LLNL RIPS Project Proposal: Discontinuous Galerkin Methods for the 1-D Spherical Neutron Transport Equation

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Motivation. The neutron transport equation in 1-D spherical geometry can model the emission of neutrons from a localized radioactive object which is hidden inside a shielded container. The equation is an important computational component of a portable detection device for two reasons. The first is that the equation is simple enough that it can be solved on a laptop. The second is that it is able to model the essential features of the flow from a localized source. The flow in one physical regime, however, has a discontinuous first derivative. This case presents problems for traditional numerical methods, because traditional methods assume smoothness which this particular form does not have. Thus the Discontinuous Galerkin method is a logical step in the direction of solving the transport equation by discontinuous methods.

Introduction. Let Ω be a rectangular domain in the two dimensional space. We consider the following simplified model problem

$$\frac{\mu}{r^2}\frac{\partial}{\partial r}(r^2\psi) + \frac{1}{r}\frac{\partial}{\partial \mu}((1-\mu^2)\psi) + \sigma\psi = f(\psi, r, \mu) \tag{1}$$

where $(r, \psi) \in \Omega$ and $\psi(r, \mu)$ is the solution to the above linear hyperbolic partial differential equation (1). This is the conservation form of the one-dimensional spherical geometry transport equation. In its most general form, however, (1) would be an integro-differential equation where the right hand side f includes an integral over all μ, which represents the scattering term. Let $n = (n_1, n_2)$ be the unit normal vector of Ω. We define the inflow boundary Γ^- and the outflow boundary Γ^+ of $\partial\Omega$ as

$$\Gamma^- := \{(r,\mu) \in \partial\Omega \mid n_1\alpha(r,\mu) + n_2\beta(r,\mu) < 0\}, \tag{2}$$

$$\Gamma^+ := \{(r,\mu) \in \partial\Omega \mid n_1\alpha(r,\mu) + n_2\beta(r,\mu) > 0\} \tag{3}$$

where $\alpha(r,\mu) = r\mu$ and $\beta(r,\mu) = 1-\mu^2$. Then we supplement equation (1) with a boundary condition

$$\psi(r,\mu) = g(r,\mu), \quad \forall (r,\mu) \in \Gamma^-. \tag{4}$$

The above setting gives a general framework for the neutron transport application. We will consider three particular cases.

Problem A. Let $\Omega = [0,b] \times [-1,1]$ and let $0 < a < b$. We consider the following equation

$$\frac{\mu}{r^2}\frac{\partial}{\partial r}(r^2\psi) + \frac{1}{r}\frac{\partial}{\partial \mu}((1-\mu^2)\psi) = \frac{q(r)}{4\pi}, \tag{5}$$

where $q(r) = 1$ for $0 < r \leq a$ and $q(r) = 0$ for $a < r < b$. The boundary condition is $\psi(r,\mu) = 0$ for $r = b$ and $\mu < 0$.

Problem B. Let $\Omega = [0,b] \times [-1,1]$ and let $0 < a < b$. We consider the following equation

$$\frac{\mu}{r^2}\frac{\partial}{\partial r}(r^2\psi) + \frac{1}{r}\frac{\partial}{\partial \mu}((1-\mu^2)\psi) + \sigma\psi = \sigma\frac{q(r)}{4\pi}, \tag{6}$$

where $q(r) = 1$ for $0 < r \leq a$ and $q(r) = 0$ for $a < r < b$ as above. The boundary condition is $\psi(r,\mu) = 0$ for $r = b$ and $\mu < 0$. The additional function σ is defined by $\sigma = \sigma_0/a$ for $0 < r \leq a$ and $\sigma = 0$ for $a < r < b$ where $\sigma_0 = 1000$

Problem C. Let $\Omega = [a,b] \times [-1,1]$ where $0 < a < b$. We consider the following equation

$$\frac{\mu}{r^2}\frac{\partial}{\partial r}(r^2\psi) + \frac{1}{r}\frac{\partial}{\partial \mu}((1-\mu^2)\psi) = 0. \tag{7}$$

The boundary condition is $\psi(r,\mu) = 0$ for $r = b$, $\mu < 0$ and $r = a$, $\mu > 0$.

