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GALERKIN-QUADRATURES FOR THE S_N METHOD IN 2D CARTESIAN GEOMETRIES AND APPLICATION TO FORWARD-PEAKED SCATTERING PARTICLE TRANSPORT PROBLEMS

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ABSTRACT

Forward-peaked-scattering problems pose a challenge for deterministic S_N schemes that utilize standard quadrature sets (e.g., level symmetric sets). Specifically, the standard quadratures do not yield accurate results and oftentimes do not converge at all in the case of highly forward-peaked scattering. Triangular Gauss-Legendre-Chebyshev (GLC) quadrature sets of the Galerkin type have been shown to improve convergence for these problems in 3D Cartesian and *rz* geometries. We present here 2D Triangular GLC quadrature sets of the Galerkin type and derive rules for the 2D Product GLC of Galerkin type. A comparison of these quadratures with standard level-symmetric sets is made using a homogenous two-dimensional domain with a one-quadrant isotropic incident source for highly forward-peaked scattering material; the scattering is modeled with a Dirac function $\delta(\mu-\mu_0)$ where μ_0=0.9, 0.95 and 0.99.

Key Words: Galerkin Angular Quadrature, Discrete Ordinate S_N method, Forward-Peaked Scattering

1. INTRODUCTION

The purpose of this paper is to define a angular quadrature sets in 2D *xy* geometries suitable for highly anisotropic problems solved deterministically using the discrete ordinate S_N method. It is well established that standard S_N quadratures, when applied to forward-peaked scattering problems, do not converge well for low orders of N and diverges for high orders of N. The Galerkin method, proposed by Morel in Ref.[1], treats the scattering matrix using a Galerkin finite element representation of the angular flux while the reminder of the transport equation is dealt with using Discrete Ordinates. In Morel's approach, the angular flux is developed on a set of interpolatory functions (the spherical harmonics). By imposing that the discrete scattering source from the interpolatory representation provides the same angular moments as the scattering source computed with the interpolatory representation of the angular flux, the discrete-to-moment matrix (D) and the moment-to-discrete matrix (M) of the Galerkin quadrature are defined such that D is the exact inverse of M. This requires that M be square and invertible, resulting in necessary rules to include enough angular moments so that the number of directions and the number of moments are equal. It can be shown that the Galerkin approach can treat a delta function in scattering exactly, while standard methods may produce an unstable scheme[2]. Galerkin quadratures for 2D *xy* Cartesian geometries are presented and implemented in Xuthus, a

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mesh adaptive S_N transport code. Xuthus code is a two-dimensional AMR deterministic particle transport code under development at Texas A&M University. It was originally developed for neutron transport, and initially contained an assortment of standard angular quadratures (e.g., level symmetric, triangular and product Gauss-Legendre-Chebyshev) unsuitable for forward-peaked scattering problems. In an effort to expand the capabilities of Xuthus, triangular Galerkin and product Galerkin sets have been implemented in the code.

Although triangular Galerkin sets have previously been tested for 2D *xy* and *rz* and 3D xyz geometries, product Galerkin sets have not yet been devised for 2D *xy* geometries. Product Galerkin quadrature set employs more directions, thus requiring additional angular moments We will show that the product Galerkin quadrature can yield more accurate results for lower quadrature orders *N* though there are no detectable benefits in computer run time for the same level of accuracy.

We begin by briefly describing the solution method employed in the Xuthus code. Then, we define the three quadrature sets to be compared: level symmetric, triangular Galerkin, and product Galerkin. Next, we present computational results obtained from Xuthus for a series of delta function scattering test cases. As a comparison, Monte Carlo results for these test cases are also included. Finally, we summarize and present conclusions.

2. THE XUTHUS CODE

Xuthus is an S_N, two-dimensional, adaptive mesh refinement code used for modeling particle transport. The code works with a 2D triangular mesh that can be automatically refined to improve the accuracy of the flux calculation while minimizing the CPU cost. A number of quadrature sets, including triangular and product sets, are already present in the code. In order to better model forward-peaked scattering problems, the triangular Galerkin and product Galerkin sets have been introduced. Xuthus solves the standard Boltzmann equation[3]:

