

**Technische Universität Graz**



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18. Workshop on  
**Fast Boundary Element Methods in  
Industrial Applications**

Söllerhaus, 8.–11.10.2020

U. Langer, M. Schanz, O. Steinbach, W. L. Wendland (eds.)

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**Berichte aus dem  
Institut für Angewandte Mathematik**



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## **Berichte aus dem Institut für Angewandte Mathematik**

Book of Abstracts 2020/11

Technische Universität Graz  
Institut für Angewandte Mathematik  
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**WWW:** <http://www.applied.math.tugraz.at>

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## Program

Thursday, October 8, 2020	
15.00	Coffee
16.30	Opening
16.40–17.10	M. Multerer (Lugano) Shape uncertainties in electrocardiology
17.10–17.40	J. Dölz (Bonn) A higher order perturbation approach for electromagnetic scattering problems on random domains
17.40–18.00	Break
18.00–18.30	C. Özdemir (Graz) A stochastic boundary element method for the wave equation in 3D
18.30	Dinner
Friday, October 9, 2020	
8.00–9.00	Breakfast
9.00–9.30	M. Zank (Wien) Space–time variational formulations and their discretisations for the wave equation
9.30–10.00	C. Urzúa–Torres (Delft) A new approach to time domain boundary integral equations for the wave equation
10.00–10.15	Break
10.15–10.45	R. Watschinger (Graz) A parallel FMM for space–time boundary element methods for the heat equation: Concept and first results
10.45–11.15	M. Merta, J. Zapletal Implementation of boundary element integration schemes for the heat equation in 3D
11.15–11.30	Break
11.30–12.00	P. Marchand (Bath) Applying GMRES to Helmholtz boundary integral equations: how do the number of iterations depend on the frequency in the presence of strong trapping
12.00–12.30	M. Averseng (Zürich) Preconditioners for integral equations on screens
12.30	Lunch
15.30	Coffee
16.00–16.30	G. Of (Graz) A finite element approximation of non-local electrostatics
16.30–17.00	R. Brügger (Basel) On the solution of a time–dependent inverse shape identification problem for the heat equation
17.00–17.15	Break
17.15–17.45	H. Yang A space–time finite element method for the inverse estimates of the initial condition for the heat equation
17.45–18.15	P. Panchal (Zürich) Adaptive shape representation
18.30	Dinner

Saturday, October 10, 2020	
8.00–9.00	Breakfast
9.00–9.30	W. L. Wendland (Stuttgart) Boundary integral equations for scattering by a perfect electrical conductor
9.30–10.00	M. Kirchhart (Aachen) Div–curl problems and stream functions in 3D Lipschitz domains
10.00–10.15	Break
10.15–10.45	H. Gimperlein (Edinburgh) High order TDBEM for the Lamé equation
10.45–11.15	I. Labarca (Zürich) Acoustic scattering with convolution quadrature and the method of fundamental solutions
11.15–11.30	Break
11.30–12.00	J. Tibaut (Graz) Fast boundary–domain integral method with the H <sup>2</sup> –matrix for numerical analysis
12.00–12.30	G. Unger (Graz) Convergence analysis of coupled finite and boundary element methods for electromagnetic scattering–resonance problems
12.30	Lunch
13.30–18.00	Hiking Tour
18.30	Dinner
Sunday, October 11, 2020	
8.00–9.00	Breakfast
9.00–9.30	H. Harbrecht (Basel) A wavelet–based approach for the optimal control of non–local operator equations
9.30–10.00	O. Steinbach (Graz) Boundary integral equations for the heat equation revisited
10.00–10.30	Coffee

## Preconditioners for integral equations on screens

M. Averseng<sup>1</sup>, F. Alouges<sup>2</sup>

<sup>1</sup>ETH Zürich, Switzerland, <sup>2</sup>Ecole Polytechnique, Palaiseau, France

This work is concerned with the integral equations arising from the resolution of the Helmholtz scattering problems by a thin screen in 2D with Dirichlet or Neumann conditions, namely the single-layer and hypersingular integral equations

$$V\lambda = f \quad \text{in } H^{1/2}(\Gamma), \quad W\mu = g \quad \text{in } H^{-1/2}(\Gamma).$$

We focus on the case where  $\Gamma$  is a smooth Jordan curve in  $\mathbb{R}^2$  (in particular, **not a Lipschitz domain**). The singularity of the geometry raises two main issues.

