

QUADRILATERAL ELEMENTS AND THE SCHARFETTER-GUMMEL METHOD

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ABSTRACT

We consider necessary conditions for convergence of the Scharfetter-Gummel method, as applied to the continuity equations associated with stationary semiconductor models. A previously determined sufficient condition on the effective widths or cross-sections of the conducting paths appears also to be necessary. However, it cannot be satisfied for all choices of underlying finite elements. For quadrilateral elements, for example, this method can be consistently applied apparently only in the special case that the four vertices lie on a circle.

1. INTRODUCTION

The discretization of the two continuity equations for stationary, numerical semiconductor device models is complicated by the fact that none of the obvious choices for the dependent variable (i.e. the carrier densities, the quasi-Fermi potentials or their exponentials) can generally be resolved on an affordable mesh. This phenomenon undermines the error estimates for both classical finite difference and projection methods, and indeed the results obtained by using such methods for these equations are often disappointing.

This difficulty is commonly overcome by using a special method, introduced in the context of numerical semiconductor models by D. L. Scharfetter and H. K. Gummel [5]. They observed that if a flux density $f = -a \frac{du}{dx}$ is constant between two mesh points x_+ and x_- , and if the function $\log a(x)$ is approximated as linear in this interval ($a(\cdot)$ is assumed uniformly positive), then the flux is given by

$$f(x) = - \frac{\log(a_-/a_+)}{a_+^{-1} - a_-^{-1}} \frac{u_+ - u_-}{X_+ - X_-}, \quad X_- < X < X_+, \quad a_+ \neq a_-, \quad (1.1)$$

in which a , a_- , u_+ , u_- are the point-values of the functions a , u at X_+ , X_- , and with the continuous extension to the case $a = a_-$. In particular, the divided difference in (1.1) does not have to approximate the derivative of u .

Little additional justifications for this method is needed for one-dimensional models. In higher dimensions, however, we wish to approximate an equation of the form $\nabla \cdot (a \nabla u) = 0$ by requiring the vanishing of a weighted sum of flux values obtained from (1.1) into each interior mesh point. (Generation-recombination of mobile carriers will be ignored in the present discussion.) Geometrically, we can consider this method as an approximation of a continuous medium by a set of one-dimensional "pipes", in the spirit of an "equivalence method" in structural mechanics [1]. However, the choice of consistent weights for these pipes - their effective widths or cross-sections - is not obvious in general. Indeed, it is not obvious that a consistent choice exists. For example in two dimensions, we know how to choose the path "widths" for rectangular or triangular meshes or domains divided into rectangular and/or triangular elements. As against this, there is no consistent choice of path "widths" for the skew-rectangular mesh shown in Fig. 1.

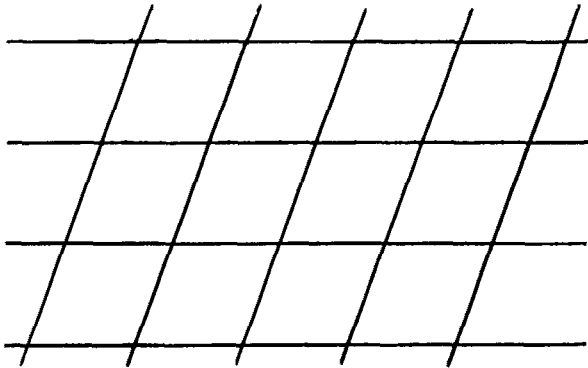


Fig. 1 Skew-rectangular mesh

To see this, it suffices to consider the special case $a = 1$, so we are trying to approximate $\Delta u = 0$. But this is impossible using a five-point difference formula on such a mesh; in the resulting Taylor expansion there are six coefficients to be controlled, those of u , u_x , u_y , u_{xx} , u_{xy} , u_{yy} , and we have only five point-values available. Approximation of $\Delta u = 0$ is certainly possible on such a mesh, but more than five points are needed in the resulting stencil.

