Comparison of different methods implementing surface integration in *KNOTOPT*

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I compared three different numerical methods for surface integral: 1. Trapezoidal 2D Rule (current used method); 2. Simpson's 2D Rule; 3. Central value. The test integrands include the total $B \cdot \vec{n}$ and an arbitrary periodic function. A basic conclusion is that the current method we used is not too bad. But we can also easily modified the code to a more accurate method, like central value or other complicated algorithms (maybe later). surface integrals (eg. reletive error less than 10^{-3}).

1 Theory backgroud

1.1 Trapezoidal 2D Rule

Trapezoidal rule for single integration is $f(x)\delta x = \frac{1}{2}(f_1(x) + f_2(x))\delta x$. Therefor the composite Trapezoidal rule has the weights pattern of $1, 2, 2, \ldots, 2, 1$. For surface integrals, it's extended to a rectangle grid with the following pattern:

$$\begin{array}{ccccccc} 1 & 2 & 2 & \ldots & 2 & 2 & 1 \\ 2 & 4 & 4 & \ldots & 4 & 4 & 2 \\ \vdots & & & \ddots & & & \vdots \\ 2 & 4 & 4 & \ldots & 4 & 4 & 2 \\ 1 & 2 & 2 & \ldots & 2 & 2 & 1 \end{array}$$

In the *KNOTOPT*, integrand for the surface normal is periodic. Thus terms on the boundary can be sumed and the new pattern is:

$$\begin{array}{ccccccc} 4 & 4 & 4 & \ldots & 4 & 4 & 0 \\ 4 & 4 & 4 & \ldots & 4 & 4 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 4 & 4 & 4 & \ldots & 4 & 4 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 & 0 \end{array}$$

Therefor the integration can be discretized as:
$E = \int_{\mathcal{S}} \frac{1}{2}(B_n)^2 \, ds = \Delta\theta \, \Delta\zeta \sum_{j=0,k=0}^{M-1,N-1} \sqrt{g}_{j,k} \frac{1}{2} \left(B_{n,j,k}\right)^2$
The error should be the second order $0(h^2)$(h denoted to the interval).

1.2 Simpson's 2D Rule

A $\frac{2}{3}$ Simpson's rule for single integration is $f(x)\, 2\delta x = \frac{1}{3}(f_1(x) + 4f_2(x) + f_3(x))\delta x$. It takes three points rather two in Trapezoidal rule. A composite Simpson's rule can be expressed as $1, 4, 2, 4, 2, \ldots, 4, 2, 1$. Thus the 2D Simpson's rule has a pattern of:

$$
\begin{array}{ccccccc}
1 & 4 & 2 & \dots & 4 & 2 & 1 \\
4 & 16 & 8 & \dots & 16 & 8 & 4 \\
2 & 8 & 4 & \dots & 8 & 4 & 2 \\
\vdots & & & \ddots & & & \vdots \\
2 & 8 & 4 & \dots & 8 & 4 & 2 \\
4 & 16 & 8 & \dots & 16 & 8 & 4 \\
1 & 4 & 2 & \dots & 4 & 2 & 1
\end{array}
$$

Considering the periodic conditions, it should follow the pattern of:

$$
\begin{array}{ccccccc}
4 & 8 & 4 & \dots & 8 & 4 & 0 \\
8 & 16 & 8 & \dots & 16 & 8 & 0 \\
4 & 8 & 4 & \dots & 8 & 4 & 0 \\
\vdots & & & \ddots & & & \vdots \\
4 & 8 & 4 & \dots & 8 & 4 & 0 \\
8 & 16 & 8 & \dots & 16 & 8 & 0 \\
0 & 0 & 0 & \dots & 0 & 0 & 0
\end{array}
$$

The error should be the fourth order $0(h^4)$(h denoted to the interval). This rule can be implemented with the same code of calculating function values at each grid point. But different weights should be included with values at different position. Here is the piece of the code.

```
        if (mod(iteta + jzeta,2) .eq. 0) then
           if (mod(iteta,2) .eq. 0) then
              total(2) = total(2) + 16 * fun    !16
           else
              total(2) = total(2) + 4 * fun    !4
           end if
        else
           total(2) = total(2) +  8 * fun    !8
        end if
```

1.3 Central value

Central value means using the function value at grid center to do surface integration. In that case, $E = \Delta\theta\,\Delta\zeta \sum_{j=0,k=0}^{M-1,N-1} \sqrt{g}_{j,k}\,\frac{1}{2}\left(B_{n,j+\frac{1}{2},k+\frac{1}{2}}\right)^2$
.

