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**UNIVERSITÀ
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Scientific Program - Timetable

Sun day 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15 30 45		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	10:15 30 45	Registration		von Mises prize lecture		
	11:15 30 45		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	12:15 30 45		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	13:15 30 45		Lunch	Lunch	Lunch	
		Opening				
		Univ. Chorus Performance				Closing
	14:15 30 45	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	15:15 30 45	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
Registration pre-opening	16:15 30 45	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	17:15 30 45	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	18:15 30 45		Public lecture Francesco D'Andria			
	19:15 30 45	Opening reception at Castle of Charles V				
	20:15 30 45			Conference dinner at Hotel Tiziano		
	21:15 30 45					

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S18: Numerical methods for differential equations

For all fields of applications the mathematical models are primarily based on differential equations. Hence, their numerical solution plays a fundamental role in numerical mathematics. This section covers mainly the construction and the behavior of numerical methods for differential equations including those of ordinary as well as of partial differential type.

Well-Balanced, Entropy Stable Discontinuous Galerkin Spectral Element Method for the Shallow Water Equations

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This contribution presents an arbitrary high-order accurate nodal discontinuous Galerkin spectral element type method for the one dimensional shallow water equations with a non-constant bottom topography

$$\begin{aligned}\frac{\partial h}{\partial t} + \frac{\partial(vh)}{\partial x} &= 0, \\ \frac{\partial(vh)}{\partial t} + \frac{\partial(v^2h + gh^2/2)}{\partial x} &= -gh \frac{\partial b}{\partial x}.\end{aligned}$$

Here, h is the height of the water and v is the velocity. The constant g is the acceleration due to gravity and the function $b = b(x)$ represents the bottom topography of the surface over which the fluid flows. The method uses a skew-symmetric formulation of the continuous problem in combination with a special numerical flux at element interfaces to exactly preserve the entropy, which is also the total energy for the shallow water equations [1].

A problem with entropy conservative formulations is they may suffer breakdown if used without dissipation to capture shocks. Physically, entropy must be dissipated at a shock. However, an isentropic algorithm does not allow the capture of this physical process, which results in the generation of large amplitude oscillations around the shock [2]. Another dire issue is that entropy conservative formulations can not converge to the weak solution as there is no mechanism to admit the dissipation physically required at the shock. We use entropy analysis techniques in the context of DG approximations to remedy any stability issues of entropy conservative schemes. We derive a minimal dissipation term to add at grid cell interfaces and stabilize the approximation. This dissipation term is the minimum required for stability, it does not and is not designed to eliminate overshoots near shocks.

Of particular importance for numerical approximations of the shallow water equations is the well-balanced property. The well-balanced property is an attribute that a numerical approximation can preserve a steady-state solution known colloquially as the “lake at rest” condition:

$$h + b = \text{constant}, \quad v = 0.$$

This steady state solution is important because relevant waves in a flow may be viewed as small perturbations of the “lake at rest,” see [3]. A good numerical method for the shallow water equations should accurately capture both the steady states and their small perturbations (quasi-steady flows). Such a property diminishes the appearance of unphysical waves with magnitude proportional to the grid size (a so-called “numerical storm”), which are normally present for numerical schemes that cannot preserve the steady-state.

Numerical tests are performed to demonstrate the theoretical findings, the high-order accuracy of the method, and the capability of the scheme to compute the solution of a rapidly varying flow over a smooth bed, and the perturbation of a stationary state.

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An Enhanced Time-Discontinuous Galerkin Method for Rotating Geometries such as Artificial Blood Pumps

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Heart failure is the main cause of death in developed countries and a heart transplant is often the only permanent medical treatment. However, the number of donor hearts is significantly lower than the number of patients in need of a transplant. Therefore, artificial blood pumps, such as Ventricular Assist Devices (VADs), are often the only alternative. State-of-the-art devices can support the failing heart for up to 5 years and can therefore function as a bridge to transplant or even as a bridge to recovery.

Computational Fluid Dynamics (CFD) has become an important development step for new VADs. It is possible to predict the hydraulic performance sufficiently with computational simulations. A change in the pump geometry can be applied easily within the simulations and its change in performance can be predicted. Therefore, CFD simulations can reduce the number of costly prototypes and experiments. The biocompatibility including hemolytic characteristics can also be estimated based on new modeling approaches [1].

Axial or centrifugal blood pumps always contain a rotating part that drives the blood flow. For time-dependent pump simulations, one has to take the mesh deformation into account, which can be done with the shear-slip mesh update method (SSMUM) [2]. With this method, we insert an update layer in the pump geometry; this layer is one element thick and created in a structured way. The update layer connects the non-moving part of the mesh with the rotating part. The elements in this layer deform with the rotation. After a certain degree of rotation, the connectivity of the mesh in the update layer is changed. This method is implemented in our in-house flow solver XNS, which is based on the time-discontinuous Galerkin finite element method. XNS is also capable of massively parallel distributed-memory simulations, which makes it suitable for the complex geometries of VADs and the high Reynolds number flows that require fine meshes.

What remained unaccounted for in the previous version of the method is that a change in connectivity between two adjacent time slabs influences the jump term that results from the discontinuous Galerkin method. The crucial step towards improved accuracy of integration is the consideration of the spatial overlap of elements from the previous and the current time slab. We will discuss the methods we use to track the elements, to compute their spatial overlap, and to handle the communication. Blood pump simulations, which are calculated using these methods, will be shown. Our results will be compared with particle image velocimetry (PIV) experimental data.

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A posteriori error estimates for IMEX schemes

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In many engineering applications physical processes acting on a wide variety of time scales need to be accounted for. One way to avoid severe time step restrictions while also (hopefully) avoiding the solution of poorly conditioned nonlinear problems in each time step is to discretize the processes acting on small time scales implicitly while those acting on slow time scales are treated explicitly. This leads to the construction of IMEX, i.e., implicit-explicit, schemes. Examples include, but are not restricted to, atmospheric flows [4] and reaction-diffusion problems [5].

