Lawrence Berkeley National Laboratory

Recent Work

Title

A PERSPECTIVE ON NUMERICAL ANALYSIS OF THE DIFFUSION EQUATION

Permalink

<https://escholarship.org/uc/item/7zg826g5>

Author

Narasimhan, T.N.

Publication Date

1976-03-01

A PERSPECTIVE ON NUMERICAL ANALYSIS
OF THE DIFFUSION EQUATION

T. N. Narasimhan

March 1976

Prepared for the U. S. Energy Research and
Development Administration under Contract W-7405-ENG-48

For Reference

Not to be taken from this room

LBL-4482
c. 1

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

A PERSPECTIVE ON NUMERICAL ANALYSIS
OF THE DIFFUSION EQUATION*

T. N. Narasimhan
Department of Civil Engineering
and
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

ABSTRACT

The diffusion equation is encountered in many branches of science and engineering. In recent years powerful integral formulations have been developed to numerically solve the diffusion equation under complex boundary conditions. Although the customary starting point for their development is the differential equation, it is shown that these integral equations can be developed directly from the basic concepts of sets, partitions and measures. The partitioning of the flow region can be explicit or implicit and the integration of fluxes in the space domain can be achieved by evaluating surface integrals or volume integrals. As a consequence of this direct approach, the weighting function of the method of weighted residuals takes on the physical meaning of a spatial partition function. It is seen in this context that for the diffusion problem, the Galerkin weighting function is a natural choice. The integral equation developed by the direct approach is compared with the Galerkin equations developed from the classical partial differential equation. It is shown that the substitution of the spatial approximating function of the dependent variable into the time derivative term (as is done in the conventional development of the Galerkin equation from the partial differential equation), leads to conceptual difficulties. It is suggested that in so far as integral numerical formulations are concerned, the direct method is simple and complete and that the differential equation may be redundant.

---

*Work partially supported by the U. S. Energy Research and Development Administration.

INTRODUCTION

The diffusion equation describes many physical phenomena such as the conduction of heat in solids or the flow of fluids through porous media. Basically, it quantifies mass or energy conservation over parts or whole of a flow region of interest. Let H denote the amount of mass or energy. For a conveniently small part A of the flow region R we can symbolically write the diffusion equation as

$$L_s(H) = L_t(H) \quad (1)$$

where L_s is an operator in space denoting spatial redistribution of H due to differences in spatial concentrations of H and L_t is an operator in the time domain representing changes of H over A as a function of time.

In practice, it is convenient to replace the dependent variable H in (1) by a scalar potential u related to H by

$$c = \frac{1}{V} \frac{dH}{du} \quad (2)$$

where V is a volume measure over A and c is a constant. In conductive heat transfer c is specific heat, V is the mass contained in A and u is temperature. In flow through porous media, V is the volume of A and u is the fluid potential. Integrating (2) we get,

$$(H-H_0) = Vc(u-u_0) \quad (3)$$

In view of (3) we replace (1) by

$$L_s(u) = L_t(u) \quad (4)$$

We will now proceed to formulate the diffusion equation from first principles. Towards this end, we introduce some elementary concepts of set theory. For further discussion of these concepts, see [1], [2], [3, pp. 612-614].

Let R be a set. A class of subsets $\{A_k : k = 1, 2, 3, \dots, N\}$ of R is said to form a partition if (a) the A_k 's are mutually exclusive or pairwise disjoint and (b) the union of this class is R . A partition of R is schematically represented in Figure 1.

XBL761-2048

Figure 1. Schematic representation of partitioning of R .

A set function is a function whose domain is a class of sets. Let $\{A_k : k = 1, 2, \dots\}$, be a partition of R . A set function F is said to be completely additive if

$$F\left(\bigcup_{k=1}^{\infty} A_k\right) = \sum_{k=1}^{\infty} F(A_k) \quad (5)$$

A set function F is called a "measure," if F is a real-valued, non-negative and completely additive set function $F(A)$ defined on a Borel field $\mathcal{F}$ of sets and satisfies the equality $F(\emptyset) = 0$. The measure F is finite if $F(R) < \infty$. The triplet $(R, \mathcal{F}, F)$ is called a measure space. If $F(R) < \infty$, the measure space is said to be finite.

In the diffusion problem we can readily verify that H satisfies the aforementioned criteria and hence H is a measure. Furthermore, it could be shown that the subregions A_k of R form a class of Borel sets and R is a Borel field of sets. Thus, the triplet $(R, \mathcal{F}, H)$ forms a finite measure space for the diffusion equation.

