A Difference Expansion Technique to Analyse the Advection/Dispersion/Sorption Equation for Phosphorous

W. D. Scott
Division of Environmental Science
Murdoch University
Perth, Western Australia 6150

J. S. Devitt
Department of Mathematics and Statistics
University of Saskatchewan
Saskatoon, Saskatchewan S7N 0W0

15 Aug 92

Murdoch University

A Difference Expansion Technique to Analyse the Advection/Dispersion/Sorption Equation for Phosphorous

W. D. Scott
Division of Environmental Science
Murdoch University
Perth, Western Australia 6150

J. S. Devitt
Department of Mathematics and Statistics
University of Saskatchewan
Saskatoon, Saskatchewan S7N 0W0

15 Aug 92

Abstract

A finite difference technique for numerical analysis of the partial differential equation for advection and dispersion with sorption is presented in detail. The sorption term is non-linear and it is difficult to simulate the breakthrough curves when the rate of change of concentration is large. A general technique is used which expands the derivatives in terms of increasing orders of finite differences. This has become possible with the advent of symbolic manipulation. It is possible to expand to any order and, importantly, separate out the terms for each order. Details are presented, together with methods for exploring the convergence and stability as well as adjusting the time and spatial differencing to lower or minimise the error.

1 Introduction

Modelling of the movement of soluble and absorbed materials in soils has long been relegated to approximation procedures, using finite approximations to the partial differential equations for transport and sorption. The procedures are outlined in the rather comprehensive articles by van Genuchten and Wierenga [16][15]. In these studies techniques are included to correct for the numerical dispersion inherent with differencing procedures. They show, quite clearly, that a better result can be obtained with the use of larger time and space differences, provided they are related to each other. This minimises the error from the numerical roundoff and numerical dispersion from the upstream (backward) difference in space. The addition of a non-linear absorption term is also considered but these terms are only estimated, partly because of the intractability of expanding the combined mass balance equation. Often the absorption term is approximated by a first order equation Munns and Fox[11]. Other models contain kinetic terms that are difficult to fit to breakthrough curves. For instance, Chien and Clayton [7] produced empirically derived sorption terms that fit the data to an logarithmic form. In contrast, some models rely on the experimental breakthrough curve to determine the forward to backward physical absorption.

The actual experimental data for absorption, without flow, is well fitted by the empirical, time dependent term of Barrow [2]; his work relies on deep background studies of the dependence of charge on the sorption properties of phosphorus ions and several related ions. He suggests that two consecutive reations occur: The first is a rapid surface absorption (or desorption). This is followed by a slow penetration into (or release from) the inner pores of the particles. The net effect is accurately predicted by a sorption term of the form:

$$S = k \cdot C^n \cdot t^m \tag{1}$$

Our work stems from that of Binh [3]; he developed implicit techniques for solving the advective dispersion equation for Phosphorus transfer in soils. Now, Notodarmojo et al [14] have included Barrow's form of the non-linear term into an advective/dispersion/sorption equation. The finite difference form has many terms that are difficult to collect and account for in the time and space steps. A small error might be ignored but their fit to the data, Fig.

10 and Fig.11, is less than satisfactory. This may be some effect of unknown physical processes or simply a result of a lack of detailed analysis of the terms in the equations. Indeed, intractable terms were dropped to allow the computation to proceed and create a stable solution. Little effort has been made to be sure these terms are unimportant and that the equations used do, indeed, converge on the infinitesimal-based partial differential equation. This is a dangerous procedure and is well known to lead to erroneous solutions even though they may be stable[8].

Today we have an advantage, symbolic manipulation with computers. One such parodos is Maple[1]. In this paper we repeat the former analyses of the equation for mass balance of phosphate.

$$\frac{\partial C}{\partial t} = D \cdot \frac{\partial^2 C}{\partial z^2} - v \cdot \frac{\partial C}{\partial z} - \frac{\rho}{\theta} \frac{\partial S}{\partial t} \tag{2}$$

without error, to many orders of expansion. Though such an analysis can conceptually be done to any order, we have truncated the terms roughly at order 5. This needs to be followed up with a refitting of the data to show the effects of preserving more terms in the expansion,

2 Finite Difference Expansion

The approach is a general one and is presented in terms of finite differences. To agree with accepted practice, we have used mixed differences. This means that first order backward differences were used in z ; first order forward differences in t and a central difference for all high order terms. Index j relates to time differences and index i , to spatial differences. This means that effectively the grid spacing for terms other than first order is halved.

[1]Maple is a registered trademark of Waterloo Maple Software

2.1 Definition of the Finite Differences

z-dependent terms:

$$\nabla_z C = C - C_{i-1}$$
$$\delta_{zz} C = \Delta_z C - \nabla_z C = \delta_z C_{i+1/2} - \delta_z C_{i-1/2}$$
$$\delta_{zzz} C = \delta_{zz} C_{i+1/2} - \delta_{zz} C_{i-1/2}$$
$$\vdots$$
$$\underbrace{\delta_{z\cdots z}}_{N} C = \underbrace{\delta_{z\cdots z}}_{N-1} C_{i+1/2} - \underbrace{\delta_{z\cdots z}}_{N-1} C_{i-1/2}$$

t-dependent terms:

$$\Delta_t C = C_{j+1} - C$$
$$\delta_{tt} C = \delta_t C_{j+1/2} - \delta_t C_{j-1/2}$$
$$\delta_{ttt} C = \delta_{tt} C_{j+1/2} - \delta_{tt} C_{j-1/2}$$
$$\vdots$$
$$\underbrace{\delta_{t\cdots t}}_{N} C = \underbrace{\delta_{t\cdots t}}_{N-1} C_{j+1/2} - \underbrace{\delta_{t\cdots t}}_{N-1} C_{j-1/2}$$

where we have used the convention that indices clearly known to be either i or j are omitted. The number of differences is N. Further,the cross terms are:

$$\delta_{zt} C = \Delta_z C_j - \nabla_z C_j = \delta_z C_{j+1/2} - \delta_z C_{j-1/2}$$
$$\delta_{zzt} C = \delta_{zz} C_{j+1/2} - \delta_{zz} C_{j-1/2}$$
$$\delta_{ztt} C = \delta_{zt} C_{j+1/2} - \delta_{zt} C_{j-1/2}$$
$$\vdots$$
$$\underbrace{\delta_{z\cdots zt\cdots t}}_{N-M\ M} C = \underbrace{\delta_{z\cdots zt\cdots t}}_{N-M\ M-1} C_{j+1/2} - \underbrace{\delta_{z\cdots zt\cdots t}}_{N-M\ M-1} C_{j+1/2}$$

where M is the number of t differencing operations. The notation uses Δ as a forward difference, ∇ as a backward difference, and δ as a central difference. The concentration of Phosphate in the liquid is C in moles/litre. There is no real reason why the differences need to be equal but here we assume equal time steps of $\Delta_t = h_t$ and equal spatial steps of $\Delta_z = h_z$.

2.2 Taylor Expansion

We proceed by considering C to be a smooth, continuous function of z and t, and expand C in a Taylor series in two dimensions about the nodal point. We write down the symbolic expressions for the value of the function at each neighbouring nodal point. Appropriate subtractions, following the differencing rules, above, produce a series of expressions for the differences. Differences of order three are obtained by subtraction of differences of order

two; differences of order two are obtained by subtraction of differences of order one; and differences of order one are obtained by subtraction of function values themselves. This produces a series of equations for the differences.

$$\nabla_z = h_z\frac{\partial C}{\partial z} - \frac{h_z^2}{2}\frac{\partial^2 C}{\partial z^2} + \frac{h_z^3}{6}\frac{\partial^3 C}{\partial z^3} - \frac{h_z^4}{24}\frac{\partial^4 C}{\partial z^4} + \frac{h_z^5}{120}\frac{\partial^5 C}{\partial z^5} - \frac{h_z^6}{720}\frac{\partial^6 C}{\partial z^6} + \frac{h_z^7}{5040}\frac{\partial^7 C}{\partial z^7} - \cdot$$

$$\Delta_t = h_t\frac{\partial C}{\partial t} + \frac{h_t^2}{2}\frac{\partial^2 C}{\partial t^2} + \frac{h_t^3}{6}\frac{\partial^3 C}{\partial t^3} + \frac{h_t^4}{24}\frac{\partial^4 C}{\partial t^4} + \frac{h_t^5}{120}\frac{\partial^5 C}{\partial t^5} + \frac{h_t^6}{720}\frac{\partial^6 C}{\partial t^6} + \frac{h_t^7}{5040}\frac{\partial^7 C}{\partial t^7} + \cdot$$

$$\delta_{zz} = h_z^2\frac{\partial^2 C}{\partial z^2} + \frac{h_z^4}{12}\frac{\partial^4 C}{\partial z^4} + \frac{h_z^6}{360}\frac{\partial^6 C}{\partial z^6} + \cdot$$

$$\delta_{tz} = h_t h_z\frac{\partial^2 C}{\partial t\partial z} + \frac{h_t h_z^3}{24}\frac{\partial^4 C}{\partial t\partial z^3} + \frac{h_t h_z^3}{24}\frac{\partial^4 C}{\partial t^3\partial z} + \frac{h_t^3 h_z^3}{576}\frac{\partial^6 C}{\partial t^3\partial z^3} + \frac{h_t^5 h_z}{1920}\frac{\partial^6 C}{\partial t^5\partial z} + \frac{h_t h_z^5}{1920}\frac{\partial^6 C}{\partial t\partial z^5} + \cdot$$

$$\delta_{tt} = h_t^2\frac{\partial^2 C}{\partial t^2} + \frac{h_t^4}{12}\frac{\partial^4 C}{\partial t^4} + \frac{h_t^6}{360}\frac{\partial^6 C}{\partial t^6} + \cdot$$

$$\vdots$$

$$\underbrace{\delta_{z\cdots z}}_{N} C = h_z^N\frac{\partial^N C}{\partial z^N} + \cdot$$

$$\underbrace{\delta_{t\cdots t}}_{N-M}\underbrace{\delta_{z\cdots z}}_{M} C = h_t^{N-M}h_z^M\frac{\partial^N C}{\partial t^{N-M}\partial z^M} + \cdot$$

$$\underbrace{\delta_{t\cdots t}}_{N} C = h_t^N\frac{\partial^N C}{\partial t^N} + \cdot$$

It is important to realise that all the derivatives are evaluated at the nodal point of concern, say (0,0); the evaluation arguments is omitted for convenience. This in no way detracts from the generality of the expansion because of the subtractions involved. That is, expanding about some arbitrary point, say (a, b), gives identically the same differences. Simply noting the nodal point as a point of expansion is sufficient.

3 Derivative Formulas to Seventh Order

The above set of equations is now solved for the derivatives in terms of the differences. The form is equivalent to a sparce matrix set and relatively easily solved. The next few listings show the results with the major differencing schemes though the present application requires mixed differences.

The other tables show the standard difference formulas and are presented for comparison purposes. Later, we see that they allow the construction of general expressions for n^th order terms.

Here we leave the partial derivative forms to conform with the Maple output. The nomenclature is such that

$\frac{\partial^2 C}{\partial t^2}$ =D[2, 2](f)(0, 0)

The expresions for all the sixth and seventh partials are omitted because they are precisely the differences divided by hz and ht.

3.1 Derivatives from Forward Differences

This is a the most common difference though it has a forward bias.

```
D[1](f)(0, 0) =

Dz       Dzz       Dzzz       Dzzzz       Dzzzzz       Dzzzzzz       Dzzzzzzz
-- - 1/2 --- + 1/3 ---- - 1/4 ----- + 1/5 ------ - 1/6 ------- + 1/7 --------,
hz       hz        hz         hz          hz           hz            hz
```

```
D[2](f)(0, 0) =

Dt       Dtt       Dttt       Dtttt       Dttttt       Dtttttt       Dttttttt
-- - 1/2 --- + 1/3 ---- - 1/4 ----- + 1/5 ------ - 1/6 ------- + 1/7 --------,
ht       ht        ht         ht          ht           ht            ht
```

```
D[1, 1](f)(0, 0) =

    Dzz   Dzzz    11  Dzzzz       Dzzzzz   137 Dzzzzzz         Dzzzzzzz
    --- - ---- + ---- ----- - 5/6 ------ + --- ------- - 7/10 --------,
      2      2   12     2            2     180     2               2
    hz     hz          hz           hz          hz              hz
```

```
                  Dzt         Dztt        Dzzt        Dzttt       Dzztt
D[1, 2](f)(0, 0) = ----- - 1/2 ----- - 1/2 ----- + 1/3 ----- + 1/4 -----
                   hz ht       hz ht       hz ht       hz ht       hz ht

      Dzzzt       Dztttt       Dzzttt       Dzzztt       Dzzzzt
+ 1/3 ----- - 1/4 ------ - 1/6 ------ - 1/6 ------ - 1/4 ------
      hz ht       hz ht        hz ht        hz ht        hz ht

      Dzttttt       Dzzttttt       Dzzzttt       Dzzzztt       Dzzzzzt
+ 1/5 ------- + 1/8 ------- + 1/9 ------- + 1/8 ------- + 1/5 -------
       hz ht         hz ht          hz ht         hz ht         hz ht
```

$$- \frac{1}{6}\,\frac{Dzttttt}{hz\ ht} - \frac{1}{10}\,\frac{Dzttttt}{hz\ ht} - \frac{1}{12}\,\frac{Dzzttttt}{hz\ ht} - \frac{1}{12}\,\frac{Dzzzttt}{hz\ ht}$$

$$- \frac{1}{10}\,\frac{Dzzzzttt}{hz\ ht} - \frac{1}{6}\,\frac{Dzzzzzzt}{hz\ ht},$$

D[2, 2](f)(0, 0) =

$$\frac{Dtt}{ht^2} - \frac{Dttt}{ht^2} + \frac{11}{12}\,\frac{Dtttt}{ht^2} - \frac{5}{6}\,\frac{Dttttt}{ht^2} + \frac{137}{180}\,\frac{Dttttt}{ht^2} - \frac{7}{10}\,\frac{Dttttttt}{ht^2},$$

