Wave Theory II — Numerical Simulation of Waves — (2) Representation of Wave Function by Using Green Function — (I) Green's Theorem and Free Space Green Function

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This lecture and the following lecture treat the Green functions to prepare for the representation of wave functions as the preparation of numerical simulations.

1 Meaning of Green Function — What to Be Concluded

Green function (or Green's function) is the wave function generated by the unit point source. As far as the law of superposition is satisfied, i.e. the system is linear, the wave function for the arbitrarily distributed source is expressed as the integration of Green function weighted by the source distribution.

Assuming the position vectors of source and observation points are $\mathbf{r}'$ and $\mathbf{r}$ respectively, the Green function of scalar Helmholtz equation $G(\mathbf{r},\ \mathbf{r}')$ is defined as

$$\nabla^2 G(\mathbf{r},\ \mathbf{r}') + k^2 G(\mathbf{r},\ \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'). \tag{1}$$

In case, the solution $\phi(\mathbf{r})$ of the general Helmholtz equation

$$\nabla^2 \phi(\mathbf{r}) + k^2 \phi(\mathbf{r}) = -\rho(\mathbf{r}) \tag{2}$$

is expressed by using Green function as

$$\phi(\mathbf{r}) = \int_V G(\mathbf{r},\ \mathbf{r}')\rho(\mathbf{r}')\mathrm{d}V' + \oint_{\partial V} \{G(\mathbf{r},\ \mathbf{r}')\nabla'\phi(\mathbf{r}') - \nabla' G(\mathbf{r},\ \mathbf{r}')\phi(\mathbf{r}')\} \cdot \mathrm{d}\mathbf{S}', \tag{3}$$

where V is the volume under consideration, ∂V is the surface of V, and $\mathrm{d}\mathbf{S}$ is the outward normal vector of ∂V. The volume integral in the right-hand side Eq. (3) corresponds to the superposition of the contribution from the source. On the other hand, the surface integral corresponds the superposition of the contribution from the equivalent sources on the boundary, which are equal to the wave function and its normal derivative. This term expresses the effect from outside the boundary, and is the formal expression of Huygens principle. Equation (3) is known as Kirchoff-Huygens principle. It is concluded from Eq. (3) that *the solution of the Helmholtz equation is uniquely solved if (i) the source distribution and (ii) the wave functions on the boundary are known.*

In the following sections, the derivation and the meaning of Eq. (3) are described. Then, the expression of $G(\mathbf{r},\ \mathbf{r}')$ in the free space is presented.

2 Green's Theorem

In an arbitrary volume V, two different scalar functions u, v satisfy the following relation.

$$\int_V (u\nabla^2 v - v\nabla^2 u)\mathrm{d}V = \oint_{\partial V} (u\nabla v - v\nabla u) \cdot \mathrm{d}\mathbf{S}, \tag{4}$$

where $\mathrm{d}\mathbf{S}$ is the outward normal vector of ∂V. This relation is known as *Green's theorem.*

[Proof]

Gauss' theorem

$$\int_V \nabla \cdot \mathbf{A}\mathrm{d}V = \oint_{\partial V} \mathbf{A} \cdot \mathrm{d}\mathbf{S} \tag{5}$$

and the vector identity

$$\begin{aligned}\nabla\cdot f\mathbf{A} &= \frac{\partial}{\partial x}(fA_x)+\frac{\partial}{\partial y}(fA_y)+\frac{\partial}{\partial z}(fA_z)\\ &= \left(\frac{\partial f}{\partial x}A_x+f\frac{\partial A_x}{\partial x}\right)+\left(\frac{\partial f}{\partial y}A_y+f\frac{\partial A_y}{\partial y}\right)+\left(\frac{\partial f}{\partial z}A_z+f\frac{\partial A_z}{\partial z}\right)\\ &= \nabla f\cdot\mathbf{A}+f\nabla\cdot\mathbf{A} \qquad (6)\end{aligned}$$

are used.

By substituting $\mathbf{A}=u\nabla v-v\nabla u$ into Eq. (5), and using vector identity (6),

$$\begin{aligned}\nabla\cdot\mathbf{A} &= \nabla u\cdot\nabla v+u\nabla^2 v\\ &\quad -\nabla v\cdot\nabla u-v\nabla^2 u \qquad (7)\end{aligned}$$

is proved.

