Differential Quadrature for Multi-dimensional Problems

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The technique of differential quadrature for the solution of partial differential equations, introduced by Bellman et al., is extended and generalized to encompass partial differential equations involving multiple space variables. Approximation formulae for a variety of first and second order partial derivatives and typical weighting coefficients are presented. Application of these formulae is demonstrated on the solution of the convection-diffusion equation for the two- and three-dimensional space dependent cases and for both the transient and steady-state dispersion of inert, neutrally buoyant pollutants from continuous sources into an unbounded atmosphere.

INTRODUCTION

Numerical solutions of partial differential equations are traditionally accomplished by some variant of the methods of finite difference and finite elements. These methods approximate the partial derivatives of a function at a grid point using only a limited number of function values in the vicinity of the grid point. The accuracy and stability of these methods depend on the sizes of the grid spacings.

In many practical applications the numerical solutions of the governing differential equations are required at only a few points in the physical domain. Frequently, for reasonable accuracy, conventional finite difference and finite element methods require the use of a large number of grid points. Therefore, even though solutions at only a few specified points may be desired, numerical solutions must be produced at all grid points.

In many cases the computational effort can be alleviated by using the method of differential quadrature, introduced by Bellman et al. [2–7] which approximates the partial space derivatives of a function by means of a polynomial expressed as a weighted linear sum of the function values at the grid points. Obviously, this method is subject to the limitations of the polynomial fit. As the order of the polynomial increases, the accuracy of the
representation increases up to the point where oscillations introduce undesirable behavior. However, the limitation on the number of grid points that may be used can be circumvented by standard numerical interpolation techniques for obtaining intermediate point solutions which are generally adequate.

Briefly, when the partial derivatives are replaced by the differential quadrature approximations, the partial differential equation is reduced to a set of algebraic equations for time-independent problems and a set of time-dependent ordinary differential equations for initial value problems and for initial and boundary value problems \([8-10]\). In all cases numerical solution methods for these resulting equations are well developed.

In the following, the method of differential quadrature is first generalized and then is demonstrated on the convection–diffusion type pollutant dispersion models.

## Differential Quadrature

Basically, the method of differential quadrature expresses a partial derivative of a function with respect to a coordinate direction as a weighted linear sum of all the function values at all mesh points along that direction. Thus, in general, the linear transformation for a derivative of order \(m\) can be expressed by

\[
\frac{\partial^m f(x_i)}{\partial x^m} = \sum_{j=1}^{N} w_{ij} f(x_j),
\]

where \(x_i: i = 1, 2, \ldots, N\), are the sample points obtained by breaking the \(x\)-variable into \(N\) discrete values, \(f(x_j)\) are the function values at these points, and \(w_{ij}\) are the weights attached to these function values. Note that the order of the quadrature must be greater than the order of the partial derivative; i.e., \(N > m\) in Eq. (1).

To determine the weighting coefficients \(w_{ij}\) the function \(f(x)\) is represented by an appropriate analytical function, such as a polynomial,

\[
f(x) = x^{k-1}; \quad k = 1, 2, \ldots, N
\]

and its \(m\)th derivative,

\[
\frac{\partial^m f(x)}{\partial x^m} = (k - 1)(k - 2)(k - 3) \cdots (k - m) x^{(k-m-1)}. \tag{3}
\]
Substituting Eqs. (2) and (3) into Eq. (1) $N$ linear algebraic equations are obtained

$$
\sum_{j=1}^{N} w_{ij} x_j^{k-1} = (k-1)(k-2)(k-3) \cdots (k-m) x_i^{(k-m-1)};
$$

$$
k = 1, 2, \ldots, N, \quad i = 1, 2, \ldots, N, \quad \text{and} \quad N > m. \quad (4)
$$

This set has a unique solution for the weighting coefficients $w_{ij}$ because the matrix elements $x_j^{k-1}$ compose a Vandermonde matrix whose inverse can be obtained analytically as shown by Hamming [14]. Typical weighting coefficient matrices for the first and second order derivatives are presented in Appendix I.

For multi-dimensional problems considering any pair of the independent variables, such as $x$ and $y$, the first order derivative approximation formula given by Eq. (1) can be expressed in closed form by the following linear transformations for the partial derivatives with respect to $x$ and $y$:

$$
\frac{\partial F}{\partial x} \cong A_x F, \quad (5)
$$

and

$$
\frac{\partial F}{\partial y} \cong A_y F, \quad (6)
$$

where $F = \{f(x_i, y_j, z_k, t)\}$ is the function matrix consisting of the function values at the grid points represented by $i = 1, 2, \ldots, N_x$, $j = 1, 2, \ldots, N_y$, and $k = 1, 2, \ldots, N_z$. $A_x$ or $A_y$ = $(a_{pq}^{x\text{or}y})$, where $p = q = 1, 2, \ldots, N_x \text{or} N_y$, is the weighting coefficient matrix whose elements are attached to those function values in the $x$ and $y$ directions, respectively, and $t$ is the time variable.

The approximation formulae for higher order partial derivatives are obtained by iterating the linear transformations given by Eqs. (5) and (6). Thus, for example, the second order partial derivatives are:

$$
\frac{\partial^2 F}{\partial x^2} \cong (A_x)^2 F, \quad (7)
$$

$$
\frac{\partial^2 F}{\partial x \partial y} \cong A_x A_y F, \quad (8)
$$

$$
\frac{\partial^2 F}{\partial y^2} \cong (A_y)^2 F. \quad (9)
$$

Obviously, Eqs. (7)–(9) require more computation than that of Eqs. (5) and (6). To economize on the computing effort for the evaluation of the second order partial derivatives (while, Eq. (8) remains unchanged for the cross partial derivative because differential quadrature expresses the partial derivatives in terms of the function values in one direction only) Eqs. (7) and (9) can be replaced by the following linear transformations which are extensions of a method inferred by Mingle [15]:

$$
\frac{\partial^2 F}{\partial x^2} \cong B_x F \quad (10)
$$
and
\[ \partial^2 F / \partial y^2 \approx B^y F, \]  
(11)

where \( B^{x,y} = (b_{pq}^{x,y}) \); \( p = q = 1, 2, \ldots, N^{x,y} \), is the weighting coefficient matrix. Extending this approach, third and higher order partials—in one coordinate direction only—can be approximated by linear transformations in a similar manner. For convenience, the approximation formulae for the first and second order partial derivatives, which are adequate for handling a wide variety of problems, are tabulated in Appendix II.

