

An Adaptive Multidimensional Integration Routine for a Vector of Integrals.

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May 29, 2014

Abstract

The specification is given for the FORTRAN implementation of a globally adaptive algorithm for the numerical integration of a vector of integrand functions over a hyper-rectangular region. Descriptions are given for use of the subroutine, the subprogram organization and the subroutine parameter list.

*Supported by the Norwegian Research Council for Humanities and Sciences and STATOIL.

[†]Supported by the Norwegian Research Council for Humanities and Sciences.

[‡]Supported by the Norwegian Marshall Fund.

1 Usage of DCUHRE

The algorithm described in [2] has been implemented in a FORTRAN 77 subroutine **DCUHRE**: a double precision adaptive cubature routine for a hyperrectangular region of integration. The single precision version has the name SCUHRE and similarly the first letter in all subroutine-names is changed to S. DCUHRE has the calling sequence:

```
CALL DCUHRE (NDIM,NUMFUN,A,B,MINPTS,MAXPTS,FUNSUB,  
             EPSABS,EPSREL,KEY,NW,RESTAR,RESULT,  
             ABSERR,NEVAL,IFAIL,WORK)
```

DCUHRE computes approximations RESULT to the integral

$$I[\text{FUNSUB}] = \int_H \text{FUNSUB } dx_{NDIM} \dots dx_1$$

where FUNSUB is a vector of integrands of length NUMFUN and H is a NDIM dimensional hyper-rectangular region with lower limits given by A and upper limits given by B.

DCUHRE attempts to compute RESULT to satisfy

$$|I[\text{FUNSUB}_k] - \text{RESULT}(k)| \leq \max(\text{EPSABS}, \text{EPSREL} * |I[\text{FUNSUB}_k]|),$$

for $k = 1, 2, \dots, \text{NUMFUN}$, and where EPSABS and EPSREL are absolute and relative tolerances, respectively. More detailed information about the parameter list is provided in the Appendix and the FORTRAN code itself. Both single and double precision versions are available. The code has been checked with the PFORT verifier in Toolpack [3]. DCUHRE has been successfully run the following computers: Alliant FX/8, SUN 3/50, CRAY-XMP/48, IBM 3090, Sequent Balance and HP-9000/840.

2 Algorithm Structure

The integration routine and the subprograms are organized according to the structure given in Figure 1.

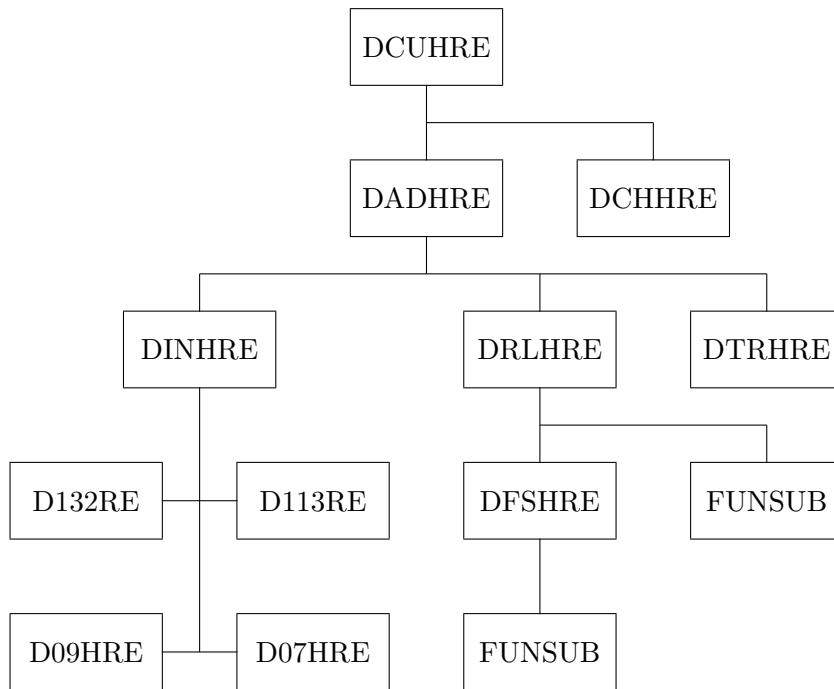


Figure 1.

The correspondence with Rice's metalgorithm (see [4]) is shown in Figure 2.

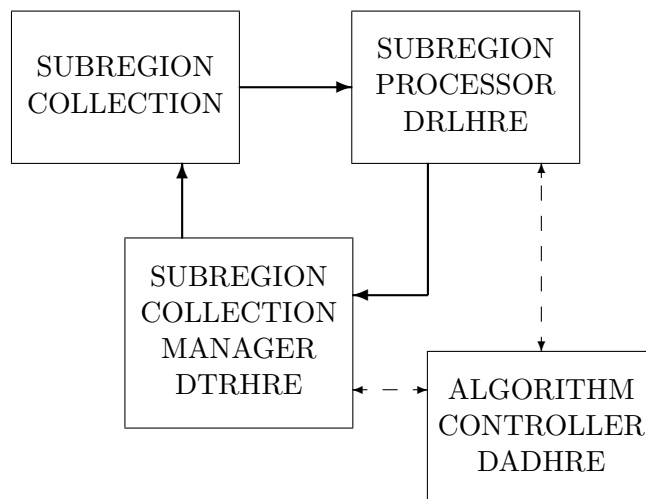


Figure 2. The metalgorithm for adaptive quadrature. The heavy lines show the flow of subregions and the dashed lines the flow of control.

In the following list we briefly describe the purpose of DCHURE and supporting subroutines.

- DCUHRE is basically a driver for the algorithm controller DADHRE. Inside DCUHRE the input to DCUHRE is checked and the workspace for DADHRE is separated into mnemonic variables.
- DCHHRE checks the validity of the input to DCUHRE.
- DADHRE is the algorithm controller which at each subdivision step decides whether to stop or continue.
- DINHRE selects the integration rule according to the value of KEY.
- D132RE is a two dimensional degree 13 rule.
- D113RE is a three dimensional degree 11 rule.
- D09HRE is a degree 9 rule for any dimension ≥ 2 .
- D07HRE is a degree 7 rule for any dimension ≥ 2 .
- DTRHRE maintains the heap of subregions.
- DRLHRE computes approximations to the integral and the error over each subregion. The integration rules are based on fully symmetric sums, and DFSHRE is called to compute these sums.

A more detailed description of the algorithm is given in [2], and results from the testing of DCUHRE (original name ADMINT) are given in [1].

References

- [1] J. Berntsen, T.O. Espelid, and A. Genz. A test of ADMINT. Reports in Informatics 31, Dept. of Informatics, Univ. of Bergen, 1988.
- [2] J. Berntsen, T.O. Espelid, and A. Genz. An Adaptive Algorithm for the Approximate Calculation of Multiple Integrals. To appear in ACM Trans. Math. Software, 1990.
- [3] W.R. Cowell and S.B. Garbow. Users Guide to Toolpack/1 (Release 2) in a Unix Environment. Technical Report ANL-87-12, Argonne National Laboratories, 1987.
- [4] J.R. Rice. A metalgorithm for adaptive quadrature. *JACM*, 22:61–82, 1975.

APPENDIX: The Parameters for DCUHRE.

Input Parameters

- NDIM** The number of variables in the integrand(s). We require $1 < NDIM \leq 15$.
- NUMFUN** The number of components in the vector integrand function.
- A** The lower limits of integration. This array has dimension NDIM.
- B** The upper limits of integration. This array has dimension NDIM.
- MINPTS** The minimum number of FUNSUB calls the code has to use.
- MAXPTS** The maximum number of FUNSUB calls the code is allowed to use. See the code for details.
- FUNSUB** An externally declared subroutine for computing all components in the vector function for the given evaluation point. It must have parameters (NDIM, X, NUMFUN, FUNVLS). The input parameters: NDIM is the dimension of the region, X is an array of dimension NDIM giving the coordinates of the evaluation point and NUMFUN is the number of components of the vector integrand. The output parameter FUNVLS is an array of dimension NUMFUN that stores NUMFUN values of the vector integrand.
- EPSABS** Requested absolute error.
- EPSREL** Requested relative error.

KEY This selects the integration rule. $KEY = 0$ is the default value. The following table gives the polynomial degrees of the different integration rules for the possible values of KEY and for dimensions 2, 3 and > 3 .

KEY	NDIM = 2	NDIM = 3	NDIM >3
0	13	11	9
1	13	-	-
2	-	11	-
3	9	9	9
4	7	7	7

NW The length of work array WORK. Let MAXSUB denote the maximum allowed number of subregions for the given value of MAXPTS, KEY and NDIM. Then $MAXSUB = (MAXPTS-NUM)/(2*NUM)+1$, where NUM is the number of FUNSUB calls over each subregion. We require $NW \geq 2*MAXSUB*(NDIM+NUMFUN+1) + 17*NUMFUN*MDIV + 1$,

where MDIV is the number of subregions that are divided in each subdivision step. Parallelism at the subregion level allows more than one subregion to be picked and processed. MDIV is default set internally in DCUHRE equal to 1. For efficient execution on parallel computers with NPROC processors MDIV should be set equal to the smallest integer such that $\text{mod}(2*\text{MDIV}, \text{NPROC}) = 0$.

RESTAR If $\text{RESTAR} = 0$, this is the first attempt to compute the integral. If $\text{RESTAR} = 1$, then we continue a previous attempt. In this case the only parameters for DCUHRE that may be changed (with respect to the previous call of DCUHRE) are MINPTS, MAXPTS, EPSABS, EPSREL and RESTAR.

Output Parameters

RESULT An array of dimension NUMFUN containing approximations to all components of the vector integral.

ABSERR An array of dimension NUMFUN of estimates for absolute errors for all components of the vector integral.

NEVAL The number of function evaluations used by DCUHRE.

IFAIL IFAIL = 0 for normal exit, with
 $\text{ABSERR}(K) \leq \max(\text{EPSABS}, \text{ABS}(\text{RESULT}(K))*\text{EPSREL})$
for $1 \leq K \leq \text{NUMFUN}$, using MAXPTS or less FUNSUB calls.
IFAIL = 1 if MAXPTS is too small for DCUHRE to obtain the requested error. In this case DCUHRE returns values of RESULT with estimated absolute errors ABSERR.
IFAIL = 2 if $\text{KEY} < 0$ or $\text{KEY} > 4$.
IFAIL = 3 if $\text{NDIM} < 2$ or $\text{NDIM} > 15$.
IFAIL = 4 if $\text{KEY} = 1$ and $\text{NDIM} \neq 2$.
IFAIL = 5 if $\text{KEY} = 2$ and $\text{NDIM} \neq 3$.
IFAIL = 6 if $\text{NUMFUN} < 1$.
IFAIL = 7 if the volume of the region of integration is zero.
IFAIL = 8 if $\text{MAXPTS} < 3*\text{NUM}$.
IFAIL = 9 if $\text{MAXPTS} < \text{MINPTS}$.
IFAIL = 10 if both $\text{EPSABS} \leq 0$ and $\text{EPSREL} \leq 0$.
IFAIL = 11 if NW is too small.
IFAIL = 12 if $\text{RESTAR} \neq 0$ and $\text{RESTAR} \neq 1$.

WORK A work array of dimension NW. See the code for details.