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Lie Group Applications to the Solution of Differential Equations

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Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The project applied Lie group techniques to the solution of differential equations (DEs) describing physical systems important to LANL's scientific mission. There were two main objectives: (1) to construct analytic or quasianalytic solutions for use as benchmark test problems; and (2) to develop improved numerical solution algorithms that possess the same symmetries (e.g. rotational, translational, and scaling invariance) as the DEs. Significant progress was achieved on both these objectives.

Background and Research Objectives

The theory of groups developed by Sophus Lie in the latter part of the 19th Century was formulated specifically for the solution of differential equations (DEs). The theory was virtually lost until it was reintroduced around the middle of this century, and the past decade has seen an explosion in its use and extension. The application of Lie group theory to the solution of DEs is described in the textbooks listed as References 1–5.

This Laboratory-Directed Research and Development (LDRD) project applied Lie group techniques to the solution of DEs describing physical systems important to the scientific mission of the Los Alamos National Laboratory (LANL). There were two main objectives: (1) to construct analytic or quasianalytic solutions for use as benchmark test problems; and (2) to develop improved numerical solution algorithms that possess the same

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symmetries (e.g. rotational, translational, and scaling invariance) as the DEs.

Importance to LANL's Science and Technology Base and National R&D Needs

In the post-cold-war era of no nuclear tests, LANL's scientific mission of maintaining nuclear weapons technology and certifying the reliability and safety of the stockpile must rely heavily on the capability of computer simulation codes. The expertise in Lie group techniques nurtured by this LDRD project is an important aid in validating these codes. Analytic solutions to complicated models of physical systems serve both to improve physics understanding and to test current numerical solution algorithms. Improved algorithms that possess the same Lie group symmetries as the model DEs increase confidence in the predictive power of numerical simulations.

The expertise developed by this project also positions LANL to work with a number of industries whose specific problems involve the solution of DEs. Lie group techniques generally are outside the scope of most commercial research programs, so LANL can now provide a unique contribution to industrial partnerships.

Scientific Approach and Accomplishments

Lie group techniques determine the continuous transformations (e.g. translations, rotations, and scale variations) under which a set of DEs is invariant. The most straightforward use of these Lie group symmetries is to identify new coordinate systems in which the equations become simpler. For ordinary DEs (ODEs), the differential order is reduced, often allowing analytic solutions. For partial DEs (PDEs), the number of independent variables is reduced, ultimately producing ODEs. During the past ten years, this procedure has been used to derive many useful analytic solutions to radiation hydrodynamics problems as described in the papers listed as References 6–8. More recently, this procedure has been applied to a class of nonlinear diffusion equations to produce analytic solutions that were used to benchmark a numerical turbulent-diffusion algorithm as described in Reference 9. The first objective of this LDRD project was to apply this procedure to produce additional analytic or quasianalytic solutions for use as benchmark test problems.

A less direct, but equally important, use of Lie group techniques is to construct

improved numerical algorithms for solving DEs. A numerical solution algorithm consists of an approximate representation of the DEs at a discrete set of values for the independent variables combined with an interpolation procedure determining the solution away from the discrete values. To be valid, discrete representations must differ from the original DEs by error terms which are in some sense small. The recent innovation provided by Lie group techniques is to construct discrete representations whose error terms have the same Lie group symmetries as the DEs. The resulting symmetric numerical algorithms produce significantly better results as demonstrated in the papers listed as References 10–12. A methodical procedure for constructing these symmetric numerical algorithms is presented in Reference 13. The second objective of this LDRD project was to determine the symmetry properties of the numerical algorithms currently used in LANL's codes and to develop algorithms with improved symmetry properties where appropriate.

During fiscal years 1994 and 1995, the LDRD project provided partial funding for technical staff member Stephen V. Coggeshall and graduate students Charles E. Knapp and D. Palmer Smitherman. Their main research accomplishments were the following:

- Four coupled ODEs were generated describing the inclusion of heat conduction in the one-dimensional Noh test problem, which describes an imploding fluid whose stagnation against a symmetry surface produces an outward-moving shock.
- A thorough and concise description of the application of Lie group techniques to the hydrodynamics equations was prepared including an exhaustive collection of 31 analytic solutions to one-, two-, and three-dimensional flow problems with and without heat conduction and shocks.
- A new Lie group technique was developed that uses a concept of hidden symmetries to reduce otherwise intractable PDEs to ODEs.
- Five coupled ODEs were generated describing the interpenetration of a simple two-fluid system.
- A new technique was developed for analyzing finite-difference representations of the one-dimensional advection equation to determine their Lie group symmetries directly from their discrete forms without first converting them to continuous forms.

During FY 1996 the LDRD project funded a four-month consulting agreement with Roy A. Axford of the University of Illinois at Urbana-Champaign. Dr. Axford's main research accomplishments were the following:

- A paper entitled "Lie Group Symmetry Properties of the Besnard-Harlow-Rauenzahn-Zemach Spectral Turbulence Transport Model" was presented at the 1996 JOWOG-32M Meeting on Mix Research held at Los Alamos, July 22–26, 1996.
- A paper entitled "Group Theory of Invariant Flux and Slope Limiters" was accepted for

presentation at the Ninth Nuclear Explosives Code Developers Conference to be held in San Diego, October 22–25, 1996.

- A general procedure was developed for finding analytic solutions to the hydrodynamic equations for fluids having more realistic equations of state than that of an ideal gas. The procedure was used to construct analytic solutions to the one-dimensional Noh test problem, which describes an imploding fluid whose stagnation against a symmetry surface produces an outward-moving shock, for both the stiff-gas and Mie-Grüneisen equations of state.
- An analytic solution was constructed for the Sedov test problem, which describes the spherical blast wave produced by a point explosion, for the case where the ambient gas has an initial density gradient in a given direction. This provides a two-dimensional generalization of the usual one-dimensional solution.

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