Summer Program on Nonlocal Continuum Models for Diffusion, Mechanics and Other Applications

Nonlocal discrete models are common in many applications. For example, molecular dynamics and other particle methods having interactions that extend beyond nearest neighbors are in common use. Less popular are nonlocal continuum models which are very much dominated in their usage by local continuum models and especially differential equation models.

However, in recent years, there has been burgeoning interest in mathematical, scientific, and engineering circles in nonlocal continuum models, especially for solid mechanics, diffusion, and wave propagation. This interest is motivated by the desire to model singular or anomalous behavior such as cracks and fracture in solids and, more generally, by the need to develop multiscale models, that is, models that are valid and tractable over a wide range of temporal and spatial scales. As a result, there are by now researchers all over the world investigating diverse aspects of nonlocal continuum models.

This Summer Program took place as a single workshop, June 25-29 2012. Participants discussed modeling, mathematical, statistical, computational, and applications issues such as

- kernel choices
- connections between nonlocal continuum models and discrete models such as Molecular Dynamics
- well posedness of the equations
- limiting behaviors of solutions
- Finite element and other discretization methods
- efficient solution methods for discretized systems
- uncertainty quantification
- applications including but not limited to mechanics, image processing, graphs, diffusion, and wave propagation

Uncertainty quantification (UQ) through nonlocal models is especially intriguing because of the very different nature of local and nonlocal models with respect to such effects as dispersion, smoothing or the lack thereof.

The format of the program was unusual, consisting of only eight invited tutorial lectures, the remainder of the time being divided into six poster sessions. This format was found to maximize the interaction among participants.

For the remainder of this report, we give (a) the workshop proposal approved by the SAMSI Directorate and National Advisory Committee, (b) the program, (c) the detailed list of posters presented.

One week Summer Program on Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications

Nonlocal discrete models are common in many applications. For example, molecular dynamics and other particle methods having interactions that extend beyond nearest neighbors are in common use. Less popular are nonlocal continuum models which are very much dominated in their usage by local continuum models, especially differential equation models. However, in recent years, there has been burgeoning interest in mathematical, scientific, and engineering circles in nonlocal continuum models, especially for solid mechanics, diffusion, and wave propagation. This interest is motivated by the desire to model singular or anomalous behavior such as cracks and fracture in solids and, more generally, by the need to develop multiscale models, that is, models that are valid and tractable over a wide range of temporal and spatial scales. As a result, there are by now researchers all over the world investigating diverse aspects of nonlocal continuum models. This Summer workshop will bring together such researchers from the mathematical, statistical, computational, scientific, and engineering communities to talk about their interests and research and establish lasting, synergistic connections that lead to new research. We are also interested in having participants who may not be involved in research into nonlocal continuum models, but that have expertise in areas that will influence future research into those models. One particular direction of that research is into uncertainty quantification which will require researchers in nonlocal continuum models to interact with statisticians so as to develop good models for Uncertainty Quantification.

Organizers

Max Gunzburger (Florida State) and Richard Lehoucq (Sandia)

SAMSI Liaison

Pierre Gremaud

Date and place

SAMSI, June 25-29, 2012

Confirmed participants as of early April 2012

Burak Aksoylu (Tobb U. Turkey), Stephen Bond (Sandia), Nathanial Burch (SAMSI), Xi Chen (Florida State U.), Marta D'Elia (Florida State), Albert Erkip (Sabanci U., Turkey), Richard Fabiano (UNC Greensboro), Greg Forrest (UNC Chapel Hill), Eliot Fried (McGill), John Fricks (Penn State), Joe Goddard (UCSD), Zhen Guan (U. Tennessee, Knoxville), Maila Hallare (U. Kansas), Steven Henke (Florida State), Xiaojie Hou (UNC Wilmington), Zhan Huang (Penn State), Lili Ju