In [2,3], sufficient conditions are obtained for the accuracy of the Scharfetter-Gummel procedure. These conditions appear to place severe restrictions on the types of mesh or elements that can be used with this procedure. Here we consider

the question of necessary conditions, in an attempt to find additional types of elements which can be used with this method. Although we find some such elements, it is questionable whether they have any practical value in terms of actual computations. Our main result is that the sufficient condition given in [3] appears to be necessary in general.

2. THE SCHARFETTER-GUMMEL METHOD IN HIGHER DIMENSIONS

As a model problem for this discussion, we consider the boundary-value problem

$$\nabla \cdot (a \nabla u) = 0, \quad x \in \Omega; \quad (2.1)$$

$$u(x) \text{ specified, } x \in \partial\Omega_D, \quad v \cdot \nabla u(x) = 0, \quad x \in \partial\Omega_N, \quad (2.2)$$

where $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ is the boundary of the region Ω , which is an open simply connected bounded set in \mathbb{R}^n . In (2.1 - 2.2), the function $a(x)$ is given, uniformly positive in Ω , v is the outward normal vector in $\partial\Omega$.

The discretization of this problem may be described as follows: the region Ω is divided into finite elements ω_i , $i = 1, \dots, N_V$. In the two dimensions, the boundary segments of these elements, assumed to be straight line segments, form a set of edges e_k , $k = 1, \dots, N_E$. In three dimensions, the edges e_k are the intersections of the faces comprising the boundary of each ω_i .

Let v_k denote a unit vector in the direction of the edge e_k , l_k the length of e_k and y_k, z_k the end points, oriented so that v_k points from y_k towards z_k . These points y_k, z_k are of course the mesh points; those mesh points in the interior of Ω or on the boundary segments $\partial\Omega_N$ will necessarily be end points of more than one edge. A simple example of such a mesh is shown in Fig. 2.

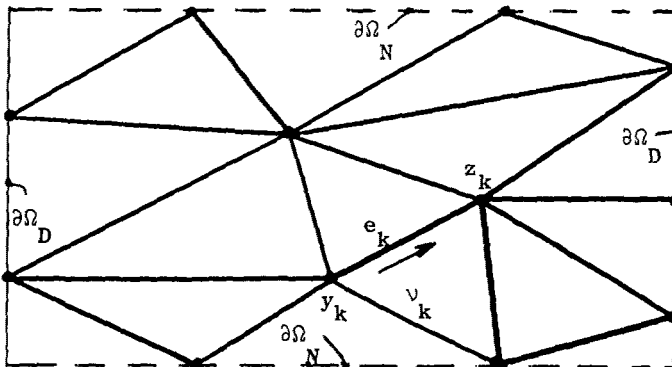


Fig. 2 Example of triangular mesh

We next denote by X a space of piecewise constant, vector-valued functions defined on the edges e_k . Thus for $g \in X$, we have

$$g|_{e_k} = g_k v_k, \quad k = 1, \dots, N_E, \quad (2.3)$$

for some constants g_k . We also define an inner product for L_2 vector-valued functions defined on the edges, by the relation

$$\langle p, q \rangle = \sum_k \sigma_k \int_{e_k} (v_k \cdot p(x)) (v_k \cdot q(x)) dx \quad (2.4)$$

In (2.4), σ_k is an effective width, in two dimensions, or cross-section, in three dimensions, assigned to the edge e_k . In general, the choice of the σ_k is not obvious, and as we shall see is an essential source of difficulty for certain choices of elements.