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi^{g}(\boldsymbol{r},\boldsymbol{\Omega})+\sigma_t\psi^{g}(\boldsymbol{r},\boldsymbol{\Omega}) = \sum_{g'=1}^{G}\int_{4\pi}\sigma_s^{g'\to g}(\boldsymbol{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\psi^{g'}(\boldsymbol{r},\boldsymbol{\Omega}')d\Omega'+S^{g}(\boldsymbol{r},\boldsymbol{\Omega}) \tag{1}$$

where:

$\psi =$ angular flux
$\boldsymbol{r} =$ position variable
$\boldsymbol{\Omega} =$ direction variable
$g =$ energy group variable
$\sigma_t =$ total macroscopic cross section
$\sigma_s =$ differential scattering cross section
$S =$ external source

The operator on the left-hand side of Eq. (1) represents the loss term, composed of particle leakage and losses due to collisions, while the right-hand side is the source term, made up of inscattering and an inhomogeneous source. The above equation is subject to appropriate boundary conditions.

Eq. (1) is solved by a standard Source Iteration (Richardson) technique or using non-stationary methods for linear algebra (in our case, GMRes). In the SI case, the iteration on the scattering source can be expressed as:

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi^{\ell+1} + \sigma_t \psi^{\ell+1} = Q^\ell + q \tag{2}$$

where

$$Q^\ell = \int_{4\pi} \sigma_s \left(\boldsymbol{r}, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}\right) \psi^\ell(\boldsymbol{r}, \boldsymbol{\Omega}') d\Omega' \tag{3}$$

and q contains the contributions from the external source and other energy groups. After spatial discretization, Eq. (2) can be written in terms of matrices as follows:

$$L\boldsymbol{\psi}^{\boldsymbol{\ell+1}} = \underline{M}\,\underline{\Sigma}\,\underline{D}\boldsymbol{\psi}^\ell + q \tag{4}$$

where L is the matrix due to streaming and total collisions, $\underline{\Sigma}$ is the scattering matrix which operates on the flux moments, $\underline{M} = M \otimes I$ is the moment-to-direction matrix, $\underline{D} = D \otimes I$ is the direction-to-moment matrix. The dimensions of L are the number of spatial degrees of freedom times the number of directions, i.e., $(N_{dof} \times N_{dir})^2$. In a discontinuous finite element method, the number of degrees of freedom N_{dof} is simply the number of elements N_{el} times the number of unknowns per element (which is $(p+1)(p+2)/2$ for a local spatial presentation of degree p on triangular cells). The dimensions of $\underline{\Sigma}$ are $(N_{dof} \times N_{mom})^2$, where N_{mom} is the number of moments employed in the spherical harmonics expansion of the angular fluxes; N_{mom} is equal to $(N_a+1)(N_a+2)/2$ in 2-D for standard angular quadratures, with N_a the anisotropic scattering order; for Galerkin quadratures, $N_{mom} = N_{dir}$. $\underline{D}$ is of dimension $(N_{dof} \times N_{mom}) \times (N_{dof} \times N_{dir})$; $\underline{M}$ is of dimension $(N_{dof} \times N_{dir}) \times (N_{dof} \times N_{mom})$. Specifically, we have employed the following (element wise) mapping[1,4].

$$\boldsymbol{\phi} = D\boldsymbol{\psi} \tag{5}$$

$$\Sigma\boldsymbol{\phi} = \Sigma D\boldsymbol{\psi} \tag{6}$$

$$\boldsymbol{Q} = M\Sigma D\boldsymbol{\psi} \tag{7}$$

$\boldsymbol{\Sigma}$ is diagonal and contains the scattering cross sections developed on Legendre polynomials. In our test cases, where a delta function scattering cross section[5] is employed, we have:

$$\sigma_{s\ell} = \frac{\alpha}{(1-\mu_s)} P_\ell(\mu_s) \tag{8}$$

where:

$\alpha =$ restricted momentum transfer
$\mu_s =$ scattering cosine

Xuthus generates the matrices M and D according to the quadrature type and order. The generation of these matrices for the three relevant quadrature sets is discussed next.

3. DEFINITION OF THE QUADRATURES

Typical quadrature sets generally fall into two classes, triangular sets, of which level-symmetric are a subset, and product sets. Triangular sets have $N/2$ polar levels per quadrant and i azimuthal angles per quadrant on level i, where the level index is numbered from 1 nearest to the pole to $N/2$ nearest the equator. Product quadrature sets analyzed here have $N/2$ polar levels per quadrant, and have $N/2$ azimuthal angles per level in each quadrant.

