Applied Mathematics and Scientific Computing Group
4 November 2010 Presentation

Tenure Track / Tenured Faculty

Benjamin Seibold (numerical PDEs: traffic modeling, simulation of flows)
Yury Grabovsky (calculus of variations, composite materials)
Daniel B. Szyld (numerical and applied linear algebra, matrix computations)

Research Assistant Professors

Prince Chidyagwai (numerical PDEs: finite elements, discontinuous Galerkin)
Fei Xue (analysis and computations for large linear systems and eigenvalues)

Graduate Students (already working on problems)

Meredith Hegg (exact relations for effective tensors of composites)
Shimao Fan (simulation of traffic flow in networks)
Zhiyong Feng (convergence of numerical methods with Shishkin meshes)
Kirk Soodhalter (Krylov subspace methods for acoustics scattering and QCD)
Dong Zhou (interface tracking; applications in medical imaging)

Importance of Applied Mathematics and Scientific Computing

- Applied mathematics and scientific computing are essential in solving many real-world problems. These fields require a fundamental mathematical approach.
- Development of new and better computational approaches (that can be used broadly in science and engineering $\rightarrow$ interaction/collaboration with other disciplines).
- Rigorous analysis of methods. *Prove* conditions for success and failure.
- New understanding of real-world phenomena by using theory and simulations in their full interplay.
- Applications and computations often inspire challenging mathematical problems which merit investigation in their own right.

Group's Activities

- 10 papers published in 2009, and 8 (so far) published in 2010
- five Ph.D. students graduated since 2007
- weekly seminar with speakers from Temple, and from other institutions in the U.S. and abroad
- group members invited speakers at several international venues
- leadership in academic societies
- editorships of leading journals in the field

Group's Accomplishments and Highlights

- an NSF CAREER Award
- several research grants from NSF and DOE (\$1.9M last 5 years)
- extensive news coverage for traffic flow research (e.g., CNN, New York Times, Financial Times (UK), Philadelphia Inquirer)
- scientific collaborations with CIS ($\times 2$) and Medical Center
- developed and ran new course (Spring 2010): Mathematical Modeling (students work on problems from industry partners)

Research in Computational Differential Equations

Benjamin Seibold

Department of Mathematics
Temple University

November 4^{th}, 2010

Traffic Modeling and Simulation

Research Projects

- Modeling of vehicular traffic flow
- Understanding of phantom traffic jams and stop-and-go waves
- Traffic forecast (volume, travel times) by combining traffic models with data mining approaches

Mathematics Personnel

Benjamin Seibold (TT AP)
Prince Chidyagwai (Research AP)
Shimao Fan (Graduate Student)

Collaborators

Morris R. Flynn (Univ. of Alberta)
Aslan Kasimov (KAUST)
Jean-Christophe Nave (McGill Univ.)
Rodolfo R. Rosales (MIT)
Slobodan Vucetic (Temple, CIS)

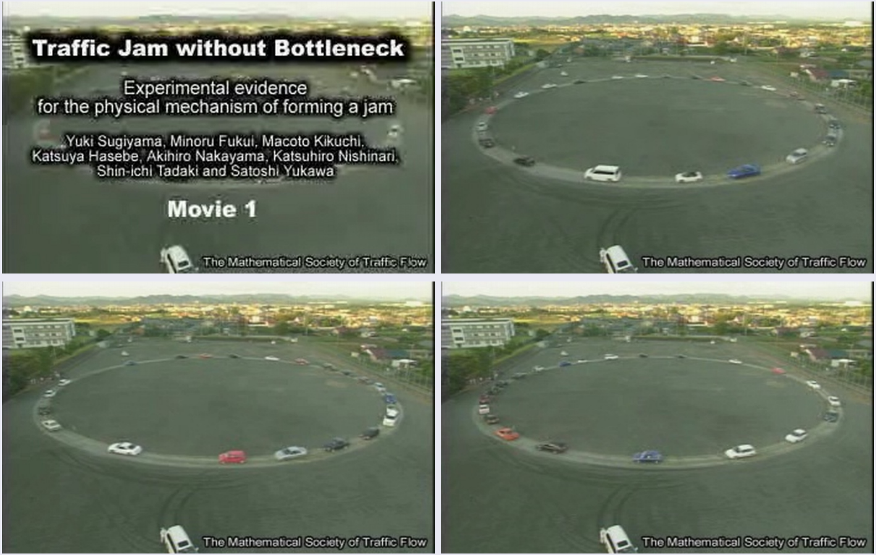
Support

NSF DMS–1007899

Phantom traffic jams, continuum modeling, and connections with detonation wave theory