The Measure $H(R)$

The diffusion problem starts with a known set of initial conditions, $u_k(t=0)$, $k = 1, 2, 3, \dots, N$ at N discrete points in R . With each discrete point k we associate a subset A_k of R so that the class $\{A_k\}$ forms a partition of R . Let N be sufficiently large so that $c_k = c(A_k)$ is constant over A_k and u_k does not vary rapidly over A_k . Then, by (3) and (5) and assuming $H_0 = 0$ at $u_0 = 0$, we get,

$$H(R) = \sum_{k=1}^N H(A_k) = \sum_{k=1}^N C_k u_k \quad (6)$$

where $C_k = V(A_k) \cdot c(A_k)$ and V is a volume measure. From (6) we see that u_k is an appropriate mean value of the scalar potential u over the set A_k . In Figure 2 R is explicitly partitioned into a class $\{A_k\}$.

However, the partition need not necessarily be explicit as in Figure 2. Instead, one could carry out an implicit partitioning as follows. First, partition R into a class $\{e_i\}$ by connecting adjacent points of the set $k = 1, 2, \dots, N$, as shown in Figure 3. Now, since each e_i is shared by points lying on its corners, we compute $H(e_i)$ by integrating H over e_i . To facilitate this, let u vary within each e_i according to,

0 0 0 0 4 4 0 6 3 4 4

-5-

XBL761-2049

Figure 2. Explicit discretization of R into partitions.

XBL761-2050

Figure 3. Partitioning of R into elements e_i .

$$u = \xi_k(x_j) u_k(t) \quad (7)$$

where ξ is a spatial function dependent on the geometry of e_i , x_j is the space coordinate system, k denotes the identification of the corner points of e_i and the repetition of the index k denotes summation over k . Moreover ξ satisfies the condition,

$$\sum_k \xi_k = 1 \quad (8)$$

at every point interior to e_i . Assuming c_{e_i} is constant over e_i we have,

$$H(e_i) = \int_{e_i} c_{e_i} \xi_k u_k dV = c_{e_i} u_k \int_{e_i} \xi_k dV \quad (9)$$

In view of (8) it is clear that $\int_{e_i} \xi_k dV$ must partition e_i into subsets whose volume measure is a fraction of V_{e_i} . Thus, if e_i is a triangle as shown shaded in Figure 3, then since ξ_k is symmetrical about each corner of the triangle, it is clear that,

$$\int_{e_i} \xi_k dV = \frac{1}{3} V_{e_i} \quad (10)$$

where V_{e_i} is the volume of e_i . Introducing (10) into (9),

$$H(e_i) = \sum_k \frac{1}{3} V_{e_i} c_{e_i} u_k = \sum_k \frac{1}{3} C_{e_i} u_k \quad (11)$$

where $C_{e_i} = V(e_i) \cdot c(e_i)$ and in which the summation is taken only over the k 's identifying the corners of e_i . Equation (11) indicates that u_k (which denotes the instantaneous potential at the point k) represents a mean value over a collection of subsets of e_i and the combined volume measure of these subsets equals $1/3 V_{e_i}$. These subsets may either be disseminated throughout e_i or may occur as a single dense subset concentrated in the immediate neighborhood of k . For simplicity we will consider these subsets to be concentrated near k . In Figure 4 G is the centroid, formed by intersecting medians and e_i is partitioned into three equal parts I, II and III, each with a volume measure of $1/3 V_{e_i}$. This indicates that u_1 , u_2 , and u_3 are mean values of the potential over the corresponding subsets I, II and III. Therefore,

XBL76I-205I

Figure 4. Sub-partitioning of triangle e_i into three equal parts.

$$H(e_i) = H(I) + H(II) + H(III) = \frac{1}{3} c_{e_i} [u_1 + u_2 + u_3] \quad (12)$$

If the integration indicated in (9) is carried out over each e_i in R and the partitioning of e_i shown in Figure 4 is implemented, the result is a new partition $\{A_k : k = 1, 2 \dots N\}$ of R as shown in Figure 5. This partition is such that (as in the case of Figure 1) interior to each A_k is located one point of the set $\{k : k = 1, 2, 3 \dots N\}$ and the potential u_k at this point represents a mean value over A_k . Thus,

$$A_k = \bigcup_{\substack{\text{all } e_i \text{ hav-} \\ \text{ing } k \text{ as a} \\ \text{corner point}}} e_{ik} \quad (13a)$$

and

$$H(A_k) = u_k \sum_{\substack{\text{all } e_i \text{ hav-} \\ \text{ing } k \text{ as a} \\ \text{corner point}}} \frac{1}{3} c_{e_i} \quad (13b)$$

Finally we have,

$$H(R) = \sum_{k=1}^N H(A_k) \quad (14)$$

The Diffusion Problem

In addition to initial conditions at $t = 0$, R is also subject to boundary conditions. These cause H to get continuously redistributed within R . Transfer of H between neighboring members of the class $\{A_k\}$ takes place across their common interface. Let $\Delta H_k = \Delta H(A_k)$ denote the change in H over A_k during an interval $\Delta t = t - t_0$. Then

$$\Delta H_k = H(A_k) \Big|_{t_0 + \Delta t} - H(A_k) \Big|_{t_0} \quad (15)$$

The consequent change $\Delta u_k = \Delta u(A_k)$ during Δt is given by,

$$\Delta u_k = \frac{\Delta H_k}{c_k} \quad (16)$$

XBL76I-2052

Figure 5. Implicit partitioning of R .

where $C_k = V(A_k) \cdot c(A_k)$ in the case of an explicit partition and $C_k = \sum_{e_i} \frac{1}{3} V(e_i) \cdot c(e_i)$, in the case of an implicit partition. The problem of diffusion, then, is to compute ΔH_k and Δu_k over each A_k of R , for a chosen $\Delta t = t - t_0$.