While the a posteriori error analysis of implicit Runge-Kutta and discontinuous Galerkin temporal discretisations is rather well-developed, see [1] and references therein, little is known for explicit and IMEX schemes. We will use an ordinary differential equation (ODE) setting (which can be understood as a semi-discretisation of a partial differential equation) to illustrate how reconstruction techniques can be employed to obtain rigorous a posteriori error estimators for certain IMEX schemes. In the past this strategy has been used successfully for implicit temporal discretisations [1], elliptic and parabolic partial differential equations [2], and hyperbolic conservation laws [3].

The fundamental idea consists in computing a reconstruction \hat{u} of the numerical solution u_h and splitting the error between u_h and the exact solution u into an error between u and \hat{u} and an error between \hat{u} and u_h . In the example at hand the reconstruction \hat{u} is explicitly computable from u_h so that it is straightforward to account for the difference $\hat{u} - u_h$. The main reason why splitting the error as described above offers an advantage is that while u_h might be defined at a finite number of time instances only, the reconstruction \hat{u} is defined in such a way that it can be inserted into the ODE. Then the appropriate stability theory of the ODE can be used to bound the difference between the exact solution u and the reconstruction \hat{u} in terms of the residual occurring when \hat{u} is inserted into the ODE. We will derive an explicit bound for the norm of the residual and show that the error estimator obtained in this way is of the same order as the error of the numerical method itself.

This is joint work with Tristan Pryer (Reading).

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Well balanced ALE: on time dependent mesh adaptation for Shallow Water flow

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The interest in the numerical simulation of water waves on moving grids lies in the accurate calculation of wave heights during the inundation stage and consequently the correct prediction of the inundated regions. Static grids are inherently not efficient for this kind of phenomena where wave fronts cross all the domain, steepen near the coastlines and spread into the land. In this paper, with the moving mesh refinement algorithm, developed among the others by [1], we redistribute cleverly the points during the computation: it is possible to follow advancing fronts through gathering nodes in the region where the wave steepens, thus avoiding excessive numerical dissipation while remaining efficient in terms of CPU time. The sharp front is followed during all the inundation stage in order to compute accurately also the inundation region which is not known a priori and for which a static refinement results, in general, less robust, see [2]. An elegant formulation to deal with balance laws on moving grids consists in writing them respect to an arbitrary moving reference system, called Arbitrary Eulerian Lagrangian framework (ALE). Shallow Water equations are discretized by means of a Residual Distribution (RD) method in an ALE framework which follows the grid distortion. The resulting scheme is interpolation free. We show that, while RD schemes on fixed grids satisfy very naturally the Well-Balanced property, with a naive extension of the same RD scheme in ALE form this property is lost. However a simple change of variable permits to recover it. With numerous benchmarks we assess the impact of the dynamic adaptation, and more in general the adaptive ALE algorithm, in terms of level of error/CPU time, proper resolution of hydraulic jumps and ability to handle complex flows where different kind of waves interact.

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Computation of state variables of one-dimensional non-stationary pipe flow at orifices on pipe ends.

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Boundary conditions of orifices in conjunction with the graphical method of characteristics given in [1] are reformulated and made ready to be used with finite difference methods. Orifice flow to the apparent narrowest cross-section is assumed conserving entropy and energy, thereafter not recovering pressure without exceeding sound speed. These conditions allow to eliminate state variables at the narrowest cross-section. Additional equations stem from mass conservation and a balance of the Riemann variable over the outgoing cross-characteristic and either further energy conservation or a balance of entropy over the outgoing particle path. They permit to determine the state at the boundary of the computational grid for usual finite difference methods. A single nonlinear equation has to be solved only in case of outflow.

References

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An adaptive space-time discontinuous Galerkin method for Maxwell's equations

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We consider a variational Petrov-Galerkin space-time discretization of linear wave equations (acoustic, elastic or electro-magnetic waves) using discontinuous Galerkin elements with upwind flux in space and continuous Galerkin elements in time. The discretization is adaptive with independent choice of polynomial degrees p in space and q in time for every space-time cell. The discretization is fully implicit, and the overall linear problem is solved with a parallel Krylov method using a multigrid preconditioner based on a subspace hierarchy with lower polynomial degrees. The adaptivity is controlled by a dual weighted residual error estimator with respect to a given linear error functional.

We present numerical examples for 2D Maxwell's equations demonstrating the efficiency of the error estimation, the adaptive strategy, and the parallel solution process.

Tracking-type Finite-Volume Schemes for Phase Transition Problems

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Systems of conservation laws can be used to model phase transitions of different kinds. One approach to solve these equations is using classical finite volume schemes. A problem encountered when using finite volume schemes for phase transition problems is the appearance of values for which the system is not hyperbolic any more due to integral averaging. Additionally, classical finite volume schemes do not resolve undercompressive phase transitions, which are non-Laxian shock waves.

This contribution shows the generalization of the scheme from [1] to the system case as well as to multiple space dimensions. The algorithm works with a sharp-interface approach, which means that the position of the phase transition is tracked with a time dependent mesh. Therefore, averaged values from two distinct phases are avoided and one can treat phase transitions separately. To solve the Riemann problem at the phase boundary, we use Riemann solvers, which allow undercompressive shock waves. Numerical examples calculated within this framework as well as properties of the scheme, such as wellposedness and conservation of the integral will be presented.

References

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Coupling Surface and Subsurface Flows

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Coupled surface-subsurface flows appear in many environmental and industrial applications, such as spreading of a contaminant by rivers and aquifers, or transport processes in fuel cells. Therefore, appropriate models that integrate free fluid flow and porous medium flow, efficient numerical methods for such models, and analysis is needed.

In this contribution coupled surface-subsurface models, consisting of the Stokes equations or shallow-water-like equations in the free flow domain, and Darcy's law or Brinkman's equation in the porous medium, are presented. Both flow regimes are coupled at a sharp interface via physically motivated coupling conditions.

To solve the coupled model efficiently, splitting schemes are applied, which allow to use already available algorithms for each flow domain and reduce the overall computational complexity.

Numerical simulation results are presented.

Multigrid preconditioning for time-periodic Navier–Stokes problems

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In science and engineering, many problems are driven by time-periodic forcing. In fluid dynamics, this occurs for example in turbines or in human blood flows. In the absence of turbulence, if a fluid is excited long enough, a time-periodic steady state establishes. In numerical models of such flows, the steady state is computed by simulating this transient phase with a time-stepping method until the periodic state is reached. In this work, we present an alternative approach by solving directly for the steady state solution, introducing periodic boundary conditions in time. This allows us to use a multi-harmonic ansatz in time for the solution of the Navier-Stokes equation. problem formulation.