Phantom Traffic Jam

Experiment on a Circular Road [Y. Sugiyama, et al., 2008]



Our Research

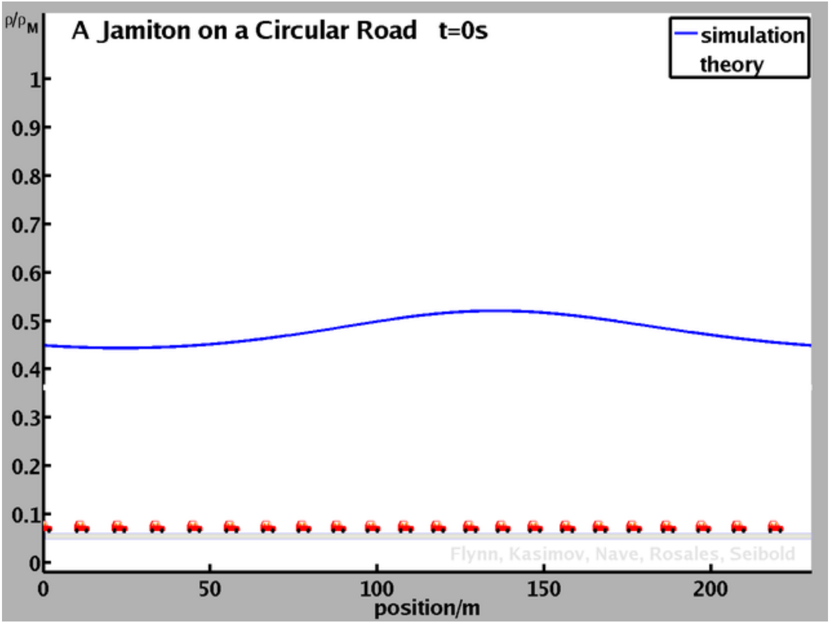
Phantom Traffic Jams and Traffic Waves

- Even in the absence of obstacles or bottlenecks, uniform traffic flow can develop instabilities.
- These grow into stop-and-go waves ("jamitons").
- Unexpected braking, stress, pollution, hot-spot for accidents.
- A deeper understanding of traffic waves is needed.

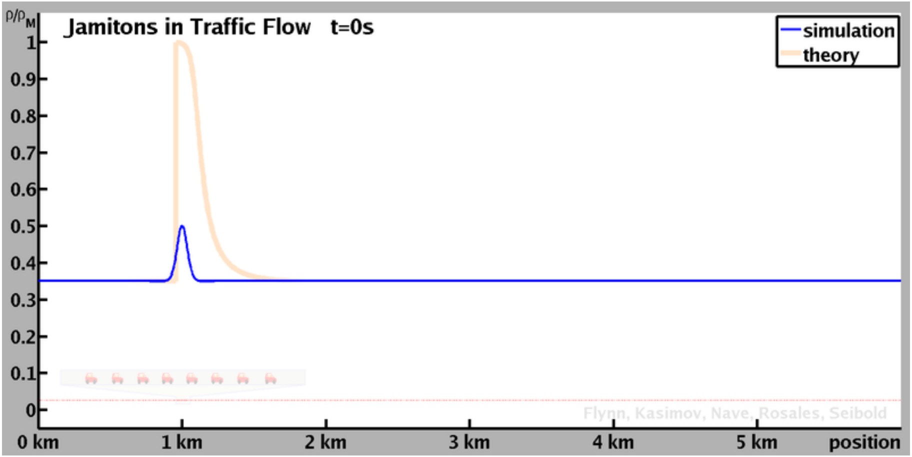
Our Research

- Consider fluid dynamical traffic models.
- Key observation: Traffic waves are analogs of detonation waves.
- Use techniques from detonation theory to predict the shape and travel speed of traffic waves.
- Comparison with numerical simulations.
- Development of countermeasures $\longrightarrow$ control of traffic.