Since u_k is a mean value over A_k and since transfer of H between adjoining A_k 's can take place only across their common interface, the strategy for setting up the diffusion equation is obvious, viz., first compute ΔH_k over A_k by algebraically summing up the fluxes across the boundary Γ_k of A_k and then compute Δu_k by (16). Thus,

$$\Delta H_k = - \Delta t \sum_m \vec{q}_{m,k} \cdot \vec{n} \Gamma_{m,k} \quad (17)$$

where $(\vec{q}_{m,k} \cdot \vec{n})$ is the specific flux along the normal to the interface $\Gamma_{m,k}$ directed away from k and m identifies a set A_m which immediately adjoins the set A_k .

In view of (17) and (16) we have,

$$C_k \frac{\Delta u_k}{\Delta t} = - \sum_m \vec{q}_{m,k} \cdot \vec{n} \Gamma_{m,k} \quad (18)$$

Or, replacing Δ by ∂ and Σ by $\int$ we can write

$$C_k \frac{\partial(u_k)}{\partial t} = - \int_{\Gamma_{A_k}} \vec{q} \cdot \vec{n} d\Gamma \quad (19)$$

On the left hand side of (19) u_k is enclosed in parenthesis to indicate that it is a mean value over A_k .

For convenience, we may define a volume normalized term "divergence*" by

$$\text{div}^* \vec{q}_k = \frac{1}{V_k} \int_{\Gamma_{A_k}} \vec{q} \cdot \vec{n} d\Gamma \quad (20)$$

so that (19) becomes,

$$c_k \frac{\partial(u_k)}{\partial t} = - V_k \operatorname{div}^* \vec{q}_k \quad (21a)$$

Or, factoring out V_k from both sides,

$$c_k \frac{\partial(u_k)}{\partial t} = - \operatorname{div}^* \vec{q}_k \quad (21b)$$

The asterisk in div^* denotes that div^* is a macroscopic concept while by convention, divergence refers to an infinitesimal volume element. Note that (21b) is of the form used in conventional finite difference schemes.

However, it is easy to see that if the cardinal number N of the set $\{k : k = 1, 2, 3, \dots, N\}$, becomes arbitrarily large, the volume measure V_k of the set $A_k \rightarrow 0$ and hence $\operatorname{div}^* \vec{q}$ indeed tends $\operatorname{div} \vec{q}$. For arbitrarily large N and for constant $c_k = c$ throughout R we can replace (21b) by

$$c \frac{\partial u_k}{\partial t} = - \operatorname{div} \vec{q}_k \quad (22)$$

Equation (22) is the differential form of the diffusion equation as it is commonly written. The subscript k is included in (22) to emphasize the fact that the time derivative pertains to u_k which is a mean value over A_k and the divergence relates to the surface integral over the surface bounding A_k . Note that in the above discussions, we have assumed that set A_k over which the conservation Equations 19 through 21b are defined, is a dense set forming the immediate neighborhood of the point k . In exactly the same manner, the differential volume element, based on which the partial differential equation of diffusion is commonly derived, is also a dense set concentrated around a point. In the light of these, we can state that the coarse or macroscopic equation defined by (21b) converges to the differential equation (22) as the cardinal number N of the set $\{k : k = 1, 2, 3, \dots, N\}$ is made arbitrarily large.

As an alternative to (19), we can make use of the divergence theorem and write,

$$c_k \frac{\partial(u_k)}{\partial t} = - \int_{A_k} \operatorname{div} \vec{q} \, dV \quad (23)$$

We now see that (19), (21b) and (23) are different expressions for the same physical concept. Each of these equations require that in order to compute $\partial u_k / \partial t$, we define a priori an exclusive subset A_k of R associated with the point k . Such indeed is the basis of the differential equation in (22), the Finite Difference Method (FDM) or the integrated form of the finite difference method [4].