3.1. Level-Symmetric Quadrature

Level symmetric quadratures are triangular sets that are rotation invariant with respect to all three axes. Once a given value of N has been selected, the choice of one cosine direction fully determines the Level-Symmetric quadrature[3]. The elements of the discrete-to-moment matrix D are given by:

$$D_{k,d} = w_d Y_{\ell,m}^{c/s}(\mathbf{\Omega}_\mathrm{d}) \tag{9}$$

for $1 \le d \le N_{dir}$, $0 \le \ell \le N_a, -\ell \le m \le \ell$. The index k is determined by a (ℓ, m) pair. For 2D Cartesian geometries, the symmetry of the angular flux with respect to the *xy* plane also imposes $\ell + m$ to be even. Finally, $Y_{\ell,m}^{c/s}(\Omega_\mathrm{d})$ represents the real cosine (c) or sin (s) spherical harmonic function evaluated for direction $\mathbf{\Omega}_\mathrm{d}$. The elements of the moment-to- discrete matrix M are given by:

$$M_{d,k} = \frac{2\ell + 1}{4\pi} Y_{\ell,m}^{c/s}(\mathbf{\Omega}_\mathrm{d}). \tag{10}$$

3.2. Galerkin Quadratures

Morel showed that by imposing that the discrete scattering source from the interpolatory representation provide the same angular moments as the scattering source computed with the interpolatory representation, the discrete-to-moment matrix (D) and the moment-to-discrete matrix (M) are defined such that D is the exact inverse of M [5]:

$$D = M^{-1} \tag{11}$$

M is defined as in Eq. (10) and Eq. (11) gives D. For Eq. (11) to hold, we require M to be square and invertible. This means that the number of angular flux moments must be the same as the number of discrete directions. Now, instead of calculating the matrix D using the direction weights, we simply calculate *M* and invert it. The spherical harmonics used to generate *M* must be carefully chosen and a typical rule is that the same number of even and odd spherical harmonics $Y_{\ell,m}^{c/s}$ are used, creating the moment basis starting from $\ell = 0$. In 2D *xy* geometry, with the polar angle θ being oriented with respect to the *z*-axis, the requirement of even (resp. odd) parity for the angular flux is an even angular flux $\psi(\boldsymbol{r},-\boldsymbol{\Omega}) = \psi(\boldsymbol{r},\boldsymbol{\Omega})$ (resp. $\psi(\boldsymbol{r},-\boldsymbol{\Omega}) = -\psi(\boldsymbol{r},\boldsymbol{\Omega})$), requiring that the moment basis contains as many ℓ even basis as ℓ odd basis (only the ℓ index determines the parity of the spherical harmonics). In addition, we imposed that the moment basis possesses an "azimuthal symmetry" by having the same number of cosine and sin spherical harmonics. This process yields the following rules for Galerkin quadratures 2D *xy* geometry, given in Table I for the triangular Galerkin set, and in Table II for the product Galerkin set. Again, recall that the requirement for $\ell + m$ to be even is a 2D geometry constraint.

Table I. Spherical harmonics used to form moment to discrete matrix for triangular Galerkin quadrature. *N* is the quadrature order S_N.

$Y_{\ell,m}^{c}(\boldsymbol{\Omega})$		$Y_{\ell,m}^{s}(\boldsymbol{\Omega})$	
ℓ	m	ℓ	m
$[0, N-1]$	$[0,\ell]$ $\ell + m$ $even$	$[1, N]$	$[1,\ell]$ $\ell + m$ $even$

Table II. Spherical harmonics used to form moment to discrete matrix for product Galerkin quadrature. *N* is the quadrature order S_N.

$Y_{\ell,m}^{c}(\boldsymbol{\Omega})$		$Y_{\ell,m}^{s}(\boldsymbol{\Omega})$	
ℓ	m	ℓ	m
$[0,2(N-1)]$	$[0,\ell]$ $\ell + m$ $even$ $m < N$ $m > (l-N)$	$[1,2(N-1)]$	$[1,\ell]$ $\ell + m$ $even$ $m \leq N$ $m > (l-N)$

