

NUMERICAL ALGORITHMS GROUP
(NAG)

Telephone: Oxford (0865) 56727
Extension 248

The NAG Central Office
Oxford University Computing
Laboratory

13 Banbury Road
Oxford OX2 6NN

Your Ref :

Our Ref : 1.A.145

17th November, 1975

Mr. A.C. Hindmarsh,
Numerical Mathematics Group, L-310,
Lawrence Livermore Laboratory,
University of California,
P.O. Box 808, Livermore,
California 94550,
U.S.A.

Dear Alan,

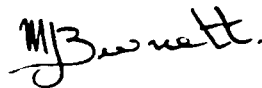
Thank you for your letter of the 17th September, which we have just received.

Thank you also for your efforts to make EPISODE available to us, one appreciates that on occasions bureaucracy hinders us all. Certainly, if anybody wants a copy of EPISODE and you are happy for them to have it from us please let me know.

It was a pleasure seeing you again. I hope we shall have more time to chat next time we meet.

Best wishes,

Yours sincerely,



B. Ford

(Dictated by B. Ford
and signed in his absence)



UNIVERSITY OF TORONTO Toronto, Canada M5S 1A7

DEPARTMENT OF COMPUTER SCIENCE
OFFICE OF THE CHAIRMAN

September 6, 1974

Dr. A.C. Hindmarsh,
Numerical Mathematics Group,
L-310,
Lawrence Livermore Laboratory,
P.O. Box 808,
Livermore, California 94550,
U.S.A.

Dear Alan:

Thank you very much for your review of the paper,
and also the times for your visit.

The best time for us is the October 28-29 one that
seems to suit you best as well. Please let me know
your flight times, and I will send you information
about the local hotel, how to get there, etc. We
will of course pay all your travel expenses from
Chicago, plus local expenses, plus an honorarium.
I hope that's okay.

We would prefer the second talk, the one on "Solution
of Large Stiff ODE Systems". Our numerical analysis
seminar is quite small, perhaps 15 or 20 people, but
they are all quite knowledgeable about solving ODEs.
However, most of them will not have had any experience
with the handling of really large systems.

We are very much looking forward to your visit.

Sincerely,

Tom

TEH:pal

Thos. E. Hull,
Chairman.

P.S. I just talked to George Byrne on the phone,
& he said they'd chosen the other time. So I
should add that Oct 7-8 is actually not possible
for us. It will have to be Oct 28-29, at least if the

you suggested.

August 30, 1974

Professor T. E. Hull
Department of Computer Science
University of Toronto
Toronto M5S 1A7
Ontario, CANADA

Dear Tom:

After talking to people at Argonne, and working out some scheduling problems at home, I've come up with the following tentative possible dates for a trip to the midwest. They are, in order of preference:

- 1) Oct. 28-29 in Toronto, Oct. 30-Nov. 1 at ANL;
- 2) Oct. 7-8 in Toronto, Oct. 9-11 at ANL.

How do these sound to you? (I realize this is somewhat sooner than I had in mind a few days ago.)

I would be delighted to give a seminar there on Tuesday (Oct. 29 or Oct. 8), and would also like time to talk to you, Art Sedgewick, and Wayne Enright. As for seminar topics, the following are possibilities that come to mind, in no particular order.

- 1) "LLL Software for ODE's." Description of GEAR, EPISODE and their descendents in terms of general software structure, user interfaces, and capabilities.
- 2) "Solution of Large Stiff ODE Systems." A more advanced description of methods in GEAR and EPISODE, with emphasis on their use for large stiff problems.
- 3) "EPISODE: A General and Powerful ODE Package." Description of methods used in EPISODE, the code's relative merits, and its appearance to the user.
- 4) Ditto (3) for GEAR.

If you could indicate which of these (or variant of one of these) seems most appropriate there, and what kind of familiarity level to expect in the audience, I'll do my best.

Thank you again for the invitation. I'll be on vacation until Sept. 16, so there is no need here to rush your response.

Best regards,



A. C. Hindmarsh
Numerical Mathematics Group
L-310

ACH: aas



3, sept., 1974.

DRS. J. G. VERWER
MATHEMATISCH CENTRUM
2-de BOERHAAVE STRAAT 49.4
AMSTERDAM
HOLLAND

Dear DR. GELINAS,

In your article "STIFF SYSTEMS OF KINETIC EQUATIONS, A PRACTITIONER'S VIEW", which appeared in J. Comp. Physics, you mention differential equations of the form

$$y_i'(t) = f_i(y_j(t), y_j'(t), t), \quad i, j = 1, \dots, N,$$

i.e. an implicit differential equation. I should like to know if Gear's method is directly applicable to this type of equation. Further I should like to know if there exists methods which are developed especially for implicit differential equations. And I would greatly appreciate receiving some information about the origin of this type of equation. I hope you are willing to send me this information if possible.