To obtain the steady state solution, a big system of nonlinear equations has to be solved, which we do by Picard iteration. We compute the Picard correction by solving a linear system with GMRES. This linear system can be written as

$$\begin{pmatrix} F & G \\ D & 0 \end{pmatrix} \begin{bmatrix} \delta \mathbf{u} \\ \delta p \end{bmatrix} = \begin{bmatrix} \mathbf{r}_u \\ r_p \end{bmatrix} . \quad (1)$$

Here, D , G , and F denote the divergence, the gradient operator, and the convection-diffusion operator, respectively. $\delta \mathbf{u}$, and δp are the velocity and pressure Picard correction containing all Fourier modes. \mathbf{r}_u and r_p are the residual vectors of the nonlinear problem. Note, that the different Fourier modes are only coupled in F , due to the nonlinearity of the convective term of the Navier–Stokes equation.

In previous work [1], a generic preconditioner was used for solving (1). In the present work, we present a new problem-specific preconditioner: a block triangular preconditioner

$$\begin{pmatrix} M_F & G \\ 0 & M_S \end{pmatrix} , \quad (2)$$

where M_S is a least squares commutator [2]. Solving with M_S amounts solving two Laplace problems of the form DG . Because the Fourier modes are not coupled in the Laplace problem, the modes can be solved in parallel.

M_F is the block diagonal of F , such that the Fourier modes are not coupled in M_F either. Thus, we have to solve a convection-diffusion problem for every Fourier mode, which can also be done concurrently. Our implementation employs the discretization and the parallelization capabilities of the well established IMPACT code [3].

We solve the convection-diffusion problems with GMRES preconditioned by a geometric multigrid using standard prolongation and restriction. Gauss–Seidel or damped Jacobi are used as smoother. The performance of the Gauss–Seidel smoother is enhanced for matrices that are close to lower triangular. This occurs, when an upwinding discretization for the convective terms is used, and the unknowns are ordered according to the convection direction. We observe sensitivity of the smoothing quality of Gauss–Seidel with regard to the numbering of unknowns depending on the convection direction.

Finally, we measure the complexity and convergence rate of our multigrid implementation, and investigate the performance of the preconditioner (2) by solving various time-periodic flow problems.

References

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Online Parameter Identification for Traffic Simulation via Lagrangian Sensing

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Macroscopic traffic simulations are based on the transport equation with a flux term governed by the speed of the flow, treating traffic as a compressible fluid. An auto-regressive model is used to solve the transport equation. We present a method to estimate model parameters based on Lagrangian measurement data that can be used for online traffic simulation. Identifiability is investigated using the Fisher Information Matrix.

In order to identify model parameters online measurement data must be collected. Two approaches are described by several authors. Commonly, Eulerian traffic data are collected by stationary loop detectors [1]. While this approach works well on highways with long sections between on- and offramps it is not ideal in urban traffic networks. The number of required stationary detectors causes relatively high installation and maintenance costs. Hence, the utilization of Lagrangian data, where the sensor moves with the flow, has recently become an area of intensive research [2]. Vehicles equipped with sensors record and transmit so-called floating car data (speed, headway, position) that can be utilized both online and offline.

The relation between driving speed and local traffic density is described by a Fundamental Diagram (FD) [3]. For simplicity the FD is generally assumed to be a convex, (linear) function with constant parameters both spatially and temporally. However, in reality these parameters may vary with environmental conditions such as weather (fog, snow, rain) and particular traffic situations (accidents, blocked lanes). For high-resolution urban traffic simulations it is therefore necessary to take the corresponding parameter changes into account.

We propose a generic FD based on a piecewise linear function, [4] that is fully defined by six parameters, which are estimated based on Lagrangian measurement data. An individual vehicle in traffic is described by an auto-regressive model where the driving speed during a time step is governed by the measured headway and the parameters of the FD. An optimization problem is formulated, where the parameters of the FD represent the decision variables, the optimization goal is to minimize the prediction error of the model. The prediction error is defined as the (mean squared) difference between the one-step-ahead-prediction and the true (measured) position of a vehicle.

Additionally, identifiability of the parameters is evaluated. The quality of the estimated parameters depends on the quality of the underlying measurement data. We use the concept of parameter sensitivity to investigate identifiability. The Fischer Information Matrix (FIM) is computed for the current set of parameters and the measurement data at hand. The singular value decomposition of the FIM provides sufficient information on identifiability. Ill conditioned singular values indicate that some parameters can not be estimated well from the data set at hand, hence, the data quality is insufficient. However, parameters that can be identified from a certain measurement data set may still be used. Utilizing both the estimated parameters found based on Lagrangian and Eulerian sensing allows for high accuracy while at the same time keeping sensor-costs low. In both cases the FIM can be utilized to determine which parameters are estimated reliably. Note here that blending algorithms must take spatial and temporal relevance into account as well.

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Robust Identification of Parametric Radiation Force Models via Impulse Response Fitting

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Hydrodynamic time-domain simulations typically use frequency-domain data in order to model radiation forces. The transformation into time-domain is based on the impulse response function method also known as Cummins Equation [1]. Due to the convolution terms in this method, the equations of motion are integro-differential equations, which are expensive to compute and unsuitable for general control purposes. In order to avoid the convolution terms, Cummins Equation can be substituted by a system of first order ordinary differential equations, a so-called state-space model. Several identification methods have been developed to obtain the state-space parameters that represent the same dynamics as the Cummins Equation [2, 3, 4]. Nevertheless, their entire application is limited to a few academic cases of low order state-space systems which is mostly due to the lacking robustness of the identification methods.

This article describes a new, straightforward and robust method to obtain state-space representations for radiation forces. In short, our method uses a prony analysis to fit the impulse response function to a state-space system of diagonal form. Particularly with regard to the robustness, this method has been found to be superior to all existing frequency-domain data identification methods.

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Numerical simulation for wine fermentation based on IDEs

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In the literature, many models, i.e. kinetic models based on ordinary differential equations and metabolic models, already exist to describe the process of wine fermentation. However, the dynamics due to yeast cell growth plays an important role in this fermentation process. This is why we take a closer look at the mass structure of yeast cells by introducing a nonlinear integro-partial differential equation for the population balance of yeast and integro-ordinary differential equations for the other substrates such as sugar, nitrogen, oxygen and the product, i.e. ethanol.

