On the Development of Discrete Calculus Methods

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ABSTRACT

A general methodology for the solution of Partial Differential Equations (PDEs) is described in which the discretization of the calculus is exact and all approximation occurs as an interpolation problem on the material constitutive equations. The fact that the calculus is exact gives these methods the ability to capture the physics of PDE systems well. For simplicity, the construction of a cell based method applied to the unsteady heat equation on an unstructured mesh is used to illustrate the Discrete Calculus approach, although the approach can be used to construct node-, face- or edge-based methods applied to any PDE system. Numerical experiments are included to reveal the accuracy and time performance of the method.

1. INTRODUCTION

Physical systems are often described by Partial Differential Equations (PDEs). It is a common belief that discretization of PDEs require approximation. This, however, need not be true and it is possible for the discrete equation system to be exact [1]. A new approach to discretization, the Discrete Calculus Approach, is presented in this paper. It exactly discretizes the calculus in a PDE and forces all approximations (or errors) into the PDEs constitutive relations. This approach has the attractive feature that it exactly captures the underlying physical properties of the system [2,3]. Every PDE can be thought of to be composed of two parts – an exact part (the conservation laws and mathematics) and an approximate part (the constitutive relations). The key to the proposed method is to *exactly* discretize the conservation laws and mathematics and introduce numerical approximations only in the constitutive relations where physical approximations are already being made.

In order to focus on the numerical scheme rather than the intricacies of the equation being solved, this work focuses on the simple unsteady heat diffusion equation to illustrate the Discrete Calculus Approach. A 'mixed' cell-based method is derived in Section 2 and the discrete operators (div, grad, curl) generated by the Discrete Calculus approach are shown to mimic all important properties of the corresponding continuous operators. Section 3 presents several numerical tests comparing the accuracy and cost of the method against a classical Finite Volume method. The paper concludes with a discussion of the results.

2. THE MIXED METHOD

2.1 Discretization Scheme

In order to make the presentation of the Discrete Calculus method concrete, a simple equation is used that is common to many fields of engineering and science – the heat equation.

$$\frac{\partial(\rho c T)}{\partial t} = \nabla \bullet k \nabla T \tag{1}$$

In heat transfer, the temperature T is the fundamental unknown, and the material properties are k, the conductivity, and ρc, the heat capacity. However, this equation, or slight variants, finds applications in many other fields with different physical interpretations for the variables.

It is convenient to consider the heat equation in an expanded form that clearly separates the physics/mathematics from the material constitutive approximations.

$$\frac{\partial i}{\partial t} = -\nabla \bullet \mathbf{q} \qquad \text{Conservation of energy} \tag{2a}$$

$$\mathbf{g} = \nabla T \qquad \text{Definition of gradient} \tag{2b}$$

$$\mathbf{q} = -k\mathbf{g} \qquad \text{Fourier's Law} \tag{2c}$$

$$i = \rho c T \qquad \text{Perfectly Caloric Material} \tag{2d}$$

This formulation introduces two new variables, i the specific internal energy and $\boldsymbol{q}$ the heat flux. The last two (algebraic) equations are physical approximations for the material. Far more complex constitutive equations, such as a tensor conductivity, could easily be substituted. All numerical approximations will also be restricted to the constitutive equations. The first two equations, containing the physics and calculus, will be discretized exactly. The advantage of discretizing the physics and calculus exactly is that the resulting numerical methods and discrete solutions cannot violate any physical or mathematical principles.

Integrating Eq, (2a) over each cell of the domain and over the time interval gives the exact discrete equation,

$$\int_c i dV^{n+1} - \int_c i dV^{n} = -\sum_f \int_n^{n+1} dt \int_f \mathbf{q}\bullet\hat{\mathbf{n}} dA \qquad (3a)$$

There is one equation for each cell in the domain. The discrete unknowns in this equation are $I_c = \int_c i dV$ the total energy in the cell at a certain time level and $Q_f = \frac{1}{\Delta t}\int dt \int_f \mathbf{q}\bullet\hat{\mathbf{n}} dA$ the time averaged heat flux through the cells faces.