Let us now turn our attention to the implicit partitioning suggested in Figure 5. In Figure 6, the dotted lines define the sets e_i which meet at the point k . The set $A_k (= \bigcup e_{ik})$ is shown enclosed by the heavy line. $e_{ik} \subset e_i$. It is obvious from Figure 6 that $A_k \subset (\bigcup e_i)$ and $V(A_k) = V_k < V(\bigcup e_i)$. Now, note from (23) that the volume integral is to be evaluated over the set A_k . However, since A_k is only defined implicitly, we could choose an alternate, "weighted" method of integration to evaluate the volume integral in (23). Thus, we could integrate $\text{div } \vec{q}$ over the entire $(\bigcup e_i)$ but "weigh" the integrand by an appropriate partition function so that the integrated quantity is distributed without residue among the corner points of the e_i 's. Thus,

$$-\int_{A_k} \text{div } \vec{q} \, dV = - \sum_{e_i} \int_{e_i} w_k [\text{div } \vec{q}] \, dV \quad (24)$$

where w_k is the weight associated with the point k . Inserting (24) into (23) and setting, $C_k = \sum_{e_i} V(e_{ik}) c_{e_i} = \sum_{e_i} c_{e_i} \int_{e_i} w_k \, dV$, we have,

$$\sum_{e_i} \int_{e_i} w_k [\text{div } \vec{q} + c \frac{\partial(u_k)}{\partial t}] \, dV = 0 \quad (25)$$

Equation (25) corresponds to a general form of the Method of Weighted Residuals [5].

We now have to search for a proper weighting function, w_k . w_k is defined on the set e_i over which (7) holds. Also, in accordance with (24) w_k must be a partition function, satisfying $\sum w_k = 1$ within e_i . Moreover, it must also satisfy the condition, $V(e_{ik}) = \frac{1}{3} V_{e_i} = \int_{e_i} w_k \, dV$.

XBL761-2053

Figure 6. Relationship between set A_k and subsets e_{ik} .

In addition, w_k must also possess a symmetry property that as long as there are no points lying on the side of the polygon, (e.g., a triangle or a quadrilateral), w_k must be symmetrical with respect to each of the corner points and hence, the integral of w_k over e_i should result in an equal partition of V_e about each corner point k .

Remembering that the partition $\{A_k\}$ of Figure 5 was implicitly defined by the introduction of the function ξ over e , and examining (7) and (10) we immediately find that the function ξ_k exactly fits the requirements of w_k that we are looking for. Letting $\xi_k = w_k$, (25) becomes

$$\sum_{e_i} \int_{e_i} \xi_k \left[\text{div } \vec{q} + c \frac{\partial(u_k)}{\partial t} \right] dV = 0 \quad (26)$$

Equation (26) is a "Galerkin" form used in developing the well known Finite Element Equations. This form has been used by [6], [7] for solving the non-linear, unsaturated groundwater flow equation. This form also corresponds to the physical development of the FEM by Wilson [8]. As will be seen in the next section, the treatment of the time derivative in (26) is somewhat different from the conventional development of the FEM equations by the Galerkin approach (GFEM).

The Galerkin weighting function ξ_k was so chosen that the partitioning achieved by it coincides with the partitioning implied in the evaluation of $H(R)$ (Figure 5). In addition, it also satisfies the symmetry condition mentioned above. Finally, it has non-zero values throughout e_i , except possibly on its boundary. Intuitively it appears that the aforesaid criteria are sufficiently stringent so that ξ_k is a unique weighting function for the type of physical problem that we are considering. It is conceivable, however, that in other physical situations (as for example, steady state heat conduction) other weighting functions may work equally well. Thus, in the case of steady flow problems $\Delta H_k = 0$, $\Delta u_k = 0$, for every subset A_k of R . Hence, for solving this type of problem one need not necessarily associate an exclusive set with each point k . One simply needs to define some subregion around k over which the equation of motion can be accurately defined. Overlapping of such subregions of adjoining points have no effect

on the solution process. Hence, in this case we do not require the artifice of a weighting function and we can simply set $w_k = 1$ over e and write

$$\sum_{e_i} \int_{e_i} \text{div } \vec{q} \, dV = 0 \quad (27)$$

Equation (27) may be called a subdomain scheme. Nevertheless, the Galerkin procedure is still followed for solving steady flow problems by the FEM because the appearance of an added weighting function leads to a convenient scheme for evaluating volume integrals.

For the numerical solution of the diffusion problem, then, we can use any one of the four equations, (19), (21b), (22) or (26), suitably partition R and solve the appropriate equation, making use of the equation of motion. The equation of motion generally used is the Darcy's law,

$$\vec{q} = -K \text{grad } u \quad (28)$$

The gradient term on the right hand side represents an average value over Δt or part of it and it can be evaluated from the known initial distribution of u over R (explicit scheme) or on the basis of the distribution of u at some average instant during the interval Δt (implicit scheme). Depending on which procedure is used one would need to satisfy appropriate criteria for stability and convergence, on which literature is extensive.

