GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF RESEARCH ADMINISTRATION

RESEARCH PROJECT INITIATION

Date: 31 October 1972

Project Title: "Irreversibility and Rate Equations for Physical Systems"

Project No: G-41-623

Principal Investigator: Dr. Joseph Ford

Sponsor: Air Force Office of Scientific Research

Agreement Period: From November 1, 1972 Until October 31, 1973

Type Agreement: Grant No. AFOSR-73-2453

Amount:
$29,969 AFOSR funds (G-41-623)
10,099 GIT Contribution (G-41-322)
$40,068 Total

Reports Required:
Final Scientific Report

Sponsor Contact Person (s):

Administrative

Marvin L. Roberts
Contracting Officer
Air Force Office of Scientific Research
1400 Wilson Boulevard
Arlington, VA 22209

Technical

Alexander A. Abela
Captain, USAF
General Physics Division
Directorate of Physics Research
Air Force Office of Scientific Res.
1400 Wilson Boulevard
Arlington, VA 22209

Assigned to: Physics

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RA-3 (6-71)

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION
RESEARCH PROJECT TERMINATION

Date: December 3, 1975

Project Title: Irreversibility and Rate Equations for Physical Systems

Project No: G-41-623

Principal Investigator: Dr. Joseph Ford

Sponsor: Air Force Office of Scientific Research

Effective Termination Date: 9/30/75(Grant Expiration; Final Tech. Report due by 11/30/75 and submitted on 10/24/75.)

Clearance of Accounting Charges: by 10/31/75

Grant/Contract Closeout Actions Remaining: Final Fiscal Report (O.F.A.)
Final Patent Report (O.C.A.)

Assigned to School of Physics

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Terminated Project File No. _____
Other _____

G-41-623

INTERIM SCIENTIFIC REPORT

1 November 1972 - 31 October 1973

Grant AFOSR 73-2453

Joseph Ford: Principal Investigator

During this report period, one student (S. Stoddard) completed his thesis work and received his Ph.D., while two students (W. Holm and T. Snyder) initiated thesis projects. Additionally, Dr. Giulio Casati, a visiting professor from the University of Milan, Italy, was actively engaged in our research effort for a period of six months.

The results of a portion of our research are discussed in the four publications listed below. Our most recent findings will be reported in four publications which are now in various stages of preparation. Additionally, our discoveries have been reported to a rather wide audience of physical scientists via the seminar presentations listed below.

Our two perhaps most important research contributions during this report period are discussed in detail in Papers 2 and 3 listed below. Aside from whatever internal merit they may possess however, their main contribution has been to germinate significant research by others. Paper 3, which was distributed in preprint form, has even before publication inspired research efforts in several countries (France, Japan, and the U. S. A.) which have already culminated in significant new results. Indeed this rapidly developing chain of new discoveries appears to be leading to a general method for completely

solving a wide class of ordinary and partial nonlinear differential equations. Equally, subsequent to its distribution in preprint form, it was realized that Paper 2 lays the foundation for determining the Kolmogorov-Sinai entropy as a function of temperature and volume for a realistic gas system. Work now underway both in England and the U. S. A. may shortly clarify the relationship between the Kolmogorov-Sinai entropy and the more usual thermodynamic entropy.

PUBLICATIONS

1. J. Ford, "The Transition from Analytic Dynamics to Statistical Mechanics," Adv. Chem. Phys. 24, 155-183 (1973).

2. S. D. Stoddard and J. Ford, "Numerical Experiments on the Stochastic Behavior of a Lennard-Jones Gas System," Phys. Rev. A8, 1504-1512 (1973).

3. J. Ford, S. D. Stoddard, and J. S. Turner, "On the Integrability of the Toda Lattice," Prog. Theor. Phys. (Accepted for publication in the November 1973 issue).

4. J. Ford, "Empirical Determination of Integrability for Nonlinear Oscillator Systems Using Area-Preserving Mappings," (To appear in 1974 in the proceedings of the International Conference on Point Mapping and Its Applications, Toulouse, France, September 10-14, 1973).

SEMINARS

1. Physics Department, Rockefeller University, New York.

2. Physics Department, Yeshiva University, New York.

3. International Conference on Point Mapping and its Applications, Toulouse, France (Speaker and Chairman of one session).

