·ARGONNE NATIONAL LABORATORY          December 7, 1973

Professor Alan Hindmarsh
Lawrence Livermore Laboratory
P.O. Box 808
Livermore, California  94550

Dear Alan:

Recent telephone conversations with you and others have encouraged us to proceed
with plans for the ODE Software Workshop.  It appears that the week of June 3
is acceptable to everyone.  "Mathematical Software II" at Purdue is the
week before.  Whether we schedule 4 or 5 days is open to discussion and I
solicit your comments.  We won't exhaust the subject in 5 days, but I'm not
sure about the participants.

The objective of the workshop can be simply stated though its accomplishment
will tax our capacities both as scientists and as diplomats.

*Objective:  Define the capability and user interface of a systematized collection**
*of routines for solving ordinary differential equations.  Propose the contents*
*of the collection which would achieve that capability.*

This is no abstract exercise.  The NATS project is interested in coordinating the
preparation, field testing and distribution of an ODE package but there are two kinds
of reasons why this is a more formidable task than the creation of EISPACK.
First, it is clear that there is far less general agreement about the nature
of such a package.  Second, collaboration with other institutions must
include work at the code development level since Argonne cannot claim the kind
of expertise in ODE software that we have in other software areas.  While the
identification of these institutional issues is not explicitly listed as an
objective of the workshop I hope we can make a start on deciding how we
might work together.

I invite each of you to nominate one or two of your colleagues to attend the
workshop with you.  We are especially eager to involve people who are experienced
in software development and who are aware of the problems involved in
creating multisystem programs.

The Laboratory will reimburse the participants for round-trip tourist class
airfare from their usual place of business to Chicago, lodging and local
transportation.  In addition, a per diem of $13 per day will cover meals
and incidentals.

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     *We use the term "systematized collection" as in Smith, B.T., Boyle, J.M.,
and Cody, W.J., The NATS Approach to Quality Software, to appear as Chapter 23
in the Proceedings of the Loughborough Conference.

We are looking forward to hearing from you.  Your suggestions about topics to be covered are important, especially at this formative stage.  I have enclosed a list of the "Core Leaders" who have indicated an interest in participating.

Yours very truly,

Wayne Cowell
Applied Mathematics Division

WC/sg
attachment

January 11, 1974

Dr. Wayne Cowell
Applied Mathematics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

Dear Wayne,

I am definitely planning on participating in the ODE Software
Workshop. In addition, I would like to invite Professor George Byrne
from the University of Pittsburgh (Departments of Mathematics and
Chemical & Petroleum Engineering) to come as my colleague. (We have
been developing an ODE code together.) Both of us will also be at
the Purdue conference.

I am contemplating inviting also Fred Fritsch from the Numerical
Mathematics Group here. He is experienced, not in ODE software develop-
ment, but in mathematical subroutine libraries and portable software
generally. If coding standards, portability, and the like are to be
major agenda items, his presence (at least part of the time) could be
helpful. I need your judgement on this.

In discussions with George about the meeting plans, some thoughts
came up which I'll pass on to you. The matter of who (and how many)
should participate in the project is one that you have no doubt given
much thought. If too many are involved at the level of setting stan-
dards and making decisions, there will be difficulty reaching a consen-
sus. If too few are involved, there might be a lack of acceptance of
the end product by the user community. I'm hopeful that the group com-
ing in June is such that both objections are met, but perhaps these
questions should be taken up again there with respect to later activi-
ties.

On the attached page I've listed some discussion topics that have
occurred to me. They are approximately in the order that they should be
covered. I would suggest that, whatever the final list of topics is,
it be sent to each participant well in advance, to allow us to give
prior thought to the issues likely to arise. In particular, regarding
code sources, I suggest that each person be advised to bring a list of
all known codes that would be relevant, and if appropriate, of any
methods that should be included but are not yet implemented in codes.

In general, I am quite optimistic about this effort. The time is
right for it. Whether 4 or 5 days is needed isn't at all clear to me,

but I'm willing to stay the full week if everyone else is. It may be a painful day or two before we come to understand each other and tolerate our mutual differences of opinion in a professional manner. But thereafter, with a generous dose of the spirit of compromise, I think we can go a long way toward the stated objective.

I will be eager to hear more about plans for the workshop when they have jelled. Also, I would appreciate your advice about inviting Fred Fritsch as soon as possible.