The derived model is solved numerically using a finite volume scheme for the discretization of the mass domain and BDF methods for the resulting system of time dependent ordinary differential equations.

In this context different flux approximation schemes and boundary conditions are studied.

Improving real-time capability of linearly-implicit solvers using structural information

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There is a growing demand for realtime simulation in automotive industry [1]. A significant challenge in this context is an efficient and stable solution of stiff ordinary differential equations [2]. The target of this work is to improve the real-time capability for a given benchmark model, i. e., to increase efficiency while keeping the stability and accuracy of the simulation within an appropriate limit. As linearly implicit methods provide adequate results for the benchmark problem, the approach of this work is to reduce the computational effort of the simulation by savings for the solution of the arising system of linear equations.

For this purpose, direct methods using structural information such as Schur complement are studied [3]. Beforehand the structure of the model equations is analysed and the findings are used for a preprocessing of the system. The direct solution by Schur complement is deployed to further profit by the knowledge about the model's structure. Furthermore the Schur complement is utilized to enable parallelization of the solution of the system of linear equations. The combination of structural preprocessing and direct solution by Schur complement delivers significant savings in computational cost. The results are verified by runtime measurements of implementations on a realtime simulation system.

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Interpolatory Model Reduction for Quadratic Bilinear Descriptor Systems

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A large class of nonlinear systems can be written as quadratic bilinear systems by using exact transformations [1], in addition to systems that naturally appear in the quadratic bilinear form. To simulate or control such nonlinear systems, we need to utilize model reduction techniques that construct a reduced system with a response comparable to the original system. We propose interpolation based projection techniques for model reduction of quadratic bilinear descriptor systems. The approach identifies projection matrices from the bilinear approximation of the original quadratic bilinear descriptor system and applies Petrov-Galerkin projection to the original system to construct the required reduced quadratic bilinear descriptor system. Two different techniques of computing the projection matrices from the bilinear approximation are proposed. One is based on linear parametric model reduction [2, 3] and the other is the bilinear rational Krylov method [4]. These methods can be used for model reduction of bilinear systems, however here we are considering their use for model reduction of descriptor systems with quadratic bilinear nonlinearities. The results are compared with the standard quadratic bilinear projection method [1] and it is observed that the approximations through the proposed methods are comparable to the standard method. An advantage of the proposed method is that the computations associated with the quadratic term in the construction of the projection matrices can be saved.

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A joint IMEX-MOR approach for Water Networks

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1 Introduction

The simulation of fluids within a large network of pipes poses several mathematical challenges. Typically after spatial discretization the resulting mathematical system is a nonlinear differential algebraic system. Standard techniques are often slow due to the stiffness of the equation. We will show a several step process on how to improve on the timing. A first and major step in order to achieve stable and fast simulators for these problems is what we call the decoupling step. In that step we are able to model the system as a discrete index 1 DAE. This step is only possible due to the chosen discretization we use. Next we use a combination of Model Order Reduction (MOR) methods in order to create a smaller scale index 1 Differential Algebraic Equation. And last but not least we use an implicit-explicit (IMEX) integration method to reduce the time-step for the stiff nonlinear differential equation. We will only present a simplified network here which includes pipes, reservoirs and so called demand nodes. This system will actually result in an ODE which simplifies the discussion.

2 Modeling

It is common to define a connected and directed simple graph $G = G(V, E)$ representing the pipe network. This allows a more compact representation of the model equations. The set V are the nodes and E are the edges and we will describe the different node and edge elements in the following. **Reservoirs** are water sources with unlimited capacity. Thus, we assume that they have a constant pressure $p = p_s$. Furthermore no balance equation holds at a reservoir, since an arbitrary amount of water may leave or enter the reservoir. In contrast to reservoirs, **tanks** have limited capacity. Never the less, pressure can in- or decrease even though the tank is full or empty respectively. We will not talk about tanks in more details here. A **demand node** has a given demand $q_s: I \rightarrow \mathbb{R}_+$. Thus, the difference between the amount of water flowing towards a node, and the amount of water flowing away from the node has to be $q_s: \sum q_{in}^i - \sum q_{out}^i = q_s(t)$ with q_{in}^i and q_{out}^i being the incoming and outgoing flow of edges connected to the demand node, respectively. It is possible that $q_s(t) = 0$ for all $t \in I$.

Now we will discuss the **pipe** model. The behavior of a pipe is described by a continuity equation and an equation describing the movement inside a pipe. We consider circular pipes with diameter D , cross-section $A = \frac{\pi}{4}D^2$ and length ℓ . The independent variables are space $x \in [0, \ell] := \Omega \subset \mathbb{R}$ and time $t \in [t_0, T] := I \subset \mathbb{R}$. The time dependent variables are the mass flow $m: \Omega \times I \rightarrow \mathbb{R}$ and the pressure $p: \Omega \times I \rightarrow \mathbb{R}$. The parameters a, ρ and c depend on material properties of the pipe and the gas. α is the angle of the pipe and g is the gravitational constant. With this, we get the following partial differential equation, which describes the behavior in pipes

$$\begin{aligned} \frac{\partial p}{\partial t}(x, t) + \frac{a^2}{A} \frac{\partial m}{\partial x}(x, t) &= 0 \\ \frac{\partial m}{\partial t}(x, t) + A \frac{\partial p}{\partial x}(x, t) + \rho A g \sin \alpha + c|m(x, t)|m(x, t) &= 0 \end{aligned} \quad (1)$$

Further edge elements are **valves** and **pumps**, which we also omit in this abstract.