4. Physics Department, University of Milan, Italy.

5. Astronomy Department, Nice Observatory, France.

6. Physics Department, University of Paris, France.

7. Physics Department, University of St. Andrews, Scotland.

8. Mathematics Department, The Open University, England.

9. Astronomical Department, University of Thessaloniki, Greece.

10. Physics Department, University of Parma, Italy.

11. Physics Department, University of Pavia, Italy.

12. Science Faculty, EURATOM, Ispra, Italy.

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G-41-623

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER	2. GOVT ACCESSION NO. / 3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle): INTERIM SCIENTIFIC REPORT- 1 NOVEMBER 1973 THROUGH 31 OCTOBER 1974	5. TYPE OF REPORT & PERIOD COVERED: INTERIM: 1 November 1973 - 31 October 1974
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): Joseph Ford	8. CONTRACT OR GRANT NUMBER(s): AFOSR-73-2453
9. PERFORMING ORGANIZATION NAME AND ADDRESS: School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: Project-Task # 9767-02
11. CONTROLLING OFFICE NAME AND ADDRESS: AFOSR/NPP, 1400 Wilson Blvd., Arlington, VA 22209	12. REPORT DATE: 27 December 1974
	13. NUMBER OF PAGES: 2
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report): UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for Public Release; Distribution Unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Research; Publications

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report describes the work performed under Grant AFOSR-73-2453 during the period 1 November 1973 through 31 October 1974.

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INTERIM SCIENTIFIC REPORT

1 November 1973 - 31 October 1974

Grant AFOSR-73-2453

Joseph Ford: Principal Investigator

During this report period, two thesis students (W. Holm and T. Snyder) decided to terminate their careers in physics. In addition, two post-doctoral students scheduled to initiate work on this research found themselves unable to come to Ga. Tech. As a consequence, the research has not proceeded as rapidly during this interim period as had been anticipated. Nonetheless, work performed during this report period in collaboration with Professor Giulio Casati of the University of Milan will result in two publications which are currently being written (Papers 4 and 5 below).

In addition to preparing the lengthy review papers listed as Papers 1 and 2 below, the Principal Investigator lectured and visited various scientists in the USSR as a guest of the Soviet Academy of Sciences during the month of May. He also lectured to and attended the six-week "Battelle Recontre" conference on mathematics and physics which was held in Seattle during June and July and organized by Jurgen Moser and Joel Lebowitz under the sponsorship of the Battelle Seattle Research Institute. Finally, he presented a series of invited lectures to the International Summerschool on Fundamental Problems in Statistical Mechanics, The Netherlands, July 29-Aug. 15, 1974.

Research papers, either published during the report period or in progress, are listed below:

1. J. Ford in Lecture Notes in Physics, Vol. 28: Lectures in Statistical Physics, W. C. Schieve, Ed. (Springer-Verlag, Berlin, 1974), p. 204 .

2. J. Ford in Fundamental Problems in Statistical Mechanics, III, Ed. by E. G. D. Cohen (North-Holland, Amsterdam, 1975).

3. J. Ford, S. D. Stoddard, J. S. Turner, Prog. Theor. Phys. 50, 1547 (1973)

4. G. Casati and J. Ford, "Ergodicity and Mixing in the Unequal Mass Hard Point Gas," J. Math. Phys. (to be submitted).

5. G. Casati and J. Ford, "Stochastic Behavior in the Toda Lattice Having Unequal Masses," J. Math. Phys. (to be submitted).

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G41-623

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE *(and Subtitle)* FINAL SCIENTIFIC REPORT - 1 NOVEMBER 1972 THROUGH 30 SEPTEMBER 1975		5. TYPE OF REPORT & PERIOD COVERED FINAL: 1 November 1972 - 30 September 1975 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Joseph Ford		8. CONTRACT OR GRANT NUMBER(s) AFOSR-73-2453
9. PERFORMING ORGANIZATION NAME AND ADDRESS School of Physics Georgia Institute of Technology		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Project-Task # 9767-02
11. CONTROLLING OFFICE NAME AND ADDRESS AFOSR/NPP 1400 Wilson Blvd., Arlington, VA 22209		12. REPORT DATE 10 October 1975 13. NUMBER OF PAGES 4
14. MONITORING AGENCY NAME & ADDRESS*(if different from Controlling Office)*		15. SECURITY CLASS. *(of this report)* UNCLASSIFIED 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

This report describes the work performed under Grant AFOSR-73-2453 during the period 1 November 1972 through 30 September 1975.

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FINAL SCIENTIFIC REPORT

1 November 1972 - 30 September 1975

Grant AFOSR-73-2453

Joseph Ford, Principal Investigator

1. ACTIVITIES

During the report period, the Principal Investigator presented invited talks at the following institutions: Rockefeller University, Yeshiva University, University of Arkansas, Moscow State University (USSR), Novosibirsk Institute for Nuclear Physics (USSR), University of Milano (Italy), Nice Observatoire (France), University of Paris (France), University of St. Andrews (Scotland), Open University (England), University of Thessaloniki (Greece), University of Parma (Italy), University of Pavia (Italy), and EURATOM (Italy). He was a participant, lecturer, and session chairman at the one-week International Conference on Point Mappings and their Applications (Toulouse, France, 1973), the six-week Battelle Recontre on Dynmaical Systems, Theory and Applications (Seattle, 1974), and the three-week International Conference on Fundamental Problems in Statistical Mechanics (Wageningen, The Netherlands, 1974). During the three fall months of 1973, he held a Senior Fellowship in Science at the University of Milano, Italy; and in the spring of 1974, he was the guest of the Soviet Academy of Science in Moscow and Novosibirsk. He has been invited to attend the International Conference on the Soliton and its Applications to be held in Tucson, Arizona, 1976.