D[1, 1, 1](f)(0, 0) =

$$\frac{Dzzz}{hz^3} - \frac{3}{2}\,\frac{Dzzzz}{hz^3} + \frac{7}{4}\,\frac{Dzzzzz}{hz^3} - \frac{15}{8}\,\frac{Dzzzzzz}{hz^3} + \frac{29}{15}\,\frac{Dzzzzzzz}{hz^3},$$

$$D[1, 1, 2](f)(0, 0) = \frac{Dzzt}{hz\ ht^2} - \frac{1}{2}\,\frac{Dzztt}{hz\ ht^2} - \frac{Dzzzt}{hz\ ht^2} + \frac{1}{3}\,\frac{Dzzttt}{hz\ ht^2} + \frac{1}{2}\,\frac{Dzzztt}{hz\ ht^2}$$

$$+ \frac{11}{12}\,\frac{Dzzzzt}{hz\ ht^2} - \frac{1}{4}\,\frac{Dzzttttt}{hz\ ht^2} - \frac{1}{3}\,\frac{Dzzzttt}{hz\ ht^2} - \frac{11}{24}\,\frac{Dzzzztt}{hz\ ht^2} - \frac{5}{6}\,\frac{Dzzzzzt}{hz\ ht^2}$$

$$+ \frac{1}{5}\,\frac{Dzttttt}{hz\ ht^2} + \frac{1}{4}\,\frac{Dzzttttt}{hz\ ht^2} + \frac{11}{36}\,\frac{Dzzzzttt}{hz\ ht^2} + \frac{5}{12}\,\frac{Dzzzzztt}{hz\ ht^2}$$

$$+ \frac{137}{180}\,\frac{Dzzzzzzt}{hz\ ht^2},$$

$$D[1, 2, 2](f)(0, 0) = \frac{Dztt}{hz\ ht^2} - \frac{Dzttt}{hz\ ht^2} - \frac{1}{2}\,\frac{Dzztt}{hz\ ht^2} + \frac{11}{12}\,\frac{Dztttt}{hz\ ht^2} + \frac{1}{2}\,\frac{Dzzttt}{hz\ ht^2}$$

$$+ \frac{1}{3}\,\frac{Dzzztt}{hz\ ht^2} - \frac{5}{6}\,\frac{Dztttttt}{hz\ ht^2} - \frac{11}{24}\,\frac{Dzzttttt}{hz\ ht^2} - \frac{1}{3}\,\frac{Dzzzttt}{hz\ ht^2} - \frac{1}{4}\,\frac{Dzzzzzt}{hz\ ht^2}$$

$$+\frac{137}{180}\frac{Dztttttt}{hz^2\,ht} + \frac{5}{12}\frac{Dzttttt}{hz^2\,ht} + \frac{11}{36}\frac{Dzzttttt}{hz^2\,ht} + \frac{1}{4}\frac{Dzzzttt}{hz^2\,ht} + \frac{1}{5}\frac{Dzzzzttt}{hz^2\,ht},$$

$$D[2, 2, 2](f)(0, 0) =$$

$$\frac{Dttt}{ht^3} - \frac{3}{2}\frac{Dtttt}{ht^3} + \frac{7}{4}\frac{Dttttt}{ht^3} - \frac{15}{8}\frac{Dtttttt}{ht^3} + \frac{29}{15}\frac{Dttttttt}{ht^3},$$

$$D[1, 1, 1, 1](f)(0, 0) = \frac{Dzzzz}{hz^4} - 2\frac{Dzzzzz}{hz^4} + \frac{17}{6}\frac{Dzzzzzz}{hz^4} - \frac{7}{2}\frac{Dzzzzzzz}{hz^4},$$

$$D[1, 1, 1, 2](f)(0, 0) = \frac{Dzzzt}{hz^3\,ht} - \frac{1}{2}\frac{Dzzztt}{hz^3\,ht} - \frac{3}{2}\frac{Dzzzzt}{hz^3\,ht} + \frac{1}{3}\frac{Dzzzttt}{hz^3\,ht} + \frac{3}{4}\frac{Dzzzztt}{hz^3\,ht} + \frac{7}{4}\frac{Dzzzzzt}{hz^3\,ht} - \frac{1}{4}\frac{Dzzzttttt}{hz^3\,ht} - \frac{1}{2}\frac{Dzzzzttt}{hz^3\,ht} - \frac{7}{8}\frac{Dzzzzztt}{hz^3\,ht} - \frac{15}{8}\frac{Dzzzzzzt}{hz^3\,ht},$$

$$D[1, 1, 2, 2](f)(0, 0) = \frac{Dzztt}{hz^2\,ht^2} - \frac{Dzzttt}{hz^2\,ht^2} - \frac{Dzzztt}{hz^2\,ht^2} + \frac{11}{12}\frac{Dzzttttt}{hz^2\,ht^2} + \frac{Dzzzttt}{hz^2\,ht^2} + \frac{11}{12}\frac{Dzzzztt}{hz^2\,ht^2} - \frac{5}{6}\frac{Dzzttttt}{hz^2\,ht^2} - \frac{11}{12}\frac{Dzzzttttt}{hz^2\,ht^2} - \frac{11}{12}\frac{Dzzzzttt}{hz^2\,ht^2} - \frac{5}{6}\frac{Dzzzzztt}{hz^2\,ht^2},$$

$$D[1,2,2,2](f)(0,0) = \frac{Dzttt}{hz^3\,ht} - \frac{3}{2}\frac{Dztttt}{hz^3\,ht} - \frac{1}{2}\frac{Dzzttt}{hz^3\,ht} + \frac{7}{4}\frac{Dzttttt}{hz^3\,ht} + \frac{3}{4}\frac{Dzttttt}{hz^3\,ht} + \frac{1}{3}\frac{Dzzzttt}{hz^3\,ht} - \frac{15}{8}\frac{Dtttttt}{hz^3\,ht} - \frac{7}{8}\frac{Dzttttt}{hz^3\,ht} - \frac{1}{2}\frac{Dzzzttt}{hz^3\,ht} - \frac{1}{4}\frac{Dzzzzttt}{hz^3\,ht},$$

$$D[2,2,2,2](f)(0,0) = \frac{Dtttt}{ht^4} - 2\frac{Dttttt}{ht^4} + \frac{17}{6}\frac{Dtttttt}{ht^4} - \frac{7}{2}\frac{Dttttttt}{ht^4},$$

$$D[1,1,1,1,1](f)(0,0) = \frac{Dzzzzz}{hz^5} - \frac{5}{2}\frac{Dzzzzzz}{hz^5} + \frac{25}{6}\frac{Dzzzzzzz}{hz^5},$$

$$D[1,1,1,1,2](f)(0,0) =$$

$$\frac{Dzzzzt}{hz^4\,ht} - \frac{1}{2}\frac{Dzzzztt}{hz^4\,ht} - 2\frac{Dzzzzzt}{hz^4\,ht} + \frac{1}{3}\frac{Dzzzzttt}{hz^4\,ht} + \frac{Dzzzzztt}{hz^4\,ht} + \frac{17}{6}\frac{Dzzzzzzt}{hz^4\,ht},$$

$$D[1,1,1,2,2](f)(0,0) =$$

$$\frac{Dzzztt}{hz^3\,ht^2} - \frac{Dzzzttt}{hz^3\,ht^2} - \frac{3}{2}\frac{Dzzzzzt}{hz^3\,ht^2} + \frac{11}{12}\frac{Dzzzttt}{hz^3\,ht^2} + \frac{3}{2}\frac{Dzzzzttt}{hz^3\,ht^2} + \frac{7}{4}\frac{Dzzzzzzt}{hz^3\,ht^2},$$

$$D[1,1,2,2,2](f)(0,0) =$$

$$\frac{Dzzttt}{hz^2\,ht^3} - \frac{3}{2}\frac{Dzzttttt}{hz^2\,ht^3} - \frac{Dzzzttt}{hz^2\,ht^3} + \frac{7}{4}\frac{Dzzttttt}{hz^2\,ht^3} + \frac{3}{2}\frac{Dzzzttttt}{hz^2\,ht^3} + \frac{11}{12}\frac{Dzzzzttt}{hz^2\,ht^3},$$

$$D[1,2,2,2,2](f)(0,0) =$$

$$\frac{Dttttt}{hz^4\,ht} - 2\,\frac{Dtttttt}{hz^4\,ht} - 1/2\,\frac{Dzttttt}{hz^4\,ht} + 17/6\,\frac{Dttttttt}{hz^4\,ht} + \frac{Dzttttt}{hz^4\,ht} + 1/3\,\frac{Dzzttttt}{hz^4\,ht},$$

$$D[2,\,2,\,2,\,2,\,2](f)(0,\,0) = \frac{Dttttt}{ht^5} - 5/2\,\frac{Dtttttt}{ht^5} + 25/6\,\frac{Dttttttt}{ht^5},$$

$$D[1,\,1,\,1,\,1,\,1,\,1](f)(0,\,0) = \frac{Dzzzzzz}{hz^6} - 3\,\frac{Dzzzzzzz}{hz^6},$$

$$D[1,\,1,\,1,\,1,\,1,\,2](f)(0,\,0) = \frac{Dzzzzzt}{hz^5\,ht} - 1/2\,\frac{Dzzzzztt}{hz^5\,ht} - 5/2\,\frac{Dzzzzzzt}{hz^5\,ht},$$

$$D[1,\,1,\,1,\,1,\,2,\,2](f)(0,\,0) = \frac{Dzzzztt}{hz^4\,ht^2} - \frac{Dzzzzttt}{hz^4\,ht^2} - 2\,\frac{Dzzzzztt}{hz^4\,ht^2},$$

$$D[1,\,1,\,1,\,2,\,2,\,2](f)(0,\,0) = \frac{Dzzttt}{hz^3\,ht^3} - 3/2\,\frac{Dzzttttt}{hz^3\,ht^3} - 3/2\,\frac{Dzzzttt}{hz^3\,ht^3},$$

$$D[1,\,1,\,2,\,2,\,2,\,2](f)(0,\,0) = \frac{Dzttttt}{hz^2\,ht^4} - 2\,\frac{Dzttttt}{hz^2\,ht^4} - \frac{Dzzttttt}{hz^2\,ht^4},$$

$$D[1,\,2,\,2,\,2,\,2,\,2](f)(0,\,0) = \frac{Dttttt}{hz\,ht^5} - 5/2\,\frac{Dtttttt}{hz\,ht^5} - 1/2\,\frac{Dzttttt}{hz\,ht^5},$$

$$D[2,\,2,\,2,\,2,\,2,\,2](f)(0,\,0) = \frac{Dttttt}{ht^6} - 3\,\frac{Dttttttt}{ht^6},$$

3.2 Derivatives from Backward Differences

These differences are identical to the forward differences, except for the sign. None of the coefficients of the backward differences have a negative sign.

Only two derivatives are shown as an example.

$$D[1](f)(0, 0) =$$

$$\frac{Dz}{hz} + 1/2\,\frac{Dzz}{hz} + 1/3\,\frac{Dzzz}{hz} + 1/4\,\frac{Dzzzz}{hz} + 1/5\,\frac{Dzzzzz}{hz} + 1/6\,\frac{Dzzzzzz}{hz} + 1/7\,\frac{Dzzzzzzz}{hz},$$

$$D[2](f)(0, 0) =$$

$$\frac{Dt}{ht} + 1/2\,\frac{Dtt}{ht} + 1/3\,\frac{Dttt}{ht} + 1/4\,\frac{Dtttt}{ht} + 1/5\,\frac{Dttttt}{ht} + 1/6\,\frac{Dtttttt}{ht} + 1/7\,\frac{Dttttttt}{ht},$$

etc.

3.3 Derivatives from Central Differences

The central difference is heuristically considered the appropriate difference. As is shown, it exhibits much better convergence.

$$D[1](f)(0, 0) = \frac{Dz}{hz} - 1/6\,\frac{Dzzz}{hz} + 3/40\,\frac{Dzzzzz}{hz} - 5/112\,\frac{Dzzzzzzz}{hz},$$

$$D[2](f)(0, 0) = \frac{Dt}{ht} - 1/6\,\frac{Dttt}{ht} + 3/40\,\frac{Dttttt}{ht} - 5/112\,\frac{Dttttttt}{ht},$$

$$D[1, 1](f)(0, 0) = \frac{Dzz}{hz^2} - 1/3\,\frac{Dzzzz}{hz^2} + 8/45\,\frac{Dzzzzzz}{hz^2},$$

$$D[1, 2](f)(0, 0) =$$

$$\frac{Dzt}{hz\,ht} - 1/6\,\frac{Dzttt}{hz\,ht} - 1/6\,\frac{Dzzzt}{hz\,ht} + 3/40\,\frac{Dztttt}{hz\,ht} + 1/36\,\frac{Dzzttt}{hz\,ht} + 3/40\,\frac{Dzzzzt}{hz\,ht}$$