From now on we consider a network with n_p many pipes and n_d many demand nodes and n_{rs} many reservoirs. For each pipe i , we get a flow $m_i: \Omega_i \times I \rightarrow \mathbb{R}$, $\Omega_i = [x_{L_i}, x_{R_i}] \subset \mathbb{R}$, $I = [t_0, T]$ and a pressure $p_i: \Omega_i \times I \rightarrow \mathbb{R}$ both depending on space $x \in \Omega_i$ and time $t \in I$. The node variables are $p_d: I \rightarrow \mathbb{R}^{n_d}$ and $p_{rs}: I \rightarrow \mathbb{R}^{n_{rs}}$, the pressures at demand nodes and reservoirs. We define

$$m_L(t) = (m_i(x_{L_i}, t))_{i \in \mathcal{A}_{pi}}, \quad m_R(t) = (m_i(x_{R_i}, t))_{i \in \mathcal{A}_{pi}}, \quad p_L(t) = (p_i(x_{L_i}, t))_{i \in \mathcal{A}_{pi}}, \quad p_R(t) = (p_i(x_{R_i}, t))_{i \in \mathcal{A}_{pi}}.$$

m_L being the vector with all pipe flows at their tail-node and m_R the flow vector at their head-nodes and similarly for p_L and p_R . Note, that the node pressures coincide with the head- and tail pressures of the pipes. We call the vector of demand and reservoir pressures by p .

Last we define the incidence matrices $A_R \in \mathbb{R}^{n_p \times n_d}$ and $A_L \in \mathbb{R}^{n_p \times n_d}$ for the demand nodes with

$$(A_R)_{ij} = \begin{cases} 1 & \text{if demand node } j \text{ is head of pipe } i \\ 0 & \text{else} \end{cases} \quad \text{and} \quad (A_L)_{ij} = \begin{cases} -1 & \text{if demand node } j \text{ is tail of flow } i \\ 0 & \text{else} \end{cases}$$

and A_R^{rs} and A_L^{rs} analogously for the reservoirs. We can combine them all and get the full incidence matrix $A := (A_R^{rs} + A_L^{rs} \quad A_R + A_L)$. With the help of these matrices we can write the spatial discretized system as

$$\begin{aligned} \dot{p}_R + D_\alpha(m_L - m_R) &= 0 \\ \dot{m}_L + D_\beta A^T p + \gamma + G(m_L)m_L &= 0 \\ A_R m_R + A_L m_L &= q_{set} \\ A_R p_d = p_R \quad A_L p_d = p_L \quad A_R^{rs} p_{rs} = p_R \quad A_L^{rs} p_{rs} = p_L \quad p_{rs} &= p_{set} \end{aligned}$$

To obtain these equation it is crucial to chose a suitable spatial discretization. D_α is a diagonal matrix containing $\alpha_i = a_i^2/A_i/\ell_i$ on the diagonal and D_β similar with $\beta_i = A_i/\ell_i$. γ is a vector with $\gamma_i = \rho_i A_i g \sin \alpha_i$ and $G(m_L)$ is a diagonal matrix function such that $G(m_L)_i = c_i m_L^i$. The vector q_{set} has an entry for every demand node showing the given demand at that particular node given by $q_s(t)$ and similar is p_{set} the vector of the given pressures p_s at the reservoirs.

By selecting a matrix A_{select} which picks one pipe for each node that has a right end in that given node we can rewrite the system of equation in the variables p_d and m_L .

$$\dot{p}_d + A_{select} D_\alpha (-C q_{set} + C A m_L) = 0, \quad \dot{m}_L + D_\beta A^T \begin{pmatrix} p_d \\ p_{set} \end{pmatrix} + \gamma + G(m_L)m_L = 0$$

We will explain in detail how we create the matrix C which is the crucial part in this decoupling process. This resulting ODE is of size $n_d + n_p$ and has the general structure

$$\dot{x} = T x + g(x, t) = f(x, t) \quad \text{with} \quad T = \begin{pmatrix} 0 & A_{select} D_\alpha C A \\ D_\beta (A_R + A_L)^T & 0 \end{pmatrix}$$

and the vector x is combined by p_d and m_L .

3 IMEX

In order to solve this stiff and nonlinear ODE we make use of implicit-explicit (IMEX) integration methods. This allow us to deal with the stiffness in an efficient way while not having to solve large-scale nonlinear problems. First order methods are of the flavor

$$\frac{x_{n+1} - x_n}{h} = (1 - \gamma)T x_n + \gamma T x_{n+1} + g(x_n, t)$$

for $\gamma \in [0, 1]$ and time step h . We study convergence properties of that by analyzing the matrix T and the function g as well as the differences for several values of γ . If $\gamma = 0$ we get explicit Euler and if $\gamma = 1$ we get a combination of implicit Euler for the linear part an explicit Euler for the nonlinear part. We will also show the differences within this class of methods as well as the difference to second order methods following [1].

4 Model Order Reduction

On the resulting ODE (2) we use the Model Order Reduction techniques Proper Orthogonal Decomposition (POD) together with Discrete Empirical Interpolation (DEIM) by [2]. POD is a projection-based method where we find a projection matrix W such that the solution of (2) $x \approx W \hat{x}$ for \hat{x} in a lower dimensional space. The resulting low-dimensional ODE is then given by

$$\dot{\hat{x}} = W^T T W \hat{x} + W^T g(W \hat{x}, t).$$

DEIM is then used to create a truly low-dimensional function approximating $W^T g(W \hat{x}, t)$.

The combination of POD-DEIM with the IMEX integration results in a significant speedup of simulation time.

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Upwind Based Parameter Uniform Convergence Analysis for Two Parametric Parabolic Convection Diffusion Problems by Moving Mesh Methods

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In this contribution, we consider the adaptive mesh generation of a two parametric parabolic convection-diffusion-reaction partial differential equation in singular perturbation context. These problems exhibit boundary layers for which one needs to generate layer adapted meshes through adaptive procedure (see [1]). The adaptive moving mesh algorithm which starts with a fixed number of mesh points and moves it in a way which can automatically detect the accurate locations and widths of the layers, is used for our analysis.

The following singularly perturbed two parametric parabolic initial-boundary-value problem (IBVP) is considered on a domain $\Omega = \Omega_x \times (0, T]$ with $\Omega_x = (0, 1)$,

$$\begin{aligned} \frac{\partial u}{\partial t} - \epsilon \frac{\partial^2 u}{\partial x^2} - \mu b(x, t) \frac{\partial u}{\partial x} + c(x, t)u &= f(x, t), \quad (x, t) \in \Omega, \\ u(x, 0) &= u_0(x), \quad x \in \overline{\Omega}_x, \quad u(0, t) = u(1, t) = 0, \quad t \in [0, T]. \end{aligned} \quad (1)$$

with sufficiently smooth $\beta_1 > b(x, t) > \beta_2 > 0$ and $c(x, t) \geq 1$. Here, β_k , $k = 1, 2$ are constants. The parameters $0 < \epsilon \ll 1$ and $0 < \mu \ll 1$ are known as the singular perturbation parameters. The presence of these parameters ensure the existence of the boundary layers.