4. RESULTS

This section will detail the results of some simple test problems solved with Xuthus using level symmetric (LS), triangular Galerkin (TG), and product Galerkin (PG) quadratures. The test case selected is a two-dimensional analog of the one used previously by Morel[6]. The problem domain is a square of 10x10 cm^2 with $\sigma_a = 0.1\,cm^{-1}$ and $\alpha = 0.25\,cm^{-1}$. An incoming stream of particles is uniformly incident on the x^- face, while vacuum conditions exist on all other faces. The incident flux is quarter-range isotropic, meaning only half the possible incoming directions have a non-zero incoming flux, i.e., the incident flux exists and is constant for all $\mu = cos(\theta) \in [0,1]$ and $\varphi \in [0, \pi/2]$ (where φ is the azithumal angle in the *xy* plane). Delta function scattering is assumed for all test cases, with polar scattering cosines of μ_s = 0.90, 0.95, and 0.99. This test problem is easily solved using Monte Carlo methods in conjunction with Xuthus. The average flux and the leakages from the x^+ face and y^- face for each quadrature type and order, as well as the Monte Carlo reference solution, are shown for $\mu_s = 0.90$, 0.95, and 0.99 in Tables III, IV, and V, respectively. The run times for each case are also included to provide an idea of how much benefit results from using the Galerkin quadrature sets.

Note that the level symmetric sets do not converge (DNC) at all for $\mu_s = 0.99$, and does not converge consistently for $\mu_s = 0.95$. This is due to the fact that the spherical harmonics orthogonality conditions are violated with significant errors, leading to spectral radii in SI that are greater than unity. The poor convergence is a clear indication that level symmetric sets are not suitable for highly anisotropic scattering. The product Galerkin quadrature also does not converge well when many directions are used. This is due to the poor conditioning number of matrix M, which resulted in lower accuracy for the coefficients of D. Indeed, the condition number for matrix M grows rapidly and for $N > 10$ the limits of machine precision are reached (in double precision REAL*8); consequently, the coefficients of matrix D are imprecise, leading to a loss of orthogonality in the numerical quadrature employed for the spherical harmonics functions.

It is also interesting to note that the leakage through the y^- face does not converge as quickly as the leakage through the x^+face. It has been suggested by Morel[6] that since the solution is not smooth, the solution near the y^-face is more rapidly varying than the solution nearer the x^+face. The solution is not smooth because if the medium was non-scattering, particles would still reach the x^+face, but not the y^-face.

Finally, we compare the run time for each quadrature. It is clear that either Galerkin quadrature will give highly accurate results while shortening run time tremendously. However, the comparison between the two Galerkin quadratures is less clear. The product quadrature yields more accurate results for lower order quadratures. However, there is no noticeable benefit in terms of computer run time. In fact, the product quadrature appears to have a longer run time in all cases, due to the increased number of directions for the same value of N.

Table III. Average flux, selected leakages, and run times for $\mu_s = 0.90$. "MC" denotes Monte Carlo, "LS" denotes level symmetric, "TG" denotes triangular Galerkin, and "PG" denotes product Galerkin.

Method	Average Flux (p/sec/cm)	Leakage x^+ face (p/sec)	Leakage y^- face (p/sec)	Convergence Time (s)
MC	5.195E-02	1.936E-02	7.124E-02	
LS S4	1.296E-01	3.556E-01	2.284E-01	6.535
LS S6	5.475E-02	3.045E-02	7.792E-02	9.212
LS S8	4.200E-02	1.243E-02	5.037E-02	23.298
LS S10	4.368E-02	1.226E-02	5.448E-02	25.503
LS S12	4.625E-02	1.421E-02	5.935E-02	52.219
LS S14	4.851E-02	1.626E-02	6.242E-02	105.523
LS S16	5.486E-02	2.302E-02	7.552E-02	242.951
TG S4	4.995E-02	1.831E-02	6.650E-02	2.077
TG S6	5.085E-02	1.891E-02	6.833E-02	6.259
TG S8	5.125E-02	1.909E-02	6.937E-02	19.189
TG S10	5.147E-02	1.919E-02	6.994E-02	27.300
TG S12	5.160E-02	1.924E-02	7.035E-02	57.601
TG S14	5.169E-02	1.928E-02	7.058E-02	132.820
TG S16	5.174E-02	1.930E-02	7.077E-02	246.139
PG S4	5.064E-02	1.870E-02	6.654E-02	3.092
PG S6	5.136E-02	1.912E-02	6.922E-02	12.107
PG S8	5.163E-02	1.924E-02	7.047E-02	33.070
PG S10	5.176E-02	1.930E-02	7.077E-02	70.566
PG S12	DNC	DNC	DNC	DNC
PG S14	DNC	DNC	DNC	DNC
PG S16	DNC	DNC	DNC	DNC

Table IV. Average flux, selected leakages, and run times for $\mu_s = 0.95$. "MC" denotes Monte Carlo, "LS" denotes level symmetric, "TG" denotes triangular Galerkin, and "PG" denotes product Galerkin.