DEVELOPMENT FROM THE DIFFERENTIAL EQUATION

In the preceding section we directly formulated the integral form of the diffusion equation starting with the elementary concepts of sets, partitions and measures. However, the conventional starting point for the development of the governing equation for numerical methods is the partial differential equation (also called the continuity equation),

$$-\text{div } \vec{q} = \nabla \cdot K \nabla u = c \frac{\partial u}{\partial t} \quad (29)$$

In order to develop the Galerkin Finite Element Equations (GFEM) from (29), one uses the mathematical approach of the weighting function and uses the Method of Weighted Residuals (MWR). In order to do this, u is replaced in (29) by $u \approx \xi_k(x_i)u_k(t)$ over e_i and $\xi_k = 0$ over the complement $\bar{e}_i$ of e_i ($\bar{e}_i \cup e_i = R$). Equation (29) is then weighted and integrated over R and the resulting set of equations solved. To obtain the GFEM equations, the weighting function is taken to be ξ itself. The logic of the Galerkin approach is that depending on how closely $\xi_k u_k$ approximates u , the weighted integral solution should yield an approximate solution for the diffusion problem. Thus,

$$\sum_{e_i} \int_{e_i} \xi_k [\nabla \cdot K \nabla \xi_m u_m - c \frac{\partial \xi_m u_m}{\partial t}] dV = 0 \quad (30)$$

Noting that $-\text{div } \vec{q} = \nabla \cdot K \nabla \xi_m u_m$, a comparison of (30) and (26) shows that the first term within the brackets is the same in both these equations and denotes the rate of accumulation of H in a set A_k associated with the point k . As suggested in Figure 5, A_k is a dense set in the neighborhood of the point k and u_k is a mean value of u over A_k . Because of these properties, if we make the cardinal number of the set $\{k : k = 1, 2, \dots, N\}$ arbitrarily large, the volume of A_k becomes arbitrarily small and A_k tends in the limit to the differential volume element which is the basis of the partial differential equation.

The two equations (30) and (26), however, differ in the manner of treating the term involving the time derivative of u . Thus, in (30), the approximating function $u \approx \xi_m u_m$ is substituted into the time derivative, and $\partial u / \partial t$ is set equal to $\partial \xi_m u_m / \partial t$. On the other hand, the direct integral formulation outlined in the first part of this paper leads to (26) in which one sets $\partial u / \partial t = \partial u_k / \partial t$ where $\partial u_k / \partial t$ is mean time rate of change of u over A_k .

We now examine the consequence of letting $\partial u / \partial t = \partial \xi_m u_m / \partial t$ in (30). As mentioned in the last paragraph, the first integrand in (30) and (26) represent the rate of accumulation of H within A_k associated with the point k . Hence,

$$\frac{\partial H(A_k)}{\partial t} = \sum_{e_i} \int_{e_i} c \xi_k \xi_m \frac{\partial u_m}{\partial t} dV \quad (31)$$

since ξ_m is independent of time. The integral on the right hand side of (31) can be evaluated according to [9] or [10] and we get,

$$\frac{\Delta H(A_k)}{\Delta t} = \frac{1}{\Delta t} \sum_{\substack{\text{all } e_i \text{ with} \\ k \text{ as a corner} \\ \text{point}}} \left\{ c \frac{Ve_i}{6} \Delta u_k + c \frac{Ve_i}{12} (\Delta u_{m_{1,i}} + \Delta u_{m_{2,i}}) \right\} \quad (32)$$

where Ve_i the volume measure of e_i and $m_{1,i}, m_{2,i}$ denote the two corner points of e_i other than k . Factoring out Δt on both sides, we can interpret (32) as follows. Figure 7A depicts a set e_i with k as a corner point. G is the centroid of e_i and the subset e_{ik} of e_i , shown by heavy lines, has a volume measure of $1/3 Ve_i$. As indicated in Figure 4, $e_{ik} \subset A_k$. Looking at Figure 7A and (32), we see that $\Delta H(A_k)$ is distributed over the set A_k in such a fashion that the distribution causes a mean change in potential equal to Δu_k over a volume of $Ve_i/6$ or one-half of the volume of e_{ik} . Over the remaining two quarters of e_{ik} , the afore-said distribution of $\Delta H(A_k)$ causes mean change in potential equal to $\Delta u_{m_{1,i}}$ and $\Delta u_{m_{2,i}}$ where $m_{1,i}, m_{2,i}$ are the other two corners of e_i besides k . If instead of (30), we use (26), then,

$$\frac{\partial H(A_k)}{\partial t} = \sum_{e_i} \int_{e_i} c \xi_k \frac{\partial u_k}{\partial t} dV = \sum_{e_i} c \frac{\partial u_k}{\partial t} \int_{e_i} \xi_k dV \quad (33)$$

In the light of (10) we then have,

$$\frac{\Delta H(A_k)}{\Delta t} = \frac{\Delta u_k}{\Delta t} \sum_{\substack{\text{all } e_i \text{ having} \\ k \text{ as a corner}}} c \frac{Ve_i}{3} \quad (34)$$

XBL761-2047

Figure 7. Distribution of ΔH_k within e_{ik} ,
 (a) weighted distribution, (b) uniform distribution.