Let A denote the L_2 projection of vector valued functions into X , i.e.

$$\langle p, q \rangle = \langle A(p), q \rangle \text{ for all } q \in X, \text{ with } A(p) \in X. \quad (2.5)$$

As a special case of (2.5), we note that for any smooth scalar function ϕ , we have

$$A(\nabla \phi)|_{e_k} = v_k \frac{\phi(z_k) - \phi(y_k)}{l_k}. \quad (2.6)$$

With this notation, the Scharfetter-Gummel procedure in higher dimensions is readily described. We rewrite (2.1) in the form

$$f = -a \nabla u \quad (2.7)$$

$$\nabla \cdot f = 0 \quad (2.8)$$

and then write the weak form of (2.8), using the boundary condition (2.2),

$$(f, \nabla \phi) = 0 \quad (2.9)$$

for all smooth ϕ vanishing on $\partial \Omega_D$. In (2.9), (\cdot, \cdot) is the ordinary L_2 inner product on Ω .

In discrete form, we first find $F \in X$, our approximation to f , by applying (1.1) to each of the edges e_k ,

$$\begin{aligned} F|_{e_k} &= F_k v_k \quad (2.10) \\ &= -v_k \frac{\log(a(y_k)/a(z_k))}{(a(z_k))^{-1} - (a(y_k))^{-1}} \frac{u(z_k) - u(y_k)}{l_k}, \quad a(z_k) \neq a(y_k); \\ F|_{e_k} &= -v_k a(y_k) \frac{u(z_k) - u(y_k)}{l_k}, \quad a(z_k) = a(y_k). \end{aligned}$$

In (2.10), $u(\cdot)$ is a mesh function, our "approximation" to u on the mesh points, and satisfying the boundary conditions for u on $\partial\Omega_D$.

The discrete form of (2.9) is given by

$$\langle F, \nabla\phi \rangle = 0 \quad (2.11)$$

for all smooth ϕ vanishing on $\partial\Omega_D$; the discrete Scharfetter-Gummel system is obtained simply by combining (2.10) and (2.11). To see this, we first note, using (2.5) and (2.6), that the number of independent equations obtained from (2.11) is N_I , the number of interior mesh points plus the number of mesh points on the insulating boundary segments $\partial\Omega_N$. Choosing ϕ in (2.11) to be equal to unity at one such mesh point and zero at all other mesh points, the usual form of the Scharfetter-Gummel stencil is recovered.

The unknowns in the system generated by (2.10), (2.11) may be taken as the point-values of u at the interior mesh points and mesh points on $\partial\Omega_N$. There are thus also N_I unknowns, and the existence and uniqueness of the discrete solution is established in [2,3].

3. COMPATIBILITY OF INNER PRODUCTS

The replacement of the continuous inner product (\cdot, \cdot) in (2.9) by the partially discrete inner product $\langle \cdot, \cdot \rangle$ in (2.11) may be viewed as the essential additional approximation required to extend the Scharfetter-Gummel method to higher dimensions. We note that in one dimension, the two inner products coincide, so that no such additional approximation is necessary. We also note that the essential step in the convergence proof of [3] is a comparison of these two inner products.

From (2.4), it is clear that the suitability of the inner product $\langle \cdot, \cdot \rangle$ depends sensitively on the choice of the σ_k . Without loss of generality, we assume at this point that the σ_k are obtained from a relation of the form

$$\sigma_k = \frac{1}{l_k} \sum_i \alpha_{ki} V_i \quad (3.1)$$

in which V_i is the area or volume of the element ω_i , the sum is over all such elements, and the α_{ki} are dimensionless numbers as yet undetermined. We wish to interpret $\alpha_{ki} V_i / l_k$ as the contribution of the element ω_i to the cross-section σ_k . Thus we set $\alpha_{ki} = 0$ if the edge e_k is not part of the boundary of ω_i . In (3.1) and below, we adopt the convention that sums on i are over the finite elements ω_i and sums on k are over the edges e_k .

