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Starlink User Note 28.1

Issued by

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NAG library - Known errors

Attached to this note is a copy of an error bulletin published by NAG which lists the known errors in the NAG library. The list refers to the the Mark 8A library. The library currently mounted at Starlink sites is Mark 8, but the information is still relevant. We will try to implement the specified corrections if time permits. Meanwhile, if you are using any of these routines, please contact Mike Lawden at RAL who may be able to give you details of the required correction.

ERROR BULLETIN - FORTRAN LIBRARY ROUTINES, MARK 9A
=====1. How to Use This Bulletin
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This Error Bulletin contains details of known errors in NAG FORTRAN Library routines. It is addressed to NAG Site Representatives, and its purpose is:

- a) to inform you of confirmed or suspected errors or defects in the Library;
- b) to assist you in notifying details of relevant errors or defects to users of the Library;
- c) to advise you in some cases how to correct such errors or defects as an interim measure before they are removed by NAG.

This Bulletin covers only those errors which have been discovered since the initial release to sites of the Mark 8 Library. Unless otherwise indicated, details apply also to earlier marks of the Library if the affected routines were present at earlier marks.

Section 2 of this Bulletin is an index of relevant error reports in order of reference number. These reference numbers (of the form IER-nnn) are allocated as part of NAG's internal maintenance procedures covering all items of library software, including many that are not relevant to this Bulletin; hence the report numbers do not form a consecutive sequence.

Not all the error reports listed in this Bulletin necessarily apply to the Library in use at your site. Each group of corrections that is incorporated by NAG in its master version of the Library, is considered to update the Library to an intermediate Mark maintenance level (e.g. 8, 8A, 8B, 8C, etc.). Libraries distributed to sites are each at a certain maintenance level, which can be determined by calling the routine A00AAF (described in the Library Support Note). For example, Mark 8 Libraries distributed to sites have all been at maintenance levels 8D, 8E or 8F; the first Mark 9 Libraries to be distributed will be at least at maintenance level 9A. Section 2 of this Bulletin states which Marks and maintenance levels a particular error report applies to. For example, if an error report applies between maintenance levels 8 and 8E, and your library is at Mark 8F, then the error report does not apply to your library: the error has already been corrected.

In addition, Section 2 states whether, to the best of NAG's knowledge, an error report applies to all implementations, or only to some.

Section 3 of this Bulletin describes the symptoms of each error or defect in terms of each primary (user-callable) Library routine that is affected. This information is suitable for publishing to users of the Library, after deleting details of errors that do not apply at your site. Those errors which may cause incorrect

1. How to Use This Bulletin (contd)

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numerical results to be returned without warning, are marked 'BEWARE', with additional exclamation marks to indicate more serious errors.

Section 4 of this Bulletin (supplied on microfiche only) contains details of corrections to the reported errors, if available, in order of routine name. These details are supplied so that corrected routines can be made available to users whose work is being hindered by existing errors or defects. NAG does not necessarily expect all the supplied corrections to be immediately included in the compiled library. It is the responsibility of site representatives to decide what action to take.

While NAG has reasonable grounds for believing that the information provided is likely to apply to all affected implementations of the Library, NAG makes no assertion that details of corrections are specifically applicable or necessarily have yet been tested and confirmed by NAG for all affected implementations.

The corrections are supplied in the form of a list of lines to be inserted or deleted in the source-text; the insertions and deletions are located by textual context (because sequence numbers in columns 73 to 80 are removed or transformed in many implementations). Before applying a correction, always check first that the correction has not already been applied; if it has, a comment will appear near the head of the source-text of the affected routine, giving the reference number of the error report and the maintenance level at which the error was corrected. After applying a correction, execute the example programs of affected primary routines as a general check on the updating process, but note that this is not an exhaustive check that no mistake has been made: great care must be taken throughout.

Normally the corrections apply to all implementations of the Library without change. However, if you have an alternative precision version of the Library, with primary routine names ending in 'E' or 'D' instead of 'F', then two systematic changes must be made to the supplied corrections:

- a) change the last letter of each NAG primary routine name from 'F' to 'E' or 'D' accordingly.
- b) interchange the first 3 and last 3 characters of each NAG auxiliary routine name, e.g. change 'D02SAU' to 'SAUD02'.