(end of proof)

3 Integral Representation of Wave Function by Using Green Function — Kirchoff-Huygens Principle

For an inhomogeneous Helmholtz equation

$$\nabla^2\phi(\mathbf{r})+k^2\phi(\mathbf{r})=-\rho(\mathbf{r}), \qquad (8)$$

Green function $G(\mathbf{r},\ \mathbf{r}')$ is given as

$$\nabla^2 G(\mathbf{r},\ \mathbf{r}')+k^2G(\mathbf{r},\ \mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}'), \qquad (9)$$

where $\mathbf{r}'$ and $\mathbf{r}$ are the position vectors of the source and the observer. Here, the Green function $G(\mathbf{r},\ \mathbf{r}')$ is assumed to satisfy the following boundary conditions[1] on $S=\partial V$.

$$A(\mathbf{r})\hat{\mathbf{n}}\cdot\nabla G(\mathbf{r},\ \mathbf{r}')+B(\mathbf{r})G(\mathbf{r},\ \mathbf{r}')=0. \qquad (10)$$

The solution $\phi(\mathbf{r})$ of the Helmholtz equation (8) is expressed by using Green function as

$$\phi(\mathbf{r})=\int_V G(\mathbf{r},\ \mathbf{r}')\rho(\mathbf{r}')\mathrm{d}V'+\oint_{\partial V}\{G(\mathbf{r},\ \mathbf{r}')\nabla'\phi(\mathbf{r}')-\nabla'G(\mathbf{r},\ \mathbf{r}')\phi(\mathbf{r}')\}\cdot\mathrm{d}\mathbf{S}'. \qquad (11)$$

Equation (11) is called Kirchoff-Huygens Principle.

[Proof]

The reciprocity of Green function is proved first. $u=G(\mathbf{r},\ \mathbf{r}_1')$ and $v=G(\mathbf{r},\ \mathbf{r}_2')$ are substituted into Green's theorem (4). Then, the integrand of the left-hand side is written as

$$\begin{aligned}u\nabla^2 v-v\nabla^2 u &= G(\mathbf{r},\ \mathbf{r}_1')\nabla^2 G(\mathbf{r},\ \mathbf{r}_2')-G(\mathbf{r},\ \mathbf{r}_2')\nabla^2 G(\mathbf{r},\ \mathbf{r}_1')\\ &= G(\mathbf{r},\ \mathbf{r}_1')\left\{-k^2G(\mathbf{r},\ \mathbf{r}_2')-\delta(\mathbf{r}-\mathbf{r}_2')\right\}\\ &\quad -G(\mathbf{r},\ \mathbf{r}_2')\left\{-k^2G(\mathbf{r},\ \mathbf{r}_1')-\delta(\mathbf{r}-\mathbf{r}_1')\right\}\\ &= -G(\mathbf{r},\ \mathbf{r}_1')\delta(\mathbf{r}-\mathbf{r}_2')+G(\mathbf{r},\ \mathbf{r}_2')\delta(\mathbf{r}-\mathbf{r}_1').\end{aligned}$$

Therefore, the Green's theorem (4) is rewritten as

$$\begin{aligned}\text{(left-hand side)} &= -G(\mathbf{r}_2',\ \mathbf{r}_1')+G(\mathbf{r}_1',\ \mathbf{r}_2'),\\ \text{(right-hand side)} &= \oint_{\partial V}\{G(\mathbf{r},\ \mathbf{r}_1')\nabla G(\mathbf{r},\ \mathbf{r}_2')-G(\mathbf{r},\ \mathbf{r}_2')\nabla G(\mathbf{r},\ \mathbf{r}_1')\}\cdot\mathrm{d}\mathbf{S},\\ &= 0 \text{ (both satisfy Eq. (10).)}\end{aligned}$$

[1] $A(\mathbf{r})=0$ is called Dirichlet condition, whereas $B(\mathbf{r})=0$ is called Neumann condition. For acoustic waves, $B(\mathbf{r})=0$ corresponds $\mathbf{v}=0$, i.e. hard surface, $A(\mathbf{r})=0$ corresponds $p=0$, i.e. soft surface, and $\frac{A(\mathbf{r})}{B(\mathbf{r})}=$ const. corresponds to impedance surface.

By rewriting the variables as $\mathbf{r}'_1 = \mathbf{r}$, $\mathbf{r}'_2 = \mathbf{r}'$,

$$G(\mathbf{r},\ \mathbf{r}') = G(\mathbf{r}',\ \mathbf{r}) \tag{12}$$

is obtained. This characteristic is called *reciprocity* of the Green function.

