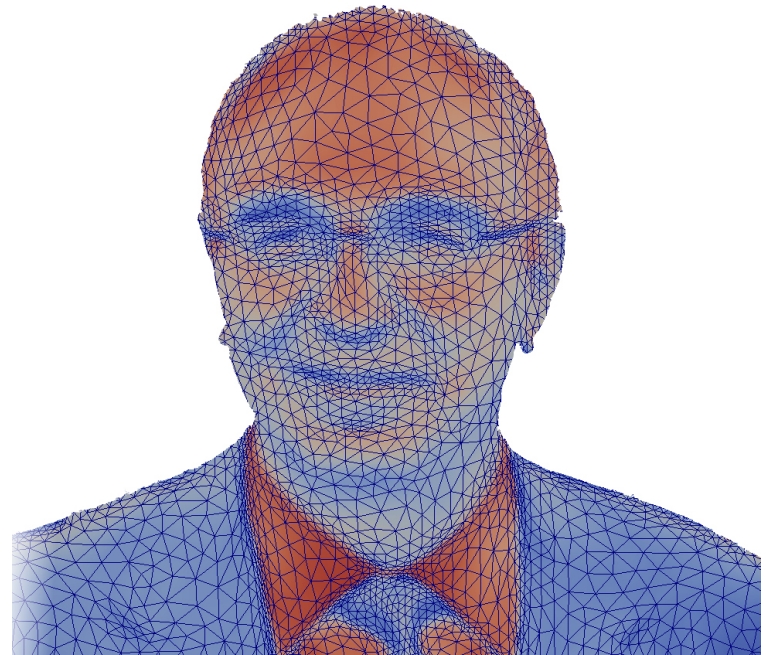


## Participants (Continued)

Stanimire Tomov, University of Tennessee  
 Vladimir Tomov, Texas A&M University  
 Tanya Vassilevska, Lawrence Livermore National Laboratory  
 Panayot Vassilevski, Lawrence Livermore National Laboratory  
 Jay Walton, Texas A&M University  
 Junping Wang, National Science Foundation  
 Xueying Wang, Texas A&M University  
 Kainan Wang, Texas A&M University  
 Jennifer Webster, Texas A&M University  
 Mary Wheeler, University of Texas at Austin  
 Joerg Willems, Texas A&M University  
 Yong Yang, Texas A&M University  
 Yangfang Yang, Texas A&M University  
 Fatma Yilmaz, Texas A&M University  
 Ivan Yotov, University of Pittsburgh  
 Anna Zemlyanova, Texas A&M University  
 Zhi Zhou, Texas A&M University  
 Ludmil Zikatanov, Pennsylvania State University

# Numerical Methods for PDEs: In Occassion of Raytcho Lazarov's 70th Birthday

Texas A&M University  
 College Station, Texas  
 Rudder Tower, Room 701  
 January 25-26, 2013



## Day 1 - January 25

8:45 a.m. - 9 a.m.	Welcome
9 a.m. - 9:30 a.m.	Svetozar Margenov, Bulgarian Academy of Sciences <i>Robust Multilevel Methods for Strongly Heterogeneous Problems</i>
9:30 a.m. - 10 a.m.	Ludmil Zikatanov, Pennsylvania State University <i>Numerical Approximation of Asymptotically Disappearing Solutions of Maxwell's Equations</i>
10 a.m. - 10:30 a.m.	Zhangxing Chen, University of Calgary <i>Numerical Simulation of Unconventional Oil and Gas Reservoirs</i>
10:30 a.m. - 11 a.m.	Break
11 a.m. - 11:30 a.m.	Hristo Kojouharov, University of Texas at Arlington <i>Dynamically Consistent Numerical Schemes for Microbial Population Models</i>
11:30 a.m. - noon	Pencho Petrushev, University of South Carolina <i>Gaussian Bounds for the Heat Kernel on the Interval, Ball, and Simplex</i>
noon - 12:20 p.m.	Victor Ginting, University of Wyoming <i>On the Application of the Continuous Galerkin Finite Element Method for Solving Multiphase Flow Problems</i>
12:20 p.m. - 2 p.m.	Lunch Break
2 p.m. - 2:30 p.m.	Mary Wheeler, University of Texas at Austin <i>Coupling Flow and Mechanics in Porous Media</i>
2:30 p.m. - 3 p.m.	Junping Wang, National Science Foundation <i>Weak Galerkin Finite Element Methods for PDEs</i>
3 p.m. - 3:30 p.m.	Peter Minev, University of Alberta <i>A Direction Splitting Algorithm for Flow Problems in Complex/Moving Geometries</i>
3:30 p.m. - 4 p.m.	Break
4 p.m. - 4:30 p.m.	Yuri Kuznetsov, University of Houston <i>Discretizations with Piece-Wise Constant Fluxes for Diffusion Equations</i>
4:30 p.m. - 5 p.m.	Ilya Mishev, Exxon Mobil Corporation <i>Mixed Multiscale Finite Volume Methods for Reservoir Simulation</i>
5 p.m. - 5:20 p.m.	Tzanio Kolev, Lawrence Livermore National Laboratory <i>High-Order Curvilinear Finite Elements for Lagrangian Hydrodynamics</i>
5:20 p.m. - 5:40 p.m.	Veselin Dobrev, Lawrence Livermore National Laboratory <i>High-Order Curvilinear ALE Hydrodynamics</i>
6:30 p.m. - 9 p.m.	Dinner Christopher's World Grille 5001 Boonville Rd., Bryan, Texas 77802 - (979)776-2181

