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NONLINEAR SYSTEMS OF PARTIAL DIFFERENTIAL EQUATIONS



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# FINAL REPORT

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## 1. INTRODUCTION

We list in the bibliography here some 40 items: research papers associated with work during the grant period — including some items which represent the continuation of work initiated during that period. These have been listed in roughly the order in which the work was done, although many of the projects overlap in timing so it is difficult to fix any precise order.

From the viewpoint of the grant, the most significant accomplishments have been, of course, those specifically related to systems of nonlinear partial differential equations with a particular emphasis on semiconductor device models. These are discussed at some length in the next two sections. We also note that *in addition* the Principal Investigator has been involved in a considerable variety of other mathematical activity — especially the work on *switching systems*, supported by the National Science Foundation under the grant ECS-8814788. Some of these collateral activities are discussed, rather more briefly, in Section .

## 2. SEMICONDUCTOR MODELLING

The initial activity<sup>1</sup> in this area was an invited talk [8] at the *AMS Summer Seminar on Computational Aspects of VLSI and Device Simulation* in the Spring of 1987. The principal result described there was well-posedness of the van Roosbroeck semiconductor model with the inclusion of source terms of the sort typically involved in the modelling of impact ionization, etc. It should be noted that all previous work on related models had assumed that the only interaction terms were recombination — essentially dissipative — without any generation terms. The treatment in [8] required some new technical machinery in order to be able to treat this more difficult problem — new estimates whose discrete analogues are now also of use for justifying convergence of a computational algorithm [39].

During the Summer of 1987 this material was presented in increasingly improved forms at ICIAM,<sup>2</sup> in Madrid, and at a conference [13] at Howard

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<sup>1</sup>While much of the technical development here represented work done before the grant period, it is fair to say that the grant and the opportunity to attend this seminar were seminal in bringing this to fruition.

<sup>2</sup>The applied Mathematics meeting in Paris, which also provided some opportunity to meet other workers in the area of semiconductor Mathematics, as Fichtner, Markowich, Polak, etc.

University. This last form [13] would seem definitive except for some restrictive conditions on the geometry for the uniqueness argument.

The present status of this line of investigation is that a further improvement has been made in the argument which makes this applicable to geometries corresponding to many of those of physical interest, including certain (re-entrant) corners.<sup>3</sup> While a still further improvement seems quite possible,<sup>4</sup> it now seems appropriate to be preparing a more detailed presentation [38] for journal publication, including the newer details of the argument together with a treatment of the coupling with temperature which did not appear in the conference versions. Further, the technical machinery which permitted the theoretical analysis is also adequate, with some modification, to justify [39] numerical computation.

The other principal line of investigation in this area has concerned a new algorithmic model originally presented [15] at a conference in Finland during the Summer of 1988 and later, with minor modification, again presented [18] at a conference on VLSI and circuit simulation held at Oberwolfach that Fall.<sup>5</sup> The point of this analysis is that van Roosbroeck's treatment of velocities and mobilities, while appropriate to the near equilibrium situations he was considering, is inadequate for the consideration of modern devices with, e.g., strongly varying fields. While *ad hoc* treatments are used in computation to handle the difficulties with 'velocity overshoot', it seems desirable to return to a more fundamental modelling effort. The unique feature of the present treatment is that it goes directly from the physical modelling to a

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<sup>3</sup>This 'corner' analysis was accomplished during the Principal Investigator's visit in Bordeaux this past Summer. It is possible that a brief note will be written concerned purely with this analysis and its computational implications in advance of the completion of [38] and [39].

<sup>4</sup>This would be based on the development of conjectured new 'weighted  $W^{1,p}(\Omega)$ ' regularity estimates for problems involving coefficients which are continuous in  $\Omega$  with controlled blowup of the modulus of continuity, e.g., near corners. While some such estimates are certainly correct, the *useful* relation between the hypotheses and conclusions has proved more elusive than originally anticipated.

<sup>5</sup>This last led to discussions with Desgondes (École Polytechnique) and others about such models, related to the underlying Boltzmann modelling of particle and energy transport. During this past Summer it was then possible to participate in a 'European' semiconductor mini-conference in Paris and continue these discussions. There has been a start made on implementation of this model but, as of now, even this preliminary one-dimensional version is not yet debugged.

computational algorithm without introducing a partial differential equation as an intermediate construct. While there is no suggestion that this model, especially in its present crude form, would be particularly efficient for computation, the idea is to have an algorithmic construction in which a variety of physical mechanisms can be inserted conveniently and yet in a less *ad hoc* fashion than in many 'engineering' treatments.

The continuing activity in this area, then, consists of (a) completing the actual writing of the papers [38] and [39], (b) continuing the development of the computer code for the new model and experimenting with (variants of) this, (c) developing further the analysis of corner effects in the interaction of the field and the conservation equations. Although this is not directly an outgrowth of the activity in this area initiated during the grant period, we note also that the investigation (discussed in the next section) of free boundary problems may lead to work on the oxydation problem arising in MOS chip fabrication.

