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**Organisers:**

**Bangti Jin, Raytcho Lazarov and Kassem Mustapha**

**Abstracts in alphabetical order**

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# RATE-DEPENDENT COHESIVE-ZONE MODELS BASED ON FRACTIONAL VISCOELASTICITY

Giulio Alfano<sup>a</sup> and Marco Musto<sup>b</sup>

Department of Mechanical, Aerospace and Civil Engineering,  
Brunel University London, UK

<sup>a</sup>`giulio.alfano@brunel.ac.uk`, <sup>b</sup>`marco.musto@brunel.ac.uk`

We present a recently developed rate-dependent cohesive-zone model which simulates crack growth along rubber interfaces. Postulating the existence of a rate-independent rupture energy, associated with the rupture of bonds, a damage variable is introduced, which is assumed to evolve as a rate-independent function of part of the elastic energy. The overall rate-dependent response is retrieved by introducing additional internal variables associated with viscous dissipation. The approach was validated against test results for a DCB made of two steel arms bonded along a rubber interface, with prescribed cross-head opening speeds ranging 5 logarithmic decades. Using a Mittag-Leffner relaxation function for the undamaged interface resulted in the first cohesive-zone model based on fractional viscoelasticity, which provides excellent correlation of experimental and numerical results across the entire range of tested speeds [3, 4].

We also discuss the accuracy and the computational cost of the numerical time integration of the fractional differential equations, which we determine via the Grünwald-Letnikov expression of the fractional derivative [2, 5].

Finally, we revisit a recently proposed thermodynamical derivation of our model [1], discussing alternative choices for the damage evolution law and how they can be physically justified for different polymeric materials.

## References

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- [3] M. Musto. *On the formulation of hereditary cohesive-zone models*. Brunel University London, 2014. PhD Thesis.
- [4] M. Musto and G. Alfano. A fractional rate-dependent cohesive-zone model. *International Journal for Numerical Methods in Engineering*, 105(5):313–341, 2015.
- [5] A. Schmidt and L. Gaul. Finite element formulation of viscoelastic constitutive equations using fractional time derivatives. *Nonlinear Dynamics*, 29(1-4):37–55, 2002.

# ENERGY EQUIVALENCE FOR THE HORIZON INDEPENDENT BOND-BASED PERIDYNAMIC SOFTENING MODEL ACCORDING TO CLASSICAL THEORY

Patrick Diehl<sup>1</sup>, Robert Lipton<sup>2</sup> and Marc Alexander Schweitzer<sup>1,3</sup>

<sup>1</sup>Institute for Numerical Simulation, University of Bonn, Germany  
`diehl@ins.uni-bonn.de`

<sup>2</sup>Department of mathematics, Louisiana State University, USA

<sup>3</sup>Meshfree Multiscale Methods, SCAI, Fraunhofer, Germany

We focus on the bond-based Peridynamic Softening [1] model with respect to small deformations. In this model the material parameters are obtained by the  $\Gamma$ -convergence and are independent of the size of the interaction zone. Thus, the length scale of the nonlocal interaction is not a discretization parameter and instead describes a length scale associated with the process zone of the material. We present how to connect the model parameters with energy equivalence to common material parameters from classical theory.

[1] R. Lipton, Dynamic Brittle Fracture as a Small Horizon Limit of Peridynamics, Journal of Elasticity, 2014, Volume 117, Issue 1, pp 21-50.

# TIME STEPPING SCHEMES FOR FRACTIONAL DIFFUSION

Bangti Jin<sup>1</sup>, Raytcho Lazarov<sup>2</sup> and Zhi Zhou<sup>3</sup>

<sup>1</sup>Department of Computer Science, University College London, UK  
`bangti.jin@gmail.com`

<sup>2</sup>Department of Mathematics, Texas A&M University, USA

<sup>3</sup>Department of Applied Mathematics and Applied Physics,  
Columbia University, USA

Fractional diffusion arises in a number of practical applications, e.g., flow in heterogeneous media, thermal diffusion in fractal domains. One mathematical model to describe the physical process is the subdiffusion equation, which involves a Caputo fractional derivative in time. The nonlocality of the fractional derivative leads to limited smoothing property, which poses significant challenge in the design and analysis of robust numerical schemes. In this talk, I shall discuss some recent progresses, e.g., the convolution quadrature and L1 scheme, for discretizing such equations in time. Error estimates and qualitative properties will be discussed.