,

$$D[2, 2](f)(0, 0) = \frac{Dtt}{ht^2} - 1/3\,\frac{Dtttt}{ht^2} + 8/45\,\frac{Dttttt}{ht^2},$$

$$D[1,1,1](f)(0,0) = \frac{Dzzz}{hz^3} - \frac{1}{2}\frac{Dzzzzz}{hz^3} + \frac{37}{120}\frac{Dzzzzzzz}{hz^3},$$

$$D[1,1,2](f)(0,0) = \frac{Dzzt}{hz^2\,ht} - \frac{1}{6}\frac{Dzztt}{hz^2\,ht} - \frac{1}{3}\frac{Dzzzzt}{hz^2\,ht} + \frac{3}{40}\frac{Dzzttttt}{hz^2\,ht} + \frac{1}{18}\frac{Dzzzzttt}{hz^2\,ht} + \frac{8}{45}\frac{Dzzzzzzt}{hz^2\,ht},$$

$$D[1,2,2](f)(0,0) = \frac{Dztt}{hz\,ht^2} - \frac{1}{3}\frac{Dzttt}{hz\,ht^2} - \frac{1}{6}\frac{Dzzztt}{hz\,ht^2} + \frac{8}{45}\frac{Dzttttt}{hz\,ht^2} + \frac{1}{18}\frac{Dzzzttt}{hz\,ht^2} + \frac{3}{40}\frac{Dzzzzzt}{hz\,ht^2},$$

$$D[2,2,2](f)(0,0) = \frac{Dttt}{ht^3} - \frac{1}{2}\frac{Dttttt}{ht^3} + \frac{37}{120}\frac{Dttttttt}{ht^3},$$

$$D[1,1,1,1](f)(0,0) = \frac{Dzzzz}{hz^4} - \frac{2}{3}\frac{Dzzzzzz}{hz^4},$$

$$D[1,1,1,2](f)(0,0) = \frac{Dzzzt}{hz^3\,ht} - \frac{1}{6}\frac{Dzzzttt}{hz^3\,ht} - \frac{1}{2}\frac{Dzzzzzt}{hz^3\,ht},$$

$$D[1,1,2,2](f)(0,0) = \frac{Dzztt}{hz^2\,ht^2} - \frac{1}{3}\frac{Dzztttt}{hz^2\,ht^2} - \frac{1}{3}\frac{Dzzzztt}{hz^2\,ht^2},$$

$$D[1,2,2,2](f)(0,0) = \frac{Dzttt}{hz\,ht^3} - \frac{1}{2}\frac{Dztttttt}{hz\,ht^3} - \frac{1}{6}\frac{Dzzzttt}{hz\,ht^3},$$

$$D[2,2,2,2](f)(0,0) = \frac{Dtttt}{ht^4} - \frac{2}{3}\frac{Dttttt}{ht^4},$$

$$D[1,1,1,1,1](f)(0,0) = \frac{Dzzzzz}{hz^5} - \frac{5}{6}\frac{Dzzzzzzz}{hz^5},$$

$$D[1,1,1,1,2](f)(0,0) = \frac{Dzzzzt}{hz\,ht^4} - \frac{1}{6}\frac{Dzzzzttt}{hz\,ht^4} - \frac{2}{3}\frac{Dzzzzzzt}{hz\,ht^4},$$

$$D[1,1,1,2,2](f)(0,0) = \frac{Dzzztt}{hz^3\,ht^2} - \frac{1}{3}\frac{Dzzzttttt}{hz^3\,ht^2} - \frac{1}{2}\frac{Dzzzzztt}{hz^3\,ht^2},$$

$$D[1,1,2,2,2](f)(0,0) = \frac{Dzzttt}{hz^2\,ht^3} - \frac{1}{2}\frac{Dzzttttt}{hz^2\,ht^3} - \frac{1}{3}\frac{Dzzzzttt}{hz^2\,ht^3},$$

$$D[1,2,2,2,2](f)(0,0) = \frac{Dzttttt}{hz\,ht^4} - \frac{2}{3}\frac{Dztttttt}{hz\,ht^4} - \frac{1}{6}\frac{Dzzztttt}{hz\,ht^4},$$

$$D[2,2,2,2,2](f)(0,0) = \frac{Dttttt}{ht^5} - \frac{5}{6}\frac{Dttttttt}{ht^5},$$

3.4 Derivatives from Mixed Differences

The following table is the solution sol as calculated using the program mdel.mpl of Section 5.1.4 for mixed differences.

$$D[1](f)(0,0) = \frac{Dz}{hz} + \frac{1}{2}\frac{Dzz}{hz} - \frac{1}{6}\frac{Dzzz}{hz} + \frac{1}{80}\frac{Dzzzzz}{hz} - \frac{3}{1792}\frac{Dzzzzzzz}{hz},$$

$$D[2](f)(0,0) = \frac{Dt}{ht} - \frac{1}{2}\frac{Dtt}{ht} - \frac{1}{6}\frac{Dttt}{ht} + \frac{1}{80}\frac{Dttttt}{ht} - \frac{3}{1792}\frac{Dttttttt}{ht},$$

$$D[1, 1](f)(0, 0) = \frac{Dzz}{hz^2} - \frac{1}{12}\frac{Dzzzz}{hz^2} + \frac{1}{90}\frac{Dzzzzzz}{hz^2},$$

$$D[1, 2](f)(0, 0) = \frac{Dzt}{hz\,ht} - \frac{1}{24}\frac{Dzttt}{hz\,ht} - \frac{1}{24}\frac{Dzzzt}{hz\,ht} + \frac{3}{640}\frac{Dztttt}{hz\,ht}$$
$$+ \frac{1}{576}\frac{Dzzzttt}{hz\,ht} + \frac{3}{640}\frac{Dzzzzzt}{hz\,ht},$$

$$D[2, 2](f)(0, 0) = \frac{Dtt}{ht^2} - \frac{1}{12}\frac{Dtttt}{ht^2} + \frac{1}{90}\frac{Dttttt}{ht^2},$$

$$D[1, 1, 1](f)(0, 0) = \frac{Dzzz}{hz^3} - \frac{1}{8}\frac{Dzzzzz}{hz^3} + \frac{37}{1920}\frac{Dzzzzzzz}{hz^3},$$

$$D[1, 1, 2](f)(0, 0) = \frac{Dzzt}{hz^2\,ht} - \frac{1}{24}\frac{Dzztt}{hz^2\,ht} - \frac{1}{12}\frac{Dzzzzt}{hz^2\,ht}$$
$$+ \frac{3}{640}\frac{Dzztttt}{hz^2\,ht} + \frac{1}{288}\frac{Dzzzzttt}{hz^2\,ht} + \frac{1}{90}\frac{Dzzzzzzt}{hz^2\,ht},$$

$$D[1, 2, 2](f)(0, 0) = \frac{Dztt}{hz\,ht^2} - \frac{1}{12}\frac{Dzttt}{hz\,ht^2} - \frac{1}{24}\frac{Dzzztt}{hz\,ht^2}$$
$$+ \frac{1}{90}\frac{Dzttttt}{hz\,ht^2} + \frac{1}{288}\frac{Dzzzttt}{hz\,ht^2} + \frac{3}{640}\frac{Dzzzzzt}{hz\,ht^2},$$

$$D[2, 2, 2](f)(0, 0) = \frac{Dttt}{ht^3} - \frac{1}{8}\frac{Dtttt}{ht^3} + \frac{37}{1920}\frac{Dttttttt}{ht^3},$$

$$D[1, 1, 1, 1](f)(0, 0) = \frac{Dzzzz}{hz^4} - \frac{1}{6}\frac{Dzzzzzz}{hz^4},$$

$$D[1,1,1,2](f)(0,0) = \frac{Dzzzt}{hz^3\,ht} - \frac{1}{24}\frac{Dzzzttt}{hz^3\,ht} - \frac{1}{8}\frac{Dzzzzzt}{hz^3\,ht},$$

$$D[1,1,2,2](f)(0,0) = \frac{Dzztt}{hz^2\,ht^2} - \frac{1}{12}\frac{Dzzttt}{hz^2\,ht^2} - \frac{1}{12}\frac{Dzzzztt}{hz^2\,ht^2},$$

$$D[1,2,2,2](f)(0,0) = \frac{Dzttt}{hz\,ht^3} - \frac{1}{8}\frac{Dzttttt}{hz\,ht^3} - \frac{1}{24}\frac{Dzzzttt}{hz\,ht^3},$$

$$D[2,2,2,2](f)(0,0) = \frac{Dtttt}{ht^4} - \frac{1}{6}\frac{Dttttt}{ht^4},$$

$$D[1,1,1,1,1](f)(0,0) = \frac{Dzzzzz}{hz^5} - \frac{5}{24}\frac{Dzzzzzzz}{hz^5},$$

$$D[1,1,1,1,2](f)(0,0) = \frac{Dzzzzt}{hz^4\,ht} - \frac{1}{24}\frac{Dzzzzttt}{hz^4\,ht} - \frac{1}{6}\frac{Dzzzzzzt}{hz^4\,ht},$$

$$D[1,1,1,2,2](f)(0,0) = \frac{Dzzztt}{hz^3\,ht^2} - \frac{1}{12}\frac{Dzzzttt}{hz^3\,ht^2} - \frac{1}{8}\frac{Dzzzzztt}{hz^3\,ht^2},$$

$$D[1,1,2,2,2](f)(0,0) = \frac{Dzzttt}{hz^2\,ht^3} - \frac{1}{8}\frac{Dzzttttt}{hz^2\,ht^3} - \frac{1}{12}\frac{Dzzzzttt}{hz^2\,ht^3},$$

$$D[1,2,2,2,2](f)(0,0) = \frac{Dzttttt}{hz\,ht^4} - \frac{1}{6}\frac{Dztttttt}{hz\,ht^4} - \frac{1}{24}\frac{Dzzzttttt}{hz\,ht^4},$$

$$D[2,2,2,2,2](f)(0,0) = \frac{Dttttt}{ht^5} - \frac{5}{24}\frac{Dttttttt}{ht^5},$$

4 Expanding the Advection/Dispersion/Sorption Equation

The finite difference expansions for the derivatives are now substituted into the Equation. First the whole linear portion of the equation is expanded into a Taylor series in the two variables. Substitution for the derivatives evaluated at (0,0) gives the finite difference expansion form for the linear part of the equation. Then the non-linear, sorption term is expanded. C^n is considered as a logarithmic Taylor Expansion and, again, a substitution converts the derivatives at (0,0) to the equivalent finite difference form. The t^m term is also expanded in a series and multiplied by the C^n term. The combined sorption term is then differentiated and subtracted from the linear form. Note that all expansions are done with reference to the start of the time step and that x and y become hx and hy at the end of the steps. Also, all the substitutions are done with the mixed difference expansion to follow normal useage. Expansions are to 5^{th} order[2].

4.1 Linear Advection/Dispersion Equation

The general form of this equation is:

$$\frac{\partial C}{\partial y} = D \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial y} \tag{3}$$

The variables x and y are purposely used instead of z and t and little 'd' is used in place of 'D'. This is essential to allow for a recognition of the order of the expansion in terms of the arbitrary variable $t \equiv 1$. It also allows the normal operator convention for 'D'.

The result of this expansion is:

[2]In this manuscript, the order of a term is defined as a combined difference level associated with the both the difference in the dependent variable and the increment in the independent variable. That is, an ordinary first derivative, approximated by finite differences would be of zero order, as would a second derivative, etc. Only when there are more differences in the numerator than the denominator does the order go to one or two or three or more. We will use the common multiplier ($t \equiv 1$) to take account of the order with t^2 multiplying a second order difference, t^3 multiplying a third order difference, etc.

Terms of order 0

$$-\frac{v\,Dx}{hx}-\frac{Dy}{hy}+\frac{d\,Dxx}{2\,hx}$$

Terms of order 1

$$\left(-3/2\,\frac{v\,Dxx}{hx}+\left(-\frac{v}{hx}-\frac{1}{hy}\right)Dxy-1/2\,\frac{Dyy}{hy}+\frac{d\,Dxxx}{2\,hx}+\frac{d\,Dxxy}{2\,hx}\right)t$$

Terms of order 2

$$\left(-1/3\,\frac{v\,Dxxx}{hx}+\left(-\frac{v}{hx}-\frac{1}{2\,hy}\right)Dxxy+\left(-1/2\,\frac{v}{hx}-\frac{1}{hy}\right)Dxyy-1/3\,\frac{Dyyy}{hy}+5/12\,\frac{d\,Dxxxx}{2\,hx}+\frac{d\,Dxxxy}{2\,hx}+1/2\,\frac{d\,Dxxyy}{2\,hx}\right)t^2$$

Terms of order 3

$$\left(-1/12\,\frac{v\,Dxxxx}{hx}+\left(-\frac{1}{8\,hy}-\frac{11}{24}\,\frac{v}{hx}\right)Dxxxy+\left(-1/2\,\frac{v}{hx}-\frac{1}{2\,hy}\right)Dxxyy+\left(\frac{11}{24\,hy}-1/8\,\frac{v}{hx}\right)Dxyyy-1/12\,\frac{Dyyyy}{hy}+1/24\,\frac{d\,Dxxxxx}{2\,hx}+5/12\,\frac{d\,Dxxxxy}{2\,hx}+1/2\,\frac{d\,Dxxxyy}{2\,hx}+1/8\,\frac{d\,Dxxyyy}{2\,hx}\right)t^3$$

Terms of order 4

$$\left(1/120\,\frac{v\,Dxxxxx}{hx}-1/12\,\frac{v\,Dxxxxy}{hx}+\left(-\frac{1}{8\,hy}-\frac{11}{48}\,\frac{v}{hx}\right)Dxxxyy+\left(\frac{11}{48\,hy}-1/8\,\frac{v}{hx}\right)Dxxyyy-1/12\,\frac{Dxyyyy}{hy}+1/120\,\frac{Dyyyyy}{hy}\right)t^4$$

Here, the 4^{th} order terms are very likely affected by the size of the chosen grid. The difference table pyramid converges at the top and becomes limited by the size chosen at the bottom. In other words, the choice of a larger base might have slightly more terms at high orders.

Nevertheless, the first order terms clearly show the numerical diffusion from the upstream spatial difference; this produces a second derivative form and effectively alters the dispersion coefficient d. Also, this differencing produces derivatives of nearly every order (see Section 3.3)

4.2 Function to a Power

Here the ln of the C^n term is expanded in a power series

Terms of order 0

$$Co^n$$

Terms of order 1

$$\frac{n\ Co^n\ t\ (Dx + Dy)}{Co}$$

Terms of order 2

$$n\ Co^n\ t^2\ ((-1/2 + 1/2\ n)\ Dx^2 + (n - 1)\ Dy\ Dx + (-1/2 + 1/2\ n)\ Dy^2 + Dxx\ Co + Dxy\ Co)\ /\ Co^2$$

Terms of order 3

$$n\ Co^n\ t^3\ ((-1/2\ n + 1/6\ n^2 + 1/3)\ Dx^3 + (-3/2\ n + 1/2\ n^2 + 1)\ Dy\ Dx^2 + ((-3/2\ n + 1/2\ n^2 + 1)\ Dy^2 + (n - 1)\ Co\ Dxx + (n - 1)\ Co\ Dxy)\ Dx + (-1/2\ n + 1/6\ n^2 + 1/3)\ Dy^3 + ((n - 1)\ Co\ Dxx + (n - 1)\ Co\ Dxy)\ Dy$$

```
                    2             2    /   3
        + 1/2 Dxxy Co  + 1/2 Dxyy Co ) /  Co
                                      /

                              Terms of order 4

    n  4  / 11          2         3      \   4
n Co  t  (|---- n - 1/4 n  + 1/24 n  - 1/4| Dx
          \ 24                            /

          2                   3          3
     + (- n  + 11/6 n + 1/6 n  - 1) Dy Dx

                              2         3    2                          2
     + ((- 3/2 + 11/4 n - 3/2 n  + 1/4 n ) Dy  + %1 Co Dxx + %1 Co Dxy) Dx  + (

        2                   3          3
    (- n  + 11/6 n + 1/6 n  - 1) Dy

          2                        2
     + ((n  + 2 - 3 n) Co Dxx + (n  + 2 - 3 n) Co Dxy) Dy

                          2                        2
     + (- 1/2 + 1/2 n) Co  Dxxy + (- 1/2 + 1/2 n) Co  Dxyy) Dx

       / 11          2         3      \   4                          2
     + |---- n - 1/4 n  + 1/24 n  - 1/4| Dy  + (%1 Co Dxx + %1 Co Dxy) Dy
       \ 24                            /

                          2                        2
     + ((- 1/2 + 1/2 n) Co  Dxxy + (- 1/2 + 1/2 n) Co  Dxyy) Dy

                          2    2              2
     + (- 1/2 + 1/2 n) Co  Dxx  + (n - 1) Co  Dxy Dxx

                          2    2              3              3              3
     + (- 1/2 + 1/2 n) Co  Dxy  + 1/8 Dxxxy Co  + 1/4 Dxxyy Co  + 1/8 Dxyyy Co

        /   4
    ) /  Co
     /

                                        2
%1 :=                       - 3/2 n + 1/2 n  + 1
```

Noteworthy here is the fact that this form has no dependence whatever on the value of the increments hx and hy. This means that the function and its powers are determined wholly by the difference values. This follows from a difference table where one makes up the function from the differences. The whole function is simply a sum of its parts; it doesn't depend on the size of the parts. All the parts are there in the sum.