The present error analysis is based on the mesh equidistribution principle [2] which starts with a error monitor function and distributes the error in a way so that each subinterval have same error measurement. In this work, we consider a curvature based monitor function $\alpha^{n+1} + \left| \frac{\partial^2 w(x, t_{n+1})}{\partial x^2} \right|$ (defined at each time step t_{n+1}), which involves the singular component $w(x, t)$ of the solution $u(x, t)$ by decomposing the solution $u(x, t) = v(x, t) + w(x, t)$. Here α^{n+1} is constant. The derivatives of $v(x, t)$ are bounded independent of perturbation parameters.

In this context, we want to note that the rigorous error analysis for time dependent problems are not available for moving mesh methods with singular perturbation framework. This work considered the discrete problem with upwind discretization for convection dominated term. A rigorous error analysis at each time interval is provided. The present analysis will generalize the adaptive method proposed in [3] (which was only for convection-diffusion problems) to reaction-diffusion as well. We have shown that the proposed method converges uniformly with respect to the perturbation parameters ϵ and μ . It converges with first-order accuracy with respect to space and time. The numerical experiments validate the theoretical findings.

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Adaptive FEM with goal-oriented error estimation and an approximation of the dual problem for inelastic problems

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Goal-oriented error estimation allows to refine meshes in space and time with respect to arbitrary quantities.[1] This approach is attractive because the quantity may be something which is actually important for the problem to be solved. The required dual problems that need to be solved usually require weak formulations and the Galerkin method in space and time to be established.[2] Unfortunately this is in conflict with structures of current finite element implementations for solid mechanics.[3] Therefore, we propose an approach to approximate the dual problem while maintaining these structures. Here, the dual problem is constructed based on the discretized primal problem. For the error estimation we apply a higher-order recovery procedure.[4] An application to elasto-plasticity is given. Numerical examples demonstrate the effectiveness of the procedure.

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An Adaptive Local Basis for Elliptic Problems with Complicated Discontinuous Coefficients

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We will present a generalized finite element method for the discretization of elliptic partial differential equations in heterogeneous media. In [1] a method has been introduced to set up an adaptive local finite element basis (AL basis) on a coarse mesh with mesh size H which, typically, does not resolve the matrix of the media while the textbook finite element convergence rates are preserved. This method requires $O(\log(1/H)^{d+1})$ basis functions per mesh point where d denotes the spatial dimension of the computational domain. Since the continuous differential operator is involved in the construction, the method presented in [1] is only semidiscrete. In our talk, we will present a fully discrete version of the method, where the AL basis is constructed by solving finite dimensional localized problems. A key tool for the discretization of the differential operator is the theory developed in [2, 3]. We will prove that the optimal convergence rates are preserved and give some complexity estimates.

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Error measurement and enhanced FEM for phase field modeling

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The analytical solution for the spatial evolution of a field variable governed by the Allen-Cahn equation

$$\lambda \frac{\partial \varphi}{\partial t} = \nabla \cdot \mu - \eta$$

serves as basis for a thorough investigation of finite element techniques on phase field modeling. A non-conserved phase field variable $\varphi \in \mathbb{R}$, free Landau energy $\psi_w(\varphi)$, and gradient energy $\psi_g(\nabla \varphi)$ constitutes the Ginzburg-Landau free energy density

$$\psi = \psi_w(\varphi) + \psi_g(\nabla \varphi) \quad (1)$$

Internal microforces η and microstresses μ balance the process of phase evolution and transition [1], defined by

$$\eta := \frac{\partial \psi_w}{\partial \varphi}, \quad \mu := \frac{\partial \psi_g}{\partial (\nabla \varphi)} \quad (2)$$

We convert the Allen-Cahn equation to a discrete problem with help of Ritz-Galerkin's method

$$G := \int_{\mathcal{B}} \mu \cdot \nabla \delta \varphi + (\eta + \lambda \dot{\varphi}) \delta \varphi \, dV - \int_{\partial \mathcal{B}} \mu \cdot n \delta \varphi \, dA = 0 \quad (3)$$

Neumann boundary conditions $\mu \cdot n = 0$ apply on all surfaces $\partial \mathcal{B}$. Thus, a numerical method has to fulfill Dirichlet boundary conditions and the left integral of Eq. 3. Linearizing G with respect to φ prepares the Newton-Raphson algorithm for numerical solution. Incremental values of the phase parameter φ are denoted with $\Delta \varphi$, thus

$$\text{Lin}G := G^* + \int_{\mathcal{B}} \left(\frac{\partial \mu}{\partial \nabla \varphi} \cdot \nabla \Delta \varphi \right) \cdot \nabla \delta \varphi + \frac{\partial \eta}{\partial \varphi} \Delta \varphi \delta \varphi + \lambda \Delta \dot{\varphi} \delta \varphi \, dV = 0 \quad (4)$$

Additionally, the backward Euler scheme is used for time integration. At time step, t and iteration, i within the Newton-Raphson method, it holds:

$$\dot{\varphi} = \frac{\varphi_t^{i+1} - \varphi_t^0}{\Delta t}, \quad \varphi_t^{i+1} = \varphi_t^i + \Delta \varphi^i, \quad \Delta \varphi^0 = 0, \quad \Delta \dot{\varphi} = \frac{\Delta \varphi^i}{\Delta t} \quad (5)$$

Time increments $\Delta t > 0$ enter the numerical formulation as regularization parameter for free energy states above the minimum. In the numerical formulation it interacts with λ via

$$\lambda \Delta \dot{\varphi} = \frac{\lambda}{\Delta t} \Delta \varphi^i \quad (6)$$

Falk [2] elaborated the analytical solution of a one dimensional phase transition ¹ reading

$$\varphi(x) = \sqrt{\frac{\beta}{\alpha}} \frac{\varphi_0 \sinh(\lambda x / \xi)}{\sqrt{A + \sinh^2(\lambda x / \xi)}} \quad (7)$$

An adaptive p-method is proposed, which is generally applicable for finite elements. The method preserves continuity of the shape functions and is particularly advantageous in the context of parallelized computing environment. Using internal wave function, the FEM shows a significant decrease of the error, e defined with help of Eq. 7.

