic wave) is not able to move. This statement can be applied to plan the vaccination of the population.

Higher spatial dimensions. Two or three dimensional epidemic models are more realistic than one-dimensional ones, hence we extended our results for such problems. Here again sufficient conditions were given that imply the validity of the qualitative properties. The DPDE models were investigated a priori in the general d-dimensional case and similar sufficient conditions were deduced. All results have been verified on test problems.

(b) Population dynamics

Preliminaries. Several theories have been constructed in the last decade to explain the ecological collapse of the Easter Island. The recent model was a system of ordinary differential equations, which describes the change of the number of people, rats and trees in some 1D subregions of the island. The movement of the human and rat populations was described by some diffusion parameters and it was shown that the increase of the diffusion parameters of people and rats makes the system unstable.

The effect of diffusion. By introducing a diffusion parameter for the tree population, we have shown that this parameter has a stabilizing effect. We have also investigated the above model with some other modifications, namely, when the amount of the rats is decreased due to some extermination. This newly added factor improves the stability property of the model and the system has a conditionally stable equilibrium point. Then we formulated a more realistic 2D ODE model. We found that a stable equilibrium can occur for some parameter values, but the ecological catastrophe is also possible.

PDE formulation. We transformed the above spatially discrete model to a continuous one, that is to a system of PDEs with homogeneous Dirichlet or Neumann boundaries, and also added diffusion terms to the equations that account for the motion of the individuals. We showed that, similarly to the discrete case, only one nontrivial stationary point exists. Moreover, large enough diffusion of the trees stabilizes the system. The theoretical results were verified on numerical test problems, where we used the FEM, here we investigated the effect of the model parameters, including the possible extinction of the trees.

(c) Tumor growth

The growth of normal and abnormal tissues can be modelled mathematically by nonlinear systems of partial differential equations, called cross-diffusion systems. We have investigated the dynamics of such systems. We showed the existence of a periodic stationary solution for proper positive initial data. The other choices of the parameters were investigated by numerical models. We also analyzed the stability of the stationary solutions. This result was a joint work with R. Kersner and M. Klincsik from the University of Pécs.

5. Investigation of first-order time-dependent problems

(a) Stability and consistency theory

We have extended our stability investigations when it is not possible to prove strictly some desirable stability, such as A-stability or L-stability, of the considered numerical method. It is still worthwhile to use it if we can show that its absolute stability region is sufficiently large. We have applied this approach for two extrapolated Runge–Kutta methods. We have also investigated discretization methods for nonlinear operator equations written as abstract nonlinear evolution equations. Motivated by the rational approximation methods for linear semigroups, we proposed a more general time discretisation method and prove its N-stability as well.

(b) Multistep methods

Zero stability. We have studied zero stability of linear multistep methods (LMMs) in case of variable stepsize methods in collaboration with Professor Söderlind (Lund University, Sweden), who is the leading expert in numerical analysis for adaptive temporal numerical methods. In order to be convergent, LMMs must be zero stable. While constant step size theory was established in the 1950's, zero stability on nonuniform grids is less well understood. Here we investigated zero stability on compact intervals and smooth nonuniform grids. In practical computations, step size control can be implemented using smooth (small) step size changes. The resulting grid can be modeled as the image of an equidistant grid under a smooth deformation map. We showed that, given any strongly stable LMM, the method is zero stable for sufficiently many grid points provided that the deformation map is smooth enough. Thus zero stability holds on these nonuniform grids.
This collaboration between I. Faragó, I. Fekete and G. Söderlind led to the extension of the published project with Miklós Mincsovics. In the previous project, we addressed this problem using a Toeplitz operator representation, showing that any strongly zero stable method remains stable for the test problem provided that the grid is smooth. In our ongoing project we work on the extension of the result to prove that the method applied to a nonlinear problem is also convergent on every smooth grid on compact intervals in the classical situation.

Stepsize control. We have also studied the estimation of the local error and control by using linear control theory for the step size for adaptive LMM. The classical asymptotic error model is based on the constant step size analysis, where all past step sizes simultaneously go to zero. This does not reflect actual computations with LMMs, where the step size control selects the next step based on error information from previously accepted steps and the recent step size history. In variable step size implementations the error model must therefore be dynamic and include past step ratios, even in the asymptotic regime. We have derived dynamic asymptotic models of the local error and its estimator. They enable the use of controllers with enhanced stability, producing more regular step size sequences.
The relevance of this has been established by the invited speaker invitation of I. Fekete for the 9th congress "The International Congress on Industrial and Applied Mathematics" in 2019.