Sincerely yours,

September 18, 1974

Dr. J. G. Verwer
 Mathematisch Centrum
 2-de Boerhaave Straat 49
 Amsterdam, HOLLAND

Dear Dr. Verwer:

Bob Gelinas relayed to me your letter of September 3, as I have developed the O.D.E. programs based on Gear's method as used at this Laboratory.

Yes, Gear's method can be used for implicit equations directly. If the implicit system is written $F(y, y', t) = 0$, then the only significant modification necessary is to replace the matrix

$I - h \lambda_0 \frac{\partial f}{\partial y}$, which occurs for the explicit case $y' = f(y, t)$, by the

matrix $\frac{\partial F}{\partial y'} + h \lambda_0 \frac{\partial F}{\partial y}$. For details, see Gear's book, "Numerical Initial

Value Problems in Ordinary Differential Equations," P. 227, and references cited there.

I do not know of any methods developed especially for implicit O.D.E.'s.

In case you are interested in our versions of Gear's program, I have attached a memorandum on how you can obtain them. I would also be glad to supply any of our reports on the subject.

I hope this is of some help to you.

Sincerely,

A C Hindmarsh

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

ACH:jat

Attachment

Dr. Ralph A Willoughby - visit

Address Jan - June 1973:
IBM Scientific Center
2670 Hanover St.
Palo Alto CA 94304

Phone: (1342) 493-3000, X3256

Called 1/9 - in Hawaii on trip
Called 1/24 - arranged visit

Arrangements here - through Terry Contreras
Bill Masson's office, 3083

Schedule of visit: Wed 3/21
Ar ~ 9:15
9:30 - 10:30 - C703 talk - 131/1274
2:00 - NM Lem. 113/1206

Honorarium (for non govt. + non UC employees) of \$50
agreed between Fred + Mel H. Doris O has check (3083)
Call for delivery or pick up or have someone else pick up.

AE's: AlH, Fred, Mel, ~~Kel~~

January 29, 1973

MEMORANDUM

TO: A. J. Hudgins
FROM: S. Fernbach
SUBJECT: Request to Invite Dr. Ralph A. Willoughby

Computation Department would like to invite Dr. Ralph A. Willoughby (a U. S. citizen), IBM, Palo Alto, to LLL on Wednesday, March 21 for the entire day. Dr. Willoughby will be giving two talks on stiff differential equations to our Numerical Mathematics Section. He will also discuss stiff differential equations and sparse matrices with various members of this Section. Dr. Willoughby is a recognized authority on these two subjects.

Approval is request to offer Dr. Willoughby a \$50 honorarium. We would like to give him this honorarium upon his departure.

Thank you.



S. Fernbach
Head, Computation Department

SF:tc

February 1, 1973

Dr. Ralph A. Willoughby
 IBM Scientific Center
 2670 Hanover Street
 Palo Alto, California 94304

Dear Ralph:

This is to confirm the arrangements for your visit to LLL, with some minor changes to the schedule I suggested in our phone conversation. The morning talk for my course is 9:30 - 10:30 and the afternoon seminar is at 2:00 (not 3:00) to roughly 3:00. (I changed the time to avoid room conflict at 4:00.) The visit has now been officially approved, and there will be a small honorarium.

Perhaps I should tell you a little more about the circumstances of your talks. The morning talk will probably be the last or next-to-last lecture of the course, and will be preceded by about 4 lectures (1 hr each) on stiff problems and stiff methods. (I've enclosed a course outline.) Considering the low level of mathematical sophistication in the class, I won't have gone very deeply at all. I will cover Gear's methods and multivalued formulations, and state the standard theorems (without proof). This gives you some freedom to talk either about the Liniger-Willoughby method (as written into the outline), or other stiff methods, or recent developments in stiff methods generally. By the way, the course is being video-taped - I hope that doesn't cramp your style too much. I'll fill you in on that later.

For the afternoon talk, a somewhat higher level can be expected, but still with a mixture of mathematicians, physicists, and other users of ODE software. Your suggested title sounds fine. I'm hoping that it draws the union of those here with ODE interests and those with sparse matrix interests, not the intersection. Incidentally, I would be interested in knowing if there are any methods developed for sparse nonlinear systems (as arise in ODE's) other than the usual quasi-Newton methods.

Thank you for sending your survey paper. I hope to have read it before we see you. But the way this course is eating up my time, nothing is certain.

About two weeks before the visit (i.e., March 7) we would like titles and abstracts of both talks, which we can use to publicize them.

I hope the enclosed maps are not too confusing. I will meet you at the West Main Gate. The 9:30 talk will be in Building 131 - about a block away, so leave a little extra time to get over there.

We're very much looking forward to your visit. Thank you in advance for taking the time and effort.