4.3 The time term y^m

This is a simple series derived from Newton's Binonial Theorem. It is only affected by changes in time and the value of hy at the end of the time increment. Remember that C^n and t^m are combined and then differentiated. The differentiation cannot be done on this form since since it has already been evaluated at $y = hy$.

$$tm := yo^m \left(1 + \frac{m\,hy}{yo} + 1/2\,\frac{m\,(m-1)\,hy^2}{yo^2} + 1/6\,\frac{m\,(m-1)\,(m-2)\,hy^3}{yo^3}\right.$$

$$+ 1/24\,\frac{m\,(m-1)\,(m-2)\,(m-3)\,hy^4}{yo^4}$$

$$+ 1/120\,\frac{m\,(m-1)\,(m-2)\,(m-3)\,(m-4)\,hy^5}{yo^5}$$

$$\left. + 1/720\,\frac{m\,(m-1)\,(m-2)\,(m-3)\,(m-4)\,(m-5)\,hy^6}{yo^6}\right)$$

The variable y (or the time) remains in this form. This term is combined with the C^n term of the last section and the kinetic constant k to make the full non-linear term.

4.4 The Non-Linear Term

The full term is a combination of the forms of the last two sections. When differentiated, it completes the mass balance requirement of the full equation (1).

```
                Terms of order 0

                  n   m /  m      Dy \
              n k Co  yo |---- + -----|
                         \yo n   hy Co/
```

Terms of order 1

$$t^{n}\,k\,Co^{m}\,yo\left(\left|\frac{1}{2}\,\frac{(2n^{2}-2n)\,Dy}{n\,Co\,hy}+\frac{m}{yo}\right|Dx+\frac{1}{2}\,\frac{(2n^{2}-2n)\,Dy^{2}}{n\,Co\,hy}+2\,\frac{Dy\,m}{yo}+\frac{Dxy}{hy}+\frac{1}{2}\,\frac{(-2m+2m^{2})\,Co\,hy}{yo^{2}\,n}+\frac{1}{2}\,\frac{Dyy}{hy}\right)/Co$$

Terms of order 2

$$t^{2}\,n\,k\,Co^{m}\,yo\left(\left|\frac{1}{6}\,\frac{(3n^{3}+6n^{2}-9n)\,Dy}{n\,Co\,hy}+\frac{1}{6}\,\frac{3mn^{2}-3mn}{n\,yo}\right|Dx^{2}+\left(\frac{1}{6}\,\frac{(6n^{3}+12n^{2}-18n^{2})\,Dy^{2}}{n\,Co\,hy}+\frac{1}{6}\,\frac{(12mn^{2}-12mn)\,Dy}{n\,yo}+\frac{1}{6}\,\frac{(-6n+6n^{2})\,Dxy}{n\,hy}+\frac{1}{6}\,\frac{(3n^{2}-3n)\,Dyy}{n\,hy}+\frac{1}{6}\,\frac{(-6mn+6mn^{2})\,Co\,hy}{n\,yo^{2}}\right)Dx+\frac{1}{6}\,\frac{(3n^{3}+6n^{2}-9n)\,Dy^{2}}{n\,Co\,hy}+\frac{1}{6}\,\frac{(9mn^{2}-9mn)\,Dy^{2}}{n\,yo}+\left(\frac{1}{6}\,\frac{(-6n+6n^{2})\,Dxx}{n\,hy}+\frac{1}{6}\,\frac{(-12n+12n^{2})\,Dxy}{n\,hy}+\frac{1}{6}\,\frac{(3n^{2}-3n)\,Dyy}{n\,hy}+\frac{1}{6}\,\frac{(9m^{2}n-9mn)\,Co\,hy}{n\,yo^{2}}\right)Dy+\frac{m\,Co\,Dxx}{yo}+2\,\frac{m\,Co\,Dxy}{yo}+\frac{1}{2}\,\frac{m\,Dyy\,Co}{yo}$$

$$+ \frac{1}{2}\frac{Co\ Dxxy}{hy} + \frac{Co\ Dxyy}{hy} + \frac{1}{6}\frac{(-9\,m^2 + 3\,m^3 + 6\,m)\,Co^2\,hy^2}{yo^3\,n^3} + \frac{1}{3}\frac{Dyyy\,Co}{hy})$$

$$\left(\frac{Co^2}{}\right.$$

Terms of order 3

$$t^3\,n^n\,k\,Co^m\,yo^m\,($$

$$\left(\frac{1/24}{n\,Co\,hy}\right.\left.\frac{(44\,n^2 - 24\,n^4 + 4\,n^3 - 24\,n^3)\,Dy}{}\right. + \left.\frac{1/24}{n\,yo}\right.\left.\frac{4\,m\,n^3 + 8\,m\,n^3 - 12\,m\,n^2}{}\right|^3 Dx)$$

$$+ \frac{(1/24}{n\,Co\,hy}\frac{(-72\,n^4 + 12\,n^2 + 132\,n^3 - 72\,n^3)\,Dy}{}$$

$$+ \frac{1/24}{n\,yo}\frac{(48\,m\,n^3 + 24\,m\,n^2 - 72\,m\,n^2)\,Dy}{} + \frac{1/24}{n\,hy}\frac{(24\,n^3 + 12\,n^2 - 36\,n^2)\,Dxy}{}$$

$$+ \frac{1/24}{n\,hy}\frac{(6\,n^3 + 12\,n^2 - 18\,n^2)\,Dyy}{}$$

$$+ \frac{1/24}{n^2\,yo^2}\frac{(-12\,m\,n^2 + 12\,m\,n^2 + 12\,m^2\,n^2 - 12\,m^2\,n)\,Co\,hy^2}{})\,Dx^2 + ($$

$$\frac{1/24}{n\,Co\,hy}\frac{(-72\,n^4 + 12\,n^2 + 132\,n^3 - 72\,n^3)\,Dy}{}$$

$$+ \frac{1/24}{n\,yo}\frac{(72\,m\,n^3 + 36\,m\,n^2 - 108\,m\,n^2)\,Dy}{} + ($$

$$1/24\ \frac{(24\,n^3 - 72\,n^2 + 48\,n)\,Dxx}{n\,hy} + 1/24\ \frac{(-144\,n^2 + 96\,n + 48\,n^3)\,Dxy}{n\,hy}$$

$$+ 1/24\ \frac{(24\,n + 12\,n^3 - 36\,n^2)\,Dyy}{n\,hy}$$

$$+ 1/24\ \frac{(36\,m\,n - 36\,m\,n^2 - 36\,m^2\,n + 36\,m^2\,n^2)\,Co\,hy}{n\,yo^2}\Big)\,Dy$$

$$+ 1/24\ \frac{(24\,m\,n^2 - 24\,m\,n)\,Co\,Dxx}{n\,yo} + 1/24\ \frac{(48\,m\,n^2 - 48\,m\,n)\,Co\,Dxy}{n\,yo}$$

$$+ 1/24\ \frac{(12\,m\,n^2 - 12\,m\,n)\,Co\,Dyy}{n\,yo} + 1/24\ \frac{(-12\,n + 12\,n^2)\,Co\,Dxxy}{n\,hy}$$

$$+ 1/24\ \frac{\%1\,Co\,Dxyy}{n\,hy} + 1/24\ \frac{(8\,n^2 - 8\,n)\,Co\,Dyyy}{n\,hy}$$

$$+ 1/24\ \frac{(-36\,m^2\,n + 12\,m^3\,n + 24\,m\,n)\,Co^2\,hy}{n\,yo^3}\Big)\,Dx$$

$$+ 1/24\ \frac{(44\,n^2 - 24\,n + 4\,n^4 - 24\,n^3)\,Dy}{n\,Co\,hy}$$

$$+ 1/24\ \frac{(16\,m\,n^3 + 32\,m\,n^2 - 48\,m\,n^3)\,Dy}{n\,yo} + (1/24\ \frac{(24\,n^3 - 72\,n^2 + 48\,n)\,Dxx}{n\,hy}$$

$$+ 1/24\ \frac{(-108\,n^2 + 36\,n^3 + 72\,n)\,Dxy}{n\,hy} + 1/24\ \frac{(6\,n^3 + 12\,n - 18\,n^2)\,Dyy}{n\,hy}$$

$$+ \frac{1}{24}\frac{(24\,m^2\,n^2 - 24\,m\,n^2 + 24\,m\,n - 24\,m^2\,n)\,Co\,hy^2}{n^2\,yo^2}\,Dy^2 + \left(\right.$$

$$\frac{1}{24}\frac{(48\,m\,n^2 - 48\,m\,n)\,Co\,Dxx}{n\,yo} + \frac{1}{24}\frac{(-72\,m\,n + 72\,m\,n^2)\,Co\,Dxy}{n\,yo}$$

$$+ \frac{1}{24}\frac{(12\,m\,n^2 - 12\,m\,n)\,Co\,Dyy}{n\,yo} + \frac{1}{24}\frac{\%1\,Co\,Dxxy}{n\,hy}$$

$$+ \frac{1}{24}\frac{(-36\,n + 36\,n^2)\,Co\,Dxyy}{n\,hy} + \frac{1}{24}\frac{(8\,n^2 - 8\,n)\,Co\,Dyyy}{n\,hy}$$

$$+ \frac{1}{24}\frac{(32\,m\,n + 16\,m^3\,n^2 - 48\,m^2\,n)\,Co^2\,hy^2}{n^3\,yo^3}\,Dy + \left(\frac{1}{24}\frac{\%1\,Co\,Dxy}{n\,hy}\right.$$

$$+ \frac{1}{24}\frac{(-12\,n + 12\,n^2)\,Co\,Dyy}{n\,hy} + \frac{1}{24}\frac{(-24\,m\,n + 24\,m^2\,n)\,Co^2\,hy^2}{n^2\,yo^2}\,Dxx$$

$$+ \frac{1}{24}\frac{\%1\,Co\,Dxy^2}{n\,hy}$$

$$+ \left|\frac{1}{24}\frac{(-12\,n + 12\,n^2)\,Co\,Dyy}{n\,hy} + \frac{1}{24}\frac{(-36\,m\,n + 36\,m^2\,n)\,Co^2\,hy^2}{n^2\,yo^2}\right|\,Dxy$$

$$+ \frac{1}{24}\frac{(6\,m^2\,n - 6\,m\,n)\,Co^2\,hy\,Dyy}{n^2\,yo^2} + \frac{m\,Co^2\,Dxxy}{yo} + \frac{3}{2}\frac{m\,Co^2\,Dxyy}{yo}$$

```
                  2          2                2               2
         m Dyyy Co         Co  Dxxxy        Co  Dxxyy    11  Co  Dxyyy
   + 1/3 ---------- + 1/8 --------- + 1/2 --------- + ---- ---------
             yo                hy               hy        24      hy

                      4        2       3    3   3                 2
         (- 24 m + 4 m  + 44 m  - 24 m ) Co  hy          Dyyyy Co       /   3
   + 1/24 --------------------------------------- + 1/12 ---------)   /  Co
                             4                                hy      /
                         yo  n

                                                 2
    %1 :=                           - 24 n + 24 n
```

Only three orders of the terms are shown to save space.