Very sincerely,

A.C. Hindmarsh
Numerical Mathematics Group, L-310
Computation Department

ACH/csm

cc: G.D. Byrne
    F.N. Fritsch

Encl.

# POSSIBLE TOPICS

1. Problem domain

   a) Initial value vs. boundary value problem

   b) Stiff vs. nonstiff

   c) 1st order vs. higher order equations

   d) Expensive vs. inexpensive $f(y,t)$ $(=\dot{y})$

   e) Expensive vs. inexpensive higher derivatives

   f) Specialized versions: differential-algebraic and implicit systems, banded or sparse Jacobian

2. Code sources

   a) Existing code candidates

   b) Unimplemented algorithm candidates

3. Programming standards

   a) Standards for EISPACK

   b) Call sequences

   c) Use of Common

   d) Modular structure

4. Testing

   a) Test problem sets

   b) Independent test centers

5. Funding

   a) Code development needs

   b) Testing needs

   c) Site selection

6. Name : ODEPACK?

U of C-AUA-USAEC

Dr. Fred N. Fritsch
Lawrence Livermore Laboratory
University of California
P.O. Box 808, L-63
Livermore, California 94550

Dear Fred:

I was pleased to have a suggestion from Alan Hindmarsh that you attend the ODE
Software Workshop at Argonne next June 3 - 7. I shall assume that Alan has
discussed the workshop with you so that you are aware of our objectives.
Although much of the workshop's work will focus rather particularly on differential
equations, we do want to consider questions of standards, portability, and
the related software engineering; and I shall attempt to arrange the agenda
so you can participate in those discussions and will have the freedom to use
your time at Argonne in conversations with Lyness and Cody and others when workshop
turns to nitty-gritty that may be outside your interests. As Jim Pool has suggested,
we wanted to attract you to Argonne for the latter purposes anyway, and may as
well capitalize on this opportunity.

It seems likely that Brian Ford will attend the workshop and participate in
the same discussions that would particularly interest you. I certainly hope you
will plan to attend.

The Laboratory will reimburse the participants for round trip tourist class air fare
from their usual place of business to Chicago, lodging and local transportation.
In addition, a per diem of $13 per day will cover meals and incidentals.

I will be writing to you very shortly concerning our plans for NATS II.

Cordially,

Wayne Cowell
Applied Mathematics Division

WC/sg
cc: Dr. Alan Hindmarsh

# ARGONNE NATIONAL LABORATORY

January 22, 1974

Professor George Byrne
Department of Mathematics
University of Pittsburgh
Pittsburgh, Pennsylvania 15213

Dear Professor Byrne:

Alan Hindmarsh has suggested that you attend the ODE Software Workshop at Argonne next June 3 - 7. We are delighted with this suggestion, and I extend to you a cordial invitation to participate.

Perhaps Alan has discussed the workshop with you, so you are likely aware of our objectives. Our purpose is to define the capability and user interface of a systematized collection* of routines for solving ordinary differential equations. We also hope to propose the contents of the collection which would achieve that capability.
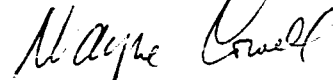
You may have heard of the NATS project which has been concerned with carrying out the systematization process for certain classes of codes notably an Eigensystem package called EISPACK and a special function package called FUNPACK. An important function of the NATS project activities is field testing in which Lawrence Livermore Laboratory has participated in a significant way. The project is interested in coordinating the preparation, field testing, and distribution of an ODE package, but there are two kinds of reasons why this is a more formidable task than was the creation of EISPACK. First, it is clear that there is far less general agreement about the nature of such a package. Second, collaboration with other institutions must include work at the code development level since Argonne cannot claim the kind of expertise in ODE software that we have in other software areas. While the identification of these institutional issues is not explicitly listed as an objective of the workshop, I hope we can make a start on deciding how we might work together.

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*We use the term "systematized collection" as in Smith, B.T., Boyle, J.M., and Cody, W. J., The NATS Approach to Quality Software, to appear as Chapter 23 in the Proceedings of the Loughborough Conference.

The Laboratory will reimburse the participants for round-trip tourist class air fare from their usual place of business to Chicago, lodging and local transportation. In addition, a per diem of $13 per day will cover meals and incidentals.