So far the method looks like a classic Finite Volume method or Discontinuous Galerkin method. The key difference in the Discrete Calculus approach lies in the discretization of Eq. (2b). In addition to discretizing (2a) exactly, it is critical that Eq. (2b), the definition of the gradient, also be discretized exactly or the advantages of exact dicretization are lost. Exact discretization of Eq. (2b) can be achieved by integrating along some line connecting the cell centers (or centroids). This gives the exact discrete equation

$$\int \mathbf{g}\bullet d\mathbf{l} = T_{c2} - T_{c1} \qquad (3b)$$

This is one equation for each face, where T_c is the value of the temperature at the cell center and $g_f = \int \mathbf{g}\bullet d\mathbf{l}$ is the average gradient along the line connecting the cell centers. Actually any path connecting the cell centers is possible, but the line joining the face centroid to the cell centroids of the two adjacent cells is considered in this work (which corresponds to the median dual mesh).

In linear algebraic terms, Eqs (3a) and (3b) may be written as

$$I_c^{n+1} - I_c^{n} = -\Delta t(DQ_f + Q_f^{BC}) \qquad (4a)$$

$$g_f^{n+1} = GT_c^{n+1} + T_f^{BC} \qquad (4b)$$

where D and G are the discrete divergence and discrete gradient operators respectively and T_f^{BC} and Q_f^{BC} are prescribed Dirichlet and Neumann boundary conditions respectively. The placement of the unknown variables is illustrated in Fig. 1.

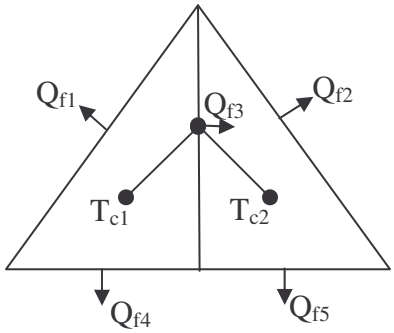

Figure 1. Placement of unknowns in the cell-based Mixed method.

2.2 Discrete Operators

The discrete divergence **D** takes information from faces and produces a result that resides on cells. The discrete gradient **G** transfers information from the cells to faces. The Discrete Calculus operators are sparse matrices whose non-zero entries are ±1. For the simple 2D mesh shown in Fig. 1, the corresponding operators are

$$\mathbf{G} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ -1 & 1 \\ -1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 & 1 \end{bmatrix} \qquad (5)$$

Note that the gradient operator **G** is a 5x2 matrix converting cell values (2 cells) into face values (5 faces). Similarly, the discrete divergence **D** converts face values into cell values. It is easy to see the symmetry between the operators (i.e.) $\mathbf{G} = -\mathbf{D}^{\mathrm{T}}$. The operators **D** and **G** are discrete versions of the continuous divergence and gradient operators. They were derived using versions of the Gauss-Green theorem and no approximation was used in their derivation. The result is that these discrete operators mimic most of the mathematical properties of the corresponding continuous operators. For example, the only solution to $\nabla\phi = 0$ on an infinite or periodic domain is ϕ is constant. Similarly, the only solution

to the discrete problem $G\phi_c = 0$ on a periodic domain is that the vector of unknowns ϕ_c is constant. In the context of heat transfer, this implies that zero heat flux results in a constant temperature solution. Similarly, $\nabla \times \nabla \phi = 0$, the gradient operator is always the null-space of the curl operator. In the Discrete Calculus approach, the sparse discrete curl operator **C** which is the (oriented) sum of edge values to face values (circulation on the face) has this same property, **CG**=0 [2].