## Participants (Continued)

Craig Gin, Texas A&M University  
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 Tzanio Kolev, Lawrence Livermore National Laboratory  
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 Peter Minev, University of Alberta  
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 Minam Moon, Texas A&M University  
 Murtazo Nazarov, Texas A&M University  
 Amir Nikooinenejad, Texas A&M University  
 Joe Pasciak, Texas A&M University  
 Guergana Petrov, Texas A&M University  
 Pencho Petrushev, University of South Carolina  
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## Organizing Committee

Wolfgang Bangerth  
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 Joseph Pasciak  
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 Bojan Popov

## Acknowledgements

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 Markus Bueg, Texas A&M University  
 Daniel Castanon, Texas A&M University  
 Zhangxing Chen, University of Calgary  
 Ulrich Colao, University of Kinshasa  
 Prabir Daripa, Texas A&M University  
 Kristy Delvo-Vela, Texas A&M University  
 Leszek Demkowicz, University of Texas at Austin  
 Denis Devaud, École Polytechnique Fédérale de Lausanne  
 Veselin Dobrev, Lawrence Livermore National Laboratory  
 Sourav Dutta, Texas A&M University  
 Yalchin Efendiev, Texas A&M University  
 Rita Ewing, Texas A&M University  
 Shubin Fu, Texas A&M University  
 Stephen Fulling, Texas A&M University  
 Arezou Gheshmati, Texas A&M University

## Day 2 - January 26

9 a.m. - 9:30 a.m.	Panayot Vassilevski, Lawrence Livermore National Laboratory <i>Improving Conservation Properties of First-Order System Least Squares Finite-Element Methods</i>
9:30 a.m. - 10 a.m.	Leszek Demkowicz, University of Texas at Austin <i>A Tutorial on Discontinuous Petrov Galerkin Method (DPG) with Optimal Test Functions</i>
10 a.m. - 10:20 a.m.	Stanimire Tomov, University of Tennessee <i>Numerical Linear Algebra for Emerging Architectures: Challenges and Approaches</i>
10:20 a.m. - 10:50 a.m.	Break
10:50 a.m. - 11:20 a.m.	Ivan Yotov, University of Pittsburgh <i>Multiscale Domain Decomposition Methods for Porous Media Flow Coupled with Geomechanics</i>
11:20 a.m. - 11:50 a.m.	Joseph Pasciak, Texas A&M University <i>An Analysis of Finite Element Approximation to the Eigenvalues of Problems Involving Fractional Order Differential Operators</i>
11:50 a.m. - noon	Closing

*Robust Multilevel Methods for Strongly Heterogeneous Problems*

**Svetozar Margenov, Bulgarian Academy of Sciences**

The first part of the talk is devoted to construction and analysis of hierarchical basis algebraic multilevel iteration (AMLI) methods in the case of coefficient jumps which are aligned with the interfaces of the initial mesh. The condition number estimates are uniform with respect to both mesh and/or coefficient anisotropy, the coefficient jumps, as well as the size of the discrete problem. The computational complexity is proportional to the number of degrees of freedom.