Next, $u = \phi(\mathbf{r})$ and $v = G(\mathbf{r},\ \mathbf{r}')$ are substituted into Green's theorem (4). Then, the integrand of the left-hand side is written as

$$\begin{aligned} u\nabla^2 v - v\nabla^2 u &= \phi(\mathbf{r})\nabla^2 G(\mathbf{r},\ \mathbf{r}') - G(\mathbf{r},\ \mathbf{r}')\nabla^2\phi(\mathbf{r}) \\ &= \phi(\mathbf{r})\left\{-k^2 G(\mathbf{r},\ \mathbf{r}') - \delta(\mathbf{r}-\mathbf{r}')\right\} - G(\mathbf{r},\ \mathbf{r}')\left\{-k^2\phi(\mathbf{r}) - \rho(\mathbf{r})\right\} \\ &= -\phi(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') + \rho(\mathbf{r})G(\mathbf{r},\ \mathbf{r}'). \end{aligned}$$

Therefore, the Green's theorem (4) is rewritten as

$$-\phi(\mathbf{r}') + \int_V G(\mathbf{r},\ \mathbf{r}')\rho(\mathbf{r})\mathrm{d}V = \oint_{\partial V} \{\phi(\mathbf{r})\nabla G(\mathbf{r},\mathbf{r}') - G(\mathbf{r},\ \mathbf{r}')\nabla\phi(\mathbf{r})\}\cdot \mathrm{d}\mathbf{S}.$$

By using the reciprocity of the Green function (12) and interchanging $\mathbf{r}$ and $\mathbf{r}'$, Eq. (11)

$$\phi(\mathbf{r}) = \int_V G(\mathbf{r},\ \mathbf{r}')\rho(\mathbf{r}')\mathrm{d}V' + \oint_{\partial V} \{G(\mathbf{r},\ \mathbf{r}')\nabla'\phi(\mathbf{r}') - \nabla' G(\mathbf{r},\ \mathbf{r}')\phi(\mathbf{r}')\}\cdot \mathrm{d}\mathbf{S}'$$

is obtained.

(end of proof)

If the Helmholtz equation (8) satisfies the same boundary condition as the Green function (10), the surface integral term of Eq. (11) becomes identically zero. *Once the Green function that satisfies the given boundary condition, the solution of the Helmholtz equation is expressed as the superposition of this Green function weighted by the source distribution.*

If the Helmholtz equation (8) does not satisfy the same boundary condition as the Green function (10), the surface integral term of Eq. (11) is nonzero in order to express the effect from outside. The first term of the integrand of this surface integral is in the same form as the source contribution in the volume integral. Therefore,

$$\rho_S(\mathbf{r}') \equiv \nabla'\phi(\mathbf{r}')\cdot\hat{\mathbf{n}}' \tag{13}$$

is called the equivalent surface (monopole) source. In the second term of the integrand, the normal derivative of the Green function is regarded as the Green function with respect to the dipole source. Therefore,

$$\hat{\boldsymbol{\mu}}_S(\mathbf{r}') \equiv -\hat{\mathbf{n}}'\phi(\mathbf{r}') \tag{14}$$

is called the equivalent surface dipole source. These equivalent sources are assumed to exist on the boundary.

When two point sources are located at $\mathbf{r}'$ and infinitesimally separated as much as $\Delta\mathbf{n}'$ with equal magnitude and alternating sign (i.e. dipole), the wave function $D(\mathbf{r},\ \mathbf{r}')$ is expressed as

$$\nabla^2 D(\mathbf{r},\ \mathbf{r}') + k^2 D(\mathbf{r},\ \mathbf{r}') = \lim_{\Delta n'\to 0}\frac{-\delta(\mathbf{r}-(\mathbf{r}'+\Delta\mathbf{n}')) + \delta(\mathbf{r}-\mathbf{r}')}{\Delta n'}. \tag{15}$$

The solution is expressed by using Green function as

$$\begin{aligned} D(\mathbf{r},\ \mathbf{r}') &= \lim_{\Delta n'\to 0}\frac{G(\mathbf{r},\ (\mathbf{r}'+\Delta\mathbf{n}')) - G(\mathbf{r},\ \mathbf{r}')}{\Delta n'} \\ &= \nabla' G(\mathbf{r},\ \mathbf{r}')\cdot\hat{\mathbf{n}}'. \end{aligned} \tag{16}$$

Therefore, $\nabla' G(\mathbf{r},\ \mathbf{r}')$ is regarded as the vector Green function with respect to the dipole source.