### Singularity of the solutions:

The solutions  $\lambda$  and  $\mu$  have edge singularities, making them unsuited to approximation by piecewise polynomials. In fact, if  $f$  and  $g$  are smooth, it is known that there exist smooth functions  $\alpha$  and  $\beta$  such that

$$\lambda = \frac{\alpha}{\omega}, \quad \mu = \omega\beta$$

where  $\omega(x) = \sqrt{d(x, \partial\Gamma)}$  is the square root of the distance to the edges of  $\Gamma$ . It is well-known that choosing a uniform mesh in the Galerkin method results in  $\mathcal{O}(\sqrt{h})$  convergence rate only.

### Ill-conditioned linear systems:

The first-kind integral equations notoriously lead to ill-conditioned linear systems. For non-Lipschitz geometries, the popular Calderón preconditioning technique is no longer optimal due to the duality mismatch  $(H^{1/2}(\Gamma))' \neq H^{-1/2}(\Gamma)$ .

Here we present an approach that overcomes both difficulties (convergence and conditioning) at the same time. As in the work of Bruno and Lintner we consider weighted versions of the layer potentials, namely

$$V_\omega : \varphi \mapsto V\left(\frac{\varphi}{\omega}\right), \quad W_\omega : \varphi \mapsto W(\omega\varphi).$$

Those weighted layer potentials are known to satisfy a Calderón-type identity, generalizing the situation that occurs in smooth geometries, so that optimal preconditioning can be achieved in this setting by simply composing the two operators. Here, we propose an alternative approach, which generalizes the analytical preconditioning method of Darbas and Antoine by introducing a symbolic calculus on the screen and creating parametrices for the layer potentials. We obtain "quasi-sparse" preconditioners. We provide numerical results illustrating the efficiency of the preconditioners.

## **On the Solution of a Time-dependent Inverse Shape Identification Problem for the Heat Equation**

Rahel Brügger

Universität Basel, Switzerland

In the talk, we treat the solution of a time-dependent shape identification problem. We specifically consider a heat-type equation on a domain, which contains a star-shaped inclusion of zero temperature. We aim at detecting this time-dependent inclusion by measuring the heat flux on the exterior boundary of the domain. Reformulation by using a Neumann data tracking functional leads to a time-dependent shape optimization problem, for which a gradient based method is considered. Numerical examples will be discussed. This is joint work with Helmut Harbrecht and Johannes Tausch.

## **A higher order perturbation approach for electromagnetic scattering problems on random domains**

Jürgen Dölz

We consider time-harmonic electromagnetic scattering problems on perfectly conducting scatterers with uncertain shape. Thus, the scattered field will also be uncertain. Based on the knowledge of the two-point correlation of the domain boundary variations around a reference domain, we derive a perturbation analysis for the mean of the scattered field. Therefore, we compute the second shape derivative of the scattering problem for a single perturbation. Taking the mean, this leads to an at least third order accurate approximation with respect to the perturbation amplitude of the domain variations. To compute the required second order correction term, a tensor product equation on the domain boundary has to be solved. We discuss its discretization and efficient solution using boundary integral equations. Numerical experiments in three dimensions are presented.

## High-order TDBEM for the Lamé equation

H. Gimperlein

Heriot-Watt University, Edinburgh, UK

We present h, p and hp-versions of the time domain boundary element method for the time dependent Lamé equation. We particularly discuss problems in polygonal domains or outside an open curve, where the solution exhibits singularities at the corners. For the h-version, graded meshes are shown to lead to optimal approximation rates for the numerical solution. For an open curve the p-version converges at twice the rate of the h-version. The hp-version exhibits exponential convergence. Numerical experiments illustrate the theory in 2d. (joint with A. Aimi, G. Di Credico, C. Guardasoni and E. P. Stephan)

## **A wavelet-based approach for the optimal control of non-local operator equations**

Helmut Harbrecht

Universität Basel, Switzerland

The purpose of this study is to propose a wavelet-based approach for the optimal control of a class of non-local equations. Namely, we consider a quadratic cost functional where the state equation involves the fractional Laplace operator in integral form. When discretizing this non-local operator with standard finite element basis functions, one arrives at a densely populated system matrix. This imposes serious obstructions to the efficient numerical treatment of such problems. Therefore, we use a wavelet basis for discretizing the state equation and apply wavelet matrix compression to arrive at a solver that has linear complexity. In particular, we show how to include box constraints to the optimal control.