4.5 The Full Expression

This is the entire equation converted to finite difference form. Note that it is rather arbitrary what is intended by order. Here we chose to attach an arbitrary factor $t \equiv 1$ to each of the differences and each hx and hy. The result is that the simpliest expansion is that of zero order. We consider later how to deal with the higher order terms. The listing below is configured to give a simplest expression but not necessarily the one that is the most useful. Note that $R - 1 = Co^{n-1} \cdot n \cdot k \cdot yo^m$.

```
                                  Terms of Order 0

                            d Dxx    v Dx    R Dy    m Co (R - 1)
                            ----- - ---- - ---- - ------------
                              2      hx      hy        n yo
                            hx

                                  Terms of Order 1
  /         2 \
  |        m  |
  |m/n - ----| Co (R - 1) hy
  \        n /                    d Dxxx    d Dxxy      m (R - 1) Dy
  -------------------------- + ------ + ------ - 2 ------------
                2                   2         2             yo
              yo                  hx        hx

       /        R - 1      1 \          /    v       1     R - 1\          m (R - 1) Dx
     + |- 1/2 ----- - ----| Dyy + |- ---- - ---- - -----| Dxy - ------------
       \          hy     2 hy/          \    hx      hy      hy /              yo
```

$$- 3/2 \frac{v\ Dxx}{hx} + \frac{\left(\frac{1}{hy} - \frac{n}{hy}\right)(R - 1)\ Dy^2}{Co} + \frac{\left(\frac{1}{hy} - \frac{n}{hy}\right)(R - 1)\ Dy\ Dx}{Co}$$

Terms of Order 2

$$\frac{\left(\frac{3}{2}\frac{m^2}{n} - m/n - 1/2\frac{m^3}{n}\right) Co\ (R - 1)\ hy^2}{yo^3} + \left(\frac{R - 1}{hy} - 1/2\frac{v}{hx} - \frac{1}{hy}\right) Dxyy$$

$$+ 1/2\frac{d\ Dxyy}{hx^2} + \frac{d\ Dxxy}{hx^2} + 5/12\frac{d\ Dxxx}{hx^2} - 1/3\frac{v\ Dxxx}{hx}$$

$$+ \left(1/3\frac{R - 1}{hy} - \frac{1}{3\ hy}\right) Dyyy + \left(1/2\frac{R - 1}{hy} - \frac{1}{2\ hy} - \frac{v}{hx}\right) Dxxy$$

$$+ \frac{(3/2\ m - 3/2\ m^2)\ (R - 1)\ hy\ Dy}{yo^2} - 1/2\frac{m\ (R - 1)\ Dyy}{yo} - 2\frac{m\ (R - 1)\ Dxy}{yo}$$

$$+ \frac{(- m^2 + m)\ (R - 1)\ hy\ Dx}{yo^2} - \frac{m\ (R - 1)\ Dxx}{yo}$$

$$+ \frac{(- 3/2\ m\ n + 3/2\ m)\ (R - 1)\ Dy^2}{Co\ yo} + \frac{(1/2\ m - 1/2\ m\ n)\ (R - 1)\ Dx^2}{Co\ yo}$$

$$+ \frac{\left(\frac{1}{hy} - \frac{n}{hy}\right)(R - 1)\ Dxy\ Dx}{Co} + \frac{\left(3\frac{n}{hy} - 2\frac{n^2}{hy}\right)(R - 1)\ Dy^2\ Dx}{Co^2}$$

$$+ \frac{\left(\frac{3}{2}\frac{n}{hy} - \frac{1}{2}\frac{n^2}{hy} - \frac{1}{hy^2}\right)(R-1)\,Dyy\,Dy\,Dx}{Co^2}$$

$$+ \frac{\left(-\frac{1}{2}\frac{n}{hy} + \frac{1}{2\,hy}\right)(R-1)\,Dyy\,Dxx}{Co} + \frac{\left(\frac{1}{hy} - \frac{n}{hy^2}\right)(R-1)\,Dxy^2}{Co}$$

$$+ \frac{\left(\frac{1}{hy} - \frac{n}{hy^2}\right)(R-1)\,Dxy\,Dxx}{Co} + \frac{\left(-\frac{1}{2}\frac{n}{hy} + \frac{1}{2\,hy}\right)(R-1)\,Dxxy\,Dx}{Co}$$

$$+ \frac{\left(\frac{3}{2}\frac{n}{hy} - \frac{1}{2}\frac{n^2}{hy} - \frac{1}{hy^2}\right)(R-1)\,Dxy\,Dx^2}{Co^2}$$

$$+ \frac{(2m - 2mn)(R-1)\,Dxy\,Dx}{Co\ yo}$$

$$+ \frac{\left(-\frac{3}{2}mn^2 + \frac{9}{2}mn - 3m\right)(R-1)\,Dy^2\,Dx}{Co^2\ yo}$$

$$+ \frac{(2m - 2mn)(R-1)\,Dy\,Dxx}{Co\ yo} + \frac{\left(\frac{1}{3\,hy} - \frac{1}{hy^2}\right)(R-1)\,Dyyy\,Dy}{Co}$$

$$+ \frac{(m - mn)(R-1)\,Dxx\,Dx}{Co\ yo} + \frac{\left(\frac{1}{hy} - \frac{n}{hy^2}\right)(R-1)\,Dxxy\,Dy}{Co}$$

$$+\frac{\left(\frac{1}{hy}-\frac{n}{hy}\right)(R-1)\,Dy\,Dxx}{Co}+\frac{\left(\frac{2}{hy}-2\,\frac{n}{hy}\right)(R-1)\,Dxy\,Dy}{Co}$$

$$+\frac{\left(3/2\,\frac{n}{hy}-1/2\,\frac{n^2}{hy}-\frac{1}{hy}\right)(R-1)\,Dy^2\,Dx}{Co^2}$$

$$+\frac{\left(-1/2\,\frac{n}{hy}+\frac{1}{2\,hy}\right)(R-1)\,Dyy\,Dx}{Co}+\frac{\left(-1/2\,\frac{n}{hy}+\frac{1}{2\,hy}\right)(R-1)\,Dyy\,Dy}{Co}$$

$$+\frac{\left(3/2\,\frac{n}{hy}-1/2\,\frac{n^2}{hy}-\frac{1}{hy}\right)(R-1)\,Dy^3}{Co^2}+\frac{(2\,m-2\,m\,n)\,(R-1)\,Dy\,Dx}{Co\;yo}$$

Terms of Order 3

$$1/2\,\frac{d\,Dxxyy}{hx^2}+1/24\,\frac{d\,Dxxxxx}{hx^2}+5/12\,\frac{d\,Dxxxxy}{hx^2}+1/8\,\frac{d\,Dxxyyy}{hx^2}-1/12\,\frac{v\,Dxxxx}{hx}$$

$$+\frac{(-4/3\,m+2\,m\,n-2/3\,m\,n^2)\,(R-1)\,Dy^3}{Co^2\;yo}$$

$$+\frac{(3/2\,m\,n-3/2\,m^2\,n-3/2\,m+3/2\,m^2)\,(R-1)\,hy\,Dy\,Dx}{Co\;yo^2}$$

$$+\frac{(-1/6\,m\,n^2+1/2\,m\,n-1/3\,m)\,(R-1)\,Dx^3}{Co^2\;yo}$$

$$+\int_{Co}\left(\frac{1}{3\,hy}-\frac{1}{3}\left(\frac{n}{hy}\right)\right)(R-1)\,Dyyy\,Dx$$

$$+\int_{Co}\left(-\frac{11}{6}\left(\frac{n}{hy}\right)^{2}+\left(\frac{n}{hy}\right)^{3}-\frac{1}{6}\left(\frac{n}{hy}\right)^{1}+\left(\frac{1}{hy}\right)^{3}\right)(R-1)\,Dy^{3}\,Dx$$

$$+\int_{Co}\left(\frac{3}{4}\left(\frac{n}{hy}\right)^{2}-\frac{1}{4}\left(\frac{n}{hy}\right)^{1}-\left(\frac{1}{2\,hy}\right)^{2}\right)(R-1)\,Dyy\,Dy^{2}$$

$$+\int_{Co}\left(\frac{1}{hy}-\left(\frac{n}{hy}\right)^{1}\right)(R-1)\,Dxyy\,Dx$$

$$+\int_{Co}\left(\frac{3}{4}\left(\frac{n}{hy}\right)^{2}-\frac{1}{4}\left(\frac{n}{hy}\right)^{1}-\left(\frac{1}{2\,hy}\right)^{2}\right)(R-1)\,Dyy\,Dx^{2}$$

$$+\int_{Co}\left(-\frac{3}{2}\left(\frac{n}{hy}\right)^{1}+\left(\frac{1}{2\,hy}\right)^{3}\right)(R-1)\,Dxyy\,Dy$$

$$+\int_{Co}\left(-\frac{1}{2}\left(\frac{n}{hy}\right)^{3}+3\left(\frac{n}{hy}\right)^{2}-\left(\frac{n}{hy}\right)^{3}-\frac{11}{2}\left(\frac{n}{hy}\right)^{1}\right)(R-1)\,Dy^{2}\,Dx^{2}$$

$$+\frac{\left(3\,\frac{n}{hy}-\frac{n^2}{hy}+\frac{n^2}{hy}\right)(R-1)\,Dxx\,Dy\,Dx}{Co^2}$$

$$+\frac{\left(3\,\frac{n}{hy}-\frac{n^2}{hy}+\frac{n^2}{hy}\right)(R-1)\,Dy^2\,Dxx}{Co^2}$$

$$+\frac{\left(-\frac{1}{2}\,m-\frac{1}{2}\,m^2\,n+\frac{1}{2}\,m\,n+\frac{1}{2}\,m^2\right)(R-1)\,hy\,Dx^2}{Co\;yo^2}$$

$$+\frac{\left(-\frac{1}{2}\,\frac{n}{hy}+\frac{1}{2\,hy}\right)(R-1)\,Dyy\,Dxy}{Co}$$

$$+\frac{\left(6\,\frac{n}{hy}-4\,\frac{n}{hy}+2\,\frac{n^2}{hy}\right)(R-1)\,Dxy\,Dy\,Dx}{Co^2}$$

$$+\frac{(3\,m-3\,m\,n)(R-1)\,Dxy\,Dy}{Co\;yo}+\frac{(-2\,m-m\,n^2+3\,m\,n)(R-1)\,Dy\,Dx^2}{Co^2\;yo}$$

$$+\frac{(1/2\,m-1/2\,m\,n)(R-1)\,Dyy\,Dx}{Co\;yo}+\frac{(1/2\,m-1/2\,m\,n)(R-1)\,Dyy\,Dy}{Co\;yo}$$

$$+\frac{\left(-\frac{3}{2}\,\frac{n^2}{hy}-3\,\frac{n}{hy}+\frac{9}{2}\,\frac{n^2}{hy}\right)(R-1)\,Dxy\,Dy^2}{Co^2}$$

$$+ \frac{\left(-\frac{1}{2}\,\frac{n^{3}}{hy} + 3\,\frac{n^{2}}{hy} + \frac{n^{3}}{hy} - \frac{11}{2}\,\frac{n}{hy}\right)(R-1)\,Dy^{3}\,Dx}{Co^{3}}$$

$$+ \frac{\left(\frac{11}{6}\,\frac{n^{2}}{hy} + \frac{n^{3}}{hy} - \frac{1}{6}\,\frac{n^{3}}{hy} + \frac{1}{hy}\right)(R-1)\,Dy^{4}}{Co^{3}} - \frac{1}{3}\,\frac{m\,(R-1)\,Dyyy}{yo}$$

$$- \frac{m\,(R-1)\,Dxxy}{yo} + \frac{(-2/3\,m^{3} + 2\,m^{2} - 4/3\,m)\,(R-1)\,hy^{2}\,Dy}{yo^{3}}$$

$$+ \frac{(1/4\,m^{2} - 1/4\,m)\,(R-1)\,hy\,Dyy}{yo^{2}} + \frac{(3/2\,m^{2} - 3/2\,m)\,(R-1)\,hy\,Dxy}{yo^{2}}$$

$$+ \frac{(-m^{3} - 1/2\,m^{2} + 3/2\,m)\,(R-1)\,hy^{2}\,Dx}{yo^{3}} + \frac{(-m^{2} + m)\,(R-1)\,hy\,Dxx}{yo^{2}}$$

$$+ \frac{(m^{2} - m + m\,n - m^{2}\,n)\,(R-1)\,hy\,Dy^{2}}{Co\,yo^{2}} - \frac{3}{2}\,\frac{m\,(R-1)\,Dxyy}{yo}$$

$$+ \left(\frac{1}{2\,hy} - \frac{1}{2}\,\frac{v}{hx} - \frac{1}{2}\,\frac{R-1}{hy}\right) Dxxyy$$

$$+ \left(\frac{1}{8}\,\frac{R-1}{hy} - \frac{1}{8\,hy} - \frac{11}{24}\,\frac{v}{hx}\right) Dxxxy + \left(\frac{1}{12\,hy} - \frac{1}{12}\,\frac{R-1}{hy}\right) Dyyyy$$

$$+ \left(\frac{11}{24\,hy} - \frac{1}{8}\,\frac{v}{hx} - \frac{11}{24}\,\frac{R-1}{hy}\right) Dxyyy$$

$$+ \frac{\left(-\frac{1}{6}\frac{m^4}{n} + \frac{m^3}{n} + \frac{m}{n} - \frac{11}{6}\frac{m^2}{n}\right) Co\,(R-1)\,hy^3}{yo^4}$$

Terms of Order 4

$$\frac{1}{120}\frac{v\,Dxxxxx}{hx} - \frac{1}{12}\frac{v\,Dxxxxy}{hx} - \frac{3}{4}\frac{m\,(R-1)\,Dxxyy}{yo} - \frac{1}{4}\frac{m\,(R-1)\,Dxxxy}{yo}$$

$$+ \frac{\left(-\frac{1}{6}m^2 + \frac{1}{6}m\right)(R-1)\,hy\,Dyyy}{yo^2} + \frac{\frac{1}{2}(R-1)\,Dxy\,Dxx\,Dx}{Co^2}$$

$$+ \frac{\left(11\frac{n}{hy} + 6\frac{n^2}{hy} + \frac{6}{hy} - \frac{n^3}{hy}\right)(R-1)\,Dxx\,Dy^2\,Dx}{Co^3}$$

$$+ \frac{\left(\frac{3}{2}mn - m - \frac{1}{2}mn^2\right)(R-1)\,Dxx\,Dx^2}{Co^2\,yo} + \frac{\frac{1}{1}(R-1)\,Dxyy\,Dx^2}{Co^2}$$

$$+ \frac{\left(\frac{2}{3}\frac{n^3}{hy} + 4\frac{n^2}{hy} + \frac{4}{hy} - \frac{22}{3}\frac{n}{hy}\right)(R-1)\,Dxy\,Dy^3}{Co^3}$$

$$+ \frac{\frac{1}{2}(R-1)\,Dxy^2\,Dx}{Co^2}$$

$$
\left/ \left| - \frac{1}{2} \frac{n^3}{hy} + 3 \frac{n^2}{hy} + \frac{n^3}{hy} - \frac{11}{2} \frac{n^3}{hy} \right| (R-1)\, Dy\, Dxx\, Dx^2 \right\backslash
$$

$$
+ \int_{Co^3}
$$

$$
\left/ \left| \frac{1}{12} \frac{n^1}{hy} - \frac{1}{12} \frac{n^1}{hy} \right| (R-1)\, Dyyyy\, Dx \right\backslash
$$

$$
+ \int_{Co}
$$

$$
\left/ \left| \frac{3}{2} \frac{n^2}{hy} - \frac{1}{4} \frac{n^3}{hy} + \frac{n^3}{2\,hy} - \frac{11}{4} \frac{n^3}{hy} \right| (R-1)\, Dyy\, Dy\, Dx^2 \right\backslash
$$

$$
+ \int_{Co^3}
$$

$$
\left/ \left| \frac{1}{2} \frac{n^2}{hy} + \frac{11}{12} \frac{n^3}{hy} - \frac{1}{12} \frac{n^3}{hy} \right| (R-1)\, Dyy\, Dx^3 \right\backslash
$$

$$
+ \int_{Co^3}
$$

$$
\left/ \left| - \frac{35}{6} \frac{n^2}{hy} - \frac{n^4}{hy} + \frac{5}{3} \frac{n^3}{hy} - \frac{1}{6} \frac{n^4}{hy} + \frac{25}{3} \frac{n^4}{hy} \right| (R-1)\, Dy^2\, Dx^3 \right\backslash
$$