APPLICATIONS

In this section the application of the method of differential quadrature to two- and three-dimensional space problems, for both the transient and steady states, will be illustrated. For this purpose the dispersion of inert, neutrally buoyant pollutants by means of convection and diffusion into an unbounded atmosphere from a continuous source is considered. For simplicity a uniform wind velocity in the convection direction and constant eddy diffusivities in the coordinate directions will be assumed. Under these circumstances the pollutant concentration distributions will be symmetric. Therefore, to save on the computational effort only one half of the physical domain for the two-dimensional case and one quarter for the three-dimensional case will be considered. In all cases, the normalized forms of the governing transport equations will be used. The quality of the numerical solutions will be established by comparing these results with those obtained from their corresponding steady state, exact analytical solutions.

FIRST PROBLEM: TWO DIMENSIONAL

The first problem deals with the solution of the following two-dimensional convection-diffusion equation
\[ \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2} + \beta \frac{\partial^2 c}{\partial y^2}, \quad 0 < x, y \leq 1, \quad t > 0, \]  
(12)

subject to the initial conditions
\[ c(x, y) = 0, \quad 0 \leq x, y \leq 1, \quad t \leq 0 \]  
(13)
and the boundary conditions for $t > 0$

\[ c(0, y) = \text{prescribed from the steady-state solutions; } 0 \leq y \leq 1, \quad (14) \]
\[ c(x, y \to \infty) \to 0, \quad (15) \]
\[ \frac{\partial c(x, 0)}{\partial y} = 0, \quad (16) \]
\[ c(x \to \infty, y) \to 0. \quad (17) \]

The quantities $\alpha$ and $\beta$ appearing in Eq. (12) are given by

\[ \alpha = \frac{1}{\text{Pe}_{xx}} \quad (18) \]

and

\[ \beta = \frac{(L/W)}{\text{Pe}_{yy}}, \quad (19) \]

where $\text{Pe}_{xx}$ and $\text{Pe}_{yy}$ are the constant Peclet numbers in the $x$ and $y$ directions and are given by

\[ \text{Pe}_{xx} = \frac{UL}{K_{xx}}, \quad (20) \]

and

\[ \text{Pe}_{yy} = \frac{UW}{K_{yy}}. \quad (21) \]

$L$ and $W$ are the length and width of the actual one half of the physical domain in which the pollutant dispersion takes place, respectively. $U$ is the uniform wind velocity in the $x$ direction. $K_{xx}$ and $K_{yy}$ are the constant numbers representing the diffusivities in the $x$ and $y$ directions, respectively.

The exact analytical solution in normalized form for the steady-state case and a line source in the $z$ direction is given by

\[ c(x, y) = K_0 \left[ \left( (x + x_0)^2 + (\alpha/\beta) y^2 \right)^{1/2} / (2\alpha) \right] \exp \left[ (x + x_0) / (2\alpha) \right], \quad (22) \]

where $K_0(\cdot)$ is the modified Bessel function of the second kind of order zero and $x_0$ is the distance of the point source to the upwind boundary. Equation (22) was actually obtained by converting the solution given by Seinfeld [18] into normalized form.

The solution function for Eq. (12) can be freed of exponential terms by transforming the dependent variable $c$ into a function $\phi$,

\[ c = \phi \exp \left[ (x + x_0) / (2\alpha) \right]. \quad (23) \]

Thus, Eqs. (12)–(17) become

\[ \frac{\partial \phi}{\partial t} + \frac{\phi}{4\alpha} = \alpha \frac{\partial^2 \phi}{\partial x^2} + \beta \frac{\partial^2 \phi}{\partial y^2}, \quad (24) \]

A. Transient-State Case

The numerical model can be obtained by replacing the partial space derivatives with the corresponding differential quadrature approximation formulae, specifically using Eqs. (114a), (115b), and (116b) presented in Appendix II. Therefore, the following equations are obtained from Eqs. (24) (29):

$$\frac{d\phi_{ij}}{dt} \approx -\frac{\phi_{ij}}{4\alpha} + a \sum_{k=1}^{N_x} b_{ik}^x \phi_{kj} + \beta \sum_{k=1}^{N_y} b_{jk}^y \phi_{ik}$$

for the unknown function values; i.e., $\phi_{ij}: i = 2, 3, ..., (N_x - 1)$ and $j = 2, 3, ..., (N_y - 1)$. The initial conditions are

$$\phi_{ij} = 0 \quad \text{at} \quad t = 0, \quad i = 1, 2, ..., N_x, \quad \text{and} \quad j = 1, 2, ..., N_y.$$  

(31)

The upwind boundary function values are prescribed using the steady-state solution given by Eq. (22),

$$\phi_{ij} = \text{prescribed}, \quad j = 1, 2, ..., N_y.$$  

(32)

The side lateral boundary function values are

$$\phi_{iN_y} = 0, \quad i = 1, 2, ..., N_x.$$  

(33)

The function values on the symmetry plane passing through the centerline can be expressed in terms of the unknown interior point function values using Eq. (28) as

$$\frac{\partial \phi_{ij}}{\partial y} \approx \sum_{k=1}^{N_y} a_{jk}^y \phi_{ik} - 0 \quad \text{at} \quad j = 1$$  

(34)
or rearranging and using the side lateral function values given by Eq. (33),

\[ \phi_{il} \cong - \left( \sum_{k=2}^{(N^x-1)} a_{ik} \phi_{lk} \right) a_{il}, \quad i = 2, 3, \ldots, (N^x - 1). \]  

(35)

The downwind function values are

\[ \phi_{N^yi} = 0, \quad j = 1, 2, \ldots, N^y. \]  

(36)

Upon substitution of the values and the expressions given above for the boundaries of the computational domain the set of time-dependent ordinary differential equations represented by Eq. (30) can be solved using a well-developed numerical method, such as Runge-Kutta.