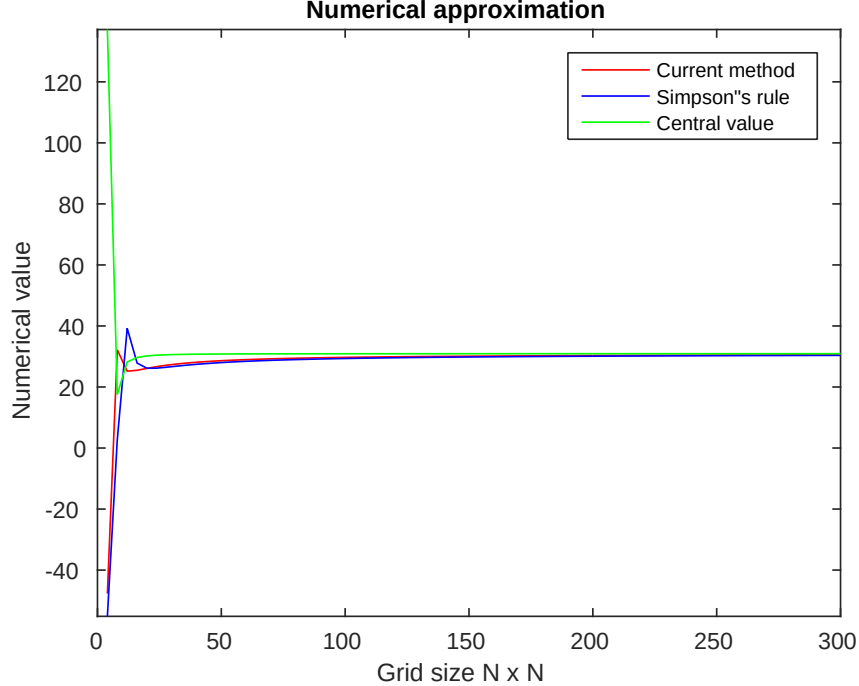
2 Results

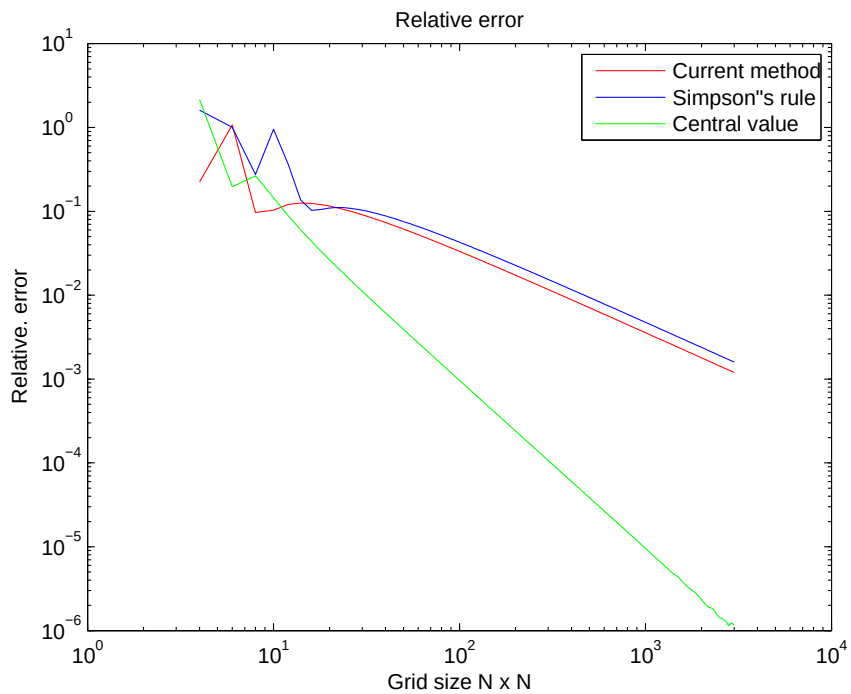
2.1 Arbitrary test function

To compare numerical approximations with analytical results, a easy testing integrand is needed. Here I take a periodic function integrated on the same grids as in the code.

$$T \;=\; \int_0^{2\pi}\int_0^{2\pi} \cos(4\theta-\zeta) + 2\zeta\sin(\frac{1}{2}\theta^2+\zeta)\;d\theta d\zeta \;=\; -12.65583063$$

The numerical approximation of the mentioned methods on the testing integrand are implemented in an individual code with the same square grid discretization as in the *Knotopt*. Numerical values and relative error $|\epsilon|/T$ vary with the grid size. Here are the details.