As shown in Figure 7B, this would mean that $\Delta H(A_k)$ is uniformly distributed over A_k so as to cause a mean change of Δu_k over entire A_k .

Now we can compute $H(A_k)$ at $t_0 + \Delta t$ by the simple relation,
 $H(A_k)|_{t_0 + \Delta t} = H(A_k)|_{t_0} + \Delta H(A_k)$. Thus, equations 30 and 32 lead to

$$H(A_k)|_{t_0 + \Delta t} = H(A_k)|_{t_0} + \sum_{\substack{\text{all } e_i \text{ having} \\ k \text{ as a corner point}}} \left\{ c \frac{Ve_i}{6} \Delta u_k + \frac{Ve_i}{12} (\Delta u_{m_{1,i}} + \Delta u_{m_{2,i}}) \right\} \quad (35)$$

On the other hand, equations 26 and 34 lead to,

$$H(A_k)|_{t_0 + \Delta t} = H(A_k)|_{t_0} + \Delta u_k \sum_{\substack{\text{all } e_i \text{ having} \\ k \text{ as a corner point}}} c \frac{Ve_i}{3} \quad (36)$$

We can also independently compute $H(A_k)|_{t_0 + \Delta t}$ with the help of the new $u_k|_{t_0 + \Delta t} = u_k|_{t_0} + \Delta u_k$ that has been calculated.
 Thus, in the light of Figures 4 and 5,

$$\begin{aligned} H(A_k)|_{t_0 + \Delta t} &= (u_k|_{t_0} + \Delta u_k) \sum_{\substack{\text{all } e_i \text{ having} \\ k \text{ as a corner point}}} c \frac{Ve_i}{3} \\ &= H(A_k)|_{t_0} + \Delta u_k \sum_{\substack{\text{all } e_i \text{ having} \\ k \text{ as a corner point}}} c \frac{Ve_i}{3} \end{aligned} \quad (37)$$

Since (36) and (37) are identical, we conclude that equation 26, which leads (36), consistently assures mass or energy balance in the set A_k associated with the point k . However, we see that (35) differs from (37).

This difference indicates that equation 30, which leads to (35) will be consistent with the independent mass or energy balance check implied by (37) only if we satisfy the following relation:

$$\sum_{\text{all } e_i \text{ with } k \text{ as a corner point}} \left\{ c \frac{Ve_i}{6} \Delta u_k + c \frac{Ve_i}{12} (\Delta u_{m_1} + \Delta u_{m_2}) \right\} = \Delta u_k \sum_{\text{all } e_i \text{ with } k \text{ as a corner point}} c \frac{Ve_i}{3} \quad (38a)$$

or

$$\sum_{\text{all } e_i \text{ with } k \text{ as a corner point}} c \frac{Ve_i}{6} \left(\frac{\Delta u_{m_1} + \Delta u_{m_2}}{2} \right) = \Delta u_k \sum_{\text{all } e_i \text{ with } k \text{ as a corner point}} c \frac{Ve_i}{6} \quad (38b)$$

From (38b) we note that in order that the equality may be satisfied, Δu_k must be an appropriate mean value of the Δu 's at all neighboring points to which k is connected. If Δu_k differs appreciably from such a mean value, (35) will differ appreciably from (37) and the procedure adopted in (32) to compute Δu_k will not be consistent with the mass or energy balance check over the set A_k as implied by (37). We have seen that if we make set A_k arbitrarily small (by arbitrarily increasing the total number of discrete points k), then the set A_k tends to the differential volume element. Now, in as much as the differential equation is an expression of mass or energy balance around of a point of interest, inconsistency in assuring mass or energy balance over the set A_k indicates inconsistency with the mass or energy balance implied by the differential equation. Therefore, we conclude that (30), which leads to (32) and (35) cannot converge, in the limit, to the differential equation of diffusion in the sense of assuring mass or energy balance in the neighborhood of a point of interest. In this respect, equation 30 is not an appropriate representation of the diffusion equation.

On the other hand we have seen that (26) which leads to (36) consistently assures mass or energy balance over the set A_k associated with the point k . By making the set A_k arbitrarily small, therefore, we can

conclude that (26) converges to the differential equation of diffusion in the sense of assuring mass or energy balance in the neighborhood of a point of interest. Hence, in this respect, equation 26 is indeed an appropriate representation of the diffusion equation. It has been shown in [11] that equation 26 converges locally to the solution of the differential equation. However, for the reasons outlined above, it is doubtful if (30) will be amenable to proof of local convergence except under some very special conditions.