### 3. OTHER NONLINEAR SYSTEMS

We note that work in this area had two principal foci of activity: free boundary problems and some problems arising from chemical engineering. There were also a variety of other items.

#### 3.1: Free Boundary Problems:

At the invitation of the organizers, the Principal Investigator participated in the Fourth International Conference on Free Boundary Problems (held at Irsee, W. Germany, in the Summer of 1987) and spoke on a controllability result for a flexible robot arm. The paper [9] is primarily concerned with controlling longitudinal vibration in an arm with a prismatic joint (using 'extension' as the control); a more recent continuation [22] of this line of investigation treats conditions for optimality in a corresponding problem for transverse vibration of an Euler-Bernoulli beam. In each case, the principal difficulty is that the control is varying the relevant length of the arm so one is comparing solutions defined on different (time-varying) spatial domains, not known *a priori*.

A conversation at this conference led to involvement with a free boundary problem for the growth/dissolution of a crystal [11], [10]. Here, Conrad had considered steady states but wanted to set this in the context of the time-dependent problem, for which no existence result was then available.

Adapting a technique developed in connection with [13], it proved possible to show well-posedness for this problem — at least in the context of (assumed) radial symmetry. Related to this are two papers [12], [17] on control-theoretic aspects of the problem. The first provides existence and compactness results (but not uniqueness) under weaker conditions than in [11] — needed to show existence of optimal controls. The second obtains the optimality conditions, gives additional regularity, and considers numerical computation.

We note that this work on free boundary problems is quite closely connected with the investigations of shape optimization which are the focus of the Principal Investigator's newer proposal. Continuing work on the problems just noted will consist of (a) a continuation of [22], (b) the extension (again joint with D. Hilhorst) of [11] to an unbounded domain with investigation of the long-time behavior, and (c) joint work with S. Jensen on numerics for the crystal problem without the assumption of radial symmetry. For this last, we note that the motion of the free boundary is now given in terms of the local curvature of the boundary and one can expect that techniques developed for this will also be applicable to a variety of other interesting free boundary problems involving such dependence.

### 3.2: Chemical Kinetics:

The first recent work in this area [16] was joint with H. Haario,<sup>6</sup> considering modelling and computation for a 'film model' for a bubble reactor. This involves coupling through the boundary conditions of a PDE diffusion-reaction system in the 'film' with an ODE system in a bulk fluid. A subsequent paper [28] considers a somewhat more complicated system of the same type, showing convergence to steady state.

During the visit to Finland, Haario arranged a consulting visit to a chemical company. At that time I proposed (as more appropriate to the actual situation) a modified model, related to treatments of age-structured population models. Haario has been working on this and I will also be involved in the continuation of that work. A question was raised at that visit about another problem, now the subject of joint investigation with Hilhorst and others in Paris, involving two reactions:  $A + B \rightarrow C$   $A + C \rightarrow [\text{product}]$ , with the first comparatively 'very fast'. Letting  $\lambda$  be the ratio of reaction

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<sup>6</sup>One of the organizers of the conference at which the semiconductor paper [15] was presented; indeed, this interaction began by e-mail in connection with that invitation.

rates, One has two interesting asymptotic problems: (possible) convergence to steady state as  $t \rightarrow \infty$  and the singular perturbation problem as  $\lambda \rightarrow \infty$  which, in fact, becomes a free boundary problem in the limit. This is also related to a boundary layer problem in electrochemistry. Some results were obtained in each direction during the Principal Investigator's visit to Orsay this past Summer and investigation continues [45], [46].

### 3.3: Various Other Problems:

Probably the most interesting 'other problem' is the success in a project with S. Antman, initiated about 10 years ago. This [32] concerns a viscoelastic rod model of 'differential equation form', i.e., not formulated in terms of material memory. We have found hypotheses on the relation between the viscosity and the elastic potential enabling us to show global existence for a genuinely nonlinear model for which one can also show a pointwise bound precluding infinite compression. The present results are for a single equation (considering only longitudinal motion of the rod) rather than a system but the extension to a full Cosserat rod model is anticipated. To the extent that this positive result could later be complemented by some 'necessity', this would be a fundamental contribution to the theory of rheology.

Of other work on nonlinear systems, we note a number of papers under revision or recently revised: [26] (recently resubmitted) and [34] on issues of controllability and stabilizability — each validates a new technique for analysis — and [33], extending earlier results, on periodic solutions of a nonlinear parabolic equation with a flux boundary condition. Another result, in a paper [21] motivated by an earlier investigation of determining the nonlinearity  $k(\cdot)$  in  $u_t = \nabla \cdot k(u)\nabla u$  from overdetermined boundary data, is that one has convergence to steady state for that equation, again in the context of a flux boundary condition.

We note finally an existence/uniqueness result [30] for a somewhat unusual parabolic equation, arising from an empirical turbulence model, in which the diffusion coefficient depends nonlinearly on the boundary trace of the derivative and [44], which provides well-posedness and some asymptotic results for the Raman scattering system.