Using (2.5), (2.6), we obtain

$$\begin{aligned}
 \langle F, \nabla \phi \rangle &= \langle F, A(\nabla \phi) \rangle \\
 &= \sum_k l_k \sigma_k F_k \frac{\phi(z_k) - \phi(y_k)}{l_k} \\
 &= \sum_i V_i \sum_k \alpha_{ki} F_k \frac{\phi(z_k) - \phi(y_k)}{l_k}
 \end{aligned} \tag{3.2}$$

using (3.1). In (3.2), we introduce the average of $\nabla \phi$ over the element ω_i ,

$$\overline{\nabla \phi} \Big|_{\omega_i} = \frac{1}{V_i} \int_{\omega_i} \nabla \phi(x) dx; \tag{3.3}$$

for ϕ a smooth function, and assuming that the elements ω_i are all of diameter $O(h)$, we have immediately

$$\frac{\phi(z_k) - \phi(y_k)}{l_k} = v_k \cdot \overline{\nabla \phi} \Big|_{\omega_i} + O(h), \tag{3.4}$$

using the fact that the edge e_k is part of the boundary of ω_i (otherwise $\alpha_{ki} = 0$). We also introduce the vector valued function \bar{F} , piecewise constant in Ω , constant within each element ω_i with value given by

$$\bar{F} \Big|_{\omega_i} = \sum_k \alpha_{ki} F_k v_k. \tag{3.5}$$

Then (3.2) becomes

$$\begin{aligned}
 \langle F, \nabla \phi \rangle &= \sum_i V_i \sum_k \alpha_{ki} F_k v_k \cdot \overline{\nabla \phi} \Big|_{\omega_i} + O(h) \\
 &= \sum_i V_i \bar{F} \Big|_{\omega_i} \cdot \overline{\nabla \phi} \Big|_{\omega_i} + O(h) \\
 &= (\bar{F}, \nabla \phi) + O(h).
 \end{aligned} \tag{3.6}$$

From (3.6) and (2.11), we see that the function \bar{F} satisfies $\nabla \cdot \bar{F} = O(h)$ weakly; we thus regard \bar{F} as our approximation to the flux f . Indeed, for the α_{ki} properly chosen, it is shown in [4] that \bar{F} approximates f to $O(h)$ in L_2 .

Substituting (2.10) in (3.5), we obtain an expression for \bar{F} , namely

$$\bar{F} \Big|_{\omega_i} = -\sum_k \alpha_{ki} v_k \left(\frac{u(z_k) - u(y_k)}{l_k} \right) \begin{cases} \frac{\log(a(y_k)/a(z_k))}{a(z_k)^{-1} - a(y_k)^{-1}}, & a(y_k) \neq a(z_k) \\ a(y_k), & a(y_k) = a(z_k). \end{cases} \tag{3.7}$$

For the overall method to be consistent, we need (3.7) to be a consistent approximation of (2.7). In the present context, it suffices to consider the special case $\alpha \equiv 1$ in (3.7). In this case, it is clear that we are effectively approximating the gradient ∇u by a piecewise constant vector-valued function D , whose value in the element ω_i is given by

$$D_i = \sum_k \alpha_{ki} \nu_k \frac{u(z_k) - u(y_k)}{l_k}, \quad i = 1, \dots, N_E. \quad (3.8)$$

As the solution of (2.1), (2.2), we know that $u \in H^1(\Omega)$; however some of the divided differences in (3.7) or (3.8) may be large, of order $O(h^{-1})$. We want the function D to approximate ∇u weakly even in this case. To this end, we identify D_i with $\overline{\nabla u}|_{\omega_i}$, the average of ∇u in ω_i , defined analogously with (3.3). Then ω_i for any smooth vector-valued function θ vanishing on the boundary $\partial\Omega$, we have

$$\begin{aligned} (D, \nabla X\theta) &= \sum_i \nu_i D_i \overline{\nabla X\theta}|_{\omega_i} \\ &= \sum_i \nu_i \overline{\nabla u}|_{\omega_i} \overline{\nabla X\theta}|_{\omega_i} \\ &= \sum_i \int_{\omega_i} \nabla u \cdot \overline{\nabla X\theta} \, dx \\ &= \sum_i \int_{\omega_i} \nabla u \cdot \nabla X\theta \, dx + O(h) \\ &= O(h) \end{aligned} \quad (3.9)$$