Robust multilevel methods for high-frequency and high-contrast problems are presented in the second part. Some advantages of the nonlinear AMLI methods including the case of element-by-element approximation of the Schur complement are discussed.

The numerical tests demonstrate: (i) robustness of the convergence estimates, and (ii) recent scalability results beyond some assumptions of the rigorous theory.

*An Analysis of Finite Element Approximation to the Eigenvalues of Problems Involving Fractional Order Differential Operators*

**Joseph Pasciak, Texas A&M University**

Co-Authors: Bangti Jin and Raytcho Lazarov, Texas A&M University

In this talk, we consider an eigenvalue problem coming from a boundary value problem involving fractional derivatives. Specifically, we consider the Caputo and Riemann-Liouville fractional differential operators and associated boundary conditions. These boundary value problems will be investigated from a variational point of view. We are interested in the case when the differential operator is of order  $\alpha$  with  $\alpha \in (1, 2)$ . These derivatives lead to non-symmetric boundary value problems. The Riemann-Liouville case is somewhat simpler as the underlying variational problem is coercive on a natural subspace of  $H^{\alpha/2}(0, 1)$  even though its solutions are less regular. The variational formulation of the Caputo derivative case is more interesting as it leads to a variational problem involving different test and trial spaces. In this case, one is required to prove variational stability on the discrete level as well.

In both cases, the analysis of the eigenvalue problem involves the derivation of “so-called” shift theorems which demonstrate that the solution of the variational problem and its adjoint are more regular, i.e., are in  $H^{\alpha/2+\gamma}(0, 1)$  with  $\gamma > 0$ . The regularity pickup enables one to prove that the norm of the solution minus that of the finite element approximation converges with  $\gamma$  dependent rates. This, in turn, can be used to deduce eigenvalue/eigenvector convergence rates. Finally, the results of numerical experiments illustrating the theory will be presented.

*Multiscale Domain Decomposition Methods for Porous Media Flow Coupled with Geomechanics*

**Ivan Yotov, University of Pittsburgh**

We consider numerical modeling of the system of poroelasticity, which describes fluid flow in deformable porous media. The focus is on locally mass conservative flow discretizations that provide efficient and accurate multiscale approximations on rough grids and for highly heterogeneous media. We employ a multiscale mortar finite element method, where the equations in the coarse elements (or subdomains) are discretized on a fine grid scale, while continuity of normal velocity and stress between coarse elements is imposed via a mortar finite element space on a coarse grid scale. With an appropriate choice of polynomial degree of the mortar space, optimal order convergence is obtained for the method on the fine scale. The algebraic system is reduced via a non-overlapping domain decomposition to a coarse scale mortar interface problem that is solved efficiently using a multiscale flux basis.

*Numerical Approximation of Asymptotically Disappearing Solutions of Maxwell's Equations*

**Ludmil Zikatanov, Pennsylvania State University**

This work is on the numerical approximation of incoming solutions to Maxwell's equations with maximally dissipative boundary conditions, whose energy decays exponentially with time. We use the standard Nedelec-Raviart-Thomas elements and a Crank-Nicholson scheme to approximate such solutions. We prove that with divergence free initial conditions, the fully discrete approximation to the electric field is weakly divergence-free for all time. We show numerically that the finite-element solution approximates well the asymptotically disappearing solutions constructed analytically when the mesh size becomes small. This is a joint work with James Adler (Tufts University) and Vesselin Petkov (University of Bordeaux 1).

*Numerical Simulation of Unconventional Oil and Gas Reservoirs*

**Zhangxing Chen, University of Calgary**

Mathematical models have widely been used to predict, understand, and optimize complex physical processes in modeling and simulation of multiphase fluid flow in petroleum reservoirs. These models are important for understanding the fate and transport of chemical species and heat. With this understanding the models are then applied to the needs of the petroleum industry to design enhanced oil and gas recovery strategies.