We are looking forward to your attendance and will in the meantime welcome your suggestions about topics to be covered. I understand that we already have input from you reflected in the list of topics in Alan's recent letter. Because of your Engineering connections you may be able to offer insight from the User community which would be very valuable.

Yours very truly,

Wayne Cowell
Applied Mathematics Division

WC/sg
cc: Dr. Alan Hindmarsh

Date:     April 2, 1974

To:       Participants in ODE Software Workshop

From:     Wayne Cowell

Attached is a list of participants in the ODE Software Workshop.
We are now working on an agenda that will occupy 4 full days,
June 3 - 6, with Friday morning, June 7, left open for ad hoc
continuation of unfinished business.

At this early stage of agenda preparation I propose that we spend
approximately one day each on the following general topics:

1. The capabilities of an ODE package;
2. The content and structure of an ODE package;
3. Testing ODE software;
4. Modes of collaboration.

To stimulate your thinking in these areas I have attached a list
of topics that Alan Hindmarsh and George Byrne constructed and a
list of leading questions I put together.  I am inviting each of
the participants to begin collecting his thoughts and assembling
program write-ups, reports, etc. that address these questions.

In 3-4 weeks I will be calling to discuss topics of particular
concern to you and to work out ways of covering your interests
adequately.  In the meantime I suggest that you circulate to all
participants, with a copy to me, any reports or comments you feel
should be studied prior to the meeting.  I expect to circulate
some thoughts on question 6 (organization and funding).

We will ask for your travel plans later so we may make local
arrangements.

WC/sg

attachment

ODE SOFTWARE WORKSHOP

Argonne National Laboratory

June 3 - 7, 1974

## List of Participants

Leonard Brown
c/o William Gear
University of Illinois
Department of Computer Science
Urbana, Illinois  61801

George Byrne
Department of Mathematics
804 Schenley Hall
University of Pittsburgh
Pittsburgh, Pennsylvania  15260

Wayne Enright
Department of Computer Science
University of Toronto
Toronto, Ontario, Canada

Fred N. Fritsch
Lawrence Livermore Laboratory
University of California
P.O. Box 808, L-63 $3'$
Livermore, California  94550

C. William Gear
University of Illinois
Department of Computer Science
Urbana, Illinois  61801

Marilyn Gordon
Applied Mathematics Division, 2642
Sandia Laboratories
Albuquerque, New Mexico  87115

Alan Hindmarsh
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Thomas E. Hull
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Fred Krogh
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Joan Walsh
Department of Mathematics
The University,
Manchester
M13 9PL
ENGLAND

## POSSIBLE TOPICS

1. Problem domain

   a) Initial value vs. boundary value problem

   b) Stiff vs. nonstiff

   c) 1st order vs. higher order equations

   d) Expensive vs. inexpensive $f(y,t)$ $(=\dot{y})$

   e) Expensive vs. inexpensive higher derivatives

   f) Specialized versions: differential-algebraic and implicit systems, banded or sparse Jacobian

2. Code sources

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   a) Standards for EISPACK

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4. Testing

   a) Test problem sets

   b) Independent test centers

5. Funding

   a) Code development needs

   b) Testing needs

   c) Site selection

6. Name : ODEPACK?

Alan Hindmarsh
George Byrne
1-11-74

ODE SOFTWARE WORKSHOP

Argonne National Laboratory

June 3 - 7, 1974

Questions for Consideration

1. Assume that the current level of effort in ODE software remains
   essentially constant over the next 5 years and that duplication
   of effort is minimal. What capabilities should ODE software possess
   in 1979?

2. Shorten the time to two years so that only software that exists
   or is in an advanced stage of completion can be considered. What
   capabilities could be exhibited by ODE software in 1976?

3. If the 1976 software could be assembled into a systematized
   collection (analogous to EISPACK) what capabilities do you
   see as having high, moderate, and low priority? (See Hindmarsh-
   Byrne Topic 1.)

4. What existing or proposed codes embody the capabilities of
   question #3? (See Hindmarsh-Byrne Topic 2.)

5. What programming conventions should be required or recommended?
   Shall the requirements apply to existing software thus implying
   restructuring or, at least, reformatting of existing code? Are
   the conventions you suggest adequate to insure that code written
   by different people in different places can be merged into a
   single package? (See Hindmarsh-Byrne Topic 3.)