Thus we wish to choose the α_{ki} so that

$$\overline{\nabla u}|_{\omega_i} = \sum_k \alpha_{ki} \nu_k \frac{u(z_k) - u(y_k)}{l_k}, \quad i = 1, \dots, N_E \quad (3.10)$$

for some H_1 interpolation of the point-values of u at the mesh points into a function of $X \in \Omega$. This apparently necessary condition on the α_{ki} is the same as the sufficient condition obtained in [3].

4. QUADRILATERAL ELEMENTS

Here we consider the types of elements ω_i for which the condition (3.10) can be satisfied. As in [3], we let Y denote the function space in which the interpolation of the mesh point-values of u lies. It is natural, of course, to choose Y to be a piecewise polynomial space on the elements ω_i . Thus for triangles ω_i , Y may be taken as piecewise linear; the value of $\alpha_{ki} \nu_i / l_k$, the contribution of ω_i to σ_k , is the perpendicular

distance from e_k to the centre of the circumscribed circle, measured positively in the direction of entering the triangle from e_k . For rectangles in two dimensions, we can take Y a space of bilinear functions and obtain $\alpha_{k1} = \frac{1}{2}$ for all i, k . For other quadrilaterals, however, this choice of Y is inappropriate, as in general such functions will not be continuous on the edges. An alternative suggests itself, based on the idea of compound finite elements; that is to partition a quadrilateral element ω_1 into two triangles, as shown in Fig. 3, and interpolate the given point-values of u as linear within each triangle.

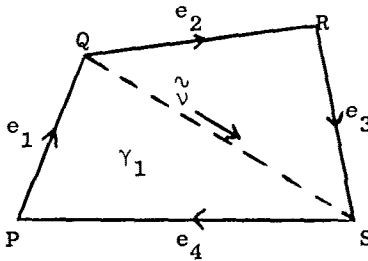


Fig. 3 Partitioning of a quadrilateral element ω_1 into triangles γ_1, γ_2 .

We number the sides of ω_1 and assign directions to the v_k as shown in Fig. 3. There are four α 's to be determined, which we call $\alpha_{1,1}$ (corresponding to edge e_1 and triangle γ_1), $\alpha_{2,2}$, $\alpha_{3,2}$ and $\alpha_{4,1}$. We can, of course, compute these by the standard method, considering each triangle γ_1, γ_2 separately. However, in so doing we will obtain two additional α 's corresponding to the created segment QS , which is part of the boundary of each of the triangles.

We have, however, the following theorem on when condition (3.10) can be satisfied for quadrilateral elements by this method.

Theorem: The following three statements are equivalent:

- (i) Condition (3.10) can be satisfied for quadrilateral elements with this choice of the space Y (i.e. u interpolated as linear within each triangle of partitioned quadrilateral).
- (ii) If the α 's are computed by the standard method (described above or in [2] or [3]) for each triangle γ_1, γ_2 separately, the "Gummel-Scharfetter width" of the created edge QS will be equal to zero, i.e.

$$\sigma_{QS} = (\alpha_{QS,1} v_1 + \alpha_{QS,2} v_2) / d(Q,S) = 0 \quad (4.1)$$

where V_1, V_2 are the areas of γ_1, γ_2 respectively and $d(Q, S)$ is the distance from Q to S .

(iii) The vertices of the quadrilateral lie on a circle.

Several comments precede the proof. We note that this argument applies to elements in two dimensions with any number of sides, not just quadrilaterals. However, the computational value of such elements for problems of this type appears extremely limited.