While mathematical modeling and computer simulation have been successful in their application to the recovery of conventional oil and gas, there still exist a lot of challenges in their application to unconventional oil and gas modeling. As conventional oil and gas reserves dwindle and oil prices rise, the recovery of unconventional oil and gas (such as heavy oil, oil sands, tight gas, and shale gas) is now the center stage. For example, enhanced heavy oil recovery technologies are an intensive research area in the petroleum industry, and have recently generated a battery of recovery methods, such as cyclic steam stimulation (CSS), steam assisted gravity drainage (SAGD), vapor extraction (VAPEX), in situ combustion (ISC), hybrid steam-solvent processes, and other emerging recovery processes, and horizontal well and hydraulic fracturing technologies have been very successful in the production of tight and shale reservoirs. This presentation will give an overview on challenges encountered in modeling and simulation of these recovery processes: insufficient physics/chemistry in current models, multi-scale phenomena, phase behavior, geomechanics, assisted history matching with closed-loop optimization, transport of solvents, wellbore modeling, and four-phase flow. It will also present some case studies for the applications of these recovery processes to real heavy oilfields and shale gas reservoirs.

*Numerical Linear Algebra for Emerging Architectures: Challenges and Approaches*

**Stanimire Tomov, University of Tennessee**

Numerical PDEs and their application in a wide range of science and engineering applications depend on the availability of high-performance linear algebra libraries; these applications will not perform well unless linear algebra libraries perform well. In the past, high-performance numerical library developers have taken for granted that each successive generation of microprocessors would make their old software run substantially faster. The emergence of the multicore and heterogeneous processor designs have brought this “free ride” to an end. Existing numerical libraries built on the old model are unable to effectively exploit these new architectures without radical modification. In this talk I will describe some of the current challenges and approaches in addressing this critical and highly disruptive situation in the area of dense linear algebra. Examples will be given with new algorithms, extending the LAPACK and ScaLAPACK libraries to efficiently support heterogeneous systems of multicore CPUs, GPUs, and/or coprocessors.



*A Tutorial on Discontinuous Petrov Galerkin Method (DPG) with Optimal Test Functions*

**Leszek Demkowicz, University of Texas at Austin**

Co-Author: Jay Gopalakrishnan, Portland State University

We will give a short tutorial on the DPG method emphasizing the main points and illustrating them with numerical examples. Here is a few of them:

1. The DPG method is a minimum-residual method with the residual evaluated in a dual norm.
2. The method can be interpreted as a Petrov-Galerkin method with optimal test functions (realizing the sup in the inf-sup condition).
3. The optimal test functions are computed on the fly by inverting approximately the Riesz operator corresponding to the test space.
4. With broken test spaces and localizable norms, the inversion is done elementwise, i.e. the optimal test functions are computed within the element routine. This is more expensive than for standard FE method but it is compatible with the standard FE technology.
5. The main price paid for the localization is the presence of additional unknowns: traces and fluxes. Compared with standard conforming FE methods or hybridizable DG methods, the number of (non-local) unknowns doubles and it is of the same range as for DG methods. Contrary to DG methods based on numerical flux, in the DPG method, the flux enters as additional unknown.
6. The method can be interpreted as a preconditioned least squares method. The stiffness matrix is hermitian and positive-definite but its condition number is the same as for standard FEs.
7. The formulation based on a first order system is very natural but not necessary. You can wish with the second order equation if you wish. The key point is to break the test functions.
8. There is nothing exotic about the ultra-weak variational formulation behind the DPG method. If the operator is well posed in the  $L^2$  sense (the operator is  $L^2$  bounded below), the ultra-weak variational formulation is also well posed with the corresponding inf-sup constant being of the same order.
9. With the use of optimal test functions, the issues of approximability and stability are fully separated. This is illustrated by using hp-adaptivity.
10. The method is especially suited for singular perturbation problems, e.g., convection-dominated diffusion, high wave number wave propagation, elasticity for thin-walled structures, etc. For problems of this type, one can systematically design a test norm to accomplish robustness, i.e., a stability uniform in the perturbation parameter.
11. If you have a hybrid FE code, converting it to a DPG code is very easy.
12. The methodology extends to nonlinear problems. We will show examples for compressible NS equations.

*Dynamically Consistent Numerical Schemes for Microbial Population Models*  
**Hristo Kojouharov, University of Texas at Arlington**

Several different mathematical models of complex biological systems involving microbial populations are briefly discussed. In addition, a finite-difference approach is presented for solving the corresponding systems of differential equations. It is based on a nonlocal modeling of the nonlinear right-hand side functions and a nonstandard discretization of the time-derivative. Positive and elementary-stable nonstandard (PESN) finite difference methods are also formulated and analyzed based on extensions of the nonstandard discretization rules. A series of numerical results are presented to demonstrate the performance of the proposed numerical methods.