6. How should an effort to create a package as in question #3 be
   organized and funded? (Note: Here "create" includes assembly
   of code from various sources into a coherent collection, carrying
   out testing procedures, disseminating and supporting the package.
   This question probes the relationship of the ODE effort to
   existing efforts.) (See Hindmarsh-Byrne Topics 4, 5.)

Wayne Cowell
4-1-74

May 8, 1974


TO:       Participants in the ODE Software Workshop,
          June 3-7, 1974

FROM:     Wayne Cowell

SUBJECT:  Collaboration and Systematized Collections

     Suppose that, as a result of discussions among leaders in the
field, there emerges a consensus as to the capabilities of an ODE
software package and agreement, at least tentatively, on existing
codes which implement that capability.  What, then, is the nature
of the process through which various groups can work together to
use such codes as raw material for the creation of a coherent pack-
age?  In my memo of April 2 I promise some remarks on this central
question.  Such remarks are necessarily very general at this time
but, as a preliminary to discussions during the workshop, I would
like to outline the structure of an ODE software task force and
to indicate the role that Argonne might play.

     In earlier correspondence I referred to a paper that Brian Smith,
Jim Boyle, and Jim Cody gave at the Loughborough Conference last year.
The proceedings of that conference will appear as Software for Numerical
Mathematics, D. J. Evans, ed., Academic Press, 1974.  Since the book
has not yet appeared, I have enclosed a copy of the paper.  It does
not deal explicitly with organization, but it offers a description of
systematized collections which can be translated into an organizational
approach to the creation of such collections.

     For individual mathematical routines the paper describes the
"quality attributes": reliability, robustness, structure, usability,
validity.  It then gives meaning to these same attributes for col-
lections of routines and defines a systematized collection to be a set
of subroutines which collectively solve a wide spectrum of problems and
which possess the quality attributes as individuals and as a collection.
The discussion in the paper is essential to an understanding of the NATS
usage of these terms, but let me present the following summary for
reference:

          Reliability is the ability of a subroutine or package
          to perform a well-defined calculation accurately and
          efficiently.  Achieving reliability requires a care-
          ful selection of underlying algorithms and their faith-
          ful implementation in software.

Robustness is the ability of a program or a package to detect and gracefully recover from abnormal situations without terminating the computer run unless precise computational results cannot be achieved, and then with provision of appropriate default numerical results and precise diagnostic information.

Good structure requires that the logical flow be easily traced. The choice of variable names, format of source code, and comments contribute to structure as does the manner of amalgamating individual programs into a coherent package. NATS did not demand the formality of what has become known as "top-down structured programming" but adopted the spirit of that movement.

Usability describes the ease with which a user can choose a program and apply it to his problem. Documentation and calling sequences are basic to this attribute.
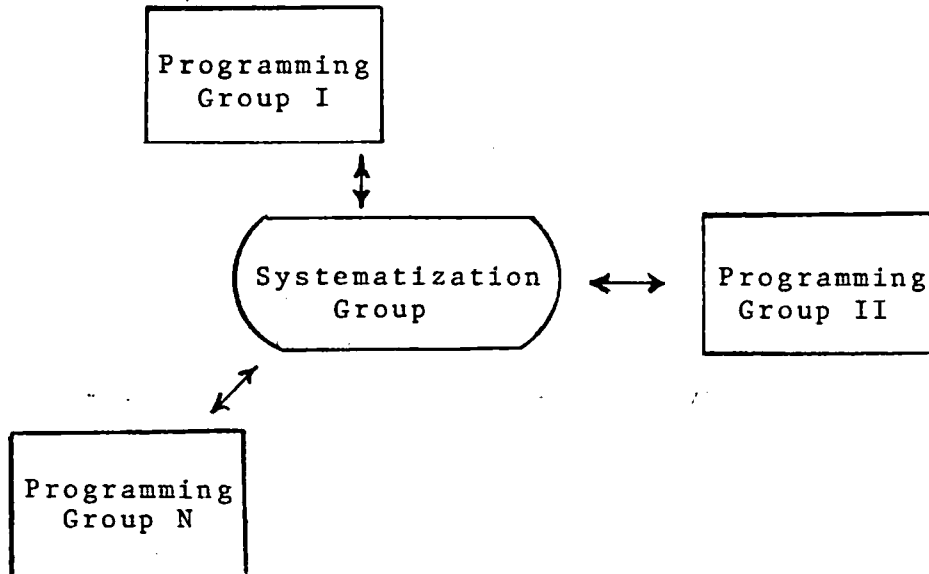
Validity refers to evidence of good performance as demonstrated by a testing process.