B. Steady-State Case

For a steady-state solution the time derivative term in Eq. (30) is dropped and then Eqs. (32)-(36) are substituted for the boundary function values. The resulting equation is rearranged to obtain the following set of linear algebraic equations for the unknown interior domain function values:

\[ \sum_{p=2}^{(N^x-1)} \sum_{q=2}^{(N^y-1)} \frac{\partial g_{ij}}{\partial \phi_{pq}} \phi_{pq} = h_{ij}, \]

\[ i = 2, 3, \ldots, (N^x - 1) \quad \text{and} \quad j = 2, 3, \ldots, (N^y - 1) \]  

(37)

for which the elements of the Jacobian matrix are given by

\[ \frac{\partial g_{ij}}{\partial \phi_{pq}} = - \frac{1}{4a} \delta_{ip} \delta_{jq} + \delta_{jq} ab_{jp} + \delta_{ip} \beta (b_{jq} - b_{jl}a_{ld}/a_{ll}). \]  

(38)

where \( \delta_{mn} \) are the Kroneker deltas which are equal to one when \( m = n \) and zero otherwise. The right side is

\[ h_{ij} = -ab_{il} \phi_{ij}. \]  

(39)

Once Eq. (37) is solved using Gaussian elimination [12] (or some other methods) the unknown function values on the symmetry plane \( \phi_{il} \) are calculated using Eq. (35).

Notice that the Jacobian matrix is not a full matrix since Eq. (38) contains Kroneker deltas. Therefore special methods could be utilized to take advantage of this situation. However, in the present study a direct elimination method was employed for all of the steady-state examples herein since it was readily available.
C. Numerical Results

For numerical calculations the source was located at a distance of \( x_0 = 0.001 \) from the upwind boundary along the centerline in the \( x \)-downwind direction. The system parameters assumed were: \( U = 1, K_{xx} = K_{yy} = 0.1, L = 2, \) and \( W = 0.5. \) All calculations were performed on an IBM 370/158.

The numerical solution of the time-dependent model was obtained by integrating simultaneously the set of ordinary differential equations represented by Eq. (30) with respect to time using a variable step Runge–Kutta–Fehlberg Four (Five) method \([11]\). For the initial step size, as well as for the tolerance limit of convergence and step size adjustment, a magnitude of \( 10^{-3} \) was prescribed, arbitrarily. Numerical solutions were carried out with a \( 7 \times 7 \), equally spaced grid system until the steady-state solutions were obtained. The final results are identical with the direct solution of the steady state formulation of the same problem as will be seen in the following.

The numerical solution of the time-independent model has been accomplished by solving simultaneously the set of algebraic equations represented by Eq. (37) using the Gaussian elimination routines DECOMP and SOLVE \([12]\) with double precision. Calculations with \( 5 \times 5, 7 \times 7, 9 \times 9, \) and

<table>
<thead>
<tr>
<th>TABLE I</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steady-State Solution of First Problem for One Half Domain Using ( 11 \times 11 ) Grid</td>
</tr>
</tbody>
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<tr>
<td>Longitudinal ( x )</td>
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<tr>
<td>0.3</td>
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<td>0.0959</td>
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<td>0.0103</td>
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<tr>
<td>0.4</td>
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<td>0.0850</td>
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<tr>
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11 × 11 equally spaced grid systems gave good solutions which improved as more grid points were used. Typical results are presented in Table I for 11 × 11 grid.

Calculations with 7 × 7 and 9 × 9 unequally spaced grid systems were also done using grid spacings which were increased progressively with increasing distances in both the x and y directions. However, in this case since the resulting solutions deteriorated completely, it was concluded that equally spaced grid points are essential for good quality solutions; this requirement has been experienced on other problems.

SECOND PROBLEM: TWO-DIMENSIONAL, STEADY STATE

The second problem is a convection–diffusion model which is given below in normalized form. (The same problem was solved by Pepper and Baker [17] using the method of fractional steps in which the convection (advection) is treated by the method of moments and diffusion by cubic splines.)

\[
\frac{\partial c}{\partial x} = \beta \frac{\partial^2 c}{\partial y^2}
\]  

subject to the boundary conditions

\[
c(0, y) = \text{prescribed}, \quad c(x, y \to \infty) \to 0, \quad \frac{\partial c(x, 0)}{\partial y} = 0,
\]

for which the exact analytic solution is given in terms of dimensionless quantities

\[
c(x, y) = x^{-1/2} \exp[-y^2/(4\beta x)],
\]

where \(\beta\) is defined as before and the dimensionless concentration is defined by

\[
c = 2(\pi K_{yy} UL)^{1/2} C/Q,
\]

where \(C\) is the actual concentration and \(Q\) is the source strength. Equations (44) and (45) were actually obtained by converting the exact analytic solution given by Seinfeld [18] into dimensionless form.