## Div-Curl Problems and Stream Functions in 3D Lipschitz Domains

Matthias Kirchhart<sup>1</sup>, Erick Schulz<sup>2</sup>

<sup>1</sup>RWTH Aachen, Germany,      <sup>2</sup>ETH Zürich, Switzerland

We consider the following problem: given a bounded Lipschitz domain  $\Omega \subset \mathbb{R}^3$  and given a vorticity field  $\mathbf{F}$ , find the velocity  $\mathbf{U} \in \mathbf{L}^2(\Omega)$  such that:

$$\begin{cases} \operatorname{curl} \mathbf{U} = \mathbf{F}, \\ \operatorname{div} \mathbf{U} = 0. \end{cases}$$

Moreover, to enforce the divergence constraint exactly, it would be desirable to represent the solution in terms of a *vector potential* (or *stream function*)  $\mathbf{A}$  as  $\mathbf{U} = \operatorname{curl} \mathbf{A}$ .

This problem naturally arises when studying the incompressible Navier–Stokes equations in their vorticity formulation and is of great practical interest in so-called vortex methods.

Last year preliminary results on this problem were presented. Important questions, however, had to be left open:

- What are the correct spaces and boundary conditions?
- What exact conditions does  $\mathbf{F}$  need to fulfil?
- How to construct a stream function  $\mathbf{A}$  of maximum regularity, given only  $\mathbf{F}$  and boundary data?

In this talk we present complete answers to the first two questions. Our solution for the third problem can be efficiently implemented on computers and relies on boundary integral formulations. It yields stream functions of higher regularity than the previous approaches. Except for certain special cases, these functions have the highest possible regularity.

# **Acoustic Scattering with Convolution Quadrature and the Method of Fundamental Solutions**

I. Labarca

Seminar für Angewandte Mathematik, ETH Zürich, Switzerland

Time-domain acoustic scattering problems in two dimensions are studied. The numerical scheme relies on the use of the Convolution Quadrature (CQ) method to reduce the time domain problem to the solution of frequency domain Helmholtz equations with complex wavenumbers. These equations are solved with the method of fundamental solutions (MFS), which approximates the solution by a linear combination of fundamental solutions defined at source points inside (outside) the scatterer for exterior (interior) problems. Numerical results show that the coupling of both methods works efficiently and accurately for multistep and multistage based CQ.

**Applying GMRES to Helmholtz boundary integral equations: how do the number of iterations depend on the frequency in the presence of strong trapping?**

P. Marchand, A. Spence, E. A. Spence

Department of Mathematical Sciences, University of Bath, UK

We are interested in solving scattering problems with strong trapping using the Combined Field Integral Equation (CFIE) and the Generalized Minimal Residual method (GMRES). In this talk, we show a new understanding of how the number of GMRES iterations depends on frequency in this situation.

The non-normal nature of CFIE makes GMRES the iterative method of choice for solving linear systems stemming from its discretisation. GMRES has the advantage of being able to solve any non-singular linear system, in particular non-normal. But the convergence analysis becomes less straightforward in this case, because it requires more information than just the spectrum. Bounds for GMRES applied to non-normal matrices can be derived using condition number of eigenvalues, numerical range or pseudo-spectrum [2, 3].

But in the case of trapping, an additional difficulty comes from the solution operator whose norm grows exponentially through a sequence of frequencies tending to infinity, with the density of these “bad” frequencies increasing as the frequency increases. In this case, the spectrum of the associated matrix has the form of a cluster with outliers near the origin. Following [1] where matrices with similar spectra are studied, we provide a new analysis of the GMRES convergence taking into account this particular distribution.