Method	Average Flux (p/sec/cm)	Leakage x^+ face (p/sec)	Leakage y^- face (p/sec)	Convergence Time (s)
MC	5.193E-02	1.927E-02	7.173E-02	
LS S4	DNC	DNC	DNC	DNC
LS S6	5.748E-01	1.551E+00	1.538E+00	120.126
LS S8	6.392E-02	5.327E-02	9.950E-02	34.444
LS S10	5.184E-02	2.504E-02	7.299E-02	60.063
LS S12	4.891E-02	1.895E-02	6.672E-02	108.761
LS S14	4.557E-02	1.450E-02	6.062E-02	181.059
LS S16	4.380E-02	1.233E-02	5.614E-02	291.52
TG S4	4.994E-02	1.826E-02	6.696E-02	3.825
TG S6	5.084E-02	1.884E-02	6.881E-02	11.012
TG S8	5.124E-02	1.902E-02	6.979E-02	25.826
TG S10	5.147E-02	1.911E-02	7.040E-02	54.111
TG S12	5.160E-02	1.917E-02	7.078E-02	103.123
TG S14	5.169E-02	1.920E-02	7.103E-02	185.25
TG S16	5.174E-02	1.922E-02	7.121E-02	312.702
PG S4	5.064E-02	1.864E-02	6.689E-02	5.9
PG S6	5.136E-02	1.905E-02	6.958E-02	21.408
PG S8	5.162E-02	1.917E-02	7.043E-02	60.394
PG S10	5.176E-02	1.923E-02	7.131E-02	146.967
PG S12	5.183E-02	1.926E-02	8.516E-02	317.414
PG S14	DNC	DNC	DNC	DNC
PG S16	DNC	DNC	DNC	DNC

Table V. Average flux, selected leakages, and run times for $\mu_s = 0.99$. "MC" denotes Monte Carlo, "LS" denotes level symmetric, "TG" denotes triangular Galerkin, and "PG" denotes product Galerkin.

Method	Average Flux (p/sec/cm)	Leakage x^+ face (p/sec)	Leakage y^- face (p/sec)	Convergence Time (s)
MC	5.192E-02	1.923E-02	7.205E-02	
LS S4	DNC	DNC	DNC	DNC
LS S6	DNC	DNC	DNC	DNC
LS S8	DNC	DNC	DNC	DNC
LS S10	DNC	DNC	DNC	DNC
LS S12	DNC	DNC	DNC	DNC
LS S14	DNC	DNC	DNC	DNC
LS S16	DNC	DNC	DNC	DNC
TG S4	4.993E-02	1.822E-02	6.732E-02	19.947
TG S6	5.083E-02	1.879E-02	6.918E-02	94.422
TG S8	5.124E-02	1.896E-02	7.012E-02	129.003
TG S10	5.147E-02	1.906E-02	7.074E-02	256.559
TG S12	5.160E-02	1.911E-02	7.112E-02	480.316
TG S14	5.168E-02	1.914E-02	7.137E-02	1205.035
TG S16	5.174E-02	1.917E-02	7.154E-02	2094.489
PG S4	5.063E-02	1.860E-02	6.717E-02	37.766
PG S6	5.136E-02	1.900E-02	6.988E-02	125.191
PG S8	5.162E-02	1.911E-02	7.059E-02	309.833
PG S10	5.175E-02	1.916E-02	6.960E-02	598.562
PG S12	5.186E-02	1.920E-02	5.651E-02	1336.93
PG S14	DNC	DNC	DNC	DNC
PG S16	DNC	DNC	DNC	DNC

5. CONCLUSIONS

The Galerkin quadrature sets can provide high levels of accuracy for problems possessing strongly forward-peaked scattering. The triangular and product Galerkin sets were presented for the 2D *xy* geometry. The product Galerkin set is an original contribution in this paper. For low-order N, this set outperforms the Triangular Galerkin set, but condition number issues caused the derivation of the D matrix to be inaccurate. This is expected since the spherical-harmonics are rotationally invariant and the product sets concentrate directions near the poles.

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