Discontinuous galerkin methods. Now, we will derive a discontinuous Galerkin formulation for equation (1). Assume Ω is a discretized domain by a family of quadrilaterals $\mathcal{T}$ such that $\Omega = \cup_{\tau\in\mathcal{T}}$. Let $\tau \in \mathcal{T}$ be a given quadrilateral. Multiplying both sides of (1) by $r^2 v$ and integrating the resulting equation on τ yields

$$\int_\tau \left\{\mu v\frac{\partial}{\partial r}(r^2\psi) + rv\frac{\partial}{\partial \mu}((1-\mu^2)\psi) + \sigma\psi r^2 v\right\} drd\mu = \int_\tau f r^2 v \, drd\mu. \tag{8}$$

Using integration by parts for the first two terms in (8),

$$\begin{aligned}
&\int_\tau \left\{\mu v\frac{\partial}{\partial r}(r^2\psi) + rv\frac{\partial}{\partial \mu}((1-\mu^2)\psi)\right\} drd\mu \\
&= -\int_\tau \left\{r^2\psi\frac{\partial}{\partial r}(\mu v) + (1-\mu^2)\psi\frac{\partial}{\partial \mu}(rv)\right\} drd\mu \\
&\quad + \int_{\partial\tau} \left\{r^2\mu\psi v n_1 + r(1-\mu^2)\psi v n_2\right\} ds.
\end{aligned}$$

Let $Q^{k,m}(\tau)$ be the space of polynomials of degree at most k in r and m in μ on τ. Define

$$\begin{aligned}
a(\psi, v) &= -\int_\tau \left\{ r^2\psi \frac{\partial}{\partial r}(\mu v) + (1-\mu^2)\psi \frac{\partial}{\partial \mu}(rv) + \sigma\psi r^2 v \right\} dr d\mu, &(9)\\
b(\psi, v) &= \int_{\partial\tau} \left\{ r^2\mu\psi v n_1 + r(1-\mu^2)\psi v n_2 \right\} ds, &(10)\\
F(v) &= \int_\tau f r^2 v \, dr d\mu. &(11)
\end{aligned}$$

The discontinuous galerkin method is: Find ψ^h such that $\psi^h|_\tau \in Q^{k,m}(\tau)$ and

$$a(\psi^h, v) + b(\hat{\psi}^h, v) = F(v), \quad (12)$$

for all v such that $v|_\tau \in Q^{k,m}(\tau)$. We remark here that we can use different polynomial degrees for the two independent variables r and μ.

Numerical flux. The above numerical scheme (12) is well-defined up to the definition of the values of ψ^h across quadrilateral interfaces. In (12), we use $\hat{\psi}^h$ to represent the value of ψ^h at the cell boundary $\partial\tau$. There are lots of ways to define this numerical flux. Consider a given cell $\tau = [r_1, r_2] \times [\mu_1, \mu_2]$. We will write $\psi^h(r,\mu) = {\psi_1}^h(r){\psi_2}^h(\mu)$ and $\hat{\psi}^h(r,\mu) = \hat{\psi_1}^h(r)\hat{\psi_2}^h(\mu)$. Then the bilinear form $b(\hat{\psi}^h, v)$ becomes

$$b(\hat{\psi}^h, v) = \int_{\partial\tau} \left\{ r^2\mu\hat{\psi_1}^h\hat{\psi_2}^h v n_1 + r(1-\mu^2)\hat{\psi_1}^h\hat{\psi_2}^h v n_2 \right\} ds.$$

As an illustration, we consider the edge $r = r_2$. Then we need to evaluate the following

$$r_2^2 \int_{\mu_1}^{\mu_2} \mu\hat{\psi_1}^h\hat{\psi_2}^h v \, d\mu. \quad (13)$$

One easy and popular choice of the numerical flux would be the upwind flux. So, in the above integral (13), the functions $\hat{\psi_1}^h$ and $\hat{\psi_2}^h$ are defined to be the upwind values on the cell interface. Here, there is a flexibility of using different fluxes for the two functions ψ_1^h and ψ_2^h. If the function ψ^h is constant in one of the two variables r and μ, we can also incorporate the WENO reconstruction technique in the computation of the numerical flux.

Outline of work planned.

(i) Familiarize the students with the equation and the numerical scheme.

(ii) Write a simple 2-D code to solve (1) using piecewise constant polynomials and no scattering term in (1). Thouroughly test, debug and tune the code. Compare against the exact solutions in Problems A, B, and C.

(iii) Raise the order of accuracy of the polynomial elements to piecewise linear. Perform grid refinement studies to verify accuracy.

(iv) Include the scattering term in (1).

(v) Thouroughly test the scheme on problems of varying complexity.

(vi) (Optional) Study the behavior of the code near the discontinuity and gauge the size of the (possible) oscillations. Add slope limiters, if necessary.

(vii) (Optional) Compare the scheme against other methods in use, including Petrov-Galerkin, simple upwind, WENO, diamond-difference, etc.

(viii) (Optional) Raise the order of accuracy to piecewise parabolic elements. Perform grid refinement studies to verify accuracy.