2.3 Discrete Equation Closure

The system comprised of algebraic equations Eq. (4a) and (4b) is discrete and exact, but closure and solution of this system requires relating the heat flux at the mesh faces, Q_f, to the temperature gradient along the line connecting the cell centers, g_f. It also requires relating the temperature at the cell-centers, T_c, to the total energy in the cells, I_c. These relationships are essentially interpolation problems. Mathematically, the desired relations are written as,

$$Q_f = -M_{(kA/L)}(\alpha g_e^{n+1} + (1-\alpha) g_e^n) \quad (4c)$$

$$I_c^{n+1} = M_{(\rho cV)} T_c^{n+1} \quad (4b)$$

where $M_{(kA/L)}$ and $M_{(\rho cV)}$ are transfer matrices that connect quantities on different meshes (the primary and dual meshes) and contain information about the material properties and specific mesh geometries. The quantity α dictates the time stepping scheme ($\alpha = 1$ will result in implicit Euler, $\alpha = 0$ will result in explicit Euler, and $\alpha = \frac{1}{2}$ will result in the second order trapezoidal time stepping scheme). We will use the shorthand notation, $\overline{g}_e = \frac{1}{\Delta t}\int g_e dt = \alpha g_e^{n+1} + (1-\alpha) g_e^n$. In the discrete calculus approach the parameter α arises from the approximation of the time integral of the gradient. The time derivative itself is integrated exactly.

Note that Eqs. (4c) and (4d) directly correspond to the material constitutive equations Eqs. (2c) and (2d). These material relations cannot be implemented exactly because the unknowns are averages over different geometric structures. For a lower (second) order method, we may assume that the heat flux is constant on faces and the divergence is constant in a polygonal cell (a first order approximation for the heat flux), then the flux can be approximated by

$$\mathbf{q}_c^{n+1/2} = \tfrac{1}{V_c}\sum_f \mathbf{r}_{fc} Q_f \quad (6)$$

where $\mathbf{r}_{fc} = \mathbf{x}_f - \mathbf{x}_c$ is the position vector from the cell centroid to the face centroid, and V_c is the cell volume. Using a first order integration along the line connecting the cell centers then gives,

$$\overline{g}_e = -\left\{ \mathbf{r}_{fc1} \bullet \frac{\mathbf{q}_{c1}^{n+1/2}}{k_1} - \mathbf{r}_{fc2} \bullet \frac{\mathbf{q}_{c2}^{n+1/2}}{k_2} \right\} \quad (7)$$

In matrix terms, Eq. (7) can be written as $\overline{g}_e = -\mathbf{R}^T \tfrac{1}{V_c k} \mathbf{R} Q_f$, so $\left(M_{(kA/L)}\right)^{-1} = \mathbf{R}^T \tfrac{1}{V_c k}\mathbf{R}$ is symmetric, positive definite and sparse.

For the other transfer matrix $M_{(\rho cV)}$, we have,

$$I_c^{n+1} = \rho c V_c T_c^{n+1} \quad (8)$$

which is second order accurate since the temperature is located at the cell centroid. Combining Eqs (4),(7) and (8), we have the coupled system,

$$\begin{bmatrix} \rho c V_c & \Delta t D \\ \alpha G & \mathbf{R}^T \tfrac{1}{Vk}\mathbf{R} \end{bmatrix} \begin{Bmatrix} T_c^{n+1} \\ Q_f \end{Bmatrix} = \begin{Bmatrix} \rho c V_c T_c^n \\ (\alpha - 1) G T_c^n \end{Bmatrix} \quad (9)$$

Because the system Eq. (9) requires the simultaneous solution of both the temperature and the heat flux, it is referred to as the Mixed Method. Since α and Δt are constant this matrix system can easily be symmetrized,

$$\begin{bmatrix} \frac{\rho c V_c}{\Delta t} & D \\ -G & \mathbf{R}^T \frac{-1}{\alpha V k}\mathbf{R} \end{bmatrix} \begin{Bmatrix} T_c^{n+1} \\ Q_f \end{Bmatrix} = \begin{Bmatrix} \frac{\rho c V_c}{\Delta t} T_c^n \\ (\frac{1}{\alpha} - 1) G T_c^n \end{Bmatrix} \quad (10)$$

As far as the authors are aware, this method is completely new and represents an example of how the Discrete Calculus approach can lead to novel numerical methods that by their very construction must capture the physics of the system well.