Very sincerely,



A. C. Hindmarsh
Numerical Mathematics Section, L-63

ACH:mr

cc:

F. N. Fritsch
V. W. Masson

March 27, 1973

Dr. Ralph A. Willoughby
IBM Scientific Center
2670 Hanover Street
Palo Alto, California 94304

Dear Ralph:

I want to express our great appreciation for your visit Wednesday. I have heard many complimentary remarks from those in my class and others who heard you in one or both of the talks. On behalf of all who heard you, many thanks.

After our conversations about large stiff system problems, I feel we are pretty much on the right track, although we have a long way to go. We will modify our treatment of Jacobians in some of the ways you suggested (more ~~use~~^{use} of analytical and polynomial-form Jacobians, more use of sparse structure).

You seemed to be saying that alternative methods for nonlinear algebraic systems (e.g., out of Ortega-Rheinboldt) are not worth our investigation. Is that right? (I'm thinking in terms of large sparse systems, with efficiency as the prime consideration.) If so, that is one less wild goose to chase.

Thank you also for the Sparse Matrix Survey (which I have already loaned out twice) and the Journal issue. We will study the Liniger-Oden paper carefully.

We appreciate your taking the time and effort to visit us.

Very sincerely,



A. C. Hindmarsh
Numerical Mathematics Section
L-63

ACH:mr

March 27, 1973

Dr. Ralph A. Willoughby
IBM Scientific Center
2570 Hanover Street
Palo Alto, California 94304

Dear Ralph:

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We appreciate your taking the time and effort to visit us.

Very sincerely,

A. C. Hindmarsh
Numerical Mathematics Section
L-63

ACh:mr

LAWRENCE LIVERMORE LABORATORY

CONTINUING EDUCATION PROGRAM LECTURE

DATE: Wednesday, March 21, 1973

TIME: 9:30 a.m.

PLACE: Bldg 131, Room 1274 (Instructional TV Studio)
Unclassified "Q" Clearance Only

SPEAKER: Dr. Ralph Willoughby, IBM, Yorktown Heights, N.Y.

TOPIC: One and Two Step Stiff Integration Methods

SUMMARY: Some special one- and two-step methods will be discussed. These methods are A-stable and contain free parameters other than the time step. The emphasis in the lecture is on how the values of these free parameters are determined. The variation of the time step will also be discussed.

* * * * *

This special guest lecture is being given for the course C703: Numerical Solution of Ordinary Differential Equations. For further information, contact Alan Hindmarsh, Ext 3330.

LAWRENCE LIVERMORE LABORATORY

SPECIAL NUMERICAL MATHEMATICS SEMINAR

Sponsored by Numerical Mathematics Section (L-63)

DATE: Wednesday, March 21, 1973

TIME: 2:00 p.m.

PLACE: Bldg. 113, Room 1206
Unclassified "Q" Clearance Only

SPEAKER: Dr. Ralph Willoughby, IBM, Yorktown Heights, N.Y.

TOPIC: Sparse Matrix Research

SUMMARY: A new class of sparse matrix problems has become important in the field of engineering design. The feasibility of fully implicit integration methods for stiff systems of ordinary differential equations was established in the late 1960's for certain classes of design problems. Progress on this type of sparse matrix problems will be described. There are a number of other problem classes in which sparse matrix research plays a central role. Some recent breakthroughs will be described.

Next LLL NMS SEMINAR: Tuesday, April 10, 1973.

September 12, 1972

Professor T. E. Hull
Department of Computer Science
University of Toronto
Toronto 181, CANADA

Dear Professor Hull:

I was pleased to receive your request for stiff ODE problems, and the accompanying memo. We have plenty of such problems, three of which are described in the attachment. You will no doubt have a considerable job paring down the final set of test problems you will have received from various people, and I hesitate to add to that task. In this connection it may be helpful to observe that these three problems are given in increasing order of both complexity and "realistic-ness." The first is entirely artificial, and so might be among the first you will want to discard. I can easily send you more information on all three problems, and/or our results with them, if that would be helpful.

Although I realize you have completed the battery of ODE solution programs, I would like to offer to you our own version of Gear's code. I recently made a lot of changes in the version we started with (which was essentially that in Gear's book), and they improved its performance greatly. (Some of these are already included in the version Gear himself is currently using). If you are interested in trying our new package in toto, it will be publicly available about November 1 (possibly too late for you). But in any case, I recommend the changes that are described in the enclosed "Preliminary Documentation ..." for your consideration.

Your project would seem to be an extremely valuable one. Please let me know if there is anything else I can do to assist in it. Thank you for your interest in our work at L.L.L.