The numerical model equations are obtained by a procedure similar to the
first problem. The resulting set of linear algebraic equations are represented by

\[ \sum_{p=2}^{N^x} \sum_{q=2}^{(N^y-1)} \frac{\partial g_{ij}}{\partial c_{pq}} c_{pq} = h_{ij}, \]

\[ i = 2, 3, \ldots, N^x \quad \text{and} \quad j = 2, 3, \ldots, (N^y - 1), \quad (46) \]

where

\[ \frac{\partial g_{ij}}{\partial c_{pq}} = \delta_{jq} a_{ip}^x + \delta_{ip} \beta (b_j^y a_{1q}^y / a_{11}^y - b_j^y) \quad (47) \]

and

\[ h_{ij} = -a_{11}^x c_{ij}. \quad (48) \]

Equations (41)–(43) for the boundary concentrations become

\[ c_{1j} = \text{prescribed}, \quad j = 1, 2, \ldots, N^y, \quad (49) \]

\[ c_{iN^y} = 0, \quad i = 1, 2, \ldots, N^x, \quad (50) \]

\[ c_{i1} = -\left( \sum_{k=2}^{(N^y-1)} a_{1k}^y c_{ik} / a_{11}^y \right), \quad i = 2, 3, \ldots, N^x. \quad (51) \]

A Gaussian elimination method was used to obtain solutions for one half of the domain considering a continuous area source consisting of four cells each having a source strength of 250 mass units/time unit/cell, a lateral diffusivity of \( K_{y_y} = 0.1 \), and a wind velocity of \( U = 1 \). The length and the width of the computational, one half domain considered were 8 and 3, respectively. The results are shown in Table II along with the analytical and published numerical results [17].

As can be seen from Table II the results obtained by the relatively simple technique of differential quadrature are as good as the steady state results reported by Pepper and Baker who used a very sophisticated technique.

**THIRD PROBLEM: THREE DIMENSIONAL**

The third problem is to solve the following three-dimensional convection–diffusion equation

\[ \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = \beta \frac{\partial^2 c}{\partial y^2} + \gamma \frac{\partial^2 c}{\partial z^2}, \quad 0 \leq x, y, z \leq 1 \quad (52) \]
TABLE II
Steady-State Solution of Second Problem for One Half Domain

| Lateral distance | Longitudinal Distance x |  |  |  |  |  |  |  |  |  |  |
|------------------|-------------------------|---|---|---|---|---|---|---|---|---|
| y                | 0.0 | 1.0 | 2.0 | 3.0 | 4.0 | 5.0 | 6.0 | 7.0 | 8.0 | 9.0 | 10.0 |
| Analytical       |     |     |     |     |     |     |     |     |     |     |     |
| 0.5              | 125 | 366 | 444 | 388 | 356 | 331 | 311 | 294 | 280 | 267 | 256 |
| 1.5              |     | 18  | 65  | 107 | 129 | 143 | 151 | 156 | 160 | 161 | 162 |
| 2.5              |     |     |     | 14  | 24  | 34  | 43  | 51  | 58  | 64  |     |
| 3.5              |     |     |     |     |     |     |     |     |     |     | 12  |
| Numerical        |     |     |     |     |     |     |     |     |     |     |     |
| Pepper & Baker (steady-state results) | | | | | | | | | | | |
| 0.5              | 111 | 340 | 426 | 392 | 363 | 339 | 319 | 302 | 287 | 273 | 262 |
| 1.5              |     | 34  | 70  | 97  | 116 | 130 | 140 | 147 | 151 | 154 | 156 |
| 2.5              |     |     |     | 12  | 19  | 27  | 35  | 43  | 49  | 56  | 61  |
| 3.5              |     |     |     |     |     |     |     |     |     |     | 11  |
| Present study ($N^r = 5$, $N^r = 7$, $L = 8$, $W = 3$) | | | | | | | | | | | |
| 0.5              | 444 |     | 353 |     | 303 |     | 272 |     |     |     | 248 |
| 1.5              | 65  |     | 127 |     | 149 |     | 155 |     |     |     | 156 |
| 2.5              |     |     | 9   |     | 27  |     | 40  |     |     |     | 47  |
| Present study ($N^r = 9$, $N^r = 7$, $L = 8$, $W = 3$) | | | | | | | | | | | |
| 0.5              | 444 | 388 | 351 | 325 | 304 | 287 | 272 | 259 | 248 |     |     |
| 1.5              | 65  | 107 | 129 | 141 | 149 | 153 | 155 | 156 | 155 |     |     |
| 2.5              |     |     | 7   | 18  | 27  | 35  | 40  | 44  | 47  |     |     |

subject to the initial conditions

$$c(x, y, z) = 0 \quad \text{everywhere for} \quad t \leq 0$$  \hspace{1cm} (53)

and the boundary conditions for $t > 0$,

$$c(0, y, z) = \text{prescribed from the exact analytical solution},$$  \hspace{1cm} (54)

$$c(x, y \to \infty, z) \to 0,$$  \hspace{1cm} (55)

$$c(x, y, z \to \infty) \to 0,$$  \hspace{1cm} (56)

$$\partial c(x, 0, z)/\partial y = 0,$$  \hspace{1cm} (57)

$$\partial c(x, y, 0)/\partial z = 0.$$  \hspace{1cm} (58)

In Eq. (52) $\beta$ is defined as before but $\gamma$ is given by

$$\gamma = (L/H)/Pe_{zz}.$$  \hspace{1cm} (59)
$H$ is the height of the actual one quarter of the physical domain in the $z$ direction, $Pe_{zz}$ is the Peclet number in the $z$ direction given by

$$Pe_{zz} = UH/K_{zz}. \quad (60)$$

The exact analytical solution in normalized form for the steady-state case and a point source is given by

$$c(x, y, z) = (x / x_0)^{-1} \exp\{-(y^2/\beta + z^2/\gamma)/[4(x / x_0)]\}, \quad (61)$$

where $x_0$ is the distance of the point source to the upwind lateral surface. Equation (61) was actually obtained by converting Seinfeld’s solution \[18\] into normalized form.