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**Implementation of boundary element integration schemes  
for the heat equation in 3D**

G. Of<sup>1</sup>, M. Merta<sup>2</sup>, R. Watschinger<sup>1</sup>, J. Zapletal<sup>2</sup>

<sup>1</sup>TU Graz, Austria,   <sup>2</sup>TU VSB Ostrava, Czech Republic

Space-time methods have attracted a lot of attention in the last couple of years. Similarly as in the case of stationary problems, the space-time boundary element method (BEM) reduces the dimensionality of the problem at the cost of dealing with singular integral operators. In the talk we focus on one of the approaches to assemble boundary element matrices stemming from the discretisation of boundary integral equations for the heat equation in three spatial dimensions. Namely, we concentrate on a semi-analytic scheme for tensor product meshes, where the temporal integrals are treated analytically, and the remaining singularities are treated by the standard numerical scheme known from stationary BEM. We conclude the talk with numerical experiments and shortly comment on alternative regularization techniques.

## Shape uncertainties in electrocardiography

Michael Multerer

Universita della Svizzera italiana, Lugano, Switzerland

joint work with Lia Gander, Rolf Krause, and Simone Pezzuto

Electrocardiographic recordings on the body surface are a direct consequence of the electric activity of the heart. In the forward problem of electrocardiography, the electric potential on the chest is uniquely determined from the pericardial potential, the torso anatomy and the electric conductivity. Conversely, in the inverse problem, or ECG imaging, the pericardial potential is recovered from a dense body surface map and an accurate description of the torso anatomy. The solution of both problems varies depending on the shape of the heart, which is typically segmented from images and therefore subject to uncertainty. In this talk, we present a model for this shape uncertainty and study its effect, both in space and time, on the forward and inverse problem of electrocardiography. To this end, the problem is first recast into the boundary integral formulation and then discretized by the collocation method. The space-time uncertainty in the potential is assessed by computing expectation and variance using an anisotropic sparse quadrature method.

## A finite element approximation of non-local electrostatics

H. Egger<sup>1</sup>, G. Of<sup>2</sup>

<sup>1</sup>TU Darmstadt, Germany, <sup>2</sup>TU Graz, Austria

We consider the non-local material response of a medium to applied electric fields in the form

$$D(x) = (\varepsilon * E)(x) = \varepsilon_0 E(x) + \int_{\Omega} \varepsilon_1(x, y) E(y) dy.$$

In the presence of charges with density  $q$ , the dielectric displacement field  $D$  is given by the Gauß-law of electrostatics

$$\operatorname{div} D = q \quad \text{in } \Omega.$$

Due to absence of alternating magnetic fields, the electric field can be expressed by

$$E = -\nabla\phi.$$

This results in the following boundary value problem for an integro-partial differential equation

$$\begin{aligned} -\operatorname{div}(\varepsilon * \nabla\phi) &= q && \text{in } \Omega, \\ \partial_{n,\varepsilon}\phi + \alpha\phi &= 0 && \text{on } \partial\Omega, \end{aligned}$$

We discuss a related finite element approximation and a data-sparse approximation of the volume integral operator.

## A stochastic boundary element method for the wave equation in 3D

H. Gimperlein, F. Meyer, C. Özdemir

TU Gaz, Austria

We consider the wave equation in an unbounded domain in 3D, where the boundary condition depends on a probability. We begin the talk by reviewing the wave equation with a space-time boundary condition. We derive a variational formulation and use a tensor product ansatz. Then we solve the resulting system with the marching-on-in time (MOT) scheme. Based on this idea, we derive a variational formulation for stochastic boundary conditions via a polynomial chaos ansatz. We present the resulting system in the stochastic space-time dimension and end the talk with numerical experiments in 3D.

## **Adaptive shape representation**

P. Panchal

Seminar für Angewandte Mathematik, ETH Zürich, Switzerland

In this work we explore an adaptive method for approximation of shapes in regard to evaluation of scalar valued shape functionals. The shapes are described by parameterizations and their closeness is induced by a Hilbert space structure on the parameter domain. We justify a heuristic for finding the best low-dimensional parameter subspace for uniformly approximating a given shape functional around a reference shape. We also propose an adaptive algorithm to find an appropriate subspace for achieving a prescribed approximation error.