Computational Results — Circular Road



Computational Results — Infinite Highway



Computation and Simulation of Flows

Research Projects

- Highly accurate methods for nonlinear flows:
  - multi-phase fluid flows
  - radiative transfer
  - porous media flows
  - ...
- Applications in medical imaging and radio-therapy

Mathematics Personnel

Benjamin Seibold (TT AP)
Prince Chidyagwai (Research AP)
Dong Zhou (Graduate Student)

Collaborators

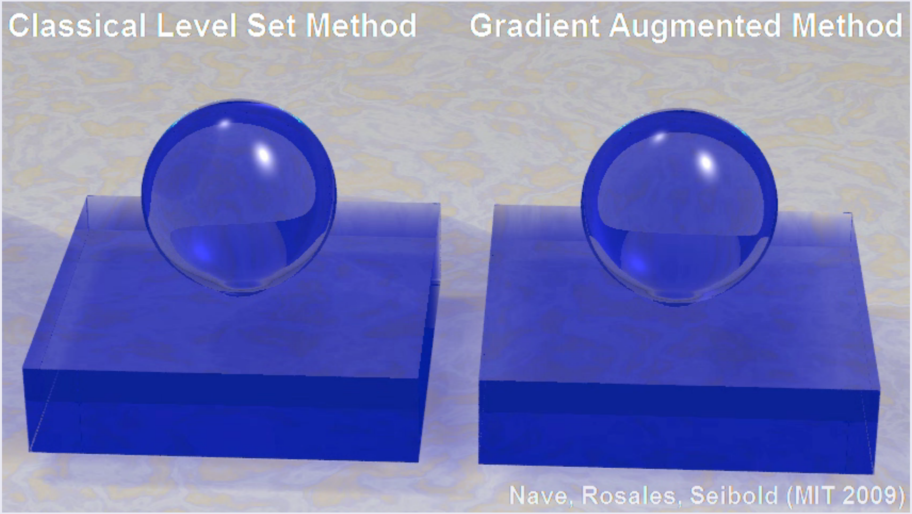
Yossi Farjoun (UC3 de Madrid)
Martin Frank (RWTH Aachen)
Feroze Mohamed (Temple, Radiology)
Jean-Christophe Nave (McGill Univ.)
Rodolfo R. Rosales (MIT)
Pallav Shah (Temple, Radiology)

Support

NSF DMS–0813648

Capturing subgrid structures with level set methods

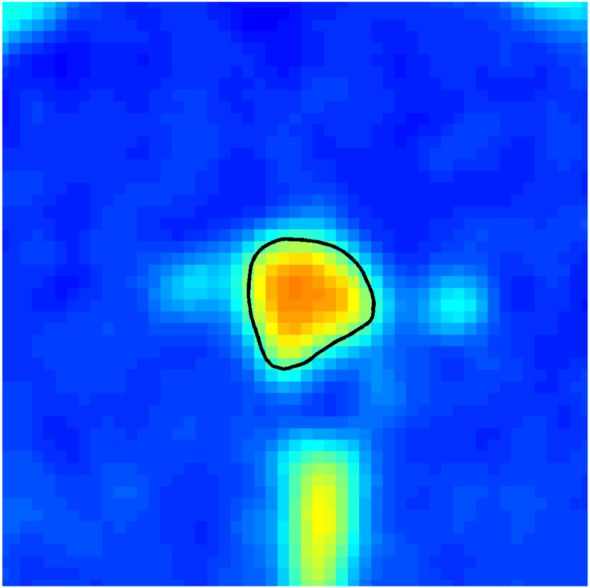
Multiphase Fluid Flow Simulations



Fundamental problem: Structures vanish when smaller than grid resolution.

New approach can track structures of subgrid size $\longrightarrow$ closer to true physics.

Medical Imaging



- User selects object by clicking on a point in the interior.
- Computer evolves curve (2D) or surface (3D) towards largest image gradient.
- Automatic computation of object's volume.

