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Quadrature Weights on Tensor-Product Nodes for Accurate Integration of Hypersingular Functions over Some Simple 3-D Geometric Shapes

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Abstract. In this paper, we present accurate and economic integration quadratures for hypersingular functions over three simple geometric shapes in $\mathbb{R}^3$ (spheres, cubes, and cylinders). The quadrature nodes are made of the tensor-product of 1-D Gauss nodes on $[-1,1]$ for non-periodic variables or uniform nodes on $[0,2\pi]$ or $[0,\pi]$ for periodic ones. The quadrature weights are converted from a brute-force integration of the hypersingular function through interpolating the smooth component of the integrand. Numerical results are presented to validate the accuracy and efficiency of computing hypersingular integrals, as in the computations of Cauchy principal values, with a minimum number of quadrature nodes. The pre-calculated quadrature tables can be then readily used to implement Nyström collocation methods of hypersingular volume integral equations such as the one for Maxwell equations.

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1 Introduction

The computation of hypersingular integrals associated with Cauchy principal values (CPVs) is the most time consuming and challenging task in solving integral equations for many mathematical physics equations, for example, Maxwell equations, elasticity equations, etc. The CPV is defined by the integration of the singular function by first excluding a small volume around the singularity, then letting the size of the exclusion volume shrink to zero to produce the CPV. Namely, the CPV is defined as

$$\text{p.v.}\int_{\Omega}\frac{f(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|^k}d\mathbf{r}=\lim_{\delta\to 0}\int_{\Omega\setminus V_\delta(\mathbf{r}')}\frac{f(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|^k}d\mathbf{r}, \tag{1.1}$$

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where Ω is a bounded domain in R^3 assumed to be a cube, rectangular prism, cylinder, or sphere in this paper and $V_\delta(\mathbf{r}')$ is an exclusion volume centered at $\mathbf{r}'$ of spherical shape of radius δ.

The objective of this paper is to develop an accurate and efficient quadrature formula to compute the integral over $\Omega\backslash V_\delta(\mathbf{r}')$ in (1.1). For any fixed $\delta>0$, the integral over domain $\Omega\backslash V_\delta(\mathbf{r}')$ can be calculated by a naive brute-force approach to a given accuracy if a large number of sample points are used. Fortunately, the function $f(\mathbf{r})$ in the numerator, which can take a general form in the integral equation method, is often smooth; therefore, $f(\mathbf{r})$ can be well represented through an interpolation of its values on the three-dimensional tensor product of 1-D Gauss quadrature or midpoint nodes. Using this simple fact, any brute-force integration quadrature involving a large number of values of $f(\mathbf{r})$ can be converted into an equivalent quadrature formula using only values at the small number of nodes of a tensor-product form in Ω. Moreover, the new weights on the tensor-product nodes can be pre-computed and tabulated to be used for a general function $f(\mathbf{r})$. This will be the approach in this paper, and the resulting weights have been used to calculate the matrix entries for a discretized Nyström volume integral equation for Maxwell equations in [1] where the issue of CPV limit is also addressed. There are other approaches in computing the CPV in (1.1), including direct evaluations of hypersingular integrals [2].

The rest of this paper will be organized as follows. In Section 2, we will describe the interpolation approach for constructing a quadrature formula for singular integrations over the domain $\Omega\backslash V_\delta(\mathbf{r}')$ on tensor-product nodes. In Sections 3 through 5, we present specific implementations of interpolated quadrature when Ω is a cube, cylinder, and sphere, respectively. In Section 6, we provide an outline of the resulting algorithm that is implemented in computer code. In Section 7, numerical tests are included for each domain. In the appendix, quadrature weights over some tensor-product nodes are given for singular integrals over each domain.

2 Quadrature formula over tensor-product nodes

Consider a hypersingular integrand formed by the product of some smooth function $f(\mathbf{r})$ with a singular kernel $1/|\mathbf{r}-\mathbf{r}'|^k$ over a domain Ω, where the singularity is at $\mathbf{r}'\in\Omega$ and k can be 1, 2, or 3, i.e.,

$$\int_{\Omega\backslash V_\delta(\mathbf{r}')}\frac{f(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|^k}d\mathbf{r}. \tag{2.1}$$

First, assume we have an N point quadrature rule that uses points $\hat{\mathbf{r}}_i$ and weights $\hat{w}_i$,

$$\int_{\Omega\backslash V_\delta(\mathbf{r}')}\frac{f(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|^k}d\mathbf{r}\approx\sum_{i=1}^{N}\frac{f(\hat{\mathbf{r}}_i)}{|\hat{\mathbf{r}}_i-\mathbf{r}'|^k}\hat{w}_i. \tag{2.2}$$

As the function $f(\mathbf{r})$ is generally smooth, it can be well approximated through an interpolation of its values over a small number of tensor-product nodes $\{\mathbf{r}_i\}|_{i=1}^{M}$. Letting