A. Transient State Case

For the numerical model the partial space derivatives in Eqs. (52)–(58) are replaced by the derivative approximation formulae, Eqs. (118a), (119a), (1110a), (1112b) and (1113b), given in Appendix II to obtain

$$\frac{dc_{ijk}}{dt} \approx - \sum_{i=1}^{N^x} a_{ij}^x c_{ijk} + \beta \sum_{l=1}^{N^y} b_{lj}^y c_{ilk} + \gamma \sum_{l=1}^{N^z} b_{kl}^z c_{ljl} \quad (62)$$

for the unknown concentration values; $c_{ijk}: i = 2, 3, ..., N^x, j = 2, 3, ..., (N^y - 1),$ and $k = 2, 3, ..., (N^z - 1).$ The initial conditions are

$$c_{ijk} = 0 \quad \text{everywhere, for} \quad t \leq 0. \quad (63)$$

The upwind boundary concentration values are prescribed using the exact analytical solution given by Eq. (61),

$$c_{ijl} : \quad j = 1, 2, ..., N^y \quad \text{and} \quad k = 1, 2, ..., N^z. \quad (64)$$

The side lateral surface boundary concentrations are

$$c_{iNyk} = 0 : \quad i = 1, 2, ..., N^x \quad \text{and} \quad k = 1, 2, ..., N^z. \quad (65)$$

Similarly the upper surface boundary concentrations are

$$c_{ijNy} = 0 : \quad i = 1, 2, ..., N^x \quad \text{and} \quad j = 1, 2, ..., N^y. \quad (66)$$

Symmetry plane boundary concentrations are expressed in terms of the unknown interior domain concentrations using Eqs. (57) and (58) as demonstrated in the first problem

$$\frac{\partial c_{ijk}}{\partial y} \approx \sum_{l=1}^{N^y} a_{jl}^y c_{ilk} = 0 \quad \text{at} \quad j = 1. \quad (67)$$
Equation (67) is combined with Eq. (65) and rearranged to obtain

$$c_{i1k} = - \left( \sum_{l=2}^{(N^y-1)} a_{il}^c c_{il} \right) \left/ a_{11}^c \right.,$$

$$i = 2, 3, \ldots, N^x \quad \text{and} \quad k = 1, 2, \ldots, (N^z - 1) \quad (68)$$

and

$$\partial c_{ijk} / \partial z \equiv \sum_{l=1}^{N^z} a_{kl}^c c_{ijkl} = 0 \quad \text{at} \quad k = 1. \quad (69)$$

Upon rearrangement of Eq. (69) with the use of Eq. (66),

$$c_{ij1} = - \left( \sum_{l=2}^{(N^y-1)} a_{il}^c c_{ijl} \right) \left/ a_{11}^c \right.,$$

$$i = 2, 3, \ldots, N^x \quad \text{and} \quad j = 1, 2, \ldots, (N^y - 1). \quad (70)$$

B. Steady-State Case

Following the procedure described in the first problem the following set of linear algebraic equations are obtained

$$\sum_{p=2}^{N^x} \sum_{q=2}^{N^y} \sum_{r=2}^{(N^z-1)} \frac{\partial g_{ijk}}{\partial c_{pqr}} c_{pqr} = h_{ijk}$$

for $i = 2, 3, \ldots, N^x$, $j = 2, 3, \ldots, (N^y - 1)$

and $k = 2, 3, \ldots, (N^z - 1) \quad (71)$

in which the Jacobian matrix elements are given by

$$\frac{\partial g_{ijk}}{\partial c_{pqr}} = \delta_{jq} \delta_{kr} a_{ip}^x + \delta_{ip} \delta_{kr} \beta (b_{jq}^y a_{1q}^x / a_{11}^x - b_{jq}^y)$$

$$+ \delta_{ip} \delta_{jq} \gamma (b_{kr}^y a_{1r}^x / a_{11}^x - b_{kr}^y) \quad (72)$$

and the right side of Eq. (71) is given by

$$h_{ijk} = -a_{11}^x c_{ijk}. \quad (73)$$

C. Numerical Results

For numerical calculations the system parameters were assumed to be $U = 1$, $K_{yy}$ and $K_{zz} = 0.1$, $L = 15$, and $W$ and $H = 3.5$. The point source was located at the centerline at a distance of $x_0 = 5$ from the upwind.

A Runge–Kutta–Fehlberg Four (Five) method was used to obtain solutions for the transient case with equally spaced $5 \times 5 \times 5$ and $7 \times 7 \times 7$. 

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grid systems; as before the numerical solutions were continued until the steady-state was reached, at which point the numerical solution and the direct solution of the steady state model—which is discussed next—were found to be identical.

The numerical solution of the time-independent model was obtained by

<table>
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<th>Dimensionless Distances</th>
<th>Longitudinal x</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.250</td>
</tr>
<tr>
<td>Lateral</td>
<td></td>
</tr>
<tr>
<td>y</td>
<td></td>
</tr>
<tr>
<td>For 5 x 5 x 5 Grid</td>
<td></td>
</tr>
<tr>
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</tr>
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<td>Numerical</td>
<td></td>
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<tr>
<td></td>
<td>0.167</td>
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<tr>
<td>Lateral</td>
<td></td>
</tr>
<tr>
<td>y</td>
<td></td>
</tr>
<tr>
<td>For 7 x 7 x 7 Grid</td>
<td></td>
</tr>
<tr>
<td>Analytical</td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>2.000</td>
</tr>
<tr>
<td>0.167</td>
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<tr>
<td>0.333</td>
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<tr>
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<td>0.721</td>
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<tr>
<td>0.667</td>
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<td>0.667</td>
<td>0.326</td>
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<td>0.833</td>
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Table continued
**DIFFERENTIAL QUADRATURE**

**TABLE III (continued)**

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<td>0.125 0.250 0.375 0.500 0.625 0.750 0.875 1.000</td>
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</tbody>
</table>

