Guangri Xue's Publication List and Abstracts

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Research Interests

My research is directed toward developing efficient and accurate solutions to multiphase, multicomponent, multidomain, multiscale and multiphysics problems encountered in modeling of real-world physical and chemical phenomena. Computational Fuel Cell Dynamics, the focus of my Ph.D. dissertation work, is one such application.

Publications and Abstracts

1. P. Sun, G. Xue, C-Y Wang and J. Xu, "New Numerical Techniques for Two-Phase Transport Model in the Cathode of Polymer Electrolyte Fuel Cell", submitted, 2007.

   Abstract. In this paper, we present some new numerical techniques for finite element methods for 2D steady-state two-phase model in the cathode of polymer electrolyte fuel cell (PEFC) that contains a gas channel and a gas diffusion layer (GDL). This two-phase PEFC model is typically modeled by a modified Navier-Stokes equation for the mass and momentum, with Darcys drag as an additional source term in momentum for flows through GDL, and a discontinuous and degenerate convection-diffusion equation for water concentration. Based on the mixed finite element method for the modified Navier-Stokes equation and standard finite element method for water equation, we design streamline-diffusion and Galerkin-least-squares to overcome the dominant convection arising from the gas channel. Meanwhile, we employ Kirchhoff transformation to deal with the discontinuous and degenerate diffusivity in water concentration. Numerical experiments demonstrate that our finite element methods, together with these new numerical techniques, are able to get accurate physical solutions with fast convergence.

2. P. Sun, G. Xue, C-Y Wang and J. Xu, "A Domain Decomposition Method for Two-Phase Transport Model in the Cathode of Polymer Electrolyte Fuel Cell", submitted, 2007.

   Abstract. In this paper, based on Kirchhoff transformation, we develop a Dirichlet-Neumann alternating iterative domain decomposition method for 2D steady-state two-phase model in the cathode of polymer electrolyte fuel cell (PEFC) that contains a gas channel and a gas diffusion layer (GDL). This two-phase PEFC model is typically presented by a modified Navier-Stokes equation with Darcys drag as an additional source term in momentum equation for flows through GDL, and a discontinuous and degenerate convection-diffusion equation for water concentration. For both cases of dry and wetted gas channel, we employ Kirchhoff transformation and Dirichlet-Neumann alternating iteration with appropriate interfacial conditions on GDL/gas channel interface to deal with the jump nonlinearities of water equation. Numerical experiments demonstrate that fast convergence as well as accurate numerical solutions are retained simultaneously in terms of these numerical techniques, along with a combined finite element-upwind finite volume discretization for automatically controlling the dominant convection terms arising in gas channel.

3. X. Xie, J. Xu and G. Xue, "Uniformly Stable Finite Element Methods for Darcy-Stokes-Brinkman Models", submitted, 2007.

   Abstarct. We consider 2D and 3D Darcy-Stokes interface problems. These equations are related to the Brinkman model that treats both Darcy's law and Stokes equations in a single form of PDE but with strongly discontinuous viscosity coefficient and zero order term coefficient. In this model relatively large viscosity coefficient and small zero-order term coefficient correspond to the Stokes equations wheres small viscosity coefficient and large zero-order term coefficient correspond to the Darcy's law. The main results of this paper are: 1. A traditional stable and uniformly-consistent Stokes element is also uniformly

stable for Darcy-Stokes-Brinkman models if and only if the pressure space contains the divergence range of the velocity space. 2. We develop several new nonconforming finite element methods that are uniformly stable (with respect to viscosity coefficient, zero order term coefficient and their jumps).

4. Y. Cao, T. Grandine, J. V. Laarhoven, O. Terlyga, J. Wu, G. Xue and P. Zhang, "WEB-Spline Finite Elements", IMA Mathematical Modeling Workshop 2006, IMA Preprint Series #2133-2.

   Abstract. B-splines are an intriguing choice of finite elements in the finite element method. B-splines form a basis for any space of piecewise polynomial functions in one variable, including those which have specified continuity conditions at the junctions between the individual polynomial pieces. However, extensions to more than one variable have been hard to come by. In our project, we implement a finite element method for an elliptic PDE by using weighted extended B-spline (WEB-spline). The WEB-spline approximation takes care of not only the boundary constraints but also the issue of well conditioning of the Galerkin systems. This choice of basis functions provides optimal approximation order with a minimal number of parameters, thus providing a natural link between geometry description and finite element simulations. We wrote Python code and tested it on Poissons equation over a 1) a circle 2) a piecewise smooth, simply connected region and 3) a region with a hole in it.

5. P. Sun, G. Xue, C-Y Wang and J. Xu, "A Combined Finite Element-Upwind Finite Volume Method for three Dimensional Simulation of Liquid Feed Direct Methanol Fuel Cell", preprint, 2007.

   Abstract. In this paper, a three-dimensional (3D), two-phase transport model of liquid feed direct methanol fuel cell (DMFC), which is based on the multiphase mixture formulation and encompasses all components in a DMFC using a single domain approach, is specifically studied and simulated by a combined finite element-upwind finite volume method together with partial Newton's linearization. Numerical simulations in 3D are carried out to explore and design efficient and robust numerical algorithms for the sake of fast and convergent nonlinear iteration. A more reasonable source term for water transport equation is given, and a series of efficient numerical algorithms and discretizations are designed and analyzed to achieve this goal. Our numerical simulations show that the convergent physical solutions can be reached within one hundred more steps. Attained reasonable numerical solutions illustrate that our numerical methods and iterative algorithms are efficient and robust.

6. G. Xue, J. Xu, C-Y Wang and R. Falgout, "Multilevel Newton's method for a two phase mixture model with nonlinear discontinuous degenerate diffusion coefficient", preprint, 2007.

   Abstract. The traditional Newton's method requires certain smoothness of the coefficients of partial differential equations to get local convergence. In this paper, multilevel and continuation Newton's methods are developed for a two phase mixture flow model in porous media with nonlinear discontinuous degenerate diffusion coefficient arising in fuel cell applications. A major finding is that the discrete algebraic equation after using linear finite element method is Lipschitz continuous. Numerical example shows the robustness of this method.

7. G. Xue, "Uniform Preconditioners for Darcy-Stokes-Brinkman Models", preprint, 2007.

   Abstract. In Darcy-Stokes-Brinkman models relatively large viscosity coefficient and small zero-order term coefficient correspond to the Stokes equations wheres small viscosity coefficient and large zero-order term coefficient correspond to the Darcy's law. The main result of this paper is that a uniform preconditioner for the Schur Complement of this

parameter dependent saddle problem is developed for the discrete models arising from the uniformly stable finite element methods [3].

8. J. Brannick, R. Falgout, J. Xu, G. Xue and L. Zikatanov, "Algebraic Multigrid Methods in Direct Methanol Fuel Cells", preprint, 2007.

Abstract. In this paper, we will develop algebraic multigrid method as a solver/preconditioner for the linear algebraic systems arising from multiphysics simulation of fuel cells [5].