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Final Technical Report
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Singular and Nonlinear Processes
in
Applied Mathematics

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I. PROJECT OVERVIEW

The original grant, "Singular and Nonlinear Processes in Applied Mathematics", supported research for the three year period 1993 - 1996 and was continued for a fourth year with a no-cost extension, ending on 31/7/97. A wide range of research topics were supported under this grant. These included:

- Complex space time singularities in nonlinear differential equations;
- Singularities in magneto-hydrodynamics;
- The dynamics of knots and curves;
- The structure and dynamics of foams and grain boundaries.

A brief summary of results achieved in each of these four areas is given below along with the associated publications acknowledging DOE support.

A. Complex space time singularities in nonlinear differential equations

In work with postdoctoral associate Alain Goriely and Applied Mathematics graduate student Craig Hyde, significant results were obtained relating the complex space time singularities of dynamical systems with the Melnikov splitting vector for the case of regular perturbations. Subsequently the technique was extended to develop new results relating the singularity structure to the case of exponentially small separatrix splitting in rapidly forced dynamical systems. Motivated by the results obtained in our studies of magnetohydrodynamics (see below) the techniques of singularity analysis were used to develop new criteria to predict the formation of finite time singularities in systems of nonlinear ordinary differential equations. The exponentially small splitting and finite time blow-up results form the bulk of Hyde's dissertation.

Resulting publications:

A. Goriely, "A simple solution to the nonlinear front problem", Phys. Rev. Lett. **75**, 2047 - 2050, (1995).

A. Goriely and M. Tabor, "The singularity analysis for nearly integrable systems: homoclinic intersections and local multivaluedness", Physica D **85**, 93-125, (1995).

A. Goriely and C. Hyde, "Necessary and sufficient conditions for finite time blow-up in ordinary differential equations", submitted to J. Diff. Equations.

C. Hyde, A. Goriely and M. Tabor, "Exponentially small separatrix splitting in rapidly forced dynamical systems", in preparation.

B. Singularities in magneto-hydrodynamics

In work with postdoctoral associate Isaac Klapper and Applied Mathematics graduate student Anita Rado we developed a new Lagrangian formulation of the full MHD equations in three dimensions. This resulted in an analytical model which demonstrated that real (finite) time singularities can occur around magnetic null points.

Resulting publications:

I. Klapper and M. Tabor, "Current sheet formation in two-dimensional incompressible MHD turbulence from a Lagrangian point of view", *Geophys. Astrophys. Fluid Dynamics*, **73**, 109 - 122 (1993).

I. Klapper and M. Tabor, "Stretching and alignment in chaotic and turbulent flows", *Chaos, Solitons and Fractals*, **4**, 1031 - 1055 (1994).

I. Klapper, A. Rado and M. Tabor, "A Lagrangian study of singularity formation at magnetic null points in ideal 3 dimensional magnetohydrodynamics", *Phys. Plasmas* **3**, 4281 - 4283 (1996).

C. The dynamics of knots and curves

Motivated by the desire to model the self-assembling behavior of bacterial macro-fibers (*Bacillus subtilis*) studied N. Mendelson (Department of Molecular and Cellular Biology at the University of Arizona) a substantial program of research was undertaken. The first phase of this program, with postdoctoral associate Isaac Klapper, consisted of the development of algorithms to simulate the motion of three dimensional elastic filaments subject to twisting forces. The algorithm was able to realistically simulate the basic writhing instabilities observed in experiments and incorporate (semi-empirically) both the viscous effects of the medium and the elongation of the filament. The second phase, carried out with postdoctoral associate Alain Goriely, consisted of major theoretical efforts in which a new perturbative technique and linear stability analysis of the time-dependent Kirchhoff equations was developed and used to study the writhing instability of rod configurations subjected to twisting forces. The linear analysis is able to provide a selection criterion for the shape of the resulting instability. The work was then extended to a *nonlinear* analysis leading to the derivation of new nonlinear evolution equations for the amplitude of the instability. As far as we know both the linear and nonlinear analyses of the full, time-dependent, Kirchhoff equations are completely new. These results enabled us to obtain new results on the stability of helical rods and, ultimately, the first *dynamical* picture of spontaneous looping (*i.e.* buckling) of twisted rods.

Resulting publications:

I. Klapper and M. Tabor, "A new twist in the kinematics and dynamics of thin filaments and ribbons", J. Phys. A. 27, 4919 - 4924 (1994).

M. Tabor and I. Klapper, "The dynamics of knots and curves (part I)", Nonlinear Science Today, 4, no. 1, 7 - 13 (1994).

M. Tabor and I. Klapper, "The dynamics of knots and curves (part II)", Nonlinear Science Today, vol 4, no. 2, 12 - 18 (1994).

J. Aldinger, I. Klapper and M. Tabor, "Formulae for the calculation and estimation of writhe", J. Knot Theory, 4, 343-372, (1995).

M. Tabor and I. Klapper, "Dynamics of twist and writhe and the modeling of bacterial fibers", IMA vol. 82, *Mathematical Approaches to Biomolecular Structure and Dynamics*, editors: J. P. Mesirov, K. Schulten, D. W. Sumners; Springer-Verlag, New York, (1995).

I. Klapper, "Biological applications of the dynamics of twisted rods", J. Comp. Phys. 125, 325 - 337 (1996).

A. Goriely and M. Tabor, "New amplitude equations for thin elastic rod", Phys. Rev. Letts 77, 3537 - 3540 (1996).

A. Goriely and M. Tabor, "Nonlinear dynamics of filaments: I. Dynamical instabilities", Physica D 105, 20 - 44 (1997).

A. Goriely and M. Tabor, "Nonlinear dynamics of filaments: II. Nonlinear analysis", Physica D 105, 20 - 44 (1997).

A. Goriely and M. Tabor, "Nonlinear dynamics of filaments: III. Instabilities of helical rods", Proc. Roy. Soc. Lond. D 105, 20 - 44 (1997).

D. The structure and dynamics of foams and grains

An algorithm to simulate the evolution of two dimensional foams was developed by graduate student J. J. Chae as part of his dissertation. This is a powerful and flexible tool that incorporates proper physical modeling of dry foams and is capable of studying the evolution of foams with and without wall rupture. Detailed studies with this algorithm were able to resolve a number of outstanding issues in the evolution of foams and give a more precise understanding of the role of topological transitions; as well as the changes in scaling laws that are observed when wall rupture is permitted. The program was also adapted to study the effects of anisotropy in grain boundary simulations and investigate nonuniversal scaling behaviors seen in grain boundary evolution.

Resulting publications:

M. Tabor and J. J. Chae, "Simulation of foam dynamics with and without wall rupture", Phys. Rev. E. 55, 598 - 610 (1997).

M. Tabor, J. J. Chae, G. Burnett and D. J. Durian, "The structure and dynamics of foams", Nonlinear Science Today (1998).

E. Dissertations supported by grant

"The Dynamics of Two Dimensional Foams", by J. J. Chae (1995)

"Dynamical Systems and Singularity Analysis", by C. Hyde (1998)

F. Postdoctoral Associates supported by grant

Alain Goriely, now Assistant Professor, Department of Mathematics, University of Arizona.

Isaac Klapper, now Assistant Professor, Department of Mathematics, Montana State University.