6. Investigation of time-dependent problems with operator splitting and extrapolation

(a) Operator splitting and symplectic integration

We focus on systems of ODEs having some characteristic properties, such as conservation of the energy, the phase space volume and the symplectic structure. We investigated Lotka—Volterra systems that conserve the energy and have the interesting property: every solution of the system lies on a closed curve. Naturally, it is important to investigate this symplectic property also for the numerical methods of such systems. We were interested in the analysis of the effect of the operator splitting techniques to the symplecticness of the numerical methods. In operator splitting techniques we split the original problem into subproblems and this subproblems are solved cyclically after each other. We gave conditions that guarantee that the combination of the Euler method and the symplectic Euler method forms a symplectic numerical method again. We verified our results on test problems.

(b) Applications of operator splitting

We have successfully applied operator splitting techniques to improve the accuracy of multi-scale Lithium-ion (Li-ion) battery models. A slightly simplified Li-ion battery model has been derived, which can be solved on one time scale and multiple time scales. Different operator splitting schemes combined with different approximations have been compared with the non-splitted reference solution in terms of stability, accuracy and processor cost.

(c) Richardson extrapolation

Richardson extrapolation is a very powerful tool to increase the order of some convergent numerical method. In the classical setting this happens by combination of the numerical results obtained on two different meshes. We have introduced the new approach when the interpolation is based on more than two meshes. This method is called as repeated Richardson extrapolation (RRE). We investigated the different properties of RRE with using different (explicit and implicit) numerical methods in the basic algorithm. We have considered absolute stability investigations when the absolute stability region is sufficiently large. We have applied our approach in the case where the active implementation of the Richardson Extrapolation is used together with particular implicit Runge–Kutta methods. Numerical examples, which were done for real-life problems (like large air-pollution process) confirmed the theoretical results. This work was done in collaboration with Aarhus University (Denmark) and Institute of Information and Communication Technologies of Bulgarian Academy of Sciences.

II. Publications

We have produced 46 refereed publications in the project period, including 3 book chapters. See details in the list of publications on the project homepage:
https://www.otka-palyazat.hu/?menuid=514

III. International contacts and cooperations

We have carried out our research in various ongoing and new cooperations, including joint work, mutual visits and co-organized workshops etc.

Our work on iterative methods is carried out in a long-run collaboration with Owe Axelsson (Ostrava, AS CR), and on Helmholtz equations it also includes Frederic Magoules (Paris, Central Supélec), with whom we have done high-performance computer experiments in Paris. In the area of Richardson extrapolation we cooperate with Zahari Zlatev (Aarhus University) and Ivan Dimov (Institute of Information and Communication Technologies at the Bulgarian Academy of Sciences). We carry out joint research with the University of Chemical Technology and Metallurgy in Sofia on shooting-projection methods for two-point boundary value problems, and on adequate iterative methods with the North-Eastern Federal University, Yakutsk (P. Vabisevich, V. Vasilev). We collaborate with Michael Radin (Rochester Institute of Technology, New York, USA) on the Easter Island model. Within a joint OTKA project we started to collaborate with Dušan D. Repovš and Vicentiu D. Radulescu (University of Ljubljana) on the topics of nonlinear PDEs.
Regarding ODE solvers, we continue our work on linear multistep methods with our co-author Gustaf Söderlind (Lund University, Sweden), and on strong stability preserving methods with Sidafa Conde and John N. Shadid (both Sandia National Laboratories, USA). The work with G. Söderlind has been more recently extended to Carmen Arévalo (Lund University, Sweden) and Yiannis Hadjimichael (Hungarian Academy of Sciences) starting with their stay in Budapest. The joint projects led to a co-supervised PhD project of G. Söderlind and I. Fekete on the computational issues of adaptive LMMs from September 2019.

We organized a joint Basque–Hungarian workshop in Bilbao in 2015, where we also gave survey talks on our results. Further, we organized two joint workshops (2017 and 2019) with the Western Norway University of Applied Sciences in Bergen, with title “Bergen-Budapest Workshop on Qualitative and Numerical Aspects of Mathematical Modelling”. These provided a forum to discuss mutual research interests for mathematicians from various Norwegian and Hungarian institutes, and also from some other countries.

We have presented our results in several other international conferences. In particular, based on our close contacts with ECMI (European Consortium for Mathematics in Industry), we have taken part in the organization of the 20th European Conference on Mathematics for Industry, held in Budapest in 2018, including memberships in the Scientific and Organizing Committes, organizing minisymposia and giving several talks.