Mathematical theory of composite materials and Calculus of Variations

Yury Grabovsky

Department of Mathematics
Temple University

November 4, 2010

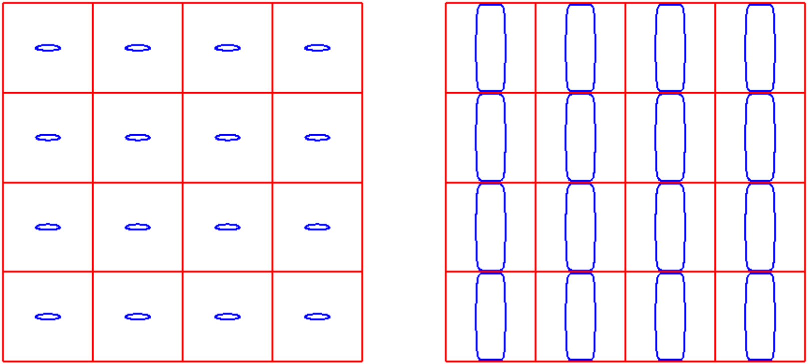
Composite materials

Composites are fine-scale mixtures of several materials which behave as homogeneous materials on a macroscopic scale

- Important in applications
- Elegant mathematical theory
- Many open fundamental questions:

  – Is a specific new material constructable as a composite of given existing materials?
  – What is the effect of the microstructure on the material properties of the product?
  – What microstructures are the optimal (extremal)?

The Vigdergauz microstructure



Exact relations are material properties that cannot be changed by means of making composites

- We developed a general theory of exact relations
- The theory combines several areas of mathematics
- The emerging results are both fundamental and beautiful

Ph.D. work of Meredith Hegg: Characterizing all exact relations for fiber-reinforced elastic composites.

Calculus of Variations

- Scalar problems: completely understood by 1930s
  - Celestial mechanics
  - Geometrical optics
  - Classical optimal control
- Vectorial problems: a lot of fundamental open questions
  - Non-linear elasticity
  - Shape memory alloys
  - Superconductivity

Recent progress

- Work with former Ph.D. student Tadele Mengesha (postdoc at Louisiana State University). We have solved a fundamental open problem about criteria for minimality in vectorial variational problems.
- Work with Prof. Lev Truskinovsky (Ecole Polytechnique, Paris). We are gaining fundamental understanding of stability of phase boundaries, observed in shape memory alloys.

Numerical and Applied Linear Algebra

Multiple areas of work

1. Large linear systems of equations
2. Eigenvalue problems
3. Matrix equations (linear and nonlinear)
4. Properties of matrices

This presentation: sample projects for each area

Funding:
Department of Energy, Office of Science, Program of Applied Mathematics

1. Linear Systems

They are ubiquitous in science and engineering problems.

Examples include

- Discretized differential equations
- Linearized nonlinear problems

Challenges include

- Size of systems: hundreds of thousands, or millions of unknowns.
- Need to Reformulate the problem to obtain solution in reasonable time.
- Design of algorithms for specific types of problems, and proofs theorems about these.
- Design of algorithms to match modern computer architectures.

Iterative Methods for Large Linear Systems

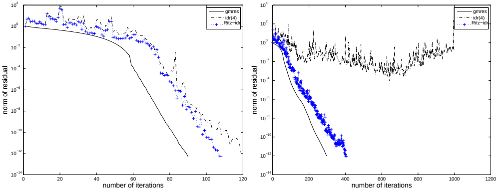
- Due to the size of the systems, we need to approximate their solution in an iterative manner. Begin with $\mathbf{x}_1$, then obtain $\mathbf{x}_2$, $\mathbf{x}_3$, etc.
- Usually the approximation $\mathbf{x}_i$ is chosen in some appropriate subspace (of growing dimension i), and with some appropriate property.
- Choice of subspace and property defines the iterative method. (Popular examples: Conjugate Gradient, GMRES)
- Preconditioning: Change problem A to problem B with same solution, but easier to solve in some sense.