(U. South Carolina), Jeremy Lechman (Sandia), Alan Lenarcic (UNC Asheville), Jiao Li (U. Wisconsin Milwaukee), Xiaofan Li (IIT), Sharon Lubkin (NCSU), Tchavdar Marinov (Southern U.), Rossitza Marinova (Concordia), Scott McKinney (U. Florida), Tadele Mengesha (Penn State), Mark Meerschaert (Michigan State), Pachenko (Washington State U.), Michael Parks (Sandia), Maria Teresa Perez-Llanos (U. Autonoma de Madrid, Spain), Petronale Radu (U. Nebraska), Michael Raghib (LANL), Naveen Ramunigari (U. Texas), Julio Rossi (U. Alicante, Spain), Ekkehard Sachs (U. Trier, Germany), Alla Sikorskii (Michigan State), Pablo Seleson (Texas at Austin), Peter Straka (Michigan State U.), Zuhal Unlu (LSU), Ying Wang (U. Minnesota), Wojbor Woyczynski (Case Western), Dexuan Xie (U. Wisconsin, Milwaukee), XiaoXia Xie (Auburn), Ling Xu (U. New Mexico), Guannan Zhang (Florida State)

We expect between 70 and 90 participants.

An example

As an example of a nonlocal continuum model, consider the equation

$$u_t = -2 \int_\Omega (u(y,t) - u(x,y))\ \gamma(x,y)\, dy \tag{1}$$

for a function $u(x,t)$; here, $\gamma(x,y)$ is a given kernel. This equation is nonlocal because interaction occurs between points x and y that are separated. This is a nonlocal diffusion equation which has applications in research areas such as fractional diffusion and fractional Laplacians, image analyses, machine learning, nonlocal Dirichlet forms, nonlocal heat conduction, dense graphs (graph Laplacians).

The model (1) and its solutions have several important features that makes them interesting. In additional to being a nonlocal, continuum model, (1) is free of spatial derivatives. For certain kernels $\gamma(x,y)$ and for smooth function u, (1) reduces, in an appropriate limit, to the heat equation. If one considers the operator on the right-hand side of (1), or if one considers the steady-state version of (1)) given by

$$-2 \int_\Omega (u(y,t) - u(x,y))\ \gamma(x,y)\, dy = b(x), \tag{2}$$

practical kernels $\gamma(x,y)$ can be defined such the solution u does not possess two more (weak) derivatives compared to the data $b(x)$ as is the case for elliptic partial differential equations. In fact, one can have, for $s \in [0,1)$, that if $b \in H^{-s}(\Omega)$, then $u \in H^s(\Omega)$. Thus, the case of no smoothing is included. Of particular interest are kernels for which $s \in [0,1/2)$ because then, equations such as (1) and (2) admit solutions with jump discontinuities so that generalizations of these equations can be used to model cracks and other discontinuous behaviors. Furthermore, for such kernels, one can discretize these equations using discontinuous finite element spaces without the need for accounting for any fluxes across element boundaries as is the case for, e.g., elliptic partial differential operators. This is just a sampling of the properties and results about nonlocal models such as (1) that have great mathematical interest and, at the same time, have deep implications to many applications.

Note that if u_t in (1) is replaced by u_{tt}, we then have a nonlocal "wave" equation. Such equations have very different character, e.g., with respect to speed of propagation, dispersion,

etc., compared the classical wave equation; these differences could have important implications to several application areas. A vector-valued form of (1) with u_t replaced by u_{tt} is equivalent to the peridynamics model for the mechanics of linear materials. Nonlinear version of (1) and (2) are also of interest, especially in the peridynamics setting.

Program topics

Participants in the workshop will discuss modeling, mathematical, statistical, computational, and applications issues such as

- choices for the kernel $\gamma(x, y)$
- connections between nonlocal continuum models and discrete models such as MD
- well posedness of the equations
- limiting behaviors of solutions
- finite element and other discretization methods
- efficient solution methods for discretized systems
- uncertainty quantification
- applications including but not limited to mechanics, image processing, graphs, diffusion, and wave propagation.

