Boundary integral numerical solution to PDEs using analytic resolution of singularities

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1 Description of the method used

Following the methodology in the paper by Bruno et al[1], we integrate the singular Green's function by resolving the singularities using partition of unity method in order to divide the integral over surface to integral over patches with periodic integrand with vanishing derivatives at the boundary allowing us to trapezoidal rule to calculate those. As an example, we take the exterior Dirichlet boundary condition with Helmholtz equation,

$$\Delta u + k^2 u = 0 \ in \ \mathbb{R}^3 \backslash \bar{\Omega}$$
$$u = g \ on \ \partial\Omega$$

The Green's function for this problem is given by $G(\mathbf{r}, \mathbf{r'}) = \frac{e^{ik|\mathbf{r}-\mathbf{r'}|}}{4\pi|\mathbf{r}-\mathbf{r'}|}$. The solution to this problem can be written in terms of single and double layer potential with surface density σ defined as follows:

$$(S\sigma)(\mathbf{r}) = \int_{\partial\Omega} G(\mathbf{r}, \mathbf{r'})\sigma(\mathbf{r'})ds(\mathbf{r'})$$
$$(D\sigma)(\mathbf{r}) = \int_{\partial\Omega} \frac{\partial G(\mathbf{r}, \mathbf{r'})}{\partial \nu(\mathbf{r'})}\sigma(\mathbf{r'})ds(\mathbf{r'})$$

where the $\nu(\mathbf{r'})$ denotes the outward normal for the surface. We can solve for the density σ on the boundary by solving the following boundary integral equation that imposes the boundary condition using jump conditions of the double layer potential.

$$\frac{1}{2}\sigma(\mathbf{r}) + (D\sigma)(\mathbf{r}) - i\gamma(S\sigma)(\mathbf{r}) = g(\mathbf{r}) \ on, \ \mathbf{r} \in \partial\Omega$$

where $\gamma \neq 0$ is a real parameter that can be used to guarantee uniqueness and can be tweaked to improve the conditioning of the system. So in order to calculate the solution, we need to be able to evaluate the singular integral involved accurately. We describe the method in particular for the sphere.

1.1 Partition of Unity and Non singular integration

We divide the sphere into six overlapping hemispherical patches (which form an open cover), say, $\{P_1, P_2, ..., P_6\}$ each of which is homeomorphic to a rectangle

$[0,\pi]\times[0,\pi]$ by the usual (θ,ϕ) parametrization. We call these parametrization maps $\phi_1,\phi_2,...,\phi_6$ with $\phi_i : [0,\pi]\times[0,\pi] \to P_i$. We use a partition of unity $\{w_1,....,w_6\}$ subordinate to this cover with $supp(w_i) \subset P_i$ and $\sum w_i = 1$. Here $w_i(\mathbf{r}) = e^{\frac{2e^{-\frac{1}{t}}}{t-1}}$ where $t = |\mathbf{r} - p_i|_g/d$. Here p_i is the pole of the hemisphere and $||_g$ denotes the geodesic distance of the point $\mathbf{r}$ from the pole p_i. If the distance is greater than d, then the $w_i(r) = 0$ otherwise it is between 1 and 0. For our experiments, we took $d = 5\pi R/12$.

Now the integral $\int_{\partial\Omega}$ can be decomposed as follows:

$$\int_{\partial\Omega} G(\mathbf{r},\mathbf{r'})\sigma(\mathbf{r'})ds(\mathbf{r'}) = \sum_{i=1}^{6}\int_{P_i} w_i(\mathbf{r})G(\mathbf{r},\mathbf{r'})\sigma(\mathbf{r'})ds(\mathbf{r'})$$

We can write double layer potential similarly as an integral over patches. Now, we can transform the coordinates for integral over each patch using the coordinate charts $\phi_i, i = 1,2,..,6$. We get the following integral

$$\sum_{i=1}^{6}\int_0^\pi\int_0^\pi w_i(\mathbf{r})G(\mathbf{r},\mathbf{r'}(u,v))\sigma(\mathbf{r'}(u,v))J_i(u,v)dudv$$

where is J_i is the Jacobian for the patch P_i.

Note the multiplication by a smooth partition of unity with vanishing derivatives at the boundary of its support makes the value of the integrand as well as the derivatives zero hence allowing us to use trapezoidal rule with high accuracy for integrating provided the integrand had no singular part which is certainly not the case. So we need to get rid of the singularity meanwhile and then handle the singular portion later separately. Note the integrand is singular only when $\mathbf{r} = \mathbf{r'}$ hence, depending on $\mathbf{r}$, we create a local floating partition of unity $\eta_{\mathbf{r},i}(\mathbf{r'}) = e^{\frac{2e^{-\frac{1}{t}}}{t-1}}$ where $t = |\phi_i^{-1}(\mathbf{r}) - \phi_i^{-1}(\mathbf{r'})|/d$. here we took $d = h$ our discretization spacing. So $(\eta_{\mathbf{r},i}, 1-\eta_{\mathbf{r},i})$ form a local smooth partition of unity with which each integral over a patch can be decomposed further as

$$\int_0^\pi\int_0^\pi (1-\eta_{\mathbf{r(u,\ v)},i})(\mathbf{r'}(u,v))w_i(\mathbf{r})G(\mathbf{r},\mathbf{r'}(u,v))\sigma(\mathbf{r'}(u,v))J_i(u,v)dudv$$

Note that now this integral has no singular part and has vanishing derivatives at the end so can be integrated using trapezoidal rule over the rectangle in parametrized space $[0,\pi]\times[0,\pi]$.