4 Free Space Green Function

The Green function in the free space, i.e. when the boundary exists infinitely far, can be derived in the following manners.

4.1 3D Green Function

When the source is assumed to be at the origin of the coordinates, the Green function $G(\mathbf{r})$ is expressed from Eq. (9) as

$$\nabla^2 G(\mathbf{r}) + k^2 G(\mathbf{r}) = -\delta(\mathbf{r}). \tag{17}$$

Since the free space is assumed, $G(\mathbf{r},\ \mathbf{r}')$ is only the function of $r = |\mathbf{r}|$ due to the symmetry. By using the Laplacian in the spherical coordinates

$$\nabla^2 \phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \phi}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \phi}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \phi}{\partial \varphi^2}, \tag{18}$$

Eq. (17) is rewritten as

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \frac{\mathrm{d}G(r)}{\mathrm{d}r}\right) + k^2 G(r) = -\delta(r). \tag{19}$$

Since the right-hand side of Eq. (19) is zero except for the origin, both sides are multiplied by r and

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}(rG(r)) + k^2(rG(r)) = 0 \tag{20}$$

is obtained. Equation (20) is easily solved to obtain

$$G(r) = M\frac{e^{-jkr}}{r}, \tag{21}$$

where M is an arbitrary constant, and only the traveling wave toward $+r$ is assumed since the source is located at the origin.

The arbitrary constant M is determined by substituting Eq. (21) into Eq. (17), and then integrating Eq. (17) within the small sphere including the origin, as (see Appendix for details)

$$\begin{aligned}
\int_V \nabla^2 G \mathrm{d}V &= \oint_{\partial V} \nabla G \cdot \mathrm{d}\mathbf{S} \\
&= 4\pi r^2 \hat{\mathbf{r}} \cdot \nabla G \\
&= -4\pi M r^2 \left(\frac{e^{-jkr}}{r^2} + jk\frac{e^{-jkr}}{r}\right) \\
\int_V k^2 G \mathrm{d}V &= 4\pi k^2 M \left\{-\frac{1}{jk} r e^{-jkr} + \frac{1}{k^2}\left(e^{-jkr} - 1\right)\right\} \\
\int_V (-\delta) \mathrm{d}V &= -1.
\end{aligned}$$

By taking the limit of $r \to 0$,

$$M = \frac{1}{4\pi} \tag{22}$$

is obtained.

When the source is located at the arbitrary position $\mathbf{r}'$, let $r = |\mathbf{r} - \mathbf{r}'|$ and the Green function $G(\mathbf{r}, \mathbf{r}')$ is expressed as

$$G_3(\mathbf{r}, \mathbf{r}') = \frac{e^{-jk|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{23}$$

4.2 2D Green Function

A 2D problem which is uniform along z direction. When the source is assumed to be at the origin of the coordinates, the Green function $G(\boldsymbol{\rho})$ is expressed from Eq. (9) as

$$\nabla^2 G(\boldsymbol{\rho}) + k^2 G(\boldsymbol{\rho}) = -\delta(\boldsymbol{\rho}). \tag{24}$$

Since the free space is assumed, $G(\boldsymbol{\rho},\ \boldsymbol{\rho}')$ is only the function of $\rho = |\rho|$ due to the symmetry. By using the Laplacian in the cylindrical coordinates

$$\nabla^2 \phi = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial \phi}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 \phi}{\partial \varphi^2} + \frac{\partial^2 \phi}{\partial z^2} \tag{25}$$

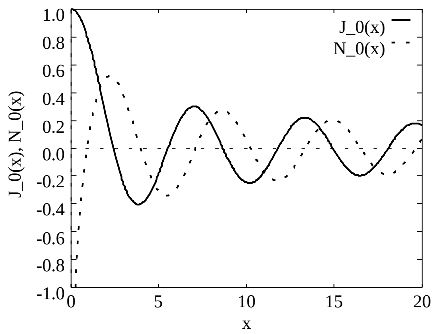

Figure 1: Bessel and Neumann functions.

Eq. (24) is rewritten as

$$\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}G(\rho)}{\mathrm{d}\rho}\right)+k^2G(\rho)=-\delta(\rho). \tag{26}$$

Since the right-hand side of Eq. (26) is zero except for the origin, Eq. (26) is rewritten as

$$\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}G(\rho)}{\mathrm{d}\rho}\right)+k^2G(\rho)=0. \tag{27}$$

This is known as the Bessel's differential equation. The two independent solutions are the Bessel function $J_0(k\rho)$ and the Neumann function $N_0(k\rho)$, which are shown in Fig. 1. Alternatively, linear combinations of these two functions, i.e. Hankel functions of first kind $H_0^{(1)}(k\rho)=J_0(k\rho)+jN_0(k\rho)$ and of second kind $H_0^{(2)}(k\rho)=J_0(k\rho)-jN_0(k\rho)$ may be used as well.

Only the traveling wave toward $+\rho$ is assumed since the source is located at the origin in the same manner as 3D case. Therefore, the solution is given as the Hankel function of second kind as

$$G(\rho)=MH_0^{(2)}(k\rho). \tag{28}$$

The arbitrary constant M is determined by substituting Eq. (28) into Eq. (24), and then integrating Eq. (24) within the small circle including the origin, as

$$\oint_{\partial S}\nabla G\cdot\mathrm{d}\mathbf{l}+\int_S k^2G\mathrm{d}S=\int_S(-\delta)\mathrm{d}S. \tag{29}$$

By taking the limit of $\rho\to 0$,

$$M=\frac{1}{4j} \tag{30}$$

is obtained.

When the source is located at the arbitrary position ρ', let $\rho=|\boldsymbol{\rho}-\boldsymbol{\rho}'|$ and the Green function $G(\boldsymbol{\rho},\ \boldsymbol{\rho}')$ is expressed as

$$G(\boldsymbol{\rho},\ \boldsymbol{\rho}')=\frac{1}{4j}H_0^{(2)}(k|\rho-\rho'|). \tag{31}$$

4.3 1D Green Function

A 1D problem which is uniform along y and z directions. In the same manner as 3D and 2D cases, the 1D free space Green function is given as

$$G(x,x')=\frac{1}{2jk}e^{-jk|x-x'|}. \tag{32}$$

A Supplements for the Derivation of Free Space Green Function

Why $\int_V\nabla^2G\mathrm{d}V$ is modified by using Gauss' theorem to avoid the singularity, while $\int_V k^2G\mathrm{d}V$ can be integrated including the singularity (i.e. the source point)? This is described in the following manner, although it is not rigorous.

The regularity means the possibility of the differentiation, and the irregularity increases by the differentiation. Therefore, $\nabla^2 G$ shall be more carefully integrated by introducing Gauss' theorem. Contrary, the integral of $k^2 G$ is finite.

These things are clarified more by considering the limiting operation which is described in this handout. That is, the variation of e^{-jkr} near the origin is very small compared with that of $\frac{1}{r}$. Therefore, the approximation $e^{-jkr} \simeq 1$ is valid. In case, the integrals are written as

$$
\begin{aligned}
\int_V \nabla^2 G \mathrm{d}V &= \oint_{\partial V} \nabla G \cdot \mathrm{d}\mathbf{S} \\
&\simeq \oint_{\partial V} \nabla \frac{M}{r} \cdot \mathrm{d}\mathbf{S} \\
&= 4\pi r^2 \left(-\frac{M}{r^2}\right), \\
&= -4\pi M \\
\int_V k^2 G \mathrm{d}V &\simeq \int_V k^2 \frac{M}{r} \mathrm{d}V \\
&= \int_0^r k^2 \frac{M}{r} 4\pi r^2 \mathrm{d}r \\
&= 2\pi M k^2 r^2,
\end{aligned}
$$

in 3D case. It is noted that the singularity in the latter integrand has been disappeared after the integration.

Report

Tokyo Tech students are requested to submit by either of the following ways:

1. by passing the lecturer before the lecture, or
2. or via the mailing post of O-okayama Minami 3 bldg. 1st floor.

Do not forget to fill out the student ID, your department and lab names, as well as your name. KMITL students shall follow the instruction of Dr. Chuwong.

The handouts as well as the copies of the slides can be downloaded from the web.

`http://mobile.ss.titech.ac.jp/~takada/waves/`

Exercises

1. Derive 1D free space Green function in cases of $x > x'$ and $x < x'$, separately.
2. Find the asymptotic formulae of the Bessel and the Neumann functions when the variable is approaching to infinity. Then, describe why the outward traveling wave is described by the Hankel function of second kind.
3. Point out the corrections of handout, if any.