Uncertainty quantification through nonlocal models is especially intriguing because of the very different nature of local and nonlocal models with respect to such effects as dispersion, smoothing or the lack thereof, etc

Program format

The format of the program will be novel. Tutorials will be given on the first 1.5 day (Monday and Tuesday morning). This will be followed by poster blitzes on Tuesday afternoon, Wednesday and Thursday (short presentations paired with posters). On Friday morning, a tutorial on available software will be offered. We expect this slightly nonstandard format to foster new discussions and interactions. The workshop will conclude with a session on future directions.

Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications
June 25-29, 2012

SCHEDULE

Monday, June 25
Radisson

8:15-8:50	Registration and Continental Breakfast
8:50-9:00	Welcoming Remarks: **Pierre Gremaud,** SAMSI
9:00-10:30	Tutorial 1: **Eliot Fried**, McGill University *"Established Continuum Approaches to Spatial Nonlocality"*
10:30-11:00	Break
11:00-12:00	Tutorial 2 (first part): **Greg Forest**, UNC *"The Dissipation Side of Fluctuation-Dissipation in Complex Fluids"*
12:00-1:30	Lunch
1:30-2:30:	Tutorial 2 (second part): **Scott McKinley**, University of Florida *"The Fluctuation Side of Fluctuation-Dissipation in Complex Fluids"*
2:30-3:00	Break
3:00-5:00	Tutorial 3: **Rich Lehoucq**, Sandia National Laboratories *"The Peridynamic Nonlocal Continuum Theory"* **Max Gunzburger**, Florida State University *"Analyses and Finite Element Methods for the Peridynamic Nonlocal Continuum Theory and Related Diffusion Models"*
5:00-7:00	Reception

Tuesday, June 26
Radisson

8:30-9:00	Registration and Continental Breakfast
9:00-11:30	Tutorial 4: **Mark Meerschaert** and **Alla Sikorskii**, Michigan State University *"Fractional Calculus Models for Anomalous Diffusion"*
11:30-11:45	Organization and schedule, **Max Gunzburger**, Florida State University and **Rich Lehoucq,** Sandia National Laboratories
11:45-1:30	Lunch
1:30-3:30	Blitz Session 1: **Xiaofan Li,** Illinois Institute of Technology **Nathanial Burch,** SAMSI **Zhen Guan,** University of Tennessee **John Fricks,** Pennsylvania State University **Jeremy Lechman,** Sandia National Laboratories **Alan Lenarcic,** University of North Carolina **Peter Straka,** Michigan State University **Lukas Zimmer**, University of Trier
3:30-5:00	Poster Session and Refreshments

Wednesday, June 27
Radisson

8:30-9:00	Registration and Continental Breakfast
9:00-10:30	Blitz Session 2: **Richard Fabiano,** University of North Carolina, Greensboro **Tchavdar Marinov,** Southern University **Rossitza Marinova,** Concordia University **Michael Raghib,** LANL **Naveen Ramunigari,** University of Texas **Arash Yavari,** Georgia Tech University
10:30-11:00	Break
11:00-1:00	Blitz Session 3: **Eliot Fried,** McGill University **Tae-Yeon Kim,** McGill University **Alexander Panchenko**, Washington State University **Yi Jiang,** University of Wisconsin **Jiao Li**, University of Wisconsin **Ying Wang,** University of Minnesota **Dexuan Xie,** University of Wisconsin **Ling Xu,** University of New Mexico
1:00-2:30	Poster Session and Lunch

Thursday, June 28
Radisson

8:30-9:00	Registration and Continental Breakfast
9:00-10:30	Blitz Session 4: **Stephen Bond,** Sandia National Laboratories **Xi Chen,** Florida State University **Steven Henke,** Florida State University **Burak Aksoylu,** Louisiana State University **Mike Parks,** Sandia National Laboratories **Zhan Huang,** Pennsylvania State University
10:30-11:00	Break
11:00-12:30	Blitz Session 5: **Maria Teresa Perez-llanos,** Univeridad Autonoma De Madrid **Lili Ju,** University of South Carolina **Petronela Radu,** University of Nebraska-Lincoln **Tadele Mengesha,** Pennsylvania State University **Pablo Seleson,** University of Texas **Marta D'Elia,** Florida State University
12:30-2:00	Lunch
2:00-3:30	Blitz Session 6: **Wojbor Woyczynski,** Case Western Reserve University **Albert Erkip,** Sabanci University **Miroslav Stoyanov,** ORNL **Guannan Zhang,** Florida State University **Xiaoxia Xie,** Auburn University **Ekkehard Sachs,** University of Trier
3:30-5:00	Poster Session and Refreshments

