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IBM-7090 GAUSSIAN INTEGRATION PACKAGE WITH OPTIONAL POINT QUADRATURE

S. K. Penny

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Abstract

A Gaussian integration package has been written for the IBM-7090. This package allows for the possibility of performing a four-fold integral and for an optional number of points in the Gaussian quadrature.

A Gaussian integration package has been written for the IBM-7090. This package consists of four FAP subroutines, GAUSS1, GAUSS2, GAUSS3, and GAUSS4. The scheme used in these routines is similar to Gaussian integration routines reported previously,[1-2] but has been generalized and made more efficient, more flexible, and simpler to use.

The generalization is the inclusion of the subroutine GAUSS4 and the option in all four routines for the use of a 2, 4, 8, or 16 point Gaussian quadrature. GAUSS4 allows for the possibility of a four-fold integral which in the author's estimation is approaching the limit of usefulness regarding computational time.

The flexibility is effected by requiring the user to write a simple FAP pseudo subroutine for the required storage area. Thus the user has complete control over the number of simultaneous integrals that he wishes to compute without touching the Gaussian package itself.

The user will find the routines simple to use because the subroutines which he must write merely use a simplified call statement to the appropriate Gaussian integration routine and then evaluate the appropriate partial integrand with no multiplication.

It is assumed that the problem is to evaluate, in general, n four-fold integrals over the same four-volume of the form:

$$\int_{L1}^{U1} F_i(x)\,dx \int_{L2}^{U2} G_i(x,y)\,dy \int_{L3}^{U3} H_i(x,y,z)\,dz \int_{L4}^{U4} J_i(x,y,z,v)\,dv$$

where $i = 1, 2, \ldots, n$.

The first thing the user must do is to decide the maximum number, NMAX, of integrals he might evaluate simultaneously and the maximum dimensional space, DMAX, over which he may wish to integrate. Then he must write the simple FAP routine and must not deviate from the symbols or scheme to follow:

```
        CØUNT   4
        ENTRY   AR9EA
        BSS     2(DMAX)(NMAX)-1
AR9EA   BSS     1
        END
```

For example, if NMAX = 50 and DMAX = 2, then one inserts the decimal number 199 in the variable field corresponding to the BSS pseudo-operation.

The user then initiates the integration, usually in a FØRTRAN main program, by using the call statement:

```
CALL GAUSS1(NI,NA,A,L1,U1,ND1,NQ1)
```

where

NI = dimension of the element over which the integration is performed ($1 \leq NI \leq DMAX \leq 4$),

NA = number of integrals to be performed ($1 \leq NA \leq NMAX$),

A = the array of integrals to be computed,

L1 = lower limit (this is a floating point number),

U1 = upper limit,

ND1 = power of two (0,1,2,etc.),

NQ1 = Gaussian quadrature desired (2,4,8, or 16).

The interval (L1,U1) is divided into 2^{ND1} equal subintervals, each of which uses NQ1 - point Gaussian quadrature.

The user must write a subroutine which if written in FØRTRAN would be denoted FX(X,ARRAY). If a single integration is to be performed, this routine merely evaluates the $F_i(x)$'s using the variable x and stores them in the array ARRAY. Since ARRAY is a parameter, the user will never see the integrand unless he stores the $F_i(x)$'s in an array defined in his routine. If at least a double integral is to be performed, a call statement to GAUSS2 must be made <u>before</u> evaluation of the $F_i(x)$'s, namely:

CALL GAUSS2 (L2,U2,ND2,NQ2)

where the parameters have the same meaning and options as those for GAUSS1 except to note that the parameters L2, U2, ND2, and NQ2 may be functions of x.

If a double integration is to be performed, the user must also write a subroutine FXY(x,y,ARRAY). This subroutine evaluates the $G_i(x,y)$'s using the variables x and y and stores them in ARRAY. If at least a triple integral is to be performed, a call statement to GAUSS3 must be made <u>before</u> evaluation of the $G_i(x,y)$'s.

CALL GAUSS3 (L3,U3,ND3,NQ3)

where the parameters' meaning is as before except that the parameters L3, U3, ND3, and NQ3 may be functions of x and y.

The triple integration requires the subroutine FXYZ (x,y,z,ARRAY). The performance of this subroutine follows precisely from the previous descriptions of FX and FXY. The call statement to GAUSS4 in case of a four-fold ingetral is:

CALL GAUSS4 (L4, U4, ND4, NQ4)

where the parameters again have the same meaning except that the parameters L4, U4, ND4, and NQ4 may be functions of x, y, and z.

A four-fold integral requires a subroutine FXYZV (x,y,z,v,ARRAY) which simply evaluates the $J_i(x,y,z,v)$'s and returns.

Some notes of warning and points of interest are in order to insure proper usage and understanding:

1. The user may delete the superfluous GAUSS2, GAUSS3, or GAUSS4 subroutines from the package depending on the n-fold integrals he is performing or else write dummy subroutines FXY, FXYZ, or FXYZV which simply return.
2. If any of the partial integrands are constant, this constant <u>must be transmitted</u> to the array ARRAY in the particular subroutine where the integrand is to be evaluated.
3. Because of the linkages involved in the routines, the user <u>must not have</u> subroutines or subroutine entries with names in the list of names to follow, but it is extremely doubtful that he will have this problem.

<u>NAME LIST</u>

WYWYW	R2R2R
QYQYQ	R3R3R
XX9XX	R4R4R
YY9YY	NI9NI
ZZ9ZZ	NA9NA

4. The integration will be correctly performed mathematically (correct sign, etc.) no matter what the relationship is between the upper and lower limits.

5. The parameters in the subroutines FX, FXY, etc. must never be inadvertently placed in CØMMØN, however, any of the parameters in GAUSS1, GAUSS2, etc. may be placed in CØMMØN if so desired.

6. The parameter NA in GAUSS1 is a time-saving device which is used internally in all the package to limit the loops involving transmittal, manipulations, etc. of the accumulated integrals.

7. The storage involved in these routines is:

GAUSS1	Octal	313
GAUSS2	"	211
GAUSS3	"	215
GAUSS4	"	205

8. Copies of these routines are available at the Central Library at the Oak Ridge Gaseous Diffusion Plant or from the author.

References

1. M. P. Lietzke, IBM-704 Gaussian Integration Routines, ORNL-CF-60-3-48 (March 14, 1960), and addendum.

2. M. B. Emmett and S. K. Penny, IBM-7090 Gaussian Integration Routines, ORNL-CF-61-5-65, Revised (Dec. 6, 1961).

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