Let us now digress a little and shift our attention from the consideration of mass or energy balance in the set A_k to that in the set e_i . Figure 8 depicts a set e_i with corner points designated as 1, 2 and 3. Now, as a consequence of (35),

$$\begin{aligned}
 H(e_i)|_{t_0+\Delta t} &= H(e_i)|_{t_0} + \sum_{k=1}^3 \Delta H(e_{ik}) \\
 &= H(e_i)|_{t_0} + c V e_i \begin{bmatrix} \frac{\Delta u_1}{6} + \frac{\Delta u_2}{12} + \frac{\Delta u_3}{12} \\ + \frac{\Delta u_1}{12} + \frac{\Delta u_2}{6} + \frac{\Delta u_3}{12} \\ + \frac{\Delta u_1}{12} + \frac{\Delta u_2}{12} + \frac{\Delta u_3}{6} \end{bmatrix} \\
 &= H(e_i)|_{t_0} + c \frac{V e_i}{3} [\Delta u_1 + \Delta u_2 + \Delta u_3] \quad (39)
 \end{aligned}$$

Alternatively, we can also compute $H(e_i)|_{t_0+\Delta t}$ using the values of $u_k|_{t_0+\Delta t} = u_k|_{t_0} + \Delta u_k$ in the manner of (37). Thus,

$$\begin{aligned}
 H(e_i)|_{t_0+\Delta t} &= c \frac{V e_i}{3} \sum_{k=1}^3 (u_k|_{t_0} + \Delta u_k) \\
 &= H(e_i)|_{t_0} + c \frac{V e_i}{3} [\Delta u_1 + \Delta u_2 + \Delta u_3] \quad (40)
 \end{aligned}$$

Figure 8. Partitioning of e_i to compute $\Delta H(e_i)$.

We immediately see from (39) and (40) that the use of equations (30) and (32) assures mass or energy balance within the set e_i and hence also over R since R is the union of $\{e_i\}$.

We thus see that although (30) does not assure mass or energy balance within each A_k , it does assure such a balance within each e_i and thus over $R = \bigcup e_i$. It follows therefore that whatever inconsistency which may exist in each $e_{ik} \subset A_k$, will be suitably compensated by opposite deviations from mass or energy balance in the sets e_{im_1} and e_{im_2} , where m_1 and m_2 are the corner points of e_i other than k . In other words, although equation 30 will lead to departures from the solution of the differential equation at individual mesh points, these errors, when integrated over R would tend to compensate each other. Thus the solution obtained using (30) will, in an overall sense, represent an approximate solution to the diffusion problem. This may perhaps be the reason why the finite element equations lead to proofs of mean convergence rather than local convergence. The well known finite difference equations, which treat the time derivative as in (26), are known, on the other hand, to be amenable to proofs of local convergence.

SOME PRACTICAL CONSEQUENCES

Apart from the purely technical consideration of the appropriateness of equations 26 and 30 considered above, it is pertinent to consider certain practical consequences of these equations. Thus, equation 26 is an inherently simpler explicit equation and is easily amenable to considerations of stability. For example, the von Neumann-type of local stability analysis of (26) has been recently applied to equation (26) by [11]. Equation 26 can therefore be solved either explicitly or implicitly depending on the size of the time step critical to stability and the size of the actual time step desired to be used in the solution process. However, equation (30) is intrinsically implicit and its local stability analysis is more involved. Moreover, as seen from (32), the occurrence of the Δu 's of all the points $m_{1,i}, m_{2,i}$ adjoining the point k leads, in this type of formulation, not only to increased requirements of computer storage but also increased number of computational steps and hence larger computer time relative to equation 34 which does not contain the time derivative of the neighboring points of k . Thus, from the point of local mass or energy balance as well as from that of lesser

computer storage and improved computational efficiency, (26) appears to be a better representation of the diffusion equation than (30).

In our discussion of the diffusion equation so far we have restricted ourselves to constant coefficients. That is, both k and c in (29) are independent of time. In certain natural systems both k and c may become functions of time and equation 29 may become nonlinear. It is customary to treat such non-linear problems as quasi-linear problems by making k and c step functions of time. In practice, the quasi-linearization procedure itself may give rise to errors of mass or energy balance which may accumulate with time and it is often necessary to keep the time steps small enough so that k and c do not vary drastically from one time step to the next. It is possible that in such problems, the local errors in mass or energy balance that may be caused as a result of using (30) may accumulate with time and render the quasi-linearization procedure either invalid or very difficult to achieve. Neuman [6,7] attempted to use equation (30) to solve the highly non-linear problem of saturated-unsaturated flow of water in soils in which both the hydraulic conductivity, K and the specific moisture capacity, c are functions of the hydraulic head or fluid potential, u . He reports that for the problem he considered, he could not get the solution to converge when he substituted the approximating function $u \approx \xi_m u_m$ into the time derivative term in equation 30. He then found that by choosing to treat the time derivative as in equation 26 (and not as in equation 30), there was no difficulty in obtaining a convergent solution to the same problem. Neuman's experience probably reinforces the inference that the inconsistency in obtaining local mass or energy balance associated with (30) may be very undesirable in extending the GFEM equations to strongly non-linear problems.