One interesting thing in the figure is that the Simpson's rule ($0(h^4)$) has the same convergence rate as the Trapezoidal rule($0(h^2)$) with slope of 1. The central value method seems having the best convergence (slope = 2.0), but it's more sensitive to the machine precision, based on the figure of relative error under single precsion (oscillation happens when grid size larger than 300×300, compared to 3000×3000 in the other two methods).

2.2 *Knotopt* denergy function

For the *Knotopt* denergy function testing, a sequence was implemented with grid size increased from 16×16 to 512×512. The number of periods of plasma boundary is set to 1. And 30 initialized coils are used. The covergence curves of the three methods are as below:

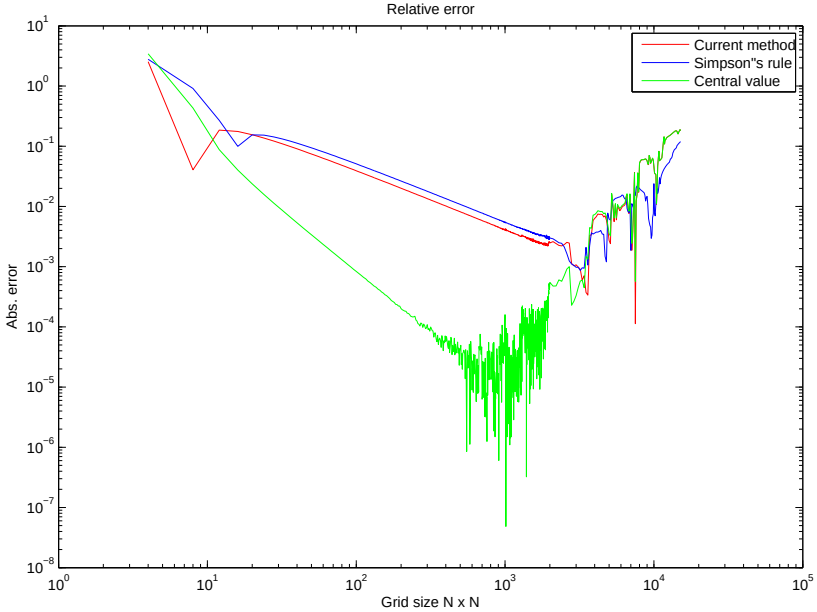
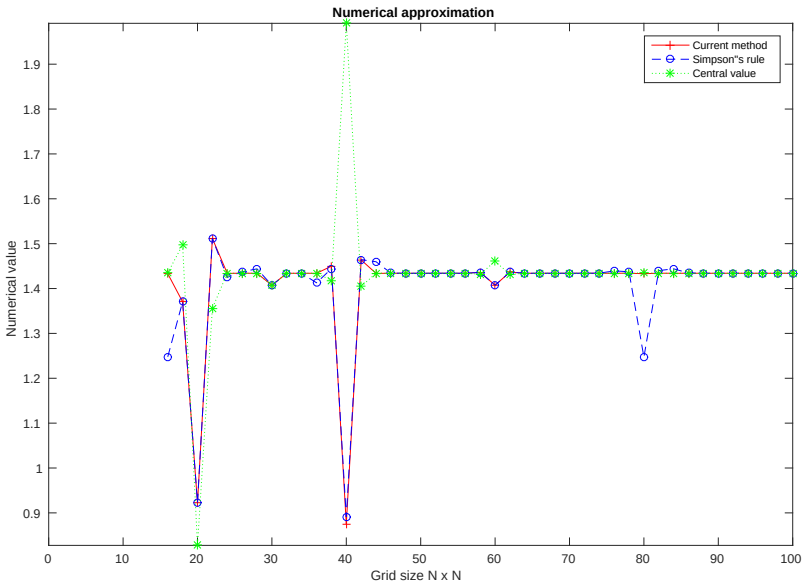


Figure 1: Relative error in single precsion



It‘s clear to see that the three methods have approximate resluts after the grid size larger than 50×50 (despite one abnormal point in Simpson‘s rule method). There are no obvious difference between the three methods. But we are convinced that central value is the best method without large modifications in the source code.