Very sincerely yours,



A. C. Hindmarsh
Numerical Analysis Group, L-63

ACH:mr



UNIVERSITY OF TORONTO *Toronto 181, Canada*

DEPARTMENT OF COMPUTER SCIENCE
OFFICE OF THE CHAIRMAN

September 1, 1972

Dr. Alan Hindmarsh,
Numerical Analysis Group,
Lawrence Livermore Laboratories,
P.O. Box 808 (L-63),
Livermore, Ca. 94550,
U.S.A.

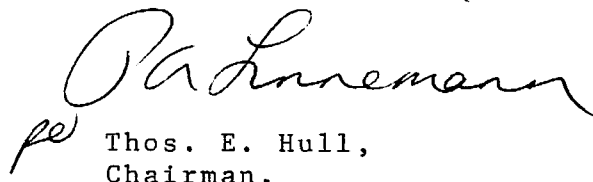
Dear Dr. Hindmarsh:

Fred Fritsch told me at a recent meeting that you had some good examples of some "real life" stiff systems that might be helpful to us in the tests that we are currently conducting.

I would very much appreciate your sending information of this sort to me. I enclose a copy of a memorandum which we sent to a number of persons interested in this area. You will see that most of our examples have been taken from the literature. We are anxious to add to this collection if it might make our tests more worthwhile. All the programming of the methods has now been completed and the results have now begun to appear this week. We will probably revise the programs somewhat further, as well as adding to or changing some of the problems, but we hope to have at least a draft of a report by Christmas time.

I will look forward to hearing from you.

Sincerely,


Thos. E. Hull,
Chairman.

TEH:pal

PURDUE UNIVERSITY
SCHOOL OF MECHANICAL ENGINEERING
WEST LAFAYETTE, INDIANA 47907

THERMAL SCIENCES & PROPULSION CENTER

August 14, 1974

Mr. A. C. Hindmarsh
Lawrence Livermore Laboratory
Livermore, California 94550

Dear Mr. Hindmarsh:

In recent conversations with Tony Oppenheim at Berkeley (where I did my graduate work), he informed me that someone (notably, you) had finally devised a successful computer program for the Gear algorithm. As part of my Ph.D. work, I devised a general program for kinetics calculations, and I would now like to revise the integrator subroutine. I would appreciate a copy of the Gear subroutine along with appropriate reports, instructions, background, etc.

I believe that by incorporating your work and mine, I can come up with a computer program second to none for kinetics calculations. I would appreciate your help here, and I will let you know of our progress.

Thanks in advance.



Normand M. Laurendeau
Assistant Professor of
Mechanical Engineering

NML:pdt

2 + 2 reports + ACC report
8/20/74

590-360 ~~FM 11/73~~ ~~RS P~~ ~~CARD~~ ~~ENC~~ ~~IC~~
 (Receipts of GEAR 7/79 thru 4/74 from A.C.C. (4))

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Mr. Luis Garcia de Viedma
Head

Requests for GEAR

relayed by Ray Chin - Dec. 1973

A. A. POURING

AEROSPACE ENGR. DEPT

U. S. NAVAL ACADEMY

ANNAPOLIS, MD. 21402

J. FERZIGER

M. E. DEPT.

STANFORD UNIVERSITY,

~~PALO ALTO~~ ^{Stanford}, CA. 94305

G. M. Homsy

CHEM. ENGR. DEPT.

STANFORD UNIVERSITY

~~PALO ALTO~~ ^{Stanford}, CA. 94305

J. M. GERSTING

ENGR / COMP. SCI

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Myron Zinsberg

Computer Science Dept.

Southern Methodist Univ.

Dallas TX 75275



E. I. DU PONT DE NEMOURS & COMPANY
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ENGINEERING DEPARTMENT

September 24, 1975

Dr. A. C. Hindmarch
Numerical Mathematics Group, L-310
Lawrence Livermore Laboratory
University of California
Livermore, California 94550

Dear Alan:

Thank you for the papers on stiff ODE's which you sent me. I am interested in the details of the modifications you have made over the past few years to DIFSUB, and have written to the Argonne Code Center requesting tapes and user's manuals of EPISODE, GEAR, and GEARB. I feel that it may be worthwhile to incorporate some of these improvements into our package here at Du Pont, although our present version is already a highly revised form of the original algorithm.

You may be interested in knowing that I have written a letter to Hal Abramson of AICHe suggesting that a continuing education course be established by the institute on the subject of stiff ODE's. Such a course would outline the theory of Gear's method and give some practical experience in using the algorithms on a few sample problems. I have discussed this possibility with George Byrne and with Professor S. W. Churchill of the University of Pennsylvania (former President of AICHe), and both were very enthusiastic about it. I suspect that the changes are good that a course of this type will be developed.

Sincerely yours,

ENGINEERING SERVICE DIVISION

Chet Miller

C. Miller, Senior Engineer
Applied Mathematics

CM/ldw