In the case that (4.1) is satisfied, application of the Scharfetter-Gummel procedure to the quadrilateral ω_1 results in the same discrete equations as would be obtained by application to the pair of triangles γ_1, γ_2 . Thus from [2] or [3] we see that this is a sufficient condition for convergence of the method, and not only for satisfying the condition (3.10).

One may conjecture that this theorem generalizes immediately to higher dimensions, e.g. that the Scharfetter-Gummel method can be applied to a solid element in three dimensions provided that all of its vertices lie on a sphere. We have no proof of this. It is interesting to note, however, that this condition is indeed satisfied for rectangles, triangular prisms, and tetrahedra, the three types of elements that we know can be used with this method [3].

Proof of theorem: Statements (ii) and (iii) are clearly both equivalent to the statement that the centre of the circumscribed circle of γ_1 , is the same point as the centre of the circumscribed circle for γ_2 .

In this case we first compute all the α 's by the procedure for triangles, for γ_1 and γ_2 separately. Then (3.10) holds for each of the triangles γ_1 and γ_2 , i.e.

$$\begin{aligned} \overline{\nabla u} \Big|_{\gamma_1} &= \alpha_{1,1} \left(\frac{u(Q)-u(P)}{l_1} \right) v_1 + \alpha_{QS,1} \left(\frac{u(S)-u(Q)}{d(Q,S)} \right) v \sim + \alpha_{4,1} \\ &\quad \left(\frac{u(P)-u(S)}{l_4} \right) v_4; \end{aligned} \tag{4.2}$$

$$\begin{aligned} \overline{\nabla u} \Big|_{\gamma_2} &= \alpha_{2,2} \left(\frac{u(R)-u(Q)}{l_2} \right) v_2 + \alpha_{3,2} \left(\frac{u(S)-u(R)}{l_3} \right) v_3 + \alpha_{QS,2} \\ &\quad \left(\frac{u(S)-u(Q)}{d(Q,S)} \right) v. \end{aligned} \tag{4.3}$$

Thus for the whole element, we have, using (4.1)

$$\begin{aligned} \overline{vu}|_{\omega_1} &= (V_1 \overline{vu}|_{\gamma_1} + V_2 \overline{vu}|_{\gamma_2}) / (V_1 + V_2) \\ &= \left(\frac{V_1 \alpha_{1,1}}{V_1 + V_2} \right) \left(\frac{u(Q) - u(P)}{l_1} \right) v_1 + \left(\frac{V_1 \alpha_{4,1}}{V_1 + V_2} \right) \left(\frac{u(P) - u(S)}{l_4} \right) v_4 \\ &\quad + \left(\frac{V_2 \alpha_{2,2}}{V_1 + V_2} \right) \left(\frac{u(R) - u(Q)}{l_2} \right) v_2 + \left(\frac{V_2 \alpha_{3,2}}{V_1 + V_2} \right) \left(\frac{u(S) - u(R)}{l_3} \right) v_3 \end{aligned}$$

which shows that (3.10) is satisfied, if each of the α_{kj} is replaced by the corresponding expression $\alpha_{kj} V_j / (V_1 + V_2)$, as appearing in (4.4). We note that this modification of the α_{kj} is just such that the α_{kj} , obtained from (3.1), are the same for the quadrilateral element as for the union of the two triangles.

Thus it suffices to show that (i) implies (ii); of course, this is the case of primary interest. In this case, we consider (3.10) applied to some special cases. We first consider the case $u(P) = 1, u(Q) = u(R) = u(S) = 0$. In this case $u \equiv 0$ in γ_2 , and is some linear function in γ_1 . Since $u(Q) = u(S) = 0$ here, (3.10) reduces to

$$\begin{aligned} \overline{vu}|_{\omega_1} &= \frac{V_1}{V_1 + V_2} \overline{vu}|_{\gamma_1} = \alpha_{1,1} \left(\frac{u(Q) - u(P)}{l_1} \right) v_1 + \alpha_{4,1} \left(\frac{u(P) - u(S)}{l_4} \right) v_4 \end{aligned} \tag{4.5}$$