$$
+ \int_{Co^4}
$$

$$
\%2\,(R-1)\, Dxxy\, Dy\, Dx + \int_{Co^2} \left/ \left| \frac{3}{4} \frac{n^2}{hy} - \frac{1}{4} \frac{n^2}{hy} - \frac{1^1}{2\,hy} \right| (R-1)\, Dxxy\, Dx^2 \right\backslash
$$

$$
+ \int_{Co^2}
$$

$$
\left/ \left| - \frac{1}{2} \frac{n^1}{hy} + \frac{1^1}{2\,hy} \right| (R-1)\, Dxxyy\, Dx \right\backslash
$$

$$
+ \int_{Co}
$$

$$+ \int_{Co^2} \left(-\frac{3}{2}\,\frac{n^2}{hy} - \frac{n^3}{hy} + \frac{9}{2}\,\frac{n^n}{hy} \right) (R-1)\, Dxyy\, Dy\, Dx$$

$$+ \int_{Co^2} \left(-\frac{3}{4}\,\frac{n^2}{hy} + \frac{9}{4}\,\frac{n^n}{hy} - \frac{n^3}{2\,hy} \right) (R-1)\, Dxy^2\, Dy^2$$

$$+ \int_{Co^2} \left(-\frac{2}{3\,hy} - \frac{1}{3}\,\frac{n^2}{hy} + \frac{n^n}{hy} \right) (R-1)\, Dyyy\, Dy\, Dx$$

$$+ \int_{Co} \left(\frac{1}{hy} - \frac{n^n}{hy} \right) (R-1)\, Dxyy\, Dxx$$

$$+ \int_{Co^4} \left(\frac{25}{12}\,\frac{n^4}{hy} - \frac{1}{24}\,\frac{n^n}{hy} + \frac{5}{12}\,\frac{n^3}{hy} - \frac{35}{24}\,\frac{n^2}{hy} - \frac{1}{hy} \right) (R-1)\, Dy^4\, Dx$$

$$+ \int_{Co} \left(\frac{11}{24\,hy} - \frac{11}{24}\,\frac{n^n}{hy} \right) (R-1)\, Dxyyy\, Dx + \int_{Co} \left(\frac{1}{3\,hy} - \frac{1}{3}\,\frac{n^n}{hy} \right) (R-1)\, Dxy\, Dyyy$$

$$+ \int_{Co} \left(-\frac{1}{4}\,\frac{n^n}{hy} + \frac{1}{4\,hy} \right) (R-1)\, Dxy^2\, Dyy$$

$$+\frac{\left(-\frac{3}{2}\frac{n^2}{hy}-\frac{n^3}{hy}+\frac{9}{2}\frac{n^n}{hy}\right)(R-1)^2\,Dxy^2\,Dy}{Co^2}$$

$$+\frac{\left(\frac{35}{4}\frac{n^2}{hy}-\frac{1}{4}\frac{n^4}{hy}+\frac{5}{2}\frac{n^3}{hy}-\frac{n^6}{hy}+\frac{25}{2}\frac{n^n}{hy}\right)(R-1)^3\,Dy^2\,Dx^2}{Co^4}$$

$$+\frac{\left(11\frac{n^2}{hy}+6\frac{n^2}{hy}+\frac{n^6}{hy}-\frac{n^3}{hy}\right)(R-1)^2\,Dxy\,Dy\,Dx^2}{Co^3}+\frac{\%1\,(R-1)^2\,Dxx^2\,Dy}{Co^2}$$

$$+\frac{\left(\frac{3}{2}\frac{n^3}{hy}-\frac{33}{2}\frac{n^n}{hy}+\frac{9}{hy}+9\frac{n^2}{hy}\right)(R-1)^2\,Dx\,Dxy\,Dy^2}{Co^3}$$

$$+\frac{\left(\frac{1}{8\,hy}-\frac{1}{8}\frac{n^n}{hy}\right)(R-1)\,Dxxxy\,Dx}{Co}+\frac{\left(-\frac{7}{12}\frac{n^n}{hy}+\frac{7}{12\,hy}\right)(R-1)\,Dxyyy\,Dy}{Co}$$

$$+\frac{\left(\frac{1}{3\,hy}+\frac{1}{2}\frac{n^n}{hy}-\frac{1}{6}\frac{n^2}{hy}\right)(R-1)^2\,Dyyy\,Dx^2}{Co^2}$$

$$+\frac{\left(-\frac{3}{2}\frac{n^n}{hy}+\frac{3}{2\,hy}\right)(R-1)\,Dxyy\,Dxy}{Co}$$

$$+ \frac{\left| -\frac{11}{6}\left(\frac{n}{hy}\right)^2 + \left(\frac{n}{hy}\right)^3 - \frac{1}{6}\left(\frac{n}{hy}\right)^3 + \left(\frac{1}{hy}\right)^3 \right| (R-1)\,Dxy\,Dx^3}{Co^3}$$

$$+ \frac{\left| \frac{1}{2hy} + \frac{1}{2}\left(\frac{n}{hy}\right)^2 - \frac{11}{12}\left(\frac{n}{hy}\right)^3 - \frac{1}{12}\left(\frac{n}{hy}\right)^3 \right| (R-1)\,Dyy\,Dy^3}{Co^3}$$

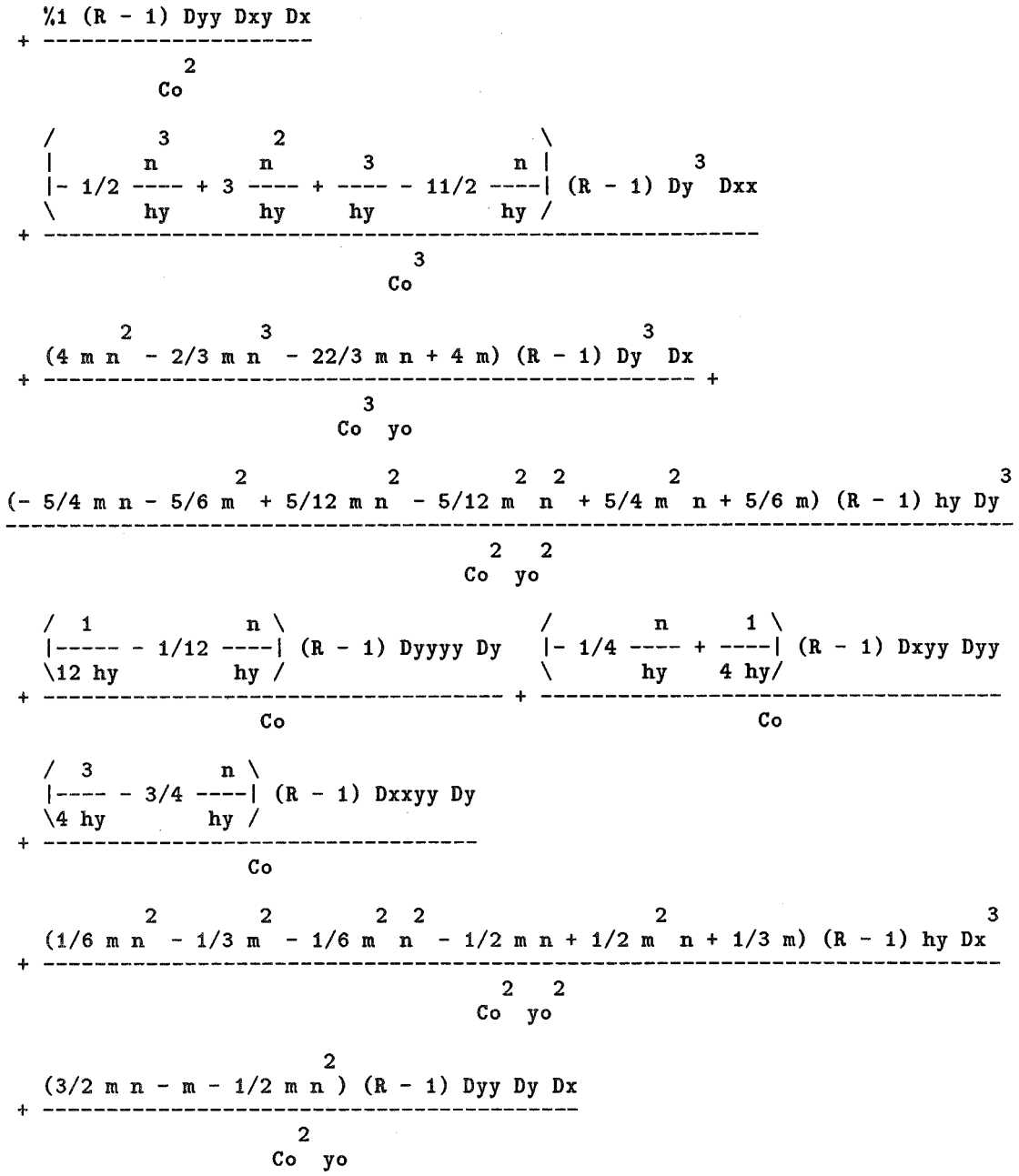
$$+ \frac{\left| \frac{1}{hy} - \frac{n}{hy} \right| (R-1)\,Dxxy\,Dxy}{Co} + \frac{\frac{1}{2}(R-1)\,Dyy\,Dxx\,Dx}{Co^2}$$

$$+ \frac{\left| 6\frac{n}{hy} - \left(\frac{n}{hy}\right)^4 - 2\left(\frac{n}{hy}\right)^2 \right| (R-1)\,Dy\,Dxx\,Dxy}{Co^2}$$

$$+ \frac{\left| -\frac{35}{6}\left(\frac{n}{hy}\right)^2 - \left(\frac{n}{hy}\right)^4 + \frac{5}{3}\left(\frac{n}{hy}\right)^3 - \frac{1}{6}\left(\frac{n}{hy}\right)^4 + \frac{25}{3}\left(\frac{n}{hy}\right)^4 \right| (R-1)\,Dx\,Dy^4}{Co^4}$$

$$+ \frac{\frac{1}{2}(R-1)\,Dy\,Dxx\,Dyy}{Co^2}$$

$$+ \frac{\left| \frac{3}{2}\left(\frac{n}{hy}\right)^2 - \frac{1}{4}\left(\frac{n}{hy}\right)^3 + \frac{3}{2hy} - \frac{11}{4}\left(\frac{n}{hy}\right)^3 \right| (R-1)\,Dyy\,Dy^2\,Dx}{Co^3}$$


%1 (R - 1) Dyy Dxy Dx
Co
(R - 1) Dy Dxx
Co
(4 m n - 2/3 m n - 22/3 m n + 4 m) (R - 1) Dy Dx
Co yo
(- 5/4 m n - 5/6 m + 5/12 m n - 5/12 m n + 5/4 m n + 5/6 m) (R - 1) hy Dy
Co yo
(R - 1) Dyyyy Dy
Co
(R - 1) Dxyy Dyy
Co
(R - 1) Dxxyy Dy
Co
(1/6 m n - 1/3 m - 1/6 m n - 1/2 m n + 1/2 m n + 1/3 m) (R - 1) hy Dx
Co yo
(3/2 m n - m - 1/2 m n) (R - 1) Dyy Dy Dx
Co yo

$$+\frac{(-3/2\,m\,n+3/2\,m)\,(R-1)\,Dxy^2}{Co\,yo}-1/12\,\frac{m\,(R-1)\,Dyyyy}{yo}$$

$$-7/12\,\frac{m\,(R-1)\,Dxyyy}{yo}+\frac{(-2\,m\,n^2+6\,m\,n-4\,m)\,(R-1)\,Dxy\,Dy^2}{Co^2\,yo}$$

$$+\frac{(2\,m^2\,n+4/3\,m-2\,m^2-4/3\,m\,n-2/3\,m^3\,n+2/3\,m^3)\,(R-1)\,hy^2\,Dy\,Dx}{Co^3\,yo}$$

$$+\frac{(1/2\,m-1/2\,m\,n)\,(R-1)\,Dyy\,Dxx}{Co\,yo}+\frac{\left(-1/2\,\frac{n}{hy}+\frac{1}{2\,hy}\right)(R-1)\,Dxxy\,Dxx}{Co}$$

$$+\frac{\left(-1/4\,\frac{n}{hy}+\frac{1}{4\,hy}\right)(R-1)\,Dxxxy\,Dy}{Co}+\frac{\left(\frac{1}{3\,hy}-1/3\,\frac{n}{hy}\right)(R-1)\,Dyyy\,Dxx}{Co}$$

$$+\frac{\%2\,(R-1)\,Dxyy\,Dy^2}{Co^2}+\frac{\left(\frac{1}{3\,hy}+1/2\,\frac{n}{hy}-1/6\,\frac{n^2}{hy}\right)(R-1)\,Dy^2\,Dyyy}{Co^2}$$

$$+\frac{\%1\,(R-1)\,Dyy\,Dxy\,Dy}{Co^2}+\frac{(9\,m\,n-6\,m-3\,m\,n^2)\,(R-1)\,Dxy\,Dy\,Dx}{Co^2\,yo}$$

$$+\frac{(2\,m-2\,m\,n)\,(R-1)\,Dxy\,Dxx}{Co\,yo}+\frac{(m-m\,n)\,(R-1)\,Dxxy\,Dx}{Co\,yo}$$

$$+\frac{(-2\,m-m\,n^2+3\,m\,n)\,(R-1)\,Dxy\,Dx^2}{Co^2\,yo}+\frac{(1/2\,m-1/2\,m\,n)\,(R-1)\,Dxx^2}{Co\,yo}$$

$$+\frac{(3/2\,m\,n - 3/2\,m^2\,n - 3/2\,m + 3/2\,m^2)\,(R-1)\,hy\,Dxy\,Dx}{Co^2\,yo^2}$$

$$+\frac{\left(1/4\,m\,n^2 - \frac{11}{24}\,m\,n - 1/24\,m\,n^3 + 1/4\,m^4\right)(R-1)\,Dx}{Co^3\,yo^3}$$

$$+\frac{(m^2 - m + m\,n - m^2\,n)\,(R-1)\,hy\,Dxx\,Dx}{Co^2\,yo^2}$$

$$\frac{(-3\,m\,n + 2\,m + 3\,m^2\,n - 2\,m^2 - m^2\,n^2 + m\,n^2)\,(R-1)\,hy\,Dy^2\,Dx}{Co^2\,yo^2}$$