Friday, June 29
Radisson

8:30-9:00	Registration and Continental Breakfast
9:00-10:30	Tutorial 5: **Michael Parks**, Sandia National Laboratories *"Computational Peridynamics"*
10:30-11:00	Break
11:00-12:00	Discussion about state-of-the art of nonlocal modeling and future directions
12:00-1:00	Lunch and Adjourn

Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications Workshop

June 25-29, 2012

POSTERS

Session 1 – Tuesday, June 26th

Nathanial Burch
SAMSI
nathanial.burch@gmail.com

"Computing the Exit-Time for a Symmetric Jump Process"

John Fricks
Pennsylvania State University
fricks@stat.psu.edu

“Detecting Heterogeneous Diffusion in Complex Fluids"

Jeremy Lechman
Sandia National Laboratories
jblechm@sandia.gov

“Diffusion of Monodisperse, Hard-Sphere Colloidal Fluids: Continuous-Time Random-Walks and Beyond”

Alan Lenarcic
University of North Carolina
AlanJazzTenor@gmail.com

“Bayes Spike High Dimensional Gibbs Selection Sampler Markov Chain”

Xiaofan Li
Illinois Institute of Technology
lix@iit.edu

“Mean Exit Time and Escape Probability for Dynamical Systems Driven by Levy Noise”

Ekkehard Sachs
University of Trier
sachs@uni-trier.de

“Nonlocal Models in Financial Applications - Theory and Numerical Analysis”

Peter Straka
Michigan State University
straka@msu.edu

"Forward and Backward Fractional Pdes for Superdiffusion"

Lukas Zimmer
University of Trier
lukasa.zimmer@online.de

“Necessary Optimality Conditions for Partial Integro-Differential Equations”

Session 2 – Wednesday, June 27th

Richard Fabiano
University of North Carolina, Greensboro
fabiano@uncg.edu

“Semidiscrete Approximation for LQR Control of Delay Systems”

Tchavdar Marinov
Southern University
tmarinov@suno.edu

"Inverse Problem for Flexural Rigidity Identification in Euler-Bernoulli Equation from Over-posed Data "

Rossitza Marinova
Concordia University
rmarinova@gmail.com

“Numerical Method for Obtaining Traveling Wave Solutions as Coefficient Identification Problem”

Michael Raghib
LANL
mraghib@lanl.gov

“Multiscale Analysis of Collective Decision-Making in Animal Groups: An Advection Diffusion Equation with Memory Approach”

Naveen Ramunigari
University of Texas
r.naveengoud@gmail.com

“Computational Design of Ceramics at Ultra High Temperatures to Compute Structural Stresses and Diffusion Variations”

Arash Yavari
Georgia Tech University

arash.yavari@ce.gatech.edu

"The Weyl Geometry and the Nonlinear Mechanics of Point Defects"

Session 3 – Wednesday, June 27th

Eliot Fried
McGill University
mechanicist@gmail.com

“Numerical Results for the Navier--Stokes-$\Alpha\Beta$ Model (co-author Tae-Yeon Kim, McGill University)

Yi Jiang
University of Wisconsin
yijiang@uwm.edu

“A Fast Finite Element Solver for a Nonlocal Dielectric Continuum Model”

Tae-Yeon Kim
McGill University
tykimsay@gmail.com

1. “Grain-Size Dependent Young's Modulus and Poisson's Ratio of Bulk Nanocrystalline Materials”