If you encounter any difficulty in correcting a routine, contact NAG Central Office.

All the corrections supplied in this Bulletin will be incorporated in any Mark 9 Libraries distributed to sites.

2. Index of Outstanding Error Reports

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Report number	Routines in error	Correction supplied?	Primary routines affected	---- Applicable to ---- Maintenance levels	Implement- ations	Note
IER-277	D03PGF	Yes	D03PGF	8 -> 8D	A11	
IER-279	G08ABF	Yes	G08ABF	8 -> 8D	A11	
IER-299	D02SAV D02SAW D02SAZ	Yes	D02SAF	8 -> 8E	A11	
IER-300	C05AGF	Yes	C05AGF	8 -> 8F	A11	
IER-301	C05AXF	Yes	C05AJF C05AXF	8 -> 8F	A11	
IER-305	D02GAF D02GBF D02RAZ	Yes	D02GAF D02GBF D02RAF	8 -> 8F	A11	
IER-308	D02QAF D02QBF	Yes	D02CBF D02CGF D02CHF D02EBF D02EGF D02EHF D02QAF D02QBF	8 -> 8F	A11	
IER-310	D02SAU	Yes	D02HAF D02HBF	8 -> 8F	A11	
IER-320	E04GBZ	Yes	E04GBF E04GCF	7 -> 8F	A11	
IER-322	E04HEX	No	E04GDF E04GEF E04HEF E04HFF	7 -> 8F	A11	
IER-331	G01ADF	Yes	G01ADF	5 -> 8F	A11	
IER-336	G08AFF	Yes	G08AFF	8 -> 8F	A11	
IER-351	E01ABF	Yes	E01ABF	5 -> 8F	A11	
IER-352	G08AAF	Yes	G08AAF	8 -> 9	A11	
IER-353	G08ABF	Yes	G08ABF	8 -> 9	A11	
IER-354	G02CJF	Yes	G02CJF	7 -> 9	A11	

2. Index of Outstanding Error Reports (contd)

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Report number	Routines in error	Correction supplied?	Primary routines affected	---- Applicable to ---- Maintenance levels	Implement- ations	Note
IER-355	D02SAU	Yes	D02HAF D02HBF	8 -> 9	All	(1)
IER-356	E02BAF	Yes	E02BAF	5 -> 9	All	
IER-357	C02ADF	Yes	C02ADF	5 -> 9	All	
IER-358	C02AEF	Yes	C02AEF	5 -> 9	All	
IER-359	F02BJZ	Yes	F02BJF	6 -> 9	All	

Notes:

- 1) The error in D02SAU described in IER-355 affects the example program results for D02HAF and D02HBF. Listings of the corrections to the results (as obtained on an ICL 2980) are supplied on microfiche at the end of the listings of corrections to the source-text. Slightly different results may be obtained on other machines.

3. Description of Outstanding Errors

Primary Routine Name	Report Number	Description of Error
CO2ADF	IER-357	may very occasionally get caught in an infinite loop in the neighbourhood of a multiple zero.
CO2AEF	IER-358	may very occasionally get caught in an infinite loop in the neighbourhood of a multiple zero.
CO5AGF	IER-300	parameter H is not unchanged on exit.
CO5AJF	IER-301	(BEWARE) may very occasionally return IFAIL = 0 when a zero has not in fact been found.
CO5AXF	IER-301	(BEWARE) may very occasionally return IFAIL = 0 when a zero has not in fact been found; also may return IFAIL = 4 instead of IFAIL = 5 .
D02CBF	IER-308	may very occasionally return IFAIL = 7 . This can only happen if the solution is required at a point in the first integration step.
D02CGF	IER-308	may very occasionally return IFAIL = 9 . This can only happen if the specified component of the solution attains the given value in the first integration step.
D02CHF	IER-308	may very occasionally return IFAIL = 8 . This can only happen if the specified function of the solution becomes zero in the first integration step.
D02EBF	IER-308	may very occasionally return IFAIL = 7 . This can only happen if the solution is required at a point in the first integration step.
D02EGF	IER-308	may very occasionally return IFAIL = 9 . This can only happen if the specified component of the solution attains the given value in the first integration step.
D02EHF	IER-308	may very occasionally return IFAIL = 8 . This can only happen if the specified function of the solution becomes zero in the first integration step.
D02GAF	IER-305	overflow occurs in D02RAY if D02GAF is called with MNP so large that $2.0^{**}(MNP-3)$ overflows, i.e. if $(MNP-3) > X02BCF(0.0)$.
D02GBF	IER-305	overflow occurs in D02RAY if D02GBF is called with MNP so large that $2.0^{**}(MNP-3)$ overflows, i.e. if $(MNP-3) > X02BCF(0.0)$.