The systematized collections thus far released by NATS, namely EISPACK and FUNPACK, were derived from single sources and the people who actually wrote the Fortran, prepared the test materials, and coordinated the field testing worked in the same hallway. They correlated their efforts through regular project meetings and many informal conversations. Programming conventions and project procedures evolved and became part of the general understanding within the group. Ensuring that the individual routines possessed the above quality attributes was not separated from work that ensured that the collection possessed them. However, I believe that it is possible for work on individual routines to be physically separated from work on systematizing the collection of such routines provided certain agreements have been reached.

We must expect that the group as a whole shall have determined what routines are to be included in the collection. Moreover, the individual routines shall have been assigned to programming groups, most likely to the group which developed the routine in the first place. Further (assuming ANSI Fortran as the source language) the group as a whole must have agreed to conventions on calling sequences, data handling, formatting, naming of variables, and documentation.

Finally, a systematization group must be formed. The task of the programming groups is to ensure that the routines assigned to them have the quality attributes. The task of the systematization

group is to build a systematized collection using the given routines.
The programming groups and the systematization group will follow the
conventions determined by the whole group.

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        ┌─────────────────┐
        │  Programming    │
        │   Group I       │
        └─────────────────┘
                 ↕
    ╭─────────────────╮         ┌─────────────────┐
    │ Systematization │  ◄────► │  Programming    │
    │     Group       │         │   Group II      │
    ╰─────────────────╯         └─────────────────┘
           ↙↗
  ┌─────────────────┐
  │  Programming    │
  │   Group N       │
  └─────────────────┘
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     In carrying out its task, the systematization group would serve
as the clearing-house for the entire effort.  The job of assembling
the pieces will require that group to remain in close contact with
each programming group as the work progresses.  The systematization
group would be responsible for field testing (part of assuring
validity) but each programming group would supply test cases for
the routines in its assignment.

     I think that funding for the activities of each programming group
should be developed by that group.  In particular, we at Argonne are
interested in setting up a systematization group which would, in effect,
be offering a service to the other groups who could then, hopefully,
justify their activity in terms of incorporating their past efforts
into a larger entity.

     There is active planning underway which, we hope, will lead to a
"mathematical software alliance".  An ODE software effort would be an
interesting prototype of the sort of thing an "alliance" would ac-
complish.

     It would be a mistake to begin a job of this size unless we thought
we had a reasonable chance to succeed.  We may conclude that the time
for an ODE software task force has not yet come.  The success of the
workshop as a forum does not depend on a positive decision to consort
further in a structured way.  But I believe that the idea is worthy of
serious consdieration and, if an organized effort toward a systematized
ODE package appears feasible, we can make a beginning in June.


WRC/dp

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*Multiple Listing
**Part-time Employee
***Temporary Employee
9/18/73

# ARGONNE NATIONAL LABORATORY

May 9, 1974

Professor Thomas E. Hull
Department of Computer Science
University of Toronto
Toronto, Ontario, Canada

Dear Tom:

The enclosed agenda is intended to be dynamic in the sense that the actual time spent on each topic will be determined by the course of the discussion. Frequent agenda reviews will enable us to allocate our time. Thursday afternoon and Friday morning will serve as buffers. I believe that each topic is essential and must be adequately covered. If your concerns are not subsumed under the listed topics, we will make necessary additions.

I have asked certain participants to make statements on various topics so as to provide a framework for well-informed discussion. Any participant is welcome and encouraged to make a statement at the beginning of the discussion of any topic. The chairpersons are people whose primary interest is not ODE software and whose task is to ensure that the discussions are conducted with reasonable order.

Again let me urge you to circulate reports, memoranda, and proposals to the participants. Please note that the name of Dr. David Sayers of Oxford has been added to the list. Also please note that I am herewith circulating a memorandum relevant to Topic VII.

Please return the enclosed housing and travel form as soon as your plans are definite.

We are looking forward to an exciting "ODE Week" at Argonne.

Cordially,

Wayne R. Cowell
Applied Mathematics Division

WRC/dp
Enclosures