Most Recent Paper Published

Interpreting IDR as a Petrov-Galerkin method, *SIAM J. Scientific Computing*, v. 438 (2010) pp. 1898–1912. With V. Simoncini (Bologna)

Induced Dimension Reduction (IDR) [Sonneveld and van Gijzen, 2008] is the most successful modern low-memory Krylov subspace method.

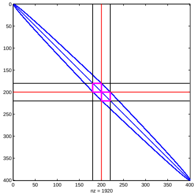
In this project, we proved why this method works, and we used the theory developed for its understanding to design a new variant of the method, which works better in most real applications.



$L(u) = -\Delta u + \beta(u_x + u_y + u_z)$ discretized in the unit cube with homogeneous Dirichlet boundary conditions, $n = 8000$: $\beta = 100$ (left), $\beta = 500$ (right)

Sample Recently Completed Project

An optimal block iterative method and preconditioner for banded matrices with applications to PDEs on irregular domains, Report 10-05-21, May 2010. With M.J. Gander (Geneva) and S. Loisel (former postdoc, now at Heriot-Watt U., Edinburgh)

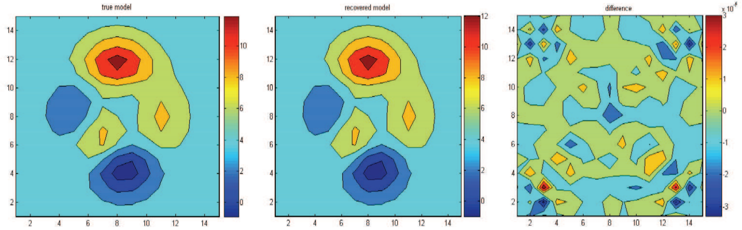


Modify certain entries in the matrix to obtain optimal preconditioner (or get an approximation to optimal and obtain a very fast one).

Sample Current Project I

Inexact and truncated Krylov subspace methods for parabolic optimal control problems, with X. Du (former Ph.D. student, now at Alfred U.), E. Haber (UBC), M. Sarkis (WPI), and C. Schaerer (Asunción)

Successful application of several strategies for the solution of certain hard control problems with temporal component.



One slice of the true and the recovered model and their difference. Note scale of difference 10^{-9}

Sample Current Project II

On short-term recurrence Krylov subspace methods for nearly-Hermitian matrices, with M. Embree (Rice), and J.A. Sifuentes (NYU), K.M. Soodhalter (current Ph.D. student)

Developed new iterative method and preconditioner for linear systems with special structure, which arise for example in Lippmann-Schwinger operators. These operators model acoustic waves as they scatter through an inhomogeneous medium.

Sample Recently Completed Project

Efficient preconditioned inner solves for inexact Rayleigh quotient iteration and their connection to the simplified Jacobi-Davidson method, Report 10-9-07, September 2010.

With F. Xue (Temple Research Assistant Professor)

Iterative methods for the solution of eigenvalue problems require at each step, the solution of a linear system (these are the "inner solves").

We provide strategies to maintain a good initial approximation to an eigenvector after preconditioning the inner solves. Theorems showing the fast convergence of the overall method are given.

Inexact Newton with Krylov projection and recycling for Riccati equations, with M. Monsalve (former postdoc, now at the U. Central de Venezuela, Caracas)

Riccati equations: Find matrix X so that

$$AX + AX^T - XBB^TX + C^TC = 0.$$

Important, e.g., in control problems.

Sample Question: Which matrices have a non-negative (or positive) dominant eigenvector (eigenvector corresponding to largest eigenvalue in modulus)?
On general matrices having the Perron-Frobenius property, *Electronic Journal on Linear Algebra*, Vol. 17 (2008) pp. 389–413. With A. Elhashash (former Ph.D. student, now in Calgary)

Sample Question: Which functions preserve the above-mentioned property?
Matrix functions preserving sets of generalized nonnegative matrices, *Electronic Journal on Linear Algebra*, Vol. 20 (2010), to appear. With A. Elhashash

Conclusion (for DBS and for the whole group)

- Breadth of research topics
- Breadth of collaborators
  (at Temple, at the national and international levels)
- Theory, computations, and applications
- Mentoring of students and postdocs,
  also through research projects