CONCLUDING REMARKS

The diffusion problem, which occurs in many branches of science and engineering, is one of mass or energy conservation. Mathematically, the conservative phenomenon is implemented based on the additive property of a measure. Extensive properties such as volume, mass or energy are true measures, while intensive properties such as temperature and fluid potential are not. Based on the elementary concepts of sets, partitions and measures

it is easy to directly formulate the complete integral form of the diffusion equation. By making the partition arbitrarily fine the integral form can be made to tend to the differential equation as a limiting case. The differential equation is an invaluable necessity for obtaining analytical solutions to idealized, simple problems. However, for setting up integral equations which form the basis of approximate, numerical methods, it is far simpler and straightforward to follow the direct approach than to use the differential equation as the starting point. For developing such integral formulations, therefore, we may consider the differential equation to be redundant.

An important difference between integral and differential formulations is the constant of integration. Fundamentally, the differential equation of diffusion concerns itself only with the time dependent changes in the measure in question over the system. The differential equation, however, ignores the total measure of the system at any instant of time. The total measure of the system at a given instant is the constant of integration. As we have seen in the preceding pages, evaluation of this constant not only provides us with an added check on appropriate measure conservation, but also focuses attention on the nature of the partition of the system which governs the basic strategy of setting up and solving the diffusion equation. In many integral formulations it is customary to neglect this constant of integration and consider only the measure change over the system as a function of time. To this extent these schemes cling to the spirit of the differential equation and fail to derive the benefit of the completeness of an integral approach.

Dr. S. Raman, Faculty of Medicine, University of Ottawa, has helped greatly with a critical review of the manuscript and with in-depth discussions. Dr. Gerald Hedstrom, Lawrence Livermore Laboratory, reviewed an earlier version of the manuscript. Drs. A. L. Edwards and A. F. Winslow of the Lawrence Livermore Laboratory and Dr. S. P. Neuman of the University of Arizona provided stimulating discussions on the subject of numerically solving the diffusion equation. My thanks are due to all of them.

REFERENCES

1. S. K. Berberian, "Measure and Integration," MacMillan, New York, 1965.
2. P. E. Pfeiffer, "Concepts of Probability Theory," McGraw Hill, New York, 1965.
3. M. Fisz, "Probability Theory and Mathematical Statistics," John Wiley, New York, 1963.
4. T. N. Narasimhan and P. A. Witherspoon, An integrated finite difference method for analyzing fluid flow through porous media, Water Resources Res. (in press).
5. B. A. Finlayson, "Method of Weighted Residuals and Variational Principles," Academic Press, New York, 1972.
6. S. P. Neuman, Saturated-unsaturated seepage by finite elements, Jour. Hydr. Div., ASCE, 99 (1973), 2233-2250.
7. S. P. Neuman, Galerkin approach to saturated-unsaturated flow in porous media, chapter 10 in "Finite Elements in Fluids," Vol. 1, Taylor et al., ed., John Wiley, London, 1975 (in press).
8. E. L. Wilson, The determination of temperatures in mass concrete structures, SESM Rept. No. 68-17, Department of Civil Engineering, University of California, Berkeley, 1968.
9. C. A. Felippa, Refined finite element analysis of linear and nonlinear two-dimensional structures, SESM Rept. No. 66-22, Structural Engineering Laboratory, University of California, Berkeley, 1966.
10. S. P. Neuman and P. A. Witherspoon, Transient flow of groundwater to wells in multiple aquifer systems, Geotechnical Engineering Report, University of California, Berkeley, 1969.
11. S. P. Neuman and T. N. Narasimhan, Mixed explicit-implicit iterative finite element scheme for diffusion-type problems: I. Theory, to be published.

NOMENCLATURE

A_k	A partition or an exclusive subregion of R associated with point k
c	Specific measure capacity of a material
div^*	Divergence defined for a finite volume element
e_i	A polygonal partition of R , whose corner points are designated by the symbol k
$\bar{e}_i$	The complement of $e_i = (R - e_i)$
e_{ik}	Subpartition of e_i associated with the corner point k
H	Measure function
K	Hydraulic conductivity or permeability
k	Designation of a point
$\vec{n}$	A unit normal to a surface
$\vec{q}$	Specific flux
R	The flow region, including its boundary
t	Time
Δt	Time interval
u	Scalar potential
V	Volume of a subregion
V_k	Volume of a partition, $V(A_k)$
V_{e_i}	Volume of an element, $V(e_i)$
$V_{e_{ik}}$	Volume of a subpartition, $V(e_{ik})$
w_k	Weighting function pertaining to point k
$\Gamma_{m,k}$	Interface between sets A_m and A_k
ξ_k	Function approximating spatial variation of u over e_i ; also the weighting function in the Galerkin scheme

0 0 0 0 4 4 0 6 3 5 6

-29-

$\cup$
 $\cap$
 $\subset$
 $\in$

Union of sets

Intersection of sets

Subset of

Element of

LEGAL NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720