*Gaussian Bounds for the Heat Kernel on the Interval, Ball, and Simplex*

**Pencho Petrushev, University of South Carolina**

We establish Gaussian upper and lower bounds for the heat kernel associated with the Jacobi operator and polynomials on the interval. Gaussian bounds are also proved for the heat kernels associated with orthogonal polynomials and respective operators on the ball and simplex with weights. The general machinery of Dirichlet spaces is utilized in this development, where the local Poincare inequality plays a crucial role. These results are used for the construction of localized frames, which in turn provide a tool for decomposition of weighted Besov and Triebel-Lizorkin spaces in the settings of interest.

*Improving Conservation Properties of First-Order System Least Squares Finite-Element Methods*

**Panayot Vassilevski, Lawrence Livermore National Laboratory**

The first-order system least-squares (FOSLS) finite element method for solving partial differential equations has many advantages, including the construction of symmetric positive definite algebraic linear systems that can be solved efficiently with multilevel iterative solvers. However, one drawback of the method is the potential lack of conservation of certain properties. One such property is conservation of mass. In this talk we describe a strategy for achieving mass conservation for a FOSLS system by changing the minimization process to that of a constrained minimization problem. If the space of corresponding Lagrange multipliers contains the piecewise constants, then local mass conservation is achieved similarly to the standard mixed finite element method. To make the strategy more robust and not add too much computational overhead to solving the resulting saddle-point system an overlapping Schwarz process is applied which we illustrate with numerical tests.

This talk is based on the report: J.H. Adler, P.S. Vassilevski, Improving conservation for first-order system least squares finite-element methods. Lawrence Livermore National Laboratory Technical Report LLNL-PROC-579552, September 6, 2012.

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*High-Order Curvilinear ALE Hydrodynamics*

**Veselin Dobrev, Lawrence Livermore National Laboratory**

Co-Authors: Robert Anderson, Tzanio Kolev, and Robert Rieben, Lawrence Livermore National Laboratory

The Arbitrary Lagrangian-Eulerian (ALE) framework forms the basis of many large-scale multi-material shock hydrodynamics codes. Current ALE discretization approaches consist of a Lagrange phase, where the hydrodynamics equations are solved on a moving mesh, followed by a three-part “advection phase” involving mesh optimization, field remap and multi-material zone treatment. While current ALE methods have been successful at extending the capability of pure Lagrangian methods, they also introduce numerical problems of their own including a lack of total energy conservation and artificial breakup of material interfaces. In this talk we will discuss the application of the curvilinear technology to the “advection phase” in order to develop new and more robust high-order ALE algorithms, while preserving the accuracy of the high-order Lagrange step. We will present some approaches for high-order extensions to classical mesh optimization algorithms, such as harmonic and equipotential smoothing, as well as the use of global mesh optimization methods. We will also discuss possible approaches to define conservative and monotonic high-order field remap and conclude the talk with some preliminary numerical results.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

*On the Application of the Continuous Galerkin Finite Element Method for Solving Multiphase Flow Problems*

**Victor Ginting, University of Wyoming**

One major drawback that prevents the use of the standard continuous Galerkin finite element method in solving conservation problems is its lack of a locally conservative flux. We present a simple post-processing for the continuous Galerkin finite element method resulting in a locally conservative flux. The post-processing requires an auxiliary fully Neumann problem to be solved independently on each finite element. Its performance is demonstrated through numerical examples of multi-phase flow in subsurface formation with triangular and quadrilateral elements along. This is a joint work with Lawrence Bush of the University of Wyoming.

*Coupling Flow and Mechanics in Porous Media*

**Mary Wheeler, University of Texas at Austin**

No abstract available.