## Boundary integral equations for the heat equation revisited

O. Steinbach  
TU Graz, Austria

The numerical analysis of boundary integral equations and boundary element methods for the heat equation is well established, see, e.g., [1] and [2] for an overview. In fact, the heat single layer boundary integral operator  $V$  turns out to be elliptic in the anisotropic Sobolev space  $H^{-1/2, -1/4}(\Sigma)$  with  $\Sigma := \partial\Omega \times (0, T)$  being the lateral boundary of the space time domain  $Q := \Omega \times (0, T)$ . While in the case of the Laplace equation the ellipticity of the single layer boundary integral operator is related to the ellipticity of the interior and exterior Dirichlet forms, this relation with a domain variational formulation as used in finite element methods for the heat equation is not obvious. This is of particular interest when considering the non-symmetric coupling of finite and boundary element methods for the heat equation, see, e.g., [3,4] for a free space transmission problem for the Poisson equation.

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- [4] O. Steinbach: A note on the stable one–equation coupling of finite and boundary elements. *SIAM J. Numer. Anal.* 49 (2011) 1521–1531.

## Fast boundary-domain integral method with the $\mathcal{H}^2$ -matrix for numerical analysis

J. Ravnik<sup>1</sup>, M. Schanz<sup>2</sup>, J. Tibaut<sup>2</sup>

<sup>1</sup>Faculty of Mechanical Engineering, University of Maribor, Slovenia

<sup>2</sup>Institut für Baumechanik, TU Graz, Austria

The Boundary Element Method (BEM) can be employed as an alternative numerical method for FEM and FVM. BEM is based on the Green's second identity. However, the method can only be employed when the fundamental solution of the partial differential equation is known. For partial differential equations that have a source or a convective part the fundamental solution is mostly not known. Thus, the Boundary-Domain Integral Method (BDIM) is employed. Portillo [1] showed a diffusion equation for inhomogeneous media with the BDIM. Verhnjak et al. [4] presented a novel two-way coupled model for the Euler-Lagrange simulation of a multiphase fluid flow. The BDIM has a computational complexity of  $\mathcal{O}(N^2)$ . Sellountos [2] used the FMM and Tibaut and Ravnik [3] the ACA, to solve the incompressible fluid flow with the BDIM. We approximate the kernel with the  $\mathcal{H}^2$ -matrix formulation and observe the influence of the approximation on the solution of the modified Helmholtz equation.

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- [3] J. Tibaut, J. Ravnik: Fast boundary-domain integral method for heat transfer simulations. *Engineering Analysis with Boundary Elements* 99 (2019) 222–232.
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## Convergence analysis of coupled finite and boundary element methods for electromagnetic scattering-resonance problems

G. Unger  
TU Graz, Austria

In this talk we present a convergence analysis of coupled finite and boundary element methods for electromagnetic scattering-resonance problems. We consider a so-called symmetric formulation of the resonance problem which is based on a coupling of a weak formulation of Maxwell's equations inside the scatterer with the Calderón projector for Maxwell's equations outside the scatterer. For the related source problem this kind of formulation and its discretization was already analyzed in [1]. It was shown that for positive frequencies and positive material parameters this kind of formulation for the source problem is weakly T-coercive and that a discretization with Nedelec elements inside the scatterer together with Raviart-Thomas boundary elements on the surface of the scatterer yields quasi-optimal convergence. We extend these results with respect to the weak T-coercivity to complex-valued frequencies and to complex-valued material parameters by introducing a frequency and material dependent operator T. The convergence of the Galerkin approximation of the resonance problem is shown by combining recent results on the regular approximation of weakly T-coercive operators [2, 5] with classical results on the approximation of eigenvalue problems for holomorphic Fredholm operator-valued functions [3, 4].

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- [5] G. Unger: Convergence analysis of a Galerkin boundary element method for electromagnetic resonance problems. Submitted, 2020.