# PETROV-GALERKIN FINITE ELEMENT METHOD FOR FRACTIONAL CONVECTION-DIFFUSION EQUATIONS

Bangti Jin<sup>1</sup>, Raytcho Lazarov<sup>2</sup> and Zhi Zhou<sup>3</sup>

<sup>1</sup>Department of Computer Science, University College London, UK  
bangti.jin@gmail.com

<sup>2</sup>Department of Mathematics,  
Texas A&M University, College Station, USA  
lazarov@math.tamu.edu

<sup>3</sup>Department of Applied Physics and Applied Mathematics,  
Columbia University, New York, USA  
zhizhou0125@gmail.com

In this work, we develop variational formulations of Petrov-Galerkin type for one-dimensional fractional boundary value problems involving either a Riemann-Liouville or Caputo derivative of order  $\alpha \in (3/2, 2)$  in the leading term and both convection and potential terms. This type of problems arise in mathematical modeling of asymmetric super-diffusion processes in highly heterogeneous media. The well-posedness of the formulations and sharp regularity pickup of the weak solutions are established.

A novel finite element method is developed, which employs continuous piecewise linear finite elements and “shifted” fractional powers for the trial and test space, respectively. The new approach has a number of distinct features as it allows deriving optimal error estimates in both  $L^2$ - and  $H^1$ -norms and produces well conditioned linear systems, since the leading term of the stiffness matrix is diagonal matrix for uniform meshes. Further, in the Riemann-Liouville case, an enriched FEM is proposed to improve the convergence. Extensive numerical results are presented to verify the theoretical analysis and robustness of the numerical scheme.

## SUBDIFFUSION IN A NONCONVEX POLYGON

William McLean<sup>1a</sup>, Kim-Ngan Le<sup>1b</sup> and Bishnu P. Lamichhane<sup>2</sup>

<sup>1</sup>School of Mathematics and Statistics,  
The University of New South Wales, Sydney 2052, AUSTRALIA  
<sup>a</sup>w.mclean@unsw.edu.au, <sup>b</sup>n.le-kim@unsw.edu.au

<sup>2</sup>School of Mathematics and Physical Sciences,  
University of Newcastle, Callaghan, NSW 2308, AUSTRALIA  
blamichha@gmail.com

We consider the spatial discretisation of a time-fractional diffusion equation in a polygonal domain  $\Omega$  using continuous, piecewise-linear finite elements. If  $\Omega$  is convex, then the method is known to be second-order accurate in  $L_2(\Omega)$ , uniformly in time, but if the domain has a re-entrant corner then the error analysis breaks down because the associated Poisson problem is no longer  $H^2$ -regular. For a quasi-uniform family of triangulations with mesh parameter  $h$ , the error is of order  $h^{2\beta}$  if largest re-entrant corner has angle  $\pi/\beta$  with  $1/2 < \beta < 1$ , but a suitable local refinement strategy restores  $h^2$  convergence.

Analogous results for the classical heat equation were proved in 2006 by Chatzipantelidis, Lazarov, Thomée and Wahlbin.