Note that while symmetric, this equation system is indefinite (it has both positive a negative eigenvalues). Also note that, $\alpha = 0$ the explicit Euler method, is not possible with this method. This is due to the fact that the continuous equation system is parabolic, and the discrete system must be at least partially implicit to capture the infinite propagation speeds associated with parabolic systems. For steady state calculations $\frac{\rho c V}{\Delta t} \to 0$ and $\alpha \to 1$.

3. NUMERICAL RESULTS

This section compares the performance of the proposed method with a classical Finite Volume method. The metric of method performance used in

this work will be the level of accuracy obtained for a given computational cost. The following subsections first present a traditional Finite Volume method, and then tests comparing the accuracy and cost of the Finite Volume method and the Discrete Calculus method.

3.1 Classical Finite Volume Method

These methods also use the conservation equation $\frac{d(\rho c V T_c)}{dt} + DQ_f = 0$ where T_c is typically located at the cell centroid. The key in these methods is to relate the face flux Q_f to the cell temperature T_c. In order to account for strong mesh distortions, typically a flux scheme is employed that relates the heat flux and temperature as

$$Q_f = \mathbf{q}_f \bullet \mathbf{n}_f - \left(kGT_c + \mathbf{q}_f \bullet \mathbf{d} \right) \frac{\mathbf{d} \bullet \mathbf{n}_f}{\mathbf{d} \bullet \mathbf{d}} \tag{11}$$

where $\mathbf{d} = \mathbf{x}_{c2} - \mathbf{x}_{c1}$ and the face heat flux vector $\mathbf{q}_f = -\left(w_1 k_1 \nabla T_1 + w_2 k_2 \nabla T_2 \right)$ is constructed using an estimate of the temperature gradient computed as

$$\nabla T = \frac{1}{V_c} \int_c \nabla T dV = \frac{1}{V_c} \sum_f T_f \mathbf{n}_f \tag{12}$$

where the face average temperature T_f is obtained by some weighted average of the cell temperatures.

On a Cartesian mesh (or equilateral triangular mesh) the correction terms involving $\mathbf{q}_f$ cancel and only $Q_f = -kGT_c$ remains. The method then becomes identical to a Discrete Calculus method based on the Veronio dual (rather than the median dual used in section 2) [2].

3.2 Discontinuous Conductivity

The discrete calculus method derived in this paper is linearly exact, even when the material properties are discontinuous across the domain. In order to illustrate this, a test problem from Shashkov [4] and Morel et. al. [5] is considered in this section. Although the theory for discontinuous coefficients only implies that the normal component of heat flux should be continuous, many numerical methods (such as the finite volume method described above) also assume that tangential flux components are continuous at a discontinuity. Such methods will have difficulties when solving for conduction that occurs at an angle to the discontinuity.

The mesh (shown in Fig. 2) is divided into two different materials with different diffusivities along the interface x=0.5. Note that the discontinuity in the material is captured by the mesh.

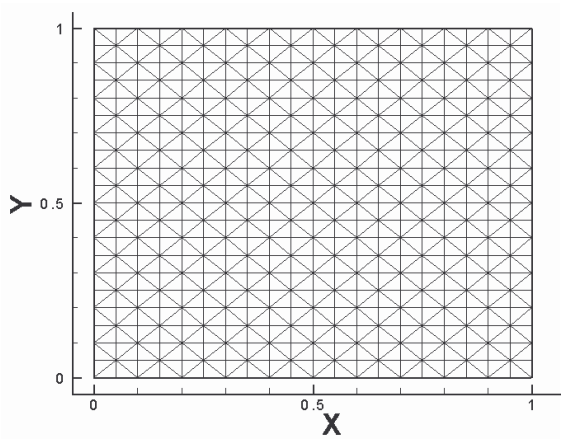

Figure 2. Mesh with different diffusivities

The diffusion coefficients are defined by,

$$k = \begin{cases} k_1 & 0 < x < 0.5 \\ k_2 & 0.5 < x < 1 \end{cases} \tag{13}$$

Dirichlet boundary conditions are enforced such that the exact steady state solution is,

$$T = \begin{cases} a + bx + cy & 0 \le x \le 0.5 \\ a - b\frac{k_1 - k_2}{2k_2} + b\frac{k_1}{k_2} x + cy & 0.5 < x \le 1 \end{cases} \tag{14}$$

This problem has a discontinuity in the tangential flux at the material interface. The normal component of the flux (bk_1) is the same across the entire domain. However, the tangential flux component is $k_1 c$ on the left side and $k_2 c$ on the right side of the interface. The numerical experiments employ a=b=c=1, k_1=4 and k_2=1. The boundary conditions are applied to the boundaries as shown below.

$$\begin{aligned} x = 0 \qquad & T = 1 + y \\ x = 1 \qquad & T = \tfrac{7}{2} + y \\ y = 0, 0 < x < 0.5 \qquad & T = 1 + x \\ y = 1, 0 < x < 0.5 \qquad & T = 2 + x \\ y = 0, 0.5 \le x < 1 \qquad & T = 4x - 0.5 \\ y = 1, 0.5 \le x < 1 \qquad & T = 4x + 0.5 \end{aligned} \tag{15}$$

The calculated temperature isolines for this problem are shown in Fig. 3. The solution obtained by the Discrete Calculus method agrees with the exact answer to machine precision.

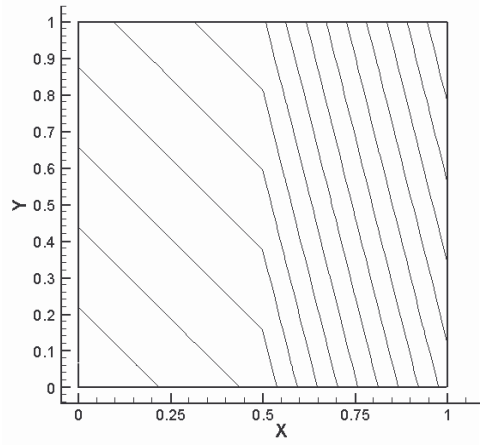

Figure 3. Isolines of temperature contours

3.3 Quadratic Problem

In this test, the accuracy of the Discrete Calculus method is compared with the Finite Volume method in a steady state heat diffusion problem ($\nabla \bullet \mathbf{q} = S$) with a constant source on a unit square domain as shown in Fig. 4.

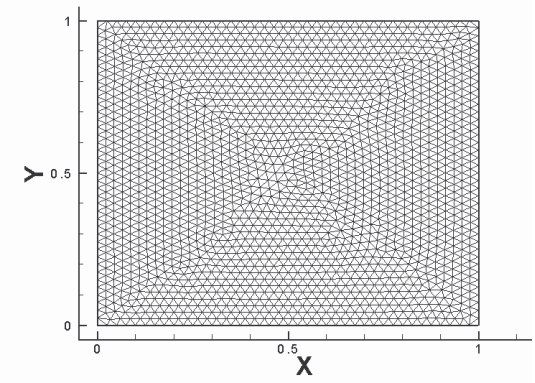

Figure 4. Typical mesh used for convergence study

Dirichlet boundary conditions are imposed on the left and right boundaries and homogeneous Neumann boundary conditions are imposed on the top and bottom boundaries. The exact solution $T(x) = 2x^2 - 2x$ is a quadratic function.

The spatial accuracy of the Mixed Method is compared against the traditional Finite Volume method in Fig. 5. The discrete L_2 norm of the temperature error at the cell centers is used as an error metric.

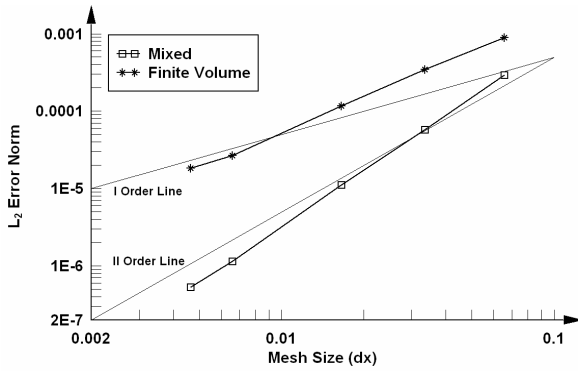

Figure 5. Accuracy of the DC and FV methods

It is seen from Fig. 5 that the Mixed method exhibits second order convergence while the Finite Volume method tends to be first order accurate with higher mesh resolution.

3.4 Computational Cost for a Desired Accuracy

Although the Discrete Calculus method was shown to be more accurate than the Finite Volume method in the previous test, it might be more important to compare the cost-effectiveness of the Discrete Calculus method against the classical method. Hence, the computational cost (in terms of the CPU time) is plotted against the L_2 error norm in Fig. 6 for the same problem considered in the previous section. This really compares the cost incurred for a desired accuracy level.

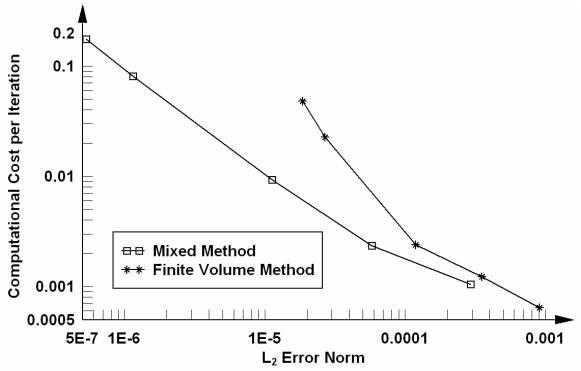

Figure 6. Cost incurred for a desired accuracy level

It is observed from Fig. 6 that for any given accuracy level, the Discrete Calculus method is always more cost-effective than the traditional FV method. Also, it is clearly seen that the cost for the corrected FV method tends to increase more rapidly than the Discrete Calculus methods as the need for accuracy increases.

3.5 Heat Transfer in a Crank Shaft

The Discrete Calculus method presented is applicable on any general 3D unstructured mesh, although the previous tests were run on 2D geometries. In order to illustrate this, a more realistic problem is considered in this section, which involves solving Eqn. (2) on a complex 3D geometry. A typical mesh considered for the analysis is shown in Fig. 7. The coarsest mesh considered has 864 nodes and 2339 cells and the finest mesh contains 73875 nodes and 360512 cells.

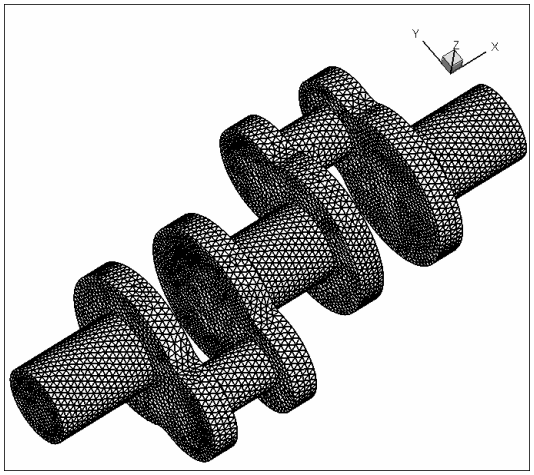

Figure 7. Crank Shaft Mesh

Fixed temperature (Dirichlet) boundary conditions are applied to the inlet and outlet faces (crankshaft ends) and the sides are insulated. Typical temperature contours are presented in Figure 8.

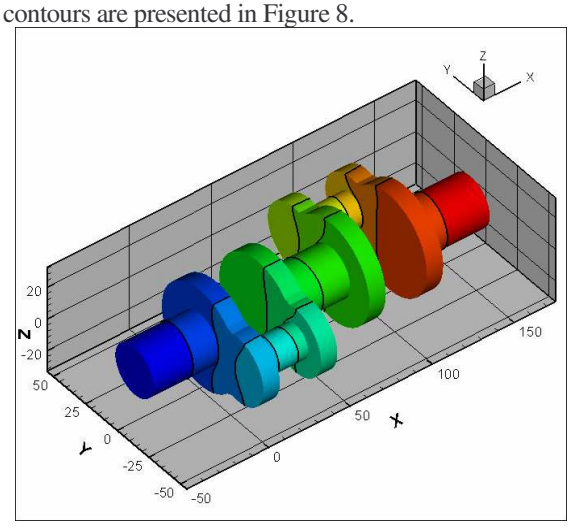

Figure 8. Temperature contours along the crank shaft

The heat flux through the inlet and outlet faces (which were verified to be equal) are measured against the mesh size for the Discrete Calculus method and extrapolated to obtain the 'exact' heat flux. This exact heat flux is then employed to compute the error in the Finite Volume and Discrete Calculus methods (Fig. 9). The mesh size (dx) is computed as the cube root of the average cell volume.

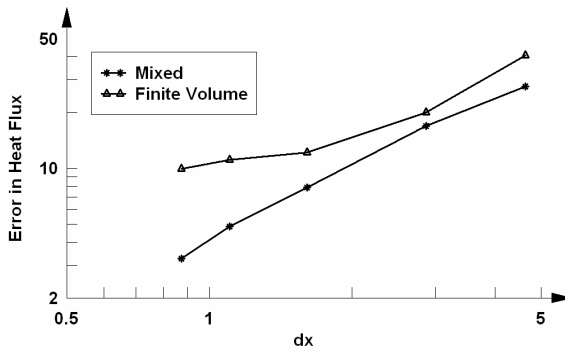

Figure 9. Accuracy of DC and FV methods

The computational time taken per solver iteration is then plotted against the percentage error, which gives the cost required to obtain a certain accuracy level (Figure 10), which is in agreement with the results of the previous section.

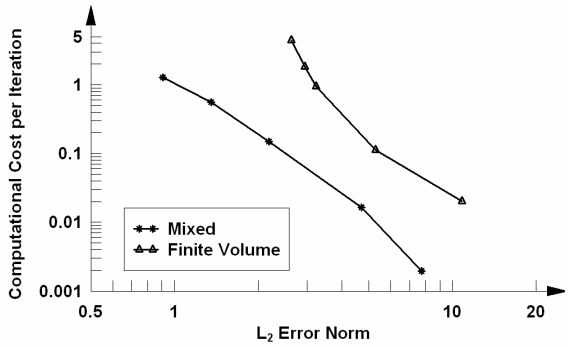

Figure 10. Cost of DC and FV methods on the Crank Shaft case

4. DISCUSSION

A new approach to discretizing Partial Differential Equation systems – the Discrete Calculus approach – is introduced that discretizes the underlying physics and mathematics of the PDEs exactly and introduces approximations only where physical approximations are also made (in the constitutive equations). An illustrative cell-based numerical method – the Mixed Method – is derived using this approach and is shown to be second order accurate on generic unstructured meshes and more cost-effective than traditional Finite Volume methods.

Although the number of unknowns is more for the Mixed method than for the classical Finite Volume

method, the memory requirements for the actual implementation for both the methods are comparable, since the correction term in the Finite Volume method also requires additional storage on mesh faces. The problem considered in Section 3.3 was used to test the memory requirements for the Mixed and the Finite Volume methods using a mesh containing 91852 cells and 138178 mesh faces, and both the methods reported an overall memory usage of 32 MB (as inferred from the Windows Task Manager).

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REFERENCES

[1] V. Subramanian and J. B. Perot. Higher-order mimetic methods for unstructured meshes. *Journal of Computational Physics*, 219:68–85, 2006.

[2] J. B. Perot, V. Subramanian, Discrete Calculus Methods for Diffusion, Journal of Computational Physics (2006), doi: 10.1016/j.jcp.2006.12.022.

[3] J. B. Perot. Conservation properties of unstructured staggered mesh schemes. *Journal of Computational Physics*, 159:59–89, 2000.

[4] M. Shashkov and S. Steinberg, Solving Diffusion Equations with Rough Coefficients in Rough Grids, J. Comput. Phys., 129, 383-405, 1996.

[5] J. M. Morel, J. E. Dendy Jr, M. L. Hall, and S. W. White, A cell-centered Lagrangian-mesh diffusion differencing scheme, J. Comput. Phys., 103, 286, 1992.