## **A New Approach to Time Domain Boundary Integral Equations for the Wave Equation**

Carolina Urzúa-Torres<sup>1</sup>, Olaf Steinbach<sup>2</sup>

<sup>1</sup>Delft Institute of Applied Mathematics, Delft University of Technology, Netherlands

<sup>2</sup>Institute of Applied Mathematics, Graz University of Technology, Austria

Different strategies have been used to derive variational methods for time domain boundary integral equations for the wave equation. The more established and succesful ones include weak formulations based on the Laplace transform, and also time-space energetic variational formulations. However, their corresponding numerical analyses are still incomplete and present difficulties that are hard to overcome, if possible at all.

In this talk, we present a new approach to formulate the boundary integral equations for the wave equation. Moreover, we discuss new results that pave the way for developing the missing mathematical analysis for space-time boundary element methods.

**A parallel FMM for space-time boundary element methods for the heat equation:  
Concept and first results**

M. Merta<sup>1</sup>, G. Of<sup>2</sup>, R. Watschinger<sup>2</sup>

<sup>1</sup>VŠB TU Ostrava, Czech Republic, <sup>2</sup>TU Graz, Austria

Space-time methods deal with the numerical solution of time-dependent partial differential equations in space and time as a whole. While this increases the computational effort it allows in particular for parallelism in space and time. In this talk we present a strategy for the parallelization of fast space-time boundary element methods for the heat equation.

The considered fast method (FMM) relies on a hierarchical approximation of the boundary element system matrix based on a clustering of the space-time boundary into axis-parallel space-time clusters. We collect clusters sharing the same temporal component and use this grouping in time to distribute the work among computational nodes. The hierarchical approximation enforces a somewhat sequential execution order of the FMM operations. Nonetheless, we can efficiently parallelize it by considering a task-based execution strategy where operations are executed when their dependencies are satisfied.

The parallelization concept is presented by means of a simple 1D model problem, which comprises the main ideas of the actual 3+1D case. In addition, first results of the solution of initial boundary value problems of the heat equation in 3+1D are shown.

**Boundary integral equations for scattering by a perfect electrical conductor**

G. C. Hsiao<sup>1</sup>, W. L. Wendland<sup>2</sup>

<sup>1</sup>University of Delaware, USA, <sup>2</sup>Universität Stuttgart, Germany

This is a lecture on the existence proof of the "EFIE" by Buffa, Costabel, Schwab and Buffa, Hiptmaier, Petersdorff, Schwab.

**A space-time finite element method for inverse estimates of the initial condition for the heat equation**

O. Steinbach<sup>1</sup>, H. Yang<sup>2</sup>

<sup>1</sup>TU Graz, Austria,   <sup>2</sup>RICAM, Linz, Austria

In this talk, we will present some numerical results for the inverse estimates of the initial data for the heat equation. This kind of inverse problems are formulated as optimal control of parabolic equations in the space-time domain. In this setting, the control is taken as initial condition and the observed data as target. The objective is a standard terminal observation functional including the Tikhonov regularization.

For such space-time optimal control problems, we then derive the first order necessary optimality system including the state and co-state as unknowns. This system is then discretized by a Galerkin-Petrov space-time finite element method proposed by O. Steinbach, 2015.

In real applications, the target at the observation time  $T$  usually contains certain noise, measured by the so-called noise level  $\delta$ . Under such circumstances, we can only fit the terminal data in a chosen norm up to such a level  $\delta$  at the best. Therefore, depending on the noise level, one needs to evaluate the optimal regularization parameter  $\varrho$ . This evaluation requires solving a nonlinear equation by Newton's method.

## Space-time variational formulations and their discretisations for the wave equation

M. Zank

Universität Wien, Austria

For the discretisation of time-dependent partial differential equations, the standard approaches are explicit or implicit time stepping schemes together with finite element methods in space. An alternative approach is the usage of space-time methods, where the space-time domain is discretised and the resulting global linear system is solved at once. In any case, CFL conditions play a decisive role for stability. In this talk, the model problem is the scalar wave equation. First, a brief overview of known results for the wave equation is presented. Second, space-time formulations are motivated and discussed. Additionally, numerical examples for a one-dimensional spatial domain and a two-dimensional spatial domain are presented. The talk is based on joint work with O. Steinbach (TU Graz).

## Participants

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