## FINITE ELEMENT METHODS FOR FRACTIONAL DIFFUSION PROBLEMS

Kassem Mustapha<sup>1</sup>, Samir Karaa<sup>2</sup> and Amiya Pani<sup>3</sup>

<sup>1</sup>Department of Mathematics and Statistics,  
King Fahd University of Petroleum and Minerals, Saudi Arabia  
kassem@kfupm.edu.saa

<sup>2</sup>Department of Mathematics and Statistics, Sultan Qaboos University, Oman,  
skaraa@squ.edu.om

<sup>3</sup> Department of Mathematics, Indian Institute of Technology Bombay, India,  
akp@math.iitb.ac.in

The Galerkin (piecewise linear) finite element method is applied to approximate the solution of a time fractional diffusion equation with variable diffusivity. By a delicate energy analysis, *a priori* error bounds in  $L^\infty(H^j)$ ,  $j = 0, 1$  and  $L^\infty(L^\infty)$ -norms are derived for both smooth and nonsmooth initial data. Our analysis is based on a repeated use of an integral operator and use of a  $t^m$  type of weights to take care of the singular behavior at  $t = 0$ . The generalized Leibniz formula for fractional derivatives is found to play a key role in our analysis. Numerical experiments are presented to illustrate the theoretical results.

# NUMERICAL APPROXIMATION OF A VARIATIONAL PROBLEM ON BOUNDED DOMAIN INVOLVING THE FRACTIONAL LAPLACIAN

Joseph E. Pasciak<sup>a</sup>, Andrea Bonito<sup>b</sup>, and Wenyu Lei<sup>c</sup>

Department of Mathematics,  
Texas A&M University, College Station TX, USA  
<sup>a</sup>pasciak@math.tamu.edu,    <sup>b</sup>bonito@math.tamu.edu,  
<sup>c</sup>wenyu@math.tamu.edu

The mathematical theory and numerical analysis of non-local operators has been a topic of intensive research in recent years. One class of applications come from replacing Brownian motion diffusion by diffusion coming from a symmetric  $\alpha$ -stable Levy process, i.e., the Laplace operator is replaced by a fractional Laplacian.

In this talk, we propose a numerical approximation of equations with this type of diffusion terms posed on bounded domains. We focus on the simplest example of an elliptic variational problem coming from the fractional Laplacian on a bounded domain with homogeneous Dirichlet boundary conditions. Although it is conceptually feasible to study the Galerkin approximation based on a standard finite element space, such a direct approach is not viable as the exact computation of the resulting stiffness matrix entries is not possible (at least in two or more spatial dimensions).

Instead, we will develop a non-conforming method by approximating the action of the stiffness matrix on a vector (sometimes referred to as a matrix free approach). The bilinear form is written as an improper integral involving the solution of parameter dependent elliptic problems on  $R^d$ . We compute an approximate action of stiffness matrix by applying a SINC quadrature rule to the improper integral, replacing the problems on  $R^d$  by problems on parameter dependent bounded domains, and the application of the finite element method to the bounded domain problems. The entire procedure can be implemented using standard finite element tools, e.g., the DEAL-II library. The analysis of the resulting algorithm is discussed. In addition, the results of numerical computations on a model problem with known solution are given.

## A PDE APPROACH TO THE FRACTIONAL OBSTACLE PROBLEM

Ricardo H. Nochetto<sup>1</sup>, Enrique Otárola<sup>2</sup> and Abner J. Salgado<sup>3</sup>

<sup>1</sup>Department of Mathematics, University of Maryland,  
College Park, MD 20742, USA  
`rhn@math.umd.edu`

<sup>2</sup>Departamento de Matemática,  
Universidad Técnica Federico Santa María, Valparaíso, Chile  
`enrique.otarola@usm.cl`

<sup>3</sup>Department of Mathematics, University of Tennessee,  
Knoxville, TN 37996, USA  
`asalgad1@utk.edu`

We study solution techniques for the elliptic and parabolic obstacle problem with fractional diffusion. The fractional diffusion operator is realized as the Dirichlet-to-Neumann map of a nonuniformly elliptic problem posed on a semi-infinite cylinder. This allows us to localize the problem and consider instead a thin obstacle problem. We present, for the elliptic case, optimal error estimates based on recent regularity results. For the parabolic case we present an error analysis with minimal smoothness and one using the best regularity results available to date.