2. “Numerical Results for the Navier--Stokes-$\Alpha\Beta$ Model (co-author Eliot Fried, McGill University)

Jiao Li
University of Wisconsin
lijiaoflying@163.com

“New Free Energy Minimization Formulation and Truncated Newton Algorithm for Solving Nonlinear Poisson-Boltzmann Equation of Protein in Ionic Solvent**”**

Co-authosr: Dexuan Xie and Yi Jiang, University of Wisconsin

Alexander Pancheko
Washington State University
anpanchenko@gmail.com

“Non-Local Continuum Models of Particle Systems”

Ying Wang
University of Minnesota
wang@umn.edu

"Interplay of Dissipation and Diffusion in Two-Phase Flow -- The Modified Buckley-Leverett Equation".

Dexuan Xie
University of Wisconsin
dxie@uwm.edu

"Advances in Nonlocal Dielectric Modeling for Protein in Water and Ionic Solvent"

Ling Xu
University of New Mexico
xuling@unm.edu

"Rock Fractures Near Tunnels Due to A Blast"

Session 4 – Thursday, June 28th

Burak Aksoylu
Louisiana State University
burak@cct.lsu.edu

"Variational Theory, Conditioning, and Domain Decomposition for Nonlocal Problems"

Stephen Bond
Sandia National Laboratories
sdbond@sandia.gov

"Quadrature for Peridynamics"

Xi Chen
Florida State University
xc07@fsu.edu

"Numerical Methods for the Nonlocal Problem - Peridynamics Model in Mechanics"

Steven Henke
Florida State University
shenke@fsu.edu

"Convergence Studies of a Peridynamic Diffusion Equation In Multiple Dimensions"

Zhan Huang
Pennsylvania State University
zhuang@math.psu.edu

"Nonlocal Convection-diffusion Equations"

Mike Parks
Sandia National Laboratories
mlparks@sandia.gov

"A New Approach for a Nonlocal, Nonlinear Conservation Law"

Session 5 – Thursday, June 28th

Marta D'Elia
Florida State University
mdelia@fsu.edu

"Optimal Control for Nonlocal Problems"

Lili Ju
University of South Carolina
ju@math.sc.edu

"A Posteriori Error Analysis of Finite Element Methods for Linear Nonlocal Diffusion and Peridynamic Models"

Tadele Mengesha
Pennsylvania State University
mengesha@math.psu.edu

"Well-Posedness of the Linear Peridynamic Model with Sign Changing Kernel"

Maria Teresa Perez-llanos
Univeridad Autonoma De Madrid
mayte.perez@uam.es

"Numerical Approximations for Nonlocal Evolution Equations"

Petronela Radu
University of Nebraska-Lincoln
pradu@math.unl.edu

"Some Mathematical Aspects Behind the Theory of Peridynamics"

Pablo Seleson
University of Texas
seleson@ices.utexas.edu

"A Force-Based Coupling Scheme for Peridynamics and Classical Elasticity"

Session 6 – Thursday, June 28th

Albert Erkip
Sabanci University
albert@sabanciuniv.edu

"On the Cauchy Problems for Some Classes of Nonlocal, Nonlinear Equations Arising in Elasticity"

Zhen Guan
University of Tennessee
zguan@math.utk.edu

"First and Second Order Unconditionally Energy Stable Schemes for the Nonlocal Cahn-Hilliard and Allen-Cahn Equations"

Miroslav Stoyanov
ORNL
mkstoyanov@gmail.com

"Gradient Based Reduced Order Approach for Uncertainty Quantification"

Wojbor Woyczynski
Case Western Reserve University
waw@case.edu

"Interplay Between the Nonlinear and Nonlocal Components of Diffusions"

Xiaoxia Xie
Auburn University
xzx0005@tigermail.auburn.edu

"Approximations of Random Dispersal Operators/Equations by Nonlocal Dispersal Operators/Equations"

Guannan Zhang
Florida State University
gzhang5@fsu.edu

"Propagation of Uncertainty through Nonlocal Models"