*High-Order Curvilinear Finite Elements for Lagrangian Hydrodynamics*

**Tzanio Kolev, Lawrence Livermore National Laboratory**

Co-Authors: Veselin Dobrev and Robert Rieben, Lawrence Livermore National Laboratory

The discretization of the Euler equations of gas dynamics in a moving Lagrangian frame is at the heart of many multi-physics simulation algorithms. In this talk, we present a general framework for high-order Lagrangian discretizations of the compressible shock hydrodynamics equations using curvilinear finite elements. This method is derived through a variational formulation of the momentum and energy conservation equations using high-order continuous finite elements for the velocity and position, and a high-order discontinuous basis for the internal energy field. The use of high-order position description enables curvilinear zone geometries allowing for better approximation of the mesh curvature which develops naturally with the flow. The semi-discrete equations involve velocity and energy mass matrices which are constant in time due to the notion of strong mass conservation. We also introduce the concept of generalized corner force matrices, which together with the strong mass conservation principle, imply the exact total energy conservation on a semi-discrete level. The fully-discrete equations are obtained by the application of a Runge Kutta-like energy conserving time stepping scheme. We review the implementation of these ideas in our research codes, and present a number of 2D, 3D and axisymmetric computational results demonstrating the benefits of the high-order approach for Lagrangian computations.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

*Mixed Multiscale Finite Volume Methods for Reservoir Simulation*

**Ilya Mishev, Exxon Mobil Corporation**

Co-Author: Lijian Jiang

Multiscale finite volume (MsFV) methods have been successfully applied to solving reservoir simulation problems with localized high heterogeneity (i.e., separable scales), but the accuracy decreases when this is not possible (non-separable scales and long-range features). We develop a mixed multiscale finite volume method (MMsFV) on a uniform mesh that can use global information in order to improve the accuracy and the robustness of the multiscale simulations of fluid flows in porous media with non-local features.

Our development starts with the observation that MPFA methods implicitly approximate the velocity and therefore any multiscale generalization also has to do the same. MsFV uses multiscale approximation of the pressure and piecewise constant approximation of the velocity. The novelty of the MMsFV method is the explicit approximation of the velocity, with a new multiscale basis being constructed to approximate the pressure with piecewise constants. The velocity basis functions can be calculated with either local information (local MMsFV) or global information (global MMsFV). We demonstrate the improved accuracy of the global MMsFV compared to the local version on several problems including the SPE 10 comparative solution problem. The error of the global MMsFv is usually several times smaller than that of the local method.

Using the same framework and the extra flexibility of the two approximation spaces, we can derive other mixed multiscale finite volume methods including extensions to unstructured meshes.

*Weak Galerkin Finite Element Methods for PDEs*

**Junping Wang, National Science Foundation**

In this talk, the speaker will introduce a new finite element technique, called Weak Galerkin (WG) finite element methods, for partial differential equations. The basic principles of WG will be thoroughly explained, and the method shall be applied to the discretization of several PDEs, including the model second order elliptic equations, Stokes, biharmonic, div-curl, and Curl4 problems. It will be seen that the WG method is widely applicable to elliptic-type problems, and the WG-FEM enjoys a great flexibility in mesh shape and generation.

*A Direction Splitting Algorithm for Flow Problems in Complex/Moving Geometries*

**Peter Minev, University of Alberta**

An extension of the direction splitting method for the incompressible Navier-Stokes equations proposed in [1], to flow problems in complex, possibly time dependent geometries will be presented. The idea stems from the idea of the fictitious domain/penalty methods for flows in complex geometry. In our case, the velocity boundary conditions on the domain boundary are approximated with a second-order of accuracy while the pressure subproblem is harmonically extended in a fictitious domain such that the overall domain of the problem is of a simple rectangular/parallelepiped shape.

The new technique is still unconditionally stable for the Stokes problem and retains the same convergence rate in both, time and space, as the Crank-Nicolson scheme. A key advantage of this approach is that the algorithm has a very impressive parallel performance since it requires the solution of one-dimensional problems only, which can be performed very efficiently in parallel by a domain decomposition Schur complement approach. Numerical results illustrating the convergence of the scheme in space and time will be presented. Finally, the implementation of the scheme for particulate flows will be discussed and some validation results for such flows will be presented.

Reference:

1. J.L. Guermond, P.D. Minev, A new class of massively parallel direction splitting for the incompressible Navier-Stokes equations. *Computer Methods in Applied Mechanics and Engineering*, 200 (2011), 2083-2093.

*Discretizations with Piece-Wise Constant Fluxes for Diffusion Equations*

**Yuri Kuznetsov, University of Houston**

In this presentation we discuss a new approach to the discretization of diffusion equations on polygonal/polyhedral meshes. The basic idea is to approximate the solution flux by piece-wise constant vector-functions which are conforming on the interfaces between mesh cells. The error estimate is derived for the solution flux in the case of special types of mesh cells. Numerical results as well as applications in geosciences are given.