## ANOMALOUS DIFFUSION WITH RESETTING

Ercília Sousa

Department of Mathematics, University of Coimbra, Portugal  
`ecs@mat.uc.pt`

We consider a fractional partial differential equation that describes the diffusive motion of a particle, performing a random walk with Lévy distributed jump lengths, on one dimension with an initial position  $x_0$ . The particle is additionally subject to a resetting dynamics, whereby its diffusive motion is interrupted at random times and is reset to  $x_0$ . A numerical method is presented for this diffusive problem with resetting. The influence of resetting on the solutions is analysed and physical quantities such as pseudo second order moments and pseudo fractional order moments will be discussed. Some comments about what happens in the presence of boundaries will be also included. This talk is based on joint work with Amal K. Das from Dalhousie University (Canada).



# ACCURATE AND FAST NUMERICAL METHODS FOR FRACTIONAL PARTIAL DIFFERENTIAL EQUATIONS

Hong Wang

Department of Mathematics, University of South Carolina, USA  
hwang@math.sc.edu

Fractional partial differential equations (FPDEs) provide a powerful tool for modeling challenging phenomena including anomalous transport, and long-range time memory or spatial interactions in nature, science, social science, and engineering. However, FPDEs present mathematical and numerical difficulties that have not been encountered in the context of integer-order PDEs.

Computationally, because of the nonlocal property of fractional differential operators, the numerical methods for space-fractional FPDEs often generate dense stiffness matrices for which widely used direct solvers have a computational complexity of  $O(N^3)$  (per time step for a time-dependent problem) and memory requirement of  $O(N^2)$  where  $N$  is the number of unknowns (per time step for a time-dependent problem). This makes numerical simulation of three-dimensional FPDE modeling computationally very expensive.

What further complicates the scenario results from the fact that the solutions to fractional elliptic PDEs with smooth data and domain may have boundary layers and poor regularity. Consequently, a fast numerical scheme discretized on a uniform mesh cannot be effective. Hence, finite-difference methods, which are obtained via a discretization of Grünwald-Letnikov fractional derivatives, are out of the question. On the other hand, a numerical scheme discretized on an adaptively refined unstructured mesh offers great flexibility in resolving the boundary layers and other singularities, it destroys the structure of the dense stiffness matrix and so the efficiency of the numerical scheme.

We derive an accurate and fast numerical scheme by balancing the flexibility and efficiency: (i) This would use a composite mesh that consists of gridded mesh near the interface regions and a structured mesh in most of the domain. (ii) This would utilize the structure of the stiffness matrices on respective subdomains. (iii) This would use low-rank approximations to the “off-diagonal” dense matrix blocks in the stiffness matrix. (iv) The resulting fast method has approximately linear computational complexity (per time step) and optimal memory requirement.

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# AN ANALYSIS OF THE MODIFIED L1 SCHEME FOR THE TIME-FRACTIONAL PARTIAL DIFFERENTIAL EQUATIONS WITH NONSMOOTH DATA

Yubin Yan<sup>a</sup>, Monzororul Khan<sup>b</sup> and Neville J. Ford<sup>c</sup>

Department of Mathematics, University of Chester, CH1 4BJ, UK

<sup>a</sup>y.yan@chester.ac.uk, <sup>b</sup>sohel\_ban@yahoo.com,

<sup>c</sup>njford@chester.ac.uk

We consider the error estimates of the modified L1 scheme for solving time fractional partial differential equation. Jin et al. (2016, An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data, IMA J. of Numer. Anal., 36, 197-221) established an  $O(k)$  convergence rate for L1 scheme for both smooth and nonsmooth initial data. We introduce a modified L1 scheme and prove that the convergence rate is  $O(k^{2-\alpha})$ ,  $0 < \alpha < 1$  for both smooth and nonsmooth initial data. We first write the time fractional partial differential equation as a Volterra integral equation which is then approximated by using two convolution quadratures, respectively. The numerical schemes obtained are equivalent to the L1 scheme and the modified L1 scheme respectively. Laplace transform method is used to prove the error estimates for the homogeneous time fractional partial differential equation for both smooth and nonsmooth data. Numerical examples are given to show that the numerical results are consistent with the theoretical results.