Numerical integration of the interaction energy of two point charges

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Abstract

We calculated numerically the energy interaction of two point charged particles. The integral has simple analytical result but is not easily solved numerically. Commercial programs as Mathematica 3.0™ and Maple V™ could not evaluate the integral and Gauss–Legendre method gave poor results. The method of Runge–Kutta integration was capable of solving it with good results. This integral showed to be a useful prototype for definite integration for double integration with poles. © 1998 IMACS/Elsevier Science B.V.

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A very simple problem of electrostatics is to calculate analytically the energy stored by two point charges. But if we try to solve it numerically by integrating the fields we are faced with a very difficult problem of numerical integration of a double integral with poles. The Gauss–Legendre method [1] showed to be unsatisfactory for this problem and also the commercial programs Mathematica 3.0™ [2] or Maple V™ could not solve it. The method of Runge–Kutta [3] succeeded as it is appropriate for treachery functions. We now proceed with the description of the analytical part and subsequently we show the numerical results.

The electric field $\mathbf{E}$ of a point charge $q$ can be described by [4]

$$
\mathbf{E} = \frac{q}{4\pi \varepsilon_0 r^2} \hat{r}
$$

where $r$ is the radial distance, $\hat{r} = \mathbf{r}/r$ and $\varepsilon_0$ is the dielectric constant. The energy stored in the field of a point charge in the volume $V$ is

$$
\mathcal{E} = \frac{\varepsilon_0}{2} \int \mathbf{E}^2 \, dV = \frac{1}{2} \frac{1}{(4\pi)^2 \varepsilon_0} \int \frac{q^2}{r^4} \, dV
$$

that is named the self-energy of a point charge.
If we have two point charges 1 and 2 separated by a distance of 2a, using the superposition principle, the resulting field will be

\[ E = E_1 + E_2. \] (3)

The total energy stored in the field generated by the two charges is given by [4]

\[ \frac{\varepsilon_0}{2} \int (E_1 + E_2)^2 \, dV = \frac{\varepsilon_0}{2} \int \left( \frac{q_1}{4\pi\varepsilon_0 r_1^2} \hat{r}_1 + \frac{q_2}{4\pi\varepsilon_0 r_2^2} \hat{r}_2 \right)^2 \, dV \]

\[ = \frac{1}{2} \frac{1}{(4\pi)^2 \varepsilon_0} \int \left( \frac{q_1^2}{r_1^4} + \frac{q_2^2}{r_2^4} + 2 \frac{q_1 q_2}{r_1^2 r_2^2} \hat{r}_1 \cdot \hat{r}_2 \right) \, dV \] (4)

where \( \hat{r}_1 = r_1/r_1 \) and \( \hat{r}_2 = r_2/r_2 \).

Removing the self-energy of each charge we have the interaction energy

\[ \varepsilon_{\text{int}} = \frac{1}{2} \frac{1}{(4\pi)^2 \varepsilon_0} \int \left( 2 \frac{q_1 q_2}{r_1^2 r_2^2} \hat{r}_1 \cdot \hat{r}_2 \right) \, dV = \frac{1}{2} \frac{1}{(4\pi)^2 \varepsilon_0} \int \left( 2 \frac{q_1 q_2}{r_1^3 r_2^3} \hat{r}_1 \cdot \hat{r}_2 \right) \, dV \] (5)

In cylindrical coordinates, \( r_1 = (\rho \cos \phi, \rho \sin \phi, z + a) \) and \( r_2 = (\rho \cos \phi, \rho \sin \phi, z - a) \). The interaction energy (5) can be written as

\[ \varepsilon_{\text{int}} = \frac{1}{2} \frac{q_1 q_2}{(4\pi)^2 \varepsilon_0} 2\pi \int_{-\infty}^{\infty} \, dz \int_0^{\infty} \rho \, d\rho \left( \frac{\rho^2 + z^2 - a^2}{[\rho^2 + (z + a)^2]^{3/2} [\rho^2 + (z - a)^2]^{3/2}} \right) \]

(6)

The interaction energy can also be calculated by the work to move the charge 2 to infinity, i.e.,

\[ \varepsilon_{\text{int}} = \text{Force} \times \text{displacement} = \int q_2 E_1 \cdot d\mathbf{l} = \int_{2a}^{\infty} q_2 \frac{q_1}{4\pi\varepsilon_0 r^2} \, dr = \frac{q_1 q_2}{4\pi\varepsilon_0} \frac{1}{2a} \]

(7)

comparing the results (6) with (7) we have

\[ \int_{-\infty}^{\infty} \, dz \int_0^{\infty} \rho \, d\rho \left( \frac{\rho^2 + z^2 - a^2}{[\rho^2 + (z + a)^2]^{3/2} [\rho^2 + (z - a)^2]^{3/2}} \right) = \frac{1}{a} \] (8)

We can define

\[ I \equiv a \int_{-\infty}^{\infty} \, dz \int_0^{\infty} \rho \, d\rho \left( \frac{\rho^2 + z^2 - a^2}{[\rho^2 + (z + a)^2]^{3/2} [\rho^2 + (z - a)^2]^{3/2}} \right) \]

(9)

that is equal to 1 for whatever value of \( a>0 \), according to Eq. (8).
So although the integral of interaction energy looks a little cumbersome, it has a very simple analytical result. We tried to solve it by Mathematica 3.0TM and by Maple VTM by analytical and by numerical methods but we do not obtain the proper results. Also using the Gauss–Legendre method with routine \textit{gauleg.f} from [3], gave poor results as shown in Table 1. As the function has poles it is considered as a treachery integral and in this case is better to use the Runge–Kutta method of integration [3]. We applied the Runge–Kutta method of integration with the subroutines \textit{odeint.f}, \textit{rkck.f}, \textit{rqck.f}, \textit{derivs.f} from [3]. Integrating first in $\rho$ and later in $z$ the method succeeded as shown in Table 2. The parameter $\textit{eps}$ is the step used in the method and the smaller the step better is the integration. The comparison for distance $a^\hat{1}$ and $a^\hat{10}$ show that the precision has little dependence on $a$. Surprisingly it could not integrate by exchanging the order of integration between $\rho$ and later in $z$.

Concluding, the energy interaction between two point charges generates a double integral with poles over the charge points. This integral has a simple analytical result. This integral can be used as a prototype for double integration with poles. Mathematica 3.0TM and Maple VTM could not solve the integral neither analytically nor numerically and Gauss–Legendre method gives poor results. Runge–Kutta method succeeded but only integrating first $\rho$ and later $z$.

The calculations were all made with double precision in a DigitalTM alpha2000 server.

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References