For $9 \times 9 \times 9$ Grid

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<tr>
<th>Lateral $y$</th>
<th>0.125</th>
<th>0.250</th>
<th>0.375</th>
<th>0.500</th>
<th>0.625</th>
<th>0.750</th>
<th>0.875</th>
<th>1.000</th>
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<tbody>
<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>2.182</td>
<td>1.714</td>
<td>1.412</td>
<td>1.200</td>
<td>1.043</td>
<td>0.923</td>
<td>0.828</td>
<td>0.750</td>
</tr>
<tr>
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<td>2.035</td>
<td>1.623</td>
<td>1.350</td>
<td>1.155</td>
<td>1.009</td>
<td>0.896</td>
<td>0.806</td>
<td>0.732</td>
</tr>
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<td>0.250</td>
<td>1.652</td>
<td>1.377</td>
<td>1.179</td>
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<td>0.913</td>
<td>0.821</td>
<td>0.745</td>
<td>0.682</td>
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<td>0.375</td>
<td>1.166</td>
<td>1.048</td>
<td>0.941</td>
<td>0.850</td>
<td>0.773</td>
<td>0.708</td>
<td>0.653</td>
<td>0.605</td>
</tr>
<tr>
<td>0.500</td>
<td>0.716</td>
<td>0.715</td>
<td>0.687</td>
<td>0.650</td>
<td>0.613</td>
<td>0.576</td>
<td>0.542</td>
<td>0.511</td>
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<td>0.625</td>
<td>0.383</td>
<td>0.437</td>
<td>0.458</td>
<td>0.461</td>
<td>0.454</td>
<td>0.442</td>
<td>0.428</td>
<td>0.412</td>
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<tr>
<td>0.750</td>
<td>0.178</td>
<td>0.239</td>
<td>0.279</td>
<td>0.302</td>
<td>0.315</td>
<td>0.320</td>
<td>0.320</td>
<td>0.317</td>
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<tr>
<td>0.875</td>
<td>0.072</td>
<td>0.118</td>
<td>0.155</td>
<td>0.184</td>
<td>0.204</td>
<td>0.218</td>
<td>0.227</td>
<td>0.232</td>
</tr>
<tr>
<td>Numerical</td>
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<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>2.152</td>
<td>1.691</td>
<td>1.395</td>
<td>1.188</td>
<td>1.033</td>
<td>0.913</td>
<td>0.817</td>
<td>0.737</td>
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<tr>
<td>0.125</td>
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<td>1.603</td>
<td>1.335</td>
<td>1.143</td>
<td>0.999</td>
<td>0.886</td>
<td>0.795</td>
<td>0.719</td>
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<tr>
<td>0.250</td>
<td>1.637</td>
<td>1.363</td>
<td>1.167</td>
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<td>0.903</td>
<td>0.810</td>
<td>0.732</td>
<td>0.666</td>
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<td>0.375</td>
<td>1.156</td>
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<td>0.932</td>
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<td>0.695</td>
<td>0.636</td>
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<td>0.500</td>
<td>0.711</td>
<td>0.708</td>
<td>0.679</td>
<td>0.641</td>
<td>0.599</td>
<td>0.558</td>
<td>0.519</td>
<td>0.482</td>
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<td>0.625</td>
<td>0.380</td>
<td>0.432</td>
<td>0.449</td>
<td>0.446</td>
<td>0.432</td>
<td>0.413</td>
<td>0.390</td>
<td>0.367</td>
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<td>0.750</td>
<td>0.176</td>
<td>0.231</td>
<td>0.262</td>
<td>0.275</td>
<td>0.276</td>
<td>0.269</td>
<td>0.259</td>
<td>0.246</td>
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<tr>
<td>0.875</td>
<td>0.066</td>
<td>0.098</td>
<td>0.118</td>
<td>0.129</td>
<td>0.133</td>
<td>0.132</td>
<td>0.128</td>
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</table>

Solving simultaneously the set of linear algebraic equations given by Eq. (71) using the method of transpose elimination with double precision as published by Wassyng [19]. Transpose elimination was selected instead of the Gaussian elimination since the method of transpose elimination requires much less storage as the number of unknowns increases. Typical numerical results, for the horizontal symmetry plane only, are presented in Table III along with the corresponding analytical solutions for equally spaced grid systems of $5 \times 5 \times 5, 7 \times 7 \times 7, \text{and } 9 \times 9 \times 9$.

**Conclusions**

The method of differential quadrature for the solution of partial differential equations, as introduced by Bellman et al., can be extended to the analysis of both time-dependent (initial or initial and boundary value) and time-independent (boundary value) problems involving multiple space dimensions.

For the multi-dimensional examples analyzed herein, the accuracy of the
numerical results via differential quadrature continued to improve as the number of equally spaced grid points was increased from 5, to 7, to 9, and to 11. A similar behavior was observed in an earlier study on the solution of the two-dimensional Poisson equation [10] when the grid points were increased from 5 to 7. However, another study involving the solution of one-dimensional convection–diffusion problems with irreversible reaction [9] clearly indicated that the accuracy of the numerical solution increased with the number of equally-spaced grid points up to 11. When the grid points were increased to 15 the accuracy dropped off which can be attributed to an ill-conditioning of the matrix according to Bellman [2]. It is conceivable, although not established, that the accuracy of the solution for multidimensional problems could very well exhibit an optimum number of grid points of approximately 11.

In the foregoing examples, the quality of the numerical solutions was obviously compromised by the arbitrary choice of dimensions for the finite domain or plume. For better results, the calculations should be repeated, utilizing dimensions which are more nearly representative of the actual unbounded domain.

APPENDIX I

Typical weighting coefficients, \( a_{pq} \) and \( b_{pq} \), for the equations given in Appendix II are shown as elements in the matrices \( A \) and \( B \) in the tabulation below for equally spaced sample points in the range \( 0 \leq x \leq 1 \). However, weighting coefficients for unequally spaced sample points can be obtained by a similar procedure.