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¹Parameters $\alpha, \beta, \varphi_0, A, \lambda, \xi$ given by own constitution in Eq. 1

Interior penalty finite element methods for high-order local boundary conditions

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Local absorbing boundary conditions are used to mimick the solution in presence of an infinite exterior in diffusion problems or time-harmonic scattering problems, in highly conducting bodies or thin layers. We consider Dirichlet-to-Neumann boundary conditions involving higher tangential derivatives. (see an analysis in [1]). If only second derivatives are present, *i.e.*, for the Neumann, Robin and Wenttzel conditions, and the boundary is smooth enough, we can incorporate the condition in usual piecewise continuous finite element methods. For higher derivatives trial and test functions with higher continuity (at least) along the boundary or auxilliary unknowns may be used. We propose as an alternative nonconforming interior penalty finite element methods for usual continuous finite element spaces in additional terms on the nodes of the boundary appear. For fourth order PDEs a similar approach has been introduced by Brenner and Sung [2]. We will present well-posedness results and *a-priori* h -convergence error estimates for uniform polynomial degrees. The theoretical convergence results are validated by a series of numerical experiments.

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Generalized approximated regular boundary element method

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Last years, numerical modeling had become universal tool and extremely important part of modern sciences, technologies and other fields of human activity. Nevertheless a number of computers and their computational opportunity are sufficiently increased, different requirements to numerical algorithms remain very serious. For example, there are an effectiveness requirement, accuracy requirement, simplicity of coding and so on. To satisfy the mentioned requirements, new numerical algorithms are developed and existing algorithms are constantly improved. Such improvement of boundary element algorithms is an aim of the present work, which continues a series of publications by the author devoted to regular boundary element algorithms. The regular boundary element method (Kupradze's functional equation method) is similar to usual collocation technique with only difference: the collocation points are situated inside or outside the solution domain. Thus well-known singularities are excluded from the algorithm. The second case of collocation point situated inside the solution domain is considered here. In contrast to other cases, exact boundary integral equation cannot be obtained in this algorithm. However, the formulated approximated boundary integral equations are always second kind and they matrices of linear algebraic equation system with better properties than in other cases. Since the collocation point is situated inside the domain, but outside the boundary, the desirable solution in this point can be formally expanded into Taylor's series. The main idea of the present work is to increase an approximation order due to using more terms of the mentioned Taylor's series. Correspondent algorithms are developed and realized as computer codes for boundary-value problems for Laplace equation and initial-boundary-value problems for heat conduction equation. Calculations are made for special sets of test problems with known analytical solutions to illustrate workability and effectiveness of the proposed approach and to determine optimal parameters of the algorithms such as collocation point positions and number of terms of the Taylor's series. As a result of computational experiments, it is shown that for rational algorithm parameters an accuracy of the calculation can be sufficiently improved due to "better properties of matrix of the linear algebraic equations". Beside of that, explicit regular boundary element algorithms are proposed for initial-boundary-value problems for heat conduction equation. The last kind of algorithms does not require a solution of linear algebraic equation, in general, saving, in the same time, enough high accuracy of whole calculations.

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Boundary element application to non-linear boundary integral equations

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Last decades, boundary element method has become a powerful tool of numerical modeling. However the boundary element method, first of all, is directed to linear boundary-value problems, for which it provides extremely high accuracy and effectiveness. There are a lot of specific difficulties, which arise under boundary element method is being applied to non-linear problem. The present work is devoted to determination and analysis of cases, when boundary element method is effective in non-linear problem application. The most important boundary element advantage is possibility of analysis boundary alone. If pure boundary formulation is not obtained, an effectiveness of boundary element algorithms is sufficiently less, than effectiveness in the first case. An evident conclusion can be made that boundary alone formulation of non-linear problems are high effective too, similar to linear problems. Thus it is necessary to find such classes of non-linear problems. First of all, boundary-value problems with linear differential operators and non-linear boundary conditions are considered. Moving boundary problem and unknown boundary problems are something like of previous class, if they have linear differential operators too. The third group of problems is the most difficult for determination and analysis, these problems have non-linear differential operators, which permit some linearization transformation (for example, substitution) giving a problem with linear differential operator, that is, the obtained problem belongs to the first class. As it is well-known, non-linear problems can have non-unique solution. The non-linear problems of all above mentioned classes arising in practical applications are usually solved using an iterative process to handle nonlinearity of boundary integral equations. It's a pity, but such approach doesn't give any opportunity to find several solutions, if the solution is not unique. The computation result in this case are completely depends on initial approximation (first step of iteration process). To make some conclusion about uniqueness of solutions, it is necessary to solve a lot of problem with great variety of initial approximations, what were made in the present work for several problems. However, there are other possible approaches to non-linear boundary integral equations based on boundary element technique, for example, Newton's method. The last direction is not developed properly yet. To illustrate the considered cases several examples of non-linear boundary integral equations are solved numerically.

Boltzmann collision operator: How to model rotational invariance

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Due to the availability of affordable computer power (CPU, GPU), discrete kinetic schemes for the simulation of the Boltzmann equation gain increasing interest. In contrast to Monte Carlo schemes, they are free of fluctuations and can resolve situations hard to calculate with stochastic methods.

Considering kinetic models on integer grids with small grid parameter h as a numerical integration scheme, their order of consistency has been investigated in a couple of papers. However, the number of grid points to be relevant for such kinds of estimates is very high – too high for efficient numerical schemes. Thus for practical purposes one has to consider models for which the grid parameter and the truncation errors when cutting the grid to a finite size are not negligible. Thus one has to adjust the collision parameters obtained as numerical weights in such a way that the overall performance in the regime of interest is acceptable. One particular point of interest is the validity of physical invariances (translational, rotational), since these are in conflict with a finite-size integer grid if the considered Mach numbers are not very small.