$$+\frac{(3/2\,m\,n - 3/2\,m^2\,n - 3/2\,m + 3/2\,m^2)\,(R-1)\,hy\,Dy\,Dxx}{Co^2\,yo^2}$$

$$+\frac{(-2\,m + 2\,m\,n - 2\,m^2\,n + 2\,m^2)\,(R-1)\,hy\,Dxy\,Dy}{Co^2\,yo^2} +$$

$$(-3/2\,m^2 + 3/4\,m\,n^2 - 3/4\,m^2\,n^2 + 9/4\,m^2\,n - 9/4\,m\,n + 3/2\,m)\,(R-1)\,hy\,Dy$$

$$Dx^2 \int \left(Co^2\,yo^2\right) + \frac{(-1/4\,m^2\,n + 1/4\,m\,n - 1/4\,m + 1/4\,m^2)\,(R-1)\,hy\,Dyy\,Dx}{Co^2\,yo^2}$$

$$+\frac{(-1/4\,m^2\,n + 1/4\,m\,n - 1/4\,m + 1/4\,m^2)\,(R-1)\,hy\,Dyy\,Dy}{Co^2\,yo^2}$$

$$+ \frac{\left(-\frac{55}{24} m n + 5/4\, m + 5/4\, m n^{2} - 5/24\, m n^{3}\right) (R - 1)\, Dy^{4}}{Co^{3}\, yo} +$$

$$\frac{(- 5/12\, m^{3} n - 5/6\, m n - 5/4\, m^{2} + 5/12\, m^{3} + 5/6\, m + 5/4\, m^{2} n) (R - 1)\, hy^{2}\, Dy^{2}}{Co\, yo^{3}}$$

$$+ \frac{(3/4\, m^{2} n - 1/2\, m n + 1/2\, m - 3/4\, m^{2} - 1/4\, m^{3} n + 1/4\, m^{3}) (R - 1)\, hy^{2}\, Dx^{2}}{Co\, yo^{3}}$$

$$+ \frac{(1/3\, m - 1/3\, m n) (R - 1)\, Dyyy\, Dx}{Co\, yo}$$

$$+ \frac{(2\, m n^{2} + 2\, m - 11/3\, m n - 1/3\, m n^{3}) (R - 1)\, Dy\, Dx^{3}}{Co^{3}\, yo}$$

$$+ \frac{(- 1/4\, m n^{2} + 3/4\, m n - 1/2\, m) (R - 1)\, Dyy\, Dy^{2}}{Co^{2}\, yo}$$

$$+ \frac{(- 2\, m n^{2} + 6\, m n - 4\, m) (R - 1)\, Dxx\, Dy\, Dx}{Co^{2}\, yo}$$

$$+ \frac{(- m - 1/2\, m^{3} + 3/2\, m^{2}) (R - 1)\, hy^{2}\, Dxx}{yo^{3}}$$

$$+ \frac{(- 3/2\, m n + 3/2\, m) (R - 1)\, Dxyy\, Dx}{Co\, yo}$$

$$+\frac{(-1/4\,m\,n^2+3/4\,m\,n-1/2\,m)\,(R-1)\,Dyy\,Dx^2}{Co^2\,yo}$$

$$+\frac{(2\,m-2\,m\,n)\,(R-1)\,Dxy\,Dy}{Co\,yo}$$

$$+\frac{(-33/4\,m\,n-3/4\,m\,n^3+9/2\,m+9/2\,m\,n^2)\,(R-1)\,Dy^2\,Dx^2}{Co^3\,yo}$$

$$+\frac{(-3/2\,m\,n^2+9/2\,m\,n-3\,m)\,(R-1)\,Dy^2\,Dxx}{Co^2\,yo}$$

$$+\frac{(1/2\,m-1/2\,m\,n)\,(R-1)\,Dyy\,Dxy}{Co\,yo}+\frac{(1/3\,m-1/3\,m\,n)\,(R-1)\,Dyyy\,Dy}{Co\,yo}$$

$$+\frac{(-3/2\,m\,n+3/2\,m)\,(R-1)\,Dxxy\,Dy}{Co\,yo}$$

$$+\frac{(-1/12\,m^3-1/6\,m+1/4\,m^2)\,(R-1)\,hy^2\,Dyy}{yo^3}$$

$$+\frac{(-2/3\,m^3+2\,m^2-4/3\,m)\,(R-1)\,hy^2\,Dxy}{yo^3}$$

$$+\frac{(m^3+m-1/6\,m^4-11/6\,m^2)\,(R-1)\,hy^3\,Dx}{yo^4}$$

$$+ \frac{\left(\frac{25}{12}\frac{n}{hy} - 1/24\,\frac{n^4}{hy} + 5/12\,\frac{n^3}{hy} - \frac{35}{24}\frac{n^2}{hy} - \frac{1}{hy}\right)(R-1)\,Dy^5}{Co^4}$$

$$+ \frac{(-3/4\,m^2 + 3/4\,m)(R-1)\,hy\,Dxxy}{yo^2}$$

$$+ \frac{\left(\frac{55}{24}m^2 + 5/4\,m^3 - 5/24\,m^4 + 5/4\,m\right)(R-1)\,hy^3\,Dy}{yo^4}$$

$$+ \frac{(-m^2 + m)(R-1)\,hy\,Dxyy}{yo^2} + \left(\frac{11}{48}\frac{v}{hx} - 1/8\,\frac{R-1}{hy} - \frac{1}{8\,hy}\right)Dxxxyy$$

$$+ \left(\frac{1}{12\,hy} - 1/12\,\frac{R-1}{hy}\right)Dxyyyy + \left(\frac{11}{48}\frac{R-1}{hy} - 1/8\,\frac{v}{hx} - \frac{11}{48\,hy}\right)Dxxyyy$$

$$+ \left(\frac{1}{120\,hy} + 1/120\,\frac{R-1}{hy}\right)Dyyyyy$$

$$+ \frac{\left(-1/24\,\frac{m^5}{n} - \frac{35}{24}\frac{m^3}{n} + 5/12\,\frac{m^4}{n} - m/n + \frac{25}{12}\frac{m^2}{n}\right)Co\,(R-1)\,hy^4}{yo^5}$$

$$\%1 := 3/2\,\frac{n}{hy} - 1/2\,\frac{n^2}{hy} - \frac{1}{hy}$$

$$\%2 := 3\,\frac{n}{hy} - \frac{2}{hy} - \frac{n^2}{hy}$$

5 Maple Codes

The codes behind the expressions are simpler and present a view of the structure of the calculations.

5.1 Derivative Formulas

The first Maple programs calculate the differences, name them, and solve for the derivatives at the nodal point. The simplest case uses forward differences. Complete versions of all these programs are presented to remove any possibility of error.

5.1.1 Forward Differences

```
# Program fdel.mpl
# Calculates the expression for the derivatives in terms of finite
#  differences for two independent variables, here named x and y,
#  to order N

# Early, workable, FORWARD DIFFERENCE routine
# Calculates a double delta expression for two variables
# set a and b, the initial x values, and N, the number of terms
#  before reading.
 a := 0; b := 0; N := 7; NP := N+1;
# NP the terms in the polynominal

readlib(mtaylor);
# usage:  tay(g(2*x,y),x,y);
tay := proc(g,x,y) local t1;
    t1 := mtaylor(g,[x=a,y=b],NP); t1 := convert(t1,polynom);
       end;

# Bookkeeping:
#  -the name of each difference is Dx..  usage: Dx Dxx Dxy Dxxx Dxyyy
#    where x is for the x direction and y, for the y direction.
#  -use primary running vector g[Dx..][i,j] to maintain the list of
#    values of the dependent values -- to be operated upon.
#  -m is the number of lower-order differences to be processed.
#  -l is the order of the difference -- outer loop
#  -the array 'nameD[i,j]' contains the name of each calculated difference.
#  -similarily 'namep[i,j]' is the indexed x,y position at which the
#    forward partial difference is formed.
```

```
# form the initial, first differences and associated tables:
   m:=0:
# counter for the calculated differences of like order
# with 2 dimensions, there are two types of differences to be produced
#  for the two directions, x & y.

   l:=0:
# 0 order is considered as the function values themselves
 for i from 0 to N do;
 for j from 0 to N do;
   m:=m+1;
   g[D][i,j]:=tay(f(i*x,j*y),x,y);
   nameD[l,m]:=D; namep[l,m]:=i,j;
 od;
 od;
```

```
# There are many different differences.  The following uses the
#  concept that once the differences are formed, the next order
#  is formed from all differences of the first
  eqns := NULL:
# Equations are built up during the calculations.
#  uses only the terms that are forward differences at position 0,0.
 nl:=N:
# nl - data points available in either directions for a given difference
for l from 1 to N do
 lm:=l-1: mm:=m: m:=0:
# with 2 dimensions, two types of differences are produced - x & y.
 for k from 1 to mm do;
  nmme:=nameD[lm,k];
  len:=length(nmme);
  nd:=substring(nmme,len..len);
  rr:=namep[lm,k]; i:=rr[1]; j:=rr[2];
  if i < nl then; if  (nd = 'D') or (nd = 'x') then;
# limits the differencing and only allows for lexigraphic order
#  i.e., Dx,Dy,Dxx,Dxy,Dyy,Dxxx,Dxxy,Dxyy,Dyyy,Dxxxx,Dxxxy,Dxxyy,Dxyyy,Dyyyy,etc.
   nmmx:=``.nmme.x;
   difference := g[nmme][i+1,j]-g[nmme][i,j];
   g[nmmx][i,j] := difference;
   if i=0 and j=0 then; eqns:=eqns,nmmx = difference; fi;
   m:=m+1; nameD[l,m]:=nmmx; namep[l,m]:=i,j;
  fi; fi;
# x difference & name stored
  if j < nl then;
   nmmy:=``.nmme.y;
   difference := g[nmme][i,j+1]-g[nmme][i,j];
   g[nmmy][i,j] := difference;
   if i=0 and j=0 then; eqns:=eqns,nmmy = difference; fi;
   m:=m+1; nameD[l,m]:=nmmy; namep[l,m]:=i,j;
  fi;
# y difference & name stored after each x difference
 od;
  www:=`Differences of order `.l.`, calculated `.m.` terms`:
  print(www); mm:=m: nl:=nl-1:
 od:

# solve the simultaneous equations for the derivatives:
 eqns := {eqns};
 nops(eqns);
  vars := select(has,indets(eqns,function),D);
  nops(vars);
   solve(eqns,vars);
   sol := expand(");
  save(sol,`fsol`);
```

5.1.2 Backward Differences

```
# Program bdel.mpl
# Calculates the expression for the derivatives in terms of finite
#  differences for two independent variables, here named x and y,
#  to order N

# BACKWARD difference form
# Calculates a double delta expression for two variables
# set a and b, the initial x values, and N, the number of terms
#  before reading.
 a := 0; b := 0; N := 7; NP := N+1;
# NP is the terms in the polynominal
#
readlib(mtaylor);
# usage:  tay(g(2*x,y),x,y);
tay := proc(g,x,y) local t1;
    t1 := mtaylor(g,[x=a,y=b],NP); t1 := convert(t1,polynom);
       end;

# Bookkeeping:
#  -the name of each difference is Dx..  usage: Dx Dxx Dxy Dxxx Dxyyy
#    where x is for the x direction and y, for the y direction.
#  -use primary running vector g[Dx..][i,j] to maintain the list of
#    values of the dependent values -- to be operated upon.
#  -m is the number of lower-order differences to be processed.
# BACKWARD DIFFERENCE routine derived from del.mpl
#  -l is the order of the difference -- outer loop
#  -the array 'nameD[i,j]' contains the name of each calculated difference.
#  -similarily 'namep[i,j]' is the indexed x,y position at which the
#    forward partial difference is formed.

# form the initial, first differences and associated tables:
   m:=0:
# counter for the calculated differences of like order
# with 2 dimensions, there are two types of differences to be produced
#  for the two directions, x & y.

   l:=0:
# 0 order is considered as the function values themselves
 for i from -N to 0 do;
 for j from -N to 0 do;
   m:=m+1;
   g[D][i,j]:=tay(f(i*x,j*y),x,y);
   nameD[l,m]:=D; namep[l,m]:=i,j;
 od;
 od;
```

```
# There are many different differences.  The following uses the
#  concept that once the differences are formed, the next order
#  is formed from all differences of the first
  eqns := NULL:
# Equations are built up during the calculations.
#  uses only the terms that are forward differences at position 0,0.
 nl:=N:
# nl - data points available in either directions for a given difference
for l from 1 to N do
 lm:=l-1: mm:=m: m:=0:
# with 2 dimensions, two types of differences are produced - x & y.
 for k from 1 to mm do;
  nmme:=nameD[lm,k];
  len:=length(nmme);
  nd:=substring(nmme,len..len);
  rr:=namep[lm,k]; i:=rr[1]; j:=rr[2];
  if -i < nl then; if  (nd = 'D') or (nd = 'x') then;
# limits the differencing and only allows for lexigraphic order
#  i.e., Dx,Dy,Dxx,Dxy,Dyy,Dxxx,Dxxy,Dxyy,Dyyy,Dxxxx,Dxxxy,Dxxyy,Dxyyy,Dyyyy,etc.
   nmmx:=``.nmme.x;
   difference := g[nmme][i,j]-g[nmme][i-1,j];
   g[nmmx][i,j] := difference;
   if i=0 and j=0 then; eqns:=eqns,nmmx = difference; fi;
   m:=m+1; nameD[1,m]:=nmmx; namep[1,m]:=i,j;
  fi; fi;
# x difference & name stored
  if j < nl then;
   nmmy:=``.nmme.y;
   difference := g[nmme][i,j]-g[nmme][i,j-1];
   g[nmmy][i,j] := difference;
   if i=0 and j=0 then; eqns:=eqns,nmmy = difference; fi;
   m:=m+1; nameD[1,m]:=nmmy; namep[1,m]:=i,j;
  fi;
# y difference & name stored after each x difference
 od;
  www:=`Differences of order `.l.`, calculated `.m.` terms`:
  print(www); mm:=m: nl:=nl-1:
 od:

# solve the simultaneous equations for the derivatives:
 eqns := {eqns};
 nops(eqns);
  vars := select(has,indets(eqns,function),D);
  nops(vars);
   solve(eqns,vars);
   sol := expand(");
  save(sol,`bsol`);
```