1.2 Singular Integration

Our next task is to evaluate the singular part of the integral remaining over each patch which is given by

$$\int_0^\pi\int_0^\pi \eta_{\mathbf{r(u,\ v)},i}(\mathbf{r'}(u,v))w_i(\mathbf{r})G(\mathbf{r},\mathbf{r'}(u,v))\sigma(\mathbf{r'}(u,v))J_i(u,v)dudv$$

We denote the integrand as succinctly as $G(\mathbf{r},\mathbf{r'(u,\ v)})\psi(u,v)$. The integrand is non zero only on a circle of radius h :discretization spacing, owing to the nature

of η constructed. This circular domain can further be parametrized using the radial coordinates $(\rho, \theta) \in [-h, h] \times [0, \pi]$. Hence, we get the integral

$$\int_0^{\pi} \int_{-h}^{h} G(\mathbf{r}, \mathbf{r'}(u(\rho,\theta), v(\rho,\theta)))\psi(u(\rho,\theta), v(\rho,\theta))|\rho| d\rho d\theta$$

where $|\rho|$ is the Jacobian. As shown in [1], the integrand is now smooth for smooth surfaces with vanishing derivatives at the boundary and hence can be integrated using trapezoidal rule again on (ρ, θ) domain. How ever to integrate over the this domain, we need ψ values at the nodes which do not fall on the Cartesian grid in the parametrization space and hence we need to interpolate the values on the Cartesian grid to obtain an approximation of the ψ values on the this nodes. For this purpose, we use make use of the periodicity of ψ obtained using partition of unity over the sphere patches and use 2D FFT interpolation with upsampling factor 16 and then perform spline interpolation to obtain values at the nodes required for integration using the trapezoidal rule on the (ρ, θ) domain. We use a spacing of $h^{\frac{3}{2}}$ on the ρ axis and $h^{\frac{1}{2}}$ on the θ axis resulting in $O(1/h)$ number of points for singular integration.

2 Evaluation of solution

For evaluation the solution, we divide the domain in three regions:
1) Well separated region: $dist(\mathbf{r}, \partial\Omega) > \sqrt{h}$

2) Intermediate region: $h < dist(\mathbf{r}, \partial\Omega) < \sqrt{h}$

3)Near singular region: $dist(\mathbf{r}, \partial\Omega) < h$

2.1 Well separated region

For this region we just use the non-singular integration routine with no floating partition of unity.

2.2 Intermediate region

For this region, we upsample the density σ by a factor of 16 and use the trapezoidal integration rule with these finer upsampled grid without any floating partition of unity.

2.3 Near singular region

For this region, we instead of directly calculating the values, we first calculate, using intermediate integration, the values at some 6 nodes lying in the intermediate region in the direction of the normal to the sphere near the node of interest and then use 1D cubic interpolation on these nodes plus the node at the boundary nearest to the point of interest to estimate the value.

3 Numerical results

3.1 Convergence of Singular integration

We evaluate the double layer potential of Laplace kernel with constant density $\sigma = 1$ with target point on the surface.

Table 1: Singular integration

h	N	L^∞ error	Rate of convergence
0.3490	486	5×10^{-3}	
0.1848	1734	1.52×10^{-4}	5.0398
0.0952	6534	1.18×10^{-6}	7.0091
0.0483	25350	1.36×10^{-8}	6.4390

3.2 Convergence of Non-singular integration

We evaluate the double layer potential of Laplace kernel with constant density $\sigma = 1$ with target point outside the surface.

Table 2: Non-singular integration

h	N	L^∞ error	Rate of convergence
0.3490	486	2.61×10^{-4}	
0.1848	1734	7.61×10^{-6}	5.1
0.0952	6534	5×10^{-9}	10.1
0.0483	25350	4.9×10^{-10}	3.4

3.3 Interior Dirichlet Laplace equation

We solved the following interior Laplace problem with Dirichlet boundary conditions,

$$-\Delta u = 0, \ \ in\ \Omega$$
$$u = 1 + y, \ \ on\ \partial\Omega$$

where R is the radius of the sphere. We took $R = 1$ for the following results.

Table 3: Interior Dirichlet Laplace problem

h	N	L^∞ error	Rate of convergence
0.9806	54	1.052×10^{-1}	
0.4487	294	2.71×10^{-2}	2
0.2856	726	7.2×10^{-3}	3.3
0.2094	1350	2×10^{-3}	3.97
0.1366	3174	5×10^{-4}	3.36

References

[1] Oscar P. Bruno and Leonid A. Kunyansky, *A Fast, High-Order Algorithm for the Solution of Surface Scattering Problems: Basic Implementation, Tests, and Applications*, Journal of Computational Physics 169, 80–110 (2001)