LA-UR-97- 3154

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Title: Phase Transitions, Nonequilibrium Dynamics,
and Critical Behavior of Strongly Interacting
Systems

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Submitted to: DOE Office of Scientific and Technical Information (OSTI)

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Phase Transitions, Nonequilibrium Dynamics, and Critical Behavior of Strongly Interacting Systems

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development project at Los Alamos National Laboratory. In this effort, large-scale simulations of strongly interacting systems were performed and a variety of approaches to the nonequilibrium dynamics of phase transitions and critical behavior were investigated. Focus areas included (1) the finite-temperature quantum chromodynamics phase transition and nonequilibrium dynamics of a new phase of matter (the quark-gluon plasma) above the critical temperature, (2) nonequilibrium dynamics of quantum fields using mean field theory, and (3) stochastic classical field theoretic models with applications to spinodal decomposition and structural phase transitions in a variety of systems, such as spin chains and shape memory alloys.

Background and Research Objectives

There is good theoretical evidence that quantum chromodynamics (QCD), the standard theory of strong nuclear interactions, undergoes a phase transition at finite temperature. Because the theory is strongly interacting, traditional analytic methods for understanding this phenomenon cannot be applied. The only universal technique available for calculating physical quantities in strongly interacting systems such as QCD is numerical simulations on a lattice. Present lattice QCD calculations estimate that this transition takes place at $T = 150$ MeV. Numerical simulations have a number of sources of systematic errors, such as finite box size, finite lattice spacing, and finite sample size. One of our goals is to reduce these systematic errors to the level of 2% or less.

The extreme conditions of temperature and density under which this phase transition takes place and a new phase of matter, namely that a quark-gluon plasma may be produced, will be realized in the laboratory and in fact existed in the early universe. Estimates of the critical baryon number density are around $n = 0.2$ inverse cubic fm and for the critical temperature $T = 150$ MeV. Such critical densities of baryon number are expected to occur at the Relativistic Heavy Ion Collider, or RHIC (now under construction at Brookhaven). An understanding of the dynamics of this process is especially important for the theoretical interpretation of the data to be produced by RHIC experiments in a few

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years. Lattice QCD calculations can only study the plasma in a static condition (i.e., equilibrium at a fixed temperature), whereas the conditions following a heavy ion collision are clearly very far from equilibrium (at least initially). One would like to understand how the plasma is produced, how efficiently it thermalizes on what time scale, how it evolves, and what are the special signatures (in terms of energy flow, particle production, correlations, etc.) of this new state of matter.

We developed large-scale numerical methods to obtain the dynamical equation-of-state of the quark-gluon plasma. This problem is challenging because of the multiple time and length scales in a highly nonequilibrium environment. We are developing field theoretic and numerical methods for attacking the general problem of quantum backreaction on classical fields, with applications to a variety of physical systems. We are involved in the first detailed calculations of energy-momentum flow, thermalization time scale, entropy production, and effective equation-of-state of the quark-gluon plasma phase of QCD for comparison with phenomenological hydrodynamic models and Boltzmann-Vlasov transport theory. As such, this work is of major importance to the field.

This theoretical effort complements the efforts of the Los Alamos Physics Division collaboration, which is presently engaged in designing experiments to be performed at RHIC. Our aim is to check which (if any) of the assumptions of the various hydrodynamical models are valid, as well as to obtain numerically the dynamical equation-of-state of the quark-gluon plasma as a function of the proper time coordinate in the future light cone of the collision event.

Our methods are applicable to a range of other physical problems. For example, the time evolution of the order parameter in a phase transition may be studied by similar techniques. These dynamics are of great interest in statistical mechanics (spinodal decomposition), where a second-order (or sometimes even fluctuation-dominated first-order) phase transition involves, by definition, multiple time and length scales. The study of this dynamics by advanced computing techniques has important consequences for materials such as amorphous metals and shape memory alloys (where the phase transition is first order). An important problem of interest is cosmological phase transitions in which there is again an interplay between several time and length scales, ranging from microscopic interaction and relaxation time scales to the expansion time scale of the universe. Large-scale numerical methods provide the only available technique to study this problem.

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

An important aspect of our project is computational: our simulations are ideal for evaluating the robustness of the hardware and software of emerging parallel architectures. Indeed, they were so used to test the CM-5 and the Cray T3D at the Advanced Computer Laboratory (ACL) at Los Alamos; they now will be ported to the next generation of supercomputers soon to arrive at the ACL.

The DOE HPCC Grand Challenge award for 1992-1996 allocated us substantial time on the CM-5 at Los Alamos. We worked in close collaboration with staff scientists at the ACL to develop hardware and software optimization tools and graphics. This symbiotic relationship between a basic science goal and computing as a tool will continue to contribute significantly to the Laboratory's growth as a front-runner in advanced computing.

Scientific Approach and Accomplishments

Los Alamos has a large experimental commitment to study heavy ion collisions at RHIC. These collisions give rise to the formation of a very large energy and entropy density in the central region. Our lattice calculations of the static properties of high-temperature QCD go toward providing a theoretical understanding of this phase and provide hints of new experimental signatures that can be detected at RHIC. We are also pursuing the study of the nonequilibrium conditions following a heavy ion collision using both analytic and numerical methods.^{1,2,3,5} In this effort we also aim to complement the Laboratory's experimental effort by predicting the dynamical behavior of the quark-gluon plasma.

Problems in statistical mechanics form the basis of our understanding of condensed matter systems and novel materials. The development of most of the numerical techniques used in lattice QCD⁷ and condensed matter originated in the study of spin models. Their study continues to provide intuition, new algorithms to overcome critical slowing down in the update, and interesting new phenomena. The study of these models is invaluable from the point of view of investigating real materials and as toy-field theoretic systems. We investigated the production of topological defects in these systems, as well as studied the statistical mechanics of nonlinear structures such as kinks in continuous spin models.⁸ We also investigated critical behavior and universality in Ising models.⁶

We developed parallel codes to take full advantage of the computer power at Los Alamos, in particular the CM-5 at the ACL. The real-time evolution of the field theoretic system was studied using $1/N$ and closed time-path methods.^{4,9} We succeeded in implementing a practical renormalization scheme that allows the solution of dynamical quantum field theoretic problems on the computer. The complexity of the computational problem for the nonequilibrium evolution of the QCD plasma may be appreciated by noting that even the simplest of our test problems requires hours of CM-5 time (the memory requirements are also very extensive).

The study of topological transitions¹⁰ and statistical mechanics of kinks⁸ (so far in one spatial dimension) uses very-large-scale, partial differential equation (PDE) simulations performed on the CM-5. In the case of kink dynamics, these simulations have revealed the existence of multiple time scales in these problems, especially in the presence of multiplicative noise. The large size of these simulations has enabled us to overcome some of the problems that bedeviled earlier work. We have applied our methods to models of shape memory alloys in 1+1 dimensions. In higher dimensions, these models display a fluctuation-dominated first-order phase transition. To see this very interesting regime, we are now in the process of extending our work to higher dimensions.

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