Weighting coefficients \( a_{pq} \) apply to the derivative approximation formulae based on the differential quadrature technique introduced by Bellman et al. [2–7] and obviously are valid for all partial derivatives regardless of order for the same set of sample points.

Weighting coefficients \( b_{pq} \) are those coefficients associated with the alternative technique based on individual quadratures for higher order derivatives, as inferred by Mingle [15]. In the following the \( b_{pq} \) weighting coefficients, which are valid only for the second order partial derivatives, are tabulated.

Weighting coefficients for individual quadrature formula approximating the third and higher order partial space derivatives can be obtained by a procedure similar to the second order partial space derivatives.

If weighting coefficients are desired for any other range, \( 0 \leq x \leq \lambda \), then the weighting coefficients matrix \( A \) as given below for \( 0 \leq x \leq 1 \) must be divided by \( \lambda \), and weighting coefficients matrix \( B \) must be divided by \( \lambda^2 \).
Typical Weighting Coefficients

3 sample points: \( x = [0 \ \frac{1}{3} \ 1] \)

\[
A = \begin{bmatrix}
-3 & 4 & -1 \\
-1 & 0 & 1 \\
1 & -4 & 3
\end{bmatrix}, \quad B = 4 \begin{bmatrix}
1 & -2 & 1 \\
1 & -2 & 1 \\
1 & -2 & 1
\end{bmatrix}
\]

4 sample points: \( x = [0 \ \frac{1}{3} \ \frac{2}{3} \ 1] \)

\[
A = \frac{1}{2} \begin{bmatrix}
-11 & 18 & -9 & 2 \\
-2 & -3 & 6 & -1 \\
1 & -6 & 3 & 2 \\
-2 & 9 & -18 & 11
\end{bmatrix}, \quad B = 9 \begin{bmatrix}
2 & -5 & 4 & -1 \\
1 & -2 & 1 & 0 \\
0 & 1 & -2 & 1 \\
-1 & 4 & -5 & 2
\end{bmatrix}
\]

5 sample points: \( x = [0 \ \frac{1}{4} \ \frac{1}{2} \ \frac{3}{4} \ 1] \)

\[
A = \frac{1}{3} \begin{bmatrix}
-25 & 48 & -36 & 16 & -3 \\
-3 & -1 & 18 & -6 & 1 \\
1 & -8 & 0 & 8 & -1 \\
1 & 6 & 18 & 1 & 3 \\
3 & -16 & 36 & -48 & 25
\end{bmatrix}, \quad B = \frac{4}{3} \begin{bmatrix}
35 & -104 & 38 & -56 & 11 \\
11 & -20 & 2 & 4 & -1 \\
-1 & 16 & -10 & 16 & -1 \\
-1 & 4 & 2 & -20 & 11 \\
11 & -56 & 38 & -104 & 35
\end{bmatrix}
\]

6 sample points: \( x = [0 \ \frac{1}{5} \ \frac{2}{5} \ \frac{3}{5} \ \frac{4}{5} \ 1] \)

\[
A = \frac{1}{12} \begin{bmatrix}
137 & 300 & -300 & 200 & -75 & 12 \\
-12 & -65 & 120 & -60 & 20 & -3 \\
3 & -30 & -20 & 60 & -15 & 2 \\
-2 & 15 & -60 & 20 & 30 & -3 \\
3 & -20 & 60 & -120 & 65 & 12 \\
-12 & 75 & -200 & 300 & -300 & 137
\end{bmatrix}, \quad B = \frac{25}{12} \begin{bmatrix}
45 & -154 & 214 & -156 & 61 & -10 \\
10 & -15 & -4 & 14 & -6 & 1 \\
-1 & 16 & -30 & 16 & -1 & 0 \\
0 & -1 & 16 & -30 & 16 & -1 \\
1 & -6 & 14 & -4 & -15 & 10 \\
-10 & 61 & -156 & 214 & -154 & 45
\end{bmatrix}
\]
7 sample points: \( x = [0 \ \frac{1}{6} \ \frac{2}{6} \ \frac{3}{6} \ \frac{4}{6} \ \frac{5}{6} \ \frac{6}{6} \ 1] \)

\[
A = \frac{1}{10}
\begin{bmatrix}
-147 & 360 & -450 & 400 & -225 & 72 & -10 \\
-10 & -77 & 150 & -100 & 50 & -15 & 2 \\
2 & -24 & -35 & 80 & -30 & -8 & -1 \\
1 & -8 & 30 & -80 & 35 & -2 \\
-2 & 15 & -50 & 100 & -150 & 77 & 10 \\
10 & -72 & 225 & -400 & 450 & -360 & 147
\end{bmatrix},
\]

\[
B = \frac{1}{10}
\begin{bmatrix}
1624 & -6264 & 10530 & -10160 & 5940 & -1944 & 274 \\
274 & -294 & -510 & 940 & -570 & 186 & -26 \\
-26 & 456 & -840 & 400 & 30 & -24 & 4 \\
4 & -54 & 540 & -980 & 540 & -54 & 4 \\
4 & -24 & 30 & 400 & -840 & 456 & -26 \\
-26 & 186 & -570 & 940 & -510 & -294 & 274 \\
274 & -1944 & 5940 & -10160 & 10530 & -6264 & 1624
\end{bmatrix}
\]

**APPENDIX II**

In the following, derivative approximation formulae based on differential quadrature are presented for both the technique introduced by Bellman et al. [2–7] (designated by the weighting coefficients, \( a_{pq} \)), and the alternative procedure of utilizing individual quadratures for the higher order derivatives (designated by the weighting coefficients \( b_{pq} \)), as inferred by Mingle [15]. It should be noted that the space variables \( x, y, \) and \( z \) which carry the connotation of Cartesian coordinates can be replaced directly by the corresponding designations for cylindrical and spherical coordinates.