One student (S. D. Stoddard) received his Ph.D. during the report period. Two students (W. Holm and T. Snyder) participated in this research work during the period, but terminated their studies short of the Ph.D. Professor Giulio Casati (University of Milano) joined our research effort for six week periods in 1973 and in 1974. This research collaboration is being continued under a two-year joint U. S. - Italy grant which has been approved by NSF with CNR approval expected. Finally an application for a joint U. S. - Japan grant (in collaboration with M. Toda, Kyoiku University, Tokyo) is being submitted.

11. PAPERS

1. S. D. Stoddard, "Numerical Experiments and Theoretical Analysis on the Source of Irreversibility in Mechanical Systems," thesis, Georgia Institute of Technology, 1973.
2. J. Ford, "The Transition from Analytic Dynamics to Statistical Mechanics," Adv. Chem. Phys. 24, 155 (1973).
3. S. D. Stoddard and J. Ford, "Numerical Experiments on the Stochastic Behavior of a Lennard-Jones Gas System," Phys. Rev. A8, 1504 (1973).
4. J. Ford, S. D. Stoddard, and J. S. Turner, "On the Integrability of the Toda Lattice," Prog. Theor. Phys. (Japan) 50, 1547 (1973).
5. J. Ford, "Stochastic Behavior in Nonlinear Oscillator Systems," in Lecture Notes in Physics, Vol. 28: Lectures in Statistical Physics, W. C. Schieve, Ed. (Springer-Verlag, Berlin, 1974), p. 204.

6. J. Ford, "The Statistical Mechanics of Classical Analytic Dynamics," in Fundamental Problems in Statistical Mechanics, Vol. III, Ed. by E. G. D. Cohen (North-Holland, Amsterdam, 1975), p. 215.

7. G. Casati and J. Ford, "Stochastic Transition in the Unequal-Mass Toda Lattice," Phys. Rev. A (to appear Oct., 1975, issue).

8. G. Casati and J. Ford, "Computer Study of Ergodicity and Mixing in a Two-Particle, Hard Point Gas System," J. Comput. Phys. (to appear in 1975 issue).

9. G. Casati and J. Ford, "Numerical Experiments on the Galogero Lattice," J. Math. Phys. (Submitted in 1975).

III. RESEARCH

Since the research performed during the report period has been given a detailed presentation in the above papers, we here confine ourselves to a brief overview. The ultimate goal of this research is to derive from first principles rate equations (and transport coefficients) governing the approach to equilibrium and to establish the validity of these rate equations via numerical (computer) experiments on increasingly realistic physical models. Most of this report period has been spent seeking and discovering suitably ergodic and mixing mechanical models, studying their properties, and verifying that they indeed approach equilibrium. Four ergodic and mixing systems have been found, namely, the monatomic Lennard-Jones gas in one-and two-dimensions, the unequal mass Toda lattice, the unequal

mass hard point gas, and the Calogero lattice with nearest neighbor interactions. Our initial efforts toward establishing rate equations has involved the study of energy transport. Our studies reveal that ergodic and mixing systems (unlike integrable systems) do yield a non-zero temperature gradient accompanying a heat current but, thus far, not as predicted by the Fourier Heat Equation, the expected rate equation for these systems. Apparently a sufficient amount of energy is still being transported via "soliton-like" pulses (waves forms which propagate without change of shape) to cause violation of proportionality between heat current and temperature gradient. It is expected that varying the available parameters for these systems, such as mass ratio, number of system particles, or interaction range, will make the "soliton-like" pulses unstable; however verification of this conjecture lies in the future.

As a sidelight in the process of performing our research, we discovered (contrary to previous belief) that the equal mass Toda lattice is integrable, and we verified that this lattice propagates energy without a temperature gradient as does the harmonic lattice. Our computer discovery of integrability subsequently led to startling new mathematical developments (by others) in analytically solving complicated nonlinear systems. In particular, the general solution to the equal mass Toda lattice has recently been discovered, and integrability has been rigorously proved for several other strongly nonlinear systems. These developments are leading to a renewal of close collaboration between pure mathematicians and physicists.