## 4. COLLATERAL ACTIVITY

In this section we discuss, somewhat more briefly, activity by the Principal Investigator during this period in *addition* to that primarily associated with *nonlinear partial differential equations*, the focus of the grant. Note that, although much of the investigation of switching systems actually *has* focussed on nonlinear partial differential equations, this has been separated out here since this activity in particular is currently being supported by the National Science Foundation (under grant ECS-8814788). The other foci of activity are ill-posed (inverse) problems and distributed parameter (control) systems but there are several more isolated items.

#### 4.1: Switching Systems:

As noted, this activity is currently being supported by the NSF (since this past Spring, somewhat overlapping the period of AFOSR-87-0190) but some of the work is of older origin. The original development of this line of investigation came from modelling a thermostat (so the initial setting was that of partial differential equations) but has since been more general. This work considers systems which evolve smoothly, e.g., by a differential equation, except for abrupt changes of 'mode'. The concern is for systems having a different switching surface for reversal of a mode change, essentially a hysteresis phenomenon; much of the work has emphasized the dynamic behavior, as existence of periodic solutions. Note that the 'switching' makes these systems inherently nonlinear.

The paper [6] develops a fundamental theory for such systems while [14] both surveys known results on periodicity and presents some new results; an expanded 'journal version' [40] of the latter is now in preparation. The two papers [7], [19] are concerned with control-theoretic aspects of this; we note that [19] introduced stochastic considerations and work has been initiated with M. Freidlin on the differentiability with respect to parameters of expectations associated with Ito equations including a (discontinuous) 'thermostat nonlinearity'. The conference presentation [23] (and the expanded version [41]) consider such systems as global 'outer' models of certain singularly perturbed nonlinear systems as well as limiting behavior as the hysteretic switching surfaces move to coincidence. Other future development of this line of investigation is expected to consider possible chaotic modes for the dynamics and the behavior of systems involving coupling of a continuum of thermostat nonlinearities.<sup>7</sup>

<sup>7</sup>This seems relevant to magnetic hysteresis (Preisach model), to phase changes in

#### **4.2: Ill-Posed Problems:**

It happens that most of the work in this area has its roots in a visit to the Centre for Mathematical Analysis (Australian National University) in the Fall of 1986. The only exception is the recent paper [21], already noted. In particular, the papers [2], [3] were largely done at ANU, although much writing and revision was done during the grant period. These concern, respectively, continuous dependence of spectral data on a 'rough' potential and the convergence of Tikhonov regularization in nonlinear contexts.

The most significant line of investigation here is the development of a theory of 'Optimal Filtering' for a class of ill-posed problems. The initial joint work with Eldén [29] was begun at ANU and continued during a visit to Linköping in 1988. The method has now also been applied to the backward heat equation [43] and a more abstract, more general treatment [47] is now being written. This theory obtains a filter of optimal accuracy for certain ill-posed problems which may be formulated as parametrized with a particular structure and suggests a novel computational approach for a somewhat more general class of problems. It is expected that future development of this line of investigation may, e.g., provide applicability to some problems of image enhancement.

The paper [25] is concerned with some 'fundamental' issues and approaches to ill-posed problems — here formulated as issues of computational complexity. A related discussion of this [42] in the context of 'system identification' will be presented at the ACC in May. The key idea is that complexity should be formulated in a way permitting concatenation of problems; it is anticipated that a treatment of more general aspects of this will be prepared for the J. of Complexity.

#### **4.3: System Theory and Control:**

While each of these items is also noted in some other context, we identify here all those papers involving control-theoretic considerations: [4], [7], [9], [12], [17], [19], [20], [21], [22], [23], [24], [26], [31], [34], [35], [42].

#### **4.4: Miscellanea:**

We begin by noting some 'holdovers': the papers [5], [4], [1] go back to before the grant period and have still not appeared. In addition, three certain history-dependent materials, and to elasto-plasticity.

papers have been 'sitting' for some while: the control-theoretic paper [35] (using semigroup methods to relate controllability and observability results to the construction of stabilizing feedback laws) and the papers [36], [37] which await new ideas, although partial results have been obtained. The papers [34], [33] have only recently been re-activated; also, [31] involves primarily older analysis of a numerical method with more recent supporting computation.

The paper [27] extends an earlier result in nonharmonic analysis by the Principal Investigator (motivated by a boundary control problem for a vibrating plate); here, a referee's suggestion for revision has led to a substantial improvement of a result on the blow-up of the 'coefficient map' as the observation interval shrinks.

Finally, we note a new line of investigation, joint with P.R. Kumar, on the stability of scheduling policies (for flexible manufacturing systems, but with results also applicable to asynchronous models of parallel computation). The initial results [20], [24] are negative (for a particular class of policies) and further investigation is in progress testing conjectures as to the construction of other classes of policies supporting positive results.

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