In the following formulae \( f = f(x, y, z, t) \) is the function; \( N^x, N^y, \) and \( N^z \) are the total number of sample points used in the \( x, y, \) and \( z \) directions, respectively; \( i, j, \) and \( k \) are the indices indicating the location of a sample point in the \( x, y, \) and \( z \) directions; and \( a_{pq}^x, a_{pq}^y, \) and \( a_{pq}^z \) are the weighting coefficients associated with the sample points in \( x, y, \) and \( z \) directions, respectively; and \( t \) is the time. Notice that for cross derivative formulae, \( N^x = N^y = N^z = N. \) Therefore, the computational domain for problems involving cross derivatives must be discretized using an equal number of sample points in each of the directions. It should be noted that these approximation formulae for the space derivatives are applicable to either time-independent or time-dependent functions.
Differential Quadrature

Derivative Approximation Formulae\textsuperscript{1,2}

**One dimensional**

First order derivative

\[
\frac{df}{dx}(i) \approx \sum_{j=1}^{N_x} a_{ij}^x f_j
\]

(II1a)

Second order derivative

\[
\frac{d^2f}{dx^2}(i) \approx \sum_{j=1}^{N_x} a_{ij}^x \sum_{k=1}^{N_x} a_{jk}^x f_k
\]

\[
\approx \sum_{j=1}^{N_x} b_{ij}^x f_j
\]

(II2b)

**Two dimensional**

First order derivatives

\[
\frac{\partial f}{\partial x}(ij) \approx \sum_{k=1}^{N_x} a_{ik}^x f_{kj}
\]

(II3a)

\[
\frac{\partial f}{\partial y}(ij) \approx \sum_{k=1}^{N_y} a_{ik}^y f_{ik}
\]

(II4a)

Second order derivatives

\[
\frac{\partial^2 f}{\partial x^2}(ij) \approx \sum_{l=1}^{N_x} a_{il}^x \sum_{k=1}^{N_x} a_{lk}^x f_{kj}
\]

\[
\approx \sum_{k=1}^{N_x} b_{ik}^x f_{kj}
\]

(II5a)

\[
\frac{\partial^2 f}{\partial y^2}(ij) \approx \sum_{l=1}^{N_y} a_{il}^y \sum_{k=1}^{N_y} a_{lk}^y f_{ik}
\]

\[
\approx \sum_{k=1}^{N_y} b_{ik}^y f_{ik}
\]

(II6b)

\[
\frac{\partial}{\partial x} \left( \frac{\partial f}{\partial y} \right)(ij) = \frac{\partial}{\partial y} \left( \frac{\partial f}{\partial x} \right)(ij)
\]

\[
\approx \sum_{l=1}^{N} a_{il} \sum_{k=1}^{N} a_{lk} f_{kl}
\]

(II7a)

\textsuperscript{1} Equations bearing the letter "a" were derived according to Bellman et al.

\textsuperscript{2} Equations bearing the letter "b" are based on a method inferred by Mingle.
Three dimensional

First order derivatives

\[
\frac{\partial f}{\partial x}_{ijk} \approx \sum_{l=1}^{N_x} a_{l}^{i} f_{ijl} \quad (118a)
\]

\[
\frac{\partial f}{\partial y}_{ijk} \approx \sum_{l=1}^{N_y} a_{l}^{j} f_{ijl} \quad (119a)
\]

\[
\frac{\partial f}{\partial z}_{ijk} \approx \sum_{l=1}^{N_z} a_{l}^{k} f_{ijl} \quad (119a)
\]

Second order derivatives

\[
\frac{\partial^2 f}{\partial x^2}_{ijk} \approx \sum_{l=1}^{N_x} a_{l}^{i} \sum_{m=1}^{N_x} a_{lm}^{i} f_{mjk} \quad (111a)
\]

\[
\approx \sum_{l=1}^{N_x} b_{l}^{i} f_{ijl} \quad (111b)
\]

\[
\frac{\partial^2 f}{\partial y^2}_{ijk} \approx \sum_{l=1}^{N_y} a_{l}^{j} \sum_{m=1}^{N_y} a_{lm}^{j} f_{imk} \quad (112a)
\]

\[
\approx \sum_{l=1}^{N_y} b_{l}^{j} f_{ijl} \quad (112b)
\]

\[
\frac{\partial^2 f}{\partial z^2}_{ijk} \approx \sum_{l=1}^{N_z} a_{l}^{k} \sum_{m=1}^{N_z} a_{lm}^{k} f_{ijm} \quad (113a)
\]

\[
\approx \sum_{l=1}^{N_z} b_{l}^{k} f_{ijl} \quad (113b)
\]

\[
\frac{\partial}{\partial x} \left( \frac{\partial f}{\partial y} \right)_{ijk} \approx \frac{\partial}{\partial y} \left( \frac{\partial f}{\partial x} \right)_{ijk} \quad (114a)
\]

\[
\approx \sum_{l=1}^{N} a_{ll}^{i} \sum_{m=1}^{N} a_{lm}^{j} f_{lmk} \quad (114a)
\]

\[
\frac{\partial}{\partial x} \left( \frac{\partial f}{\partial z} \right)_{ijk} \approx \frac{\partial}{\partial z} \left( \frac{\partial f}{\partial x} \right)_{ijk} \quad (115a)
\]

\[
\approx \sum_{l=1}^{N} a_{ll}^{i} \sum_{m=1}^{N} a_{km}^{j} f_{lm} \quad (115a)
\]

\[
\frac{\partial}{\partial y} \left( \frac{\partial f}{\partial z} \right)_{ijk} \approx \frac{\partial}{\partial z} \left( \frac{\partial f}{\partial y} \right)_{ijk} \quad (116a)
\]

\[
\approx \sum_{l=1}^{N} a_{jl}^{i} \sum_{m=1}^{N} a_{km}^{j} f_{li} \quad (116a)
\]
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References