In recent years kinetic models on integer grids have been investigated systematically [1, 2]. The present contribution reports on the continuation of these studies following a new approach based on so-called multilayer systems. These are composed of single layers each of which considers only collisions $(v + p, v + q) \leftrightarrow (v, v + p + q)$ with fixed vectors p and q . This point of view reveals a couple of interesting properties of a large class of discrete kinetic models. In particular, it allows to derive without too much effort the correct numerical weights by considering each layer as a specific integration point of the numerical quadrature rule.

Furthermore, it is possible to apply the results of previous works [4, 3] concerning the structure of the solutions to the Milne and Kramers problems. This allows to constitute a relation between the weights attached to each of the layers and the flow parameters (viscosity, heat conduction) in the regime close to the Navier-Stokes domain. The knowledge of these relations allows to fit flow properties in order to cut down truncation effects and to restore invariance properties like rotational symmetry of solutions.

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Fully-Implicit Log-Conformation Formulation of Viscoelastic Constitutive Laws

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The robust and stable simulation of viscoelastic flows has been and still is a struggle of computational rheology. This fact, which is usually referred to as the High Weissenberg Number Problem, is not fully understood and the origin of the problem, i.e., whether it is an insufficiency of the numerical discretization or the model itself, is yet to be determined. One approach to tackle the problem from the numerical side is the so-called log-conformation formulation. The latter, which has first been proposed in 2004 by Fattal and Kupferman [1], owes much of its popularity to the circumstance that it was found to be crucial for numerical discretizations to resemble the analytical solution in the preservation of the positive-definiteness of the conformation tensor. The log-conformation formulation simply achieves this by using $\Psi = \log \sigma$ as the primal variable of the simulation instead of the conformation tensor σ . However, the corresponding set of constitutive equations derived in [1] carry the small intricacy that the formulation of the constitutive equation requires an algebraic decomposition of the velocity gradient field. In addition to hindering the closed formulation of the full system of partial differential equations in combination with the Navier–Stokes equations, this also complicates the application of further analytical tools. One of these tools with particular importance for numerical simulations is the Newton–Raphson algorithm, which promises quadratic convergence for the solution of the whole system.

In this talk we will present our recent development of a fully-implicit log-conformation formulation [2]. The key concept is the same as in the original log-conformation formulation: We substitute the polymeric stress or the conformation tensor as our primal variables by the logarithm of the conformation tensor. As such we also inherit the property that the conformation tensor is positive-definite by design. The substantial difference to the original method is that we can formulate a constitutive equation in the new variable that completely avoids the algebraic decomposition of the velocity gradient and thus paves the way for the Newton–Raphson algorithm. Following the theoretical description of the method, the talk will subsequently cover results of an implementation in our in-house FEM flow solver, ranging from benchmark problems to die swell simulations [3].

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Approximate exponential time integration for diffusion problems

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We develop a class of numerical methods for the time integration of the unsteady diffusion equation, based on an approximation of the Exponential Time Integration (ETI). ETI has gained importance following the work of Cox and Matthews [1] and with recent developments in efficient methods for computing the matrix exponential [2]. The formulation of this Approximate Exponential Time Integration (AETI) makes use of a combination of the Von Neumann analysis and the Taylor series expansion. We describe schemes with second and higher order of accuracy, and extend the method to show how it can be transformed into a new algorithmic structure. We benchmark the method with respect to classical explicit numerical schemes that treat time integration and spatial approximation separately. Our analysis and numerical tests demonstrate that the new formulation is more accurate and efficient than combinations of Explicit Euler and Runge-Kutta (RK) methods of second, third and fourth order with explicit differencing schemes up to sixths order and allows for considerably larger time integration steps.

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On multi-dimensional discrete equations of convolution type

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We consider a special class of integral operators of convolution type, namely a simplest variant of Calderon - Zygmund operators. Such operators arise in a lot of applied problems, and the studying their properties is of a special interest. We start from the Calderon-Zygmund operator [1]

$$K : u(x) \mapsto v.p. \int_D K(x-y)u(y), \quad x \in D,$$

and its discrete analogue

$$K_d : u_d(\tilde{x}) \mapsto \sum_{\tilde{y} \in D \cap \mathbf{Z}^m} K(\tilde{x} - \tilde{y})u_d(\tilde{y}), \quad \tilde{x} \in D \cap \mathbf{Z}^m,$$

where D is one of canonical domains \mathbf{R}^m , $\mathbf{R}_+^m = \{x \in \mathbf{R}^m : x_m > 0\}$, $C_+^a = \{x \in \mathbf{R}^m : x_m > a|x'|, a > 0, x' = (x_1, \dots, x_{m-1})\}$, \mathbf{Z}^m is integer lattice in the space \mathbf{R}^m , and study the invertibility properties for such operators. These considerations are based on symbol properties of Calderon - Zygmund operators, discrete Fourier transform, and periodic analogue of classical Riemann boundary problem [2, 3, 4, 5].

According to classical symbol of the Calderon - Zygmund operator K [1]

$$\sigma(\xi) = v.p. \int_{\mathbf{R}^m} K(x)e^{-ix \cdot \xi} dx, \quad \xi \in \mathbf{R}^m \setminus \{0\},$$

we define a symbol for the discrete operator K_d by multi-dimensional Fourier series

$$\sigma_d(\xi) = \lim_{N \rightarrow +\infty} \sum_{\tilde{x} \in Q_N \cap \mathbf{Z}^m} K(\tilde{x})e^{-i\tilde{x} \cdot \xi}, \quad \xi \in \mathbf{T}^m,$$

where $Q_N = \{x \in \mathbf{R}^m : \max_{1 \leq k \leq m} |x_k| \leq N\}$, $\mathbf{T}^m = [-\pi, \pi]^m$ is basic cube of periods.

A correlation between the symbols $\sigma(\xi)$ and $\sigma_d(\xi)$ for the case $\mathbf{R}^m, \mathbf{R}_+^m$ was considered in papers [3, 4, 5]. For studying convolution equations with the operator K_d for the case $D = C_+^a$ authors develop the theory of multi-dimensional Riemann boundary problem which has its continual analogue [2]. It was found that the existence of a wave factorization for the symbol $\sigma(\xi)$ with respect to the cone C_+^a implies the existence of required factorization for the symbol $\sigma_d(\xi)$. For this purpose the authors consider a certain class of holomorphic functions in special tube domains over cones.

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