5.1.3 Central Differences

```
# Program cdel.mpl
# Calculates the expression for the derivatives in terms of finite
#  differences for two independent variables, here named x and y,
#  to order N

# CENTRAL difference form 4Jun92
# Calculates a double delta expression for two variables
#  set a and b are left as offsets in x and y in the series

  N := 7; NP := N+1: a := 0: b:= 0:
# N is the number of orders of the differences
# NP the terms in the polynominal
#  a and b are set to zero -- this should make no difference because all
#  the expansions are relative to the initial point anyway.

readlib(mtaylor);
# usage:  tay(g(2*x,y),x,y);
tay := proc(g,x,y) local t1;
    t1 := mtaylor(g,[x=a,y=b],NP); t1 := convert(t1,polynom);
       end;

# Bookkeeping:
#  -the name of each difference is Dx..  usage: Dx Dxx Dxy Dxxx Dxyyy
#    where x is for the x direction and y, for the y direction.
#  -use primary running vector g[Dx..][i,j] to maintain the list of
#    values of the dependent values -- to be operated upon.
#  -m is the number of lower-order differences to be processed.
#  -l is the order of the difference -- outer loop
#  -the array 'nameD[i,j]' contains the name of each calculated difference.
#  -similarily 'namep[i,j]' is the indexed x,y position at which the
#    forward partial difference is formed.

# form the initial, first differences and associated tables:
   m:=0:
# counter for the calculated differences of like order
# with 2 dimensions, there are two types of differences to be produced
#  for the two directions, x & y.

   l:=0:
# 0 order is considered as the function values themselves
 for i from -N to N do;
 for j from -N to N do;
   m:=m+1;
   g[D][i,j]:=tay(f(i*x,j*y),x,y);
   nameD[l,m]:=D; namep[l,m]:=i,j;
 od;
 od;
```

```
# There are many different differences.  The following uses the
#  concept that once the differences are formed, the next order
#  is formed from all differences of the first
  eqns := NULL:
# Equations are built up during the calculations.
#  uses only the terms that are forward differences at position 0,0.
 nl:=N:
# nl - data points available in either direction for a given difference
for l from 1 to N do
 lm:=l-1: mm:=m: m:=0:
# with 2 dimensions, two types of differences are produced - x & y.
 for k from 1 to mm do;
  nmme:=nameD[lm,k];
  len:=length(nmme);
  nd:=substring(nmme,len..len);
  rr:=namep[lm,k]; i:=rr[1]; j:=rr[2];
  if (-nl < i and i < nl) then; if  (nd = 'D') or (nd = 'x') then;
# limits the differencing and only allows for lexigraphic order
#  i.e., Dx,Dy,Dxx,Dxy,Dyy,Dxxx,Dxxy,Dxyy,Dyyy,Dxxxx,Dxxxy,Dxxyy,Dxyyy,Dyyyy,etc.
   nmmx:=``.nmme.x;
   difference := (g[nmme][i+1,j]-g[nmme][i-1,j])/2;
   g[nmmx][i,j] := difference;
   if i=0 and j=0 then; eqns:=eqns,nmmx = difference; fi;
   m:=m+1; nameD[1,m]:=nmmx; namep[1,m]:=i,j;
  fi; fi;
# x difference & name stored
  if (-nl < j and j < nl) then;
   nmmy:=``.nmme.y;
   difference := (g[nmme][i,j+1]-g[nmme][i,j-1])/2;
   g[nmmy][i,j] := difference;
   if i=0 and j=0 then; eqns:=eqns,nmmy = difference; fi;
   m:=m+1; nameD[1,m]:=nmmy; namep[1,m]:=i,j;
  fi;
# y difference & name stored after each x difference
 od;
  www:=`Differences of order `.l.`, calculated `.m.` terms`:
  print(www); mm:=m: nl:=nl-1:
 od:

# solve the simultaneous equations for the derivatives:
 eqns := {eqns};
 nops(eqns);
  vars := select(has,indets(eqns,function),D);
  nops(vars);
   solve(eqns,vars);
   sol := expand(");
  save(sol,`csol`):
```

5.1.4 Mixed Differences

```
# Program mdel.mpl
# Calculates the expression for the derivatives in terms of finite
#  differences for two independent variables, here named x and y,
#  to order N

# MIXED difference form for the phorphorus problem 9Jun92
#
#  This is the central difference form called cdel.mpl
#   except:
#     - initial functional values are derived for half the spacing
#     - the differences formed are not divided by two
#       (this gives the same effect as the differences used by
#         Notodarmojo et al, with All higher order differences
#         considered as central differences)
#     - first order differences are corrupted so that:
#        Dx is a backward difference
#        Dy is a forward difference

  N := 5; NP := N+1: NH := N/2: a := 0: b:= 0:
# N is the number of orders of differences
# NP the terms in the polynominal; NH the number of half differences
#  a and b are offsets in x and y of the Taylor series expansion
#  They are set to zero -- this should produce no limitation on the
#  validity of the expressions because the approximation process is
#  always relative to the initial notal point.

readlib(mtaylor);
# usage:  tay(g(2*x,y),x,y);
tay := proc(g,x,y) local t1;
    t1 := mtaylor(g,[x=a,y=b],NP); t1 := convert(t1,polynom);
       end;

# Bookkeeping:
#  -the name of each difference is Dx..  usage: Dx Dxx Dxy Dxxx Dxyyy
#    where x is for the x direction and y, for the y direction.
#  -use primary running vector g[Dx..][i,j] to maintain the list of
#    values of the dependent values -- to be operated upon.
#  -m is the number of lower-order differences to be processed.
#  -l is the order of the difference -- outer loop
#  -the array 'nameD[i,j]' contains the name of each calculated difference.
#  -similarily 'namep[i,j]' is the indexed x,y position at which the
#    forward partial difference is formed.

# form the initial, first differences and associated tables:
   m:=0:
# counter for the calculated differences of like order
#  with 2 dimensions, there are two types of differences to be produced
#  for the two directions, x & y.
```

```
   l:=0:
# Here 0 order is considered as the function values themselves
 for i from -NH by 1/2 to NH do;
 for j from -NH by 1/2 to NH do;
   m:=m+1;
   g[D][i,j]:= tay(f(i*x,j*y),x,y);
   nameD[l,m]:=D; namep[l,m]:=i,j;
 od;
 od;

# We first calculate the functional values, the 0 order differences.
# Then the first order differences, second order differences, etc.
# are formed
 eqns := NULL:
# Equations are built up during the calculations.
#  only the terms at position 0,0 are collected.
 nl:=NH:
# nl - data points available in a given direction

for l from 1 to N do
 lm:=l-1: mm:=m: m:=0:
# with 2 dimensions, two types of differences are produced - x & y.

 for k from 1 to mm do;
  nmme:=nameD[lm,k];
  len:=length(nmme);
  nd:=substring(nmme,len..len);
  rr:=namep[lm,k]; i:=rr[1]; j:=rr[2];

  # first calculate the x difference
  if (-nl < i and i < nl) then; if  (nd = 'D') or (nd = 'x') then;
   # limits the differencing and only allows lexigraphic order,
   #  i.e., Dx,Dy,Dxx,Dxy,Dyy,Dxxx,Dxxy,Dxyy,Dyyy,etc.
   nmmx:=``.nmme.x;
   difference := (g[nmme][i+1/2,j]-g[nmme][i-1/2,j]);
   g[nmmx][i,j] := difference;
   if i=0 and j=0 then;
    if l = 1 then; difference := (g[nmme][i,j]-g[nmme][i-1,j]); fi;
    # backward difference corruption to match Phosphorus calculation
    eqns:=eqns,nmmx = difference; fi;
    m:=m+1; nameD[l,m]:=nmmx; namep[l,m]:=i,j;
   fi;
  fi;
```

```
  # then calculate the y difference
  if (-nl < j and j < nl) then;
   nmmy:=``.nmme.y;
   difference := (g[nmme][i,j+1/2]-g[nmme][i,j-1/2]);
   g[nmmy][i,j] := difference;
   if i=0 and j=0 then:
    if l = 1 then; difference := (g[nmme][i,j+1]-g[nmme][i,j]); fi;
    # forward difference corruption to match Phosphorus calculation
    eqns:=eqns,nmmy = difference;
   fi;
   m:=m+1; nameD[l,m]:=nmmy; namep[l,m]:=i,j;
  fi;
  # y difference & name stored after each x difference

 od;
  www:='Differences of order '.l.', calculated '.m.' terms':
  print(www); mm:=m: nl:=nl-1/2:
 od:

# solve the simultaneous equations for the derivatives:
 eqns := {eqns};
 nops(eqns);
  vars := select(has,indets(eqns,function),D);
 eee := collect(eqns,vars):
# save eee, 'eqn.m';
   solve(eqns,vars):
   sol := expand(");
  save sol,'msol.m';
 quit;
```

5.2 Full Equation

Basically, the above expressions produce a set of solutions for the derivatives at the nodal point $(0,0)$. The P.D.E. is expanded as a whole and substitutions made for the derivatives. This is done in two parts, the linear, advective/dispersion portion to the equation and, separately, the non-linear absorption term.

```
# Program sf.ml
# Expands the Phosphorus advection/dispersion/sorption equation and
#  substitutes for the derivatives at the nodal point.

    read msol.m:
# To change to other differences, replace this line.
# File produced by mdel.mpl contains the finite difference
#  solutions for the derivatives, called sol

   N := 5: NP := N+1:
```

```
# Build a list of equations marking the differences by
#  t^(Order of difference)
   Assign := proc(a,b) a=b; end:
   tot := NULL:
   for i from 0 to N do
   for j from 0 to N do
        tname := cat(D,x$i,y$j);
        tot := tot,tname =t^(i+j)*tname;
   od: od;
   sol := subs({f=C,tot},sol):
   sol := subs(x=t*hx,y=t*hy,sol):
# C is now the dependent variable
#  the t is to keep track of the order
#  the x&y in sol are really increments.

   readlib(mtaylor):

   pde := - v*diff(C(x,y),x) + d*diff(C(x,y),x,x) - diff(C(x,y),y);
# Note the signs and the order of the terms
# the non-linear term dSdt with S = k C^m t^n is subtracted later
   mtaylor(pde,[x=0,y=0],NP):
   convert( " ,polynom):
   subs(sol, " ):
   subs(C(0,0)=Co, " ):
   subs(C=proc(x,y) 0 end , " ):  # removes unwanted high order terms
   subs(x=t*x,y=t*y, " ):
# remember t is a dummy variable (=1) just to keep track of orders
   subs(x=hx,y=hy, " ); #remove to preserve x & y dependence
   taylor( " ,t,NP):
   result := convert( " ,polynom);
#  save result, 'result.m';

   read 'fn.m':

# The function f^n is returned as a double taylor series fn from
#  program fn.mpl
   subs(f=C,fn):
   subs(sol, " ):
   subs(C(0,0)=Co, " ):
   Cn := convert( " ,polynom);
#  save Cn, 'Cn.m';

# the generation  of the time term tm
   (1+yy)^m:
   series( " ,yy,NP+1): convert( " ,polynom):
   tm := yo^m*subs(yy=y/yo, " );
#  save tm, 'tm.m';
# The term is written this way to allow an expansion about yo,
#  the value of time at the start of the time step.


# The non-linear sorption isotherm for the concentration
#  on the solid:
```

```
    S := k*Cn*tm:

# Substitute into the non-linear term in the full equation
    diff(S,y):
    subs(y=t*y,x=t*x, " ):
    subs(x=hx,y=hy, " ): #remove to preserve x & y
#  remember t is a dummy variable (=1) just to keep track of orders
    series(",t,NP):
    term := convert( " ,polynom);
#   save term, 'term.m';

# The final result is:

   series(result-term,t,NP):
   convert( " ,polynom):
   expand( " ):
   F := collect( " ,t):
   save F,'F.m';
quit;
```

This file is run in a Unix environment with the command

```
>maple <sf.ml >sf.out
```

though many variations are possible depending on the amount of interaction intermediate results or checkout required. Several intermediate forms may need to be explored; these are obtained by activating the lines that save files result.m, Cn.m, tm.m, and F.m. Important is the factor t which is used to mark the order of the difference, defined such that each delta, independent and dependent is prefaced with a single t.

The first routine, builds a list of names with the t attached. The next routine expands the linear, advection/dispersion portion of the equation. Then the C^n term is formed as a taylor series in x and y. This function is made up from a combination of exponential and logarithmic forms and is obtained from separate program fn.mpl and read in as fn. The time power t^m is formed from a simple binomial series, note that it is expanded about the initial time, here yo. The sorption term is then formed, differentiated, and, through substitution, converted to the expanded, difference form. A final subtraction of the differentiated, sorption term gives the final expanded form of the P.D.E. A little cleanup along the way is required to keep the size of the expressions minimal and make the final result clear.

5.3 Other Codes

The function C^n is obtained indirectly from program fn.mpl. It uses a double expansion of an exponential and logarithm.

```
# Program fn.mpl
#  creates an series expansion for (f(x,y))^n
   N := 5: NP := N+1:
# NP is the number of terms in the polynominal

expr := f(x,y)^n;

# The working form is exp(ln(expr)).  The technique uses the 'homogenous
#  form' x->xt and y->yt to construct a multidimensional series from a single
#  dimensional series.  This automatically carries the x and y along even
#  though the expansion is in terms of t.  later, t is set equal to 1.

# The ln(expr) series
subs({x=x*t,y=y*t},expr);
expand(ln(''));
series('',t,NP):
convert('',polynom):
A := expand(''):
A := subs(ln(t)=0,A):

# The exp(u) series
series(exp(A),t,NP):
B := convert('',polynom):
B := expand(''):
B := collect('', t): nops(B);
#B := map(factor,B):
subs(t=1,B):
fn := simplify('');
save(fn,'fn.m'):
```

All of the expressions need some cleanup, depending on how they are to be analysed. The following are the main programs, somewhat combined. Note that finites, printlevel and removal of garbage collection gc(0) are common to most of the cleanup, as is N, the number of terms.

```
# Program fix.mpl
#  used to clean up the terms

#-----Organise differences and derivatives-----
printlevel := 0:
words(0) : gc(0):
 tt := collect('',t);

 finites:= [Dx,Dy, Dxx,Dxy,Dyy, Dxxx,Dxxy,Dxyy,Dyyy,
  Dxxxx,Dxxxy,Dxxyy,Dxyyy,Dyyyy, Dxxxxx,Dