Examples and advice for using fm_integrate.

```
type (fm), save :: a, b, check, err, pi, r1, r2, result, seven, tol
type (fm), external :: f
integer :: k, kprt, n, n_errors, nw
character(80) :: st1
n_errors = 0
```

1. Start with an integral without singularities on the interval of integration. integrate $\log (t) * \cos (t)$ from pi/4 to pi/2.

Set the tolerance to get at least 40 significant digits. fm_integrate does a sequence of iterations using the tanh-sinh quadrature formula. Each iteration uses more points until the last two iterates agree within the specified tolerance. Since the next-to-last iterate satisfies the tolerance and the last iterate (returned as result) is even more accurate, the value returned from fm_integrate is usually slightly more accurate than requested. In this case, the error check below shows that result is actually correct to about 60 digits.

It is usually best to set FM's precision level to be slightly higher than the number of digits requested with the tolerance. Here we set precision to 20 more digits.
$\mathrm{n}=1$

Call fm_set to define FM's precision level before any multiple precision variables are defined. This sets 60-digit precision and tol is 1.0e-40.
$k=40$
call fm_set $(k+20)$
tol $=$ to_fm(10) ${ }^{* *}$ (-k)
write (*, "(//)")
call fm_pi(pi)
$a$ and $b$ are the limits for the integral.
$a=p i / 4$
$b=p i / 2$
kprt controls trace printing in fm_integrate. Setting it to 1 will print a summary of the call, giving the result, number of function evaluations, and time.
nw is the unit number for this trace output.
kprt $=1$
$n w=6$
call fm_integrate(f, $n, a, b$, tol, result, kprt, nw)

For these sample problems the integrals have known closed-form results, so we can check the accuracy of fm_integrate.

```
check = log(pi/2) - log(pi/4)/sqrt(to_fm(2)) + sin_integral(pi/4) - sin_integral(pi/2)
err = abs( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
```

2. Next do an integral with a singularity at zero (from "Integrals of Powers of LogGamma" by T. Amdeberhan, M. Coffey, O. Espinosa, C. Koutschan, D. Manna, and V. Moll, in Proc. Amer. Math. Soc., \#139, 2011)
integrate $\log (\operatorname{gamma}(t))$ from 0 to 1.

Leave precision and tolerance the same as above.

The tanh-sinh algorithm is good at handling singularities at the endpoints, so this case takes about the same number of function evaluations as case 1.

```
n = 2
write (*, "(//)")
a = 0
b = 1
tol = to_fm(10) ** (-k)
kprt = 1
nw = 6
call fm_integrate(f, n, a, b, tol, result, kprt, nw)
check = log( sqrt( 2*pi ) )
err = abs( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
```

3. This integral has a pole at pi/2 and a sqrt singularity at zero. (from "a Comparison of Three High-Precision Quadrature Schemes" by D. H. Bailey, K. Jeyabalan, and X. S. Li, in Experimental Mathematics, Vol 14 (2005), No. 3)
integrate sqrt( $\tan (\mathrm{t})$ ) from 0 to $\mathrm{pi} / 2$.

Set tolerance to give 100 digits.

Here the fact that the pi/2 endpoint is not exactly representable in floating point form causes a problem. fm_integrate will increase precision above the user's level while computing the integral. But the endpoints $a$ and $b$ are input values that were defined at the user's precision, and their extra digits will be zeros when precision is raised in fm_integrate.

That is fine for $a=0$, but $b=p i / 2$ will still be accurate only to the user's precision, not to the higher intermediate precision. The fact that $b$ is $a$
singularity for the function means that fm_integrate will need to know the position of $b$ to higher precision to evaluate the integral accurately.

The fix is to make a change of variables to get an equivalent integral where both endpoints are exact in floating point. Leaving a singular endpoint inexact will usually cause fm_integrate to run much slower, and sometimes fail.

Let $u=t * 2 / p i$. Then $t=u * p i / 2$ and $d t=p i / 2 d u$. The new form of this integral becomes:
integrate $\operatorname{sqrt}(\operatorname{abs}(\tan (u * p i / 2))) * p i / 2$ from 0 to 1.
Now pi will be computed inside function $f$, so it will be done at whatever higher precision fm_integrate uses.

When changing variables in this case, we also need to defend against rounding errors when computing $u^{*} \mathrm{pi} / 2$. When $u$ is very close to 1 , rounding could cause $u^{*} \mathrm{pi} / 2$ to round up, giving a value slightly greater than pi/2.
Then tan would return a negative value and then sqrt would return unknown, causing the integration to fail. The fix is to take the absolute value before doing the square root.

```
n = 3
k = 100
call fm_set(k+20)
    Precision has increased, so we must get pi at the new precision.
call fm_pi(pi)
write (*, "(//)")
a = 0
b = 1
tol = to_fm(10) ** (-k)
kprt = 1
nw = 6
call fm_integrate(f, n, a, b, tol, result, kprt, nw)
check = pi * sqrt( to_fm(2) ) / 2
err = abs( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
```

4. integrate $\exp \left(-t^{* * 2} / 2\right)$ from 0 to infinity.
(from "a Comparison of Three High-Precision Quadrature Schemes" by D. H. Bailey, K. Jeyabalan, and X. S. Li, in Experimental Mathematics, Vol 14 (2005), No. 3)

Set tolerance to give 100 digits.

Infinite regions must be converted to finite ones. Let $u=1 /(t+1)$ to get:
integrate $\exp (-(1 / u-1) * * 2 / 2) / u^{* * 2}$ from 0 to 1.
Exponential functions pose another problem for fm_integrate. When $u$ is very close to zero the exponential can underflow. FM does not flush
underflows to zero like most floating point systems, so when that value is then divided by the small $u^{* *} 2 \mathrm{FM}$ detects the possibility that this result could be above the underflow threshold. Since FM can't be sure whether the true function value is below the underflow threshold, unknown is returned.

The fix in this case is to see that whenever underflow occurs in this integration the final function value is too small to change the integral. That is the usual situation whenever $f$ underflows and the final value of the integral is greater than $10^{* *}\left(-10^{* *} 6\right)$ in magnitude, because FM 's underflow is less than $10^{* *}\left(-10^{* *} 8\right)$. So we check for underflow after doing the exponential in function $f$ and replace underflowed function values by zero.

Starting with the 2022 version of FM this check for intermediate underflow can usually be skipped. Some extra information is now included in underflowed or overflowed results, so that usually the program can tell in cases like this that when the exp function underflows, after dividing by $u^{* *} 2$ for a small $u$ the function value is still in the underflow region. Then FM can return underflow for the function value instead of the unknown result in previous versions.

The old check for underflow has been left in the $f(x)$ routine in this program, since there are still some rare cases where it might be needed.

```
n = 4
k = 100
call fm_set(k+20)
call fm_pi(pi)
write (*, "(//)")
a = 0
b = 1
tol = to_fm(10) ** (-k)
kprt = 1
nw = 6
```

call fm_integrate(f, $n, a, b$, tol, result, kprt, nw)
check $=\operatorname{sqrt}(\mathrm{pi} / 2)$
err $=$ abs ( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
5. integrate $\log (\operatorname{abs}((\tan (t)+\operatorname{sqrt}(7)) /(\tan (t)-\operatorname{sqrt}(7))))$ from pi/3 to pi/2.
(from "High-Precision Numerical Integration: Progress and Challenges" by D. H. Bailey and J. M. Borwein (2009))

Set tolerance to give 150 digits.
There is only one singularity, but it is atan(sqrt(7)), which is not an endpoint. fm_integrate will initially have very slow convergence and then will try to isolate the singularity and split into two integrals with the singularity at endpoints.

This strategy works here, but it is slower and doesn't always succeed. Case 6 shows a better way to handle interior singularities.

```
n = 5
k = 150
call fm_set(k+20)
call fm_pi(pi)
write (*, "(//)")
a = pi/3
b = pi/2
tol = to_fm(10) ** (-k)
kprt = 1
nw = 6
call fm_integrate(f, n, a, b, tol, result, kprt, nw)
seven = 7
check = ( sqrt(seven) / 168 ) * ( polygamma(1, 1/seven) + polygamma(1, 2/seven) - &
                                    polygamma(1, 3/seven) + polygamma(1, 4/seven) - &
                                    polygamma(1, 5/seven) - polygamma(1, 6/seven) )
err = abs( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
```

6. Same integral as case 5 .
integrate $\log (\operatorname{abs}((\tan (t)+\operatorname{sqrt}(7)) /(\tan (t)-\operatorname{sqrt}(7))))$
from pi/3 to pi/2.

Set tolerance to give 150 digits.

Split into two integrals and change variables to make the endpoints exact. This will be faster than making fm_integrate search for the interior singularity as in case 5.
Call the two function numbers 61 and 62.

1. from $\mathrm{pi} / 3$ to atan(sqrt(7)).

Let $u=(t-p i / 3) /(\operatorname{atan}(\operatorname{sqrt}(7))-p i / 3)$
2. from $\operatorname{atan}(\operatorname{sqrt}(7))$ to $\mathrm{pi} / 2$.

Let $v=(t-\operatorname{atan}(s q r t(7))) /(p i / 2-\operatorname{atan}(\operatorname{sqrt}(7)))$

This gives two integrals from 0 to 1 , then we add the two results.

```
n = 6
k = 150
call fm_set(k+20)
call fm_pi(pi)
write (*, "(//)")
a = 0
b = 1
tol = to_fm(10) ** (-k)
kprt = 1
nw = 6
call fm_integrate(f, 61, a, b, tol, r1, kprt, nw)
call fm_integrate(f, 62, a, b, tol, r2, kprt, nw)
result = r1 + r2
```

```
write (*,*) ' '
```

write (*,*) ' Adding these last two integrals gives the case 6 result:'
write (*,*) ' '
call fm_print(result)

```
seven = 7
check = ( sqrt(seven) / 168 ) * ( polygamma(1, 1/seven) + polygamma(1, 2/seven) - &
    polygamma(1, 3/seven) + polygamma(1, 4/seven) - &
    polygamma(1, 5/seven) - polygamma(1, 6/seven) )
err = abs( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
```

7. Same integral as cases 5 and 6.

Combine these two integrals into one, so only one call to fm_integrate is needed. This will be faster than doing two calls as in case 6.

```
integrate log(abs( ( tan(t) + sqrt(7) ) / ( tan(t) - sqrt(7) ) ) )
```

    from pi/3 to pi/2.
    Set tolerance to give 150 digits.

Split into two integrals and change variables to make the endpoints exact. Both new integrals are from 0 to 1.

1. from $\mathrm{pi} / 3$ to atan(sqrt(7)).
Let $u=(t-p i / 3) /(\operatorname{atan}(\operatorname{sqrt}(7))-p i / 3)$
2. from $\operatorname{atan}(\operatorname{sqrt}(7))$ to $\mathrm{pi} / 2$.
Let $v=(t-\operatorname{atan}(s q r t(7))) /(p i / 2-\operatorname{atan}(\operatorname{sqrt}(7)))$
$\mathrm{n}=7$
$\mathrm{k}=150$
call fm_set $(k+20)$
call fm_pi(pi)
write (*, "(//)")
$a=0$
b $=1$
tol $=$ to_fm(10) ${ }^{* *}(-k)$
kprt $=1$
$n w=6$
call fm_integrate(f, 7, $a, b$, tol, result, kprt, nw)
seven $=7$
check $=(\operatorname{sqrt}($ seven $) / 168){ }^{*}($ polygamma(1, 1/seven) + polygamma(1, 2/seven) - \&
polygamma(1, 3/seven) + polygamma(1, 4/seven) - \&
polygamma(1, 5/seven) - polygamma(1, 6/seven) )
err $=$ abs ( result - check )
call fm_form('es12.4', err, st1)
write (*, "(/10x, a, i2, a, a)") ' Error for case ', n, ' = ', trim(st1)
if (err > tol) n_errors = n_errors + 1
```
write (*,*) ' '
write (*,*) ' '
if (n_errors == 0) then
    write (*,*) ' All results were ok -- no errors were found.'
else
    write (*,*) n_errors, ' error(s) were found.'
endif
write (*,*) ' '
stop
end program test
function f(x, n) result (return_value)
use fmzm
implicit none
type (fm) :: return_value, x
integer :: n
intent (in) :: x, n
type (fm), save :: c1, c2, pi, sqrt7, tanx
if (n == 1) then
    return_value = log(x) * cos(x)
else if (n == 2) then
    return_value = log( gamma( x ) )
else if (n == 3) then
```

The original limits from 0 to pi/2 have been changed to 0 to 1 .
call fm_pi(pi)
return_value $=$ pi * sqrt $(\operatorname{abs}(\tan (p i * x / 2))) / 2$
else if ( $n==4$ ) then
Before the 2023 version of $F M$, exp could underflow and then make $f$ unknown.
The previous code here checked for underflow and set $f=0$ in that case.

```
        return_value = exp( -(1 - 1/x)**2 / 2 )
        if ( is_underflow(return_value) ) then
            return_value = 0
        else
            return_value = return_value / x**2
        endif
```

            Starting with the 2023 version, \(F M\) 's exception handling is stronger, so
            now these undeflows in exp don't need to be trapped and the integration
            works as intented.
    return_value \(=\exp \left(-(1-1 / x)^{* * 2} / 2\right) / x^{* * 2}\)
    else if ( $n==5$ ) then
sqrt7 $=$ sqrt(to_fm(7))
$\tan \mathrm{x}=\tan (\mathrm{x})$
return_value $=\log (\operatorname{abs}((\tan x+\operatorname{sqrt7}) /(\tan x-\operatorname{sqrt7})))$
else if ( $n==61$ ) then
call fm_pi(pi)

It is tempting to compute constants like c1, c2, sqrt7 once and then save them for use in subsequent calls to $f$. That can be done, but it is trickier than it seems,
since fm_integrate may call $f$ with different precision levels during one integration, so it is easy to not have the right precision in a saved variable.
Here we just compute them each time, making the logic straightforward while the function evaluations are somewhat slower.

```
    sqrt7 = sqrt(to_fm(7))
    c1 = atan(sqrt7) - pi/3
    tanx = tan( c1*x + pi/3 )
    return_value = c1 * log( abs( ( tanx + sqrt7 ) / ( tanx - sqrt7 ) ) )
else if (n == 62) then
    call fm_pi(pi)
    sqrt7 = sqrt(to_fm(7))
    c2 = atan(sqrt7)
    c1 = pi/2 - c2
    tanx = tan( c1*x + c2 )
    return_value = c1 * log( abs( ( tanx + sqrt7 ) / ( tanx - sqrt7 ) ) )
else if (n == 7) then
```

        Combine the two integrals into one.
    call fm_pi(pi)
    sqrt7 \(=\) sqrt(to_fm(7))
    c2 = atan(sqrt7)
    \(\mathrm{c} 1=\mathrm{c} 2-\mathrm{pi} / 3\)
    \(\tan x=\tan \left(c 1^{*} x+p i / 3\right)\)
    return_value \(=c 1{ }^{*} \log (\operatorname{abs}((\tan x+\operatorname{sqrt7}) /(\operatorname{tanx}-\operatorname{sqrt7})))\)
    \(\mathrm{c} 1=\mathrm{pi} / 2-\mathrm{c} 2\)
    \(\tan x=\tan \left(c 1^{*} x+c 2\right)\)
    return_value \(=\) return_value \(+c 1 * \log (\operatorname{abs}((\tan x+\operatorname{sqrt7}) /(\operatorname{tanx}-\operatorname{sqr} t 7)))\)
    endif
end function $f$