3. Description of Outstanding Errors (contd)

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Primary

Routine Report

Name	Number	Description of Error
D02HAF	IER-310	array bound error in D02SAU if D02HAF is called with $M1 = 2$.
D02HAF	IER-355	(BEWARE!) returns incorrect values in the array SOLN if called with $M1 > 1$.
D02HBF	IER-310	array bound error in D02SAU if D02HBF is called with $M1 = 2$.
D02HBF	IER-355	(BEWARE!) returns incorrect values in the array SOLN if called with $M1 > 1$.
D02QAF	IER-308	may very occasionally return with COUT(4) and COUT(5) incorrectly set. This can only happen if an interrupt occurs in the first integration step.
D02QBF	IER-308	may very occasionally return with COUT(4) and COUT(5) incorrectly set. This can only happen if an interrupt occurs in the first integration step.
D02RAF	IER-305	overflow occurs in D02RAY if D02RAF is called with MNP so large that $2.0^{**}(MNP-3)$ overflows, i.e. if $(MNP-3) > X02BCF(0.0)$.
D02SAF	IER-299	may not converge to the solution nearest to the initial estimates, or may occasionally return IFAIL = 14 or 15 when this could be avoided.
D03PGF	IER-277	does not return IFAIL = 7 if called with $M < 0$ or $M > 2$, but attempts to compute with unpredictable consequences.
E01ABF	IER-351	array bound error if called with $N = 1$
E02BAF	IER-356	overflow may occur very occasionally.
E04GBF	IER-320	slow convergence may occur in problems where rank-deficient Jacobians are encountered.
E04GCF	IER-320	slow convergence may occur in problems where rank-deficient Jacobians are encountered.
E04GDF	IER-322	may incorrectly return IFAIL = 0 when the Hessian matrix at the final point is not positive-definite.
E04GEF	IER-322	may incorrectly return IFAIL = 0 when the Hessian matrix at the final point is not positive-definite.

3. Description of Outstanding Errors (contd)

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Primary Routine Name	Report Number	Description of Error
E04HEF	IER-322	may incorrectly return IFAIL = 0 when the Hessian matrix at the final point is not positive-definite.
E04HFF	IER-322	may incorrectly return IFAIL = 0 when the Hessian matrix at the final point is not positive-definite.
F02BJF	IER-359	overflow may occur in F02BJZ during normalization of the eigenvectors.
G01ADF	IER-331	does not return IFAIL = 2 if on entry $X(K-1) > X(K)$.
G02CJF	IER-354	(BEWARE!) returns incorrect results in the array C (the rows and columns of C being incorrectly permuted), if any columns are interchanged during the QR-factorization of X, i.e. if on exit IPIV(I) .NE. I for any I.
G08AAF	IER-352	(BEWARE) the value of P returned is not correct for use in 2-tailed or upper 1-tailed tests of significance on small samples (see (i) and (ii) in Section 3 of routine document). To avoid fault, ensure that $P < 0.5$ by interchanging the samples if necessary.
G08ABF	IER-279	(BEWARE) may occasionally return an incorrect value for P when there are tied ranks.
G08ABF	IER-353	(BEWARE) the value of P returned is not correct for use in 2-tailed or upper 1-tailed tests of significance on small samples (see (i) and (ii) in Section 3 of routine document). To avoid fault, ensure that $P < 0.5$ by interchanging the samples if necessary.
G08AFF	IER-336	may occasionally fail to return IFAIL = 4 .

4. Corrections to Source-text

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