Since (4.5) is a vector equation, it gives two independent equations (v_1 and v_4 are assumed not parallel, of course) in the two unknowns $\alpha_{1,1}$ and $\alpha_{4,1}$, which are thus uniquely determined. But we know one solution of (4.5), that is to ignore γ_2 , and to find the $\alpha_{1,1}, \alpha_{4,1}$ so that (3.10) holds on γ_1 , and finally multiplying these values by $V_1 / (V_1 + V_2)$ to compensate for the additional area of γ_2 . By uniqueness this is the solution of (4.5).

Applying the same argument to Γ_2 , i.e. with $u(P) = u(Q) = u(S) = 0, u(R) = 1$, we find that the values of $\alpha_{2,2}$ and $\alpha_{3,2}$ are those that would be obtained for the triangle γ_2 alone, multiplied by $V_2 / (V_1 + V_2)$. Thus we see that the α_{kj} corresponding to the sides of ω_1 have to be the values obtained previously, but this is still not sufficient to show that (4.1) is satisfied.

Let $\alpha_{QS,1}$ and $\alpha_{QS,2}$ be the values of α obtained by considering the triangles γ_1, γ_2 separately. We consider the case where u is linear on all of ω_1 (in this case only three of the four vertex values are independent). With the other α 's determined as above, we have in this case

$$\begin{aligned} \overline{v u} \Big|_{\omega_i} &= \alpha_{1,1} \left(\frac{u(Q)-u(P)}{l_1} \right) v_1 + \alpha_{2,2} \left(\frac{u(R)-u(Q)}{l_2} \right) v_2 + \alpha_{3,2} \\ &\quad \left(\frac{u(S)-u(R)}{l_3} \right) v_3 + \alpha_{4,1} \left(\frac{u(P)-u(S)}{l_4} \right) v_4 \end{aligned} \quad (4.6)$$

$$\begin{aligned} \overline{v u} \Big|_{\gamma_1} &= \alpha_{1,1} \left(\frac{v_1+v_2}{v_1} \right) \left(\frac{u(Q)-u(P)}{l_1} \right) v_1 + \alpha_{4,1} \left(\frac{v_1+v_2}{v_1} \right) \left(\frac{u(P)-u(S)}{l_4} \right) v_4 \\ &\quad + \alpha_{QS,1} \left(\frac{u(S)-u(Q)}{d(Q,S)} \right) \tilde{v}, \end{aligned} \quad (4.7)$$

$$\begin{aligned} \overline{v u} \Big|_{\gamma_2} &= \alpha_{2,2} \left(\frac{v_1+v_2}{v_1} \right) \left(\frac{u(R)-u(Q)}{l_2} \right) v_2 + \alpha_{3,2} \left(\frac{v_1+v_2}{v_2} \right) \left(\frac{u(S)-u(R)}{l_3} \right) v_3 \\ &\quad + \alpha_{QS,2} \left(\frac{u(S)-u(Q)}{d(Q,S)} \right) \tilde{v}, \end{aligned} \quad (4.8)$$

holding simultaneously, with $\overline{v u} \Big|_{\omega_i} = \overline{v u} \Big|_{\gamma_1} = \overline{v u} \Big|_{\gamma_2}$. Choosing u

such that $u(s) \neq u(Q)$, we note that

$$\overline{v u} \Big|_{\omega_i} = \left(\frac{v_1}{v_1+v_2} \right) \overline{v u} \Big|_{\gamma_1} + \left(\frac{v_2}{v_1+v_2} \right) \overline{v u} \Big|_{\gamma_2}; \quad (4.9)$$

substituting (4.7) and (4.8) into (4.9) and comparing with (4.6), we obtain (4.1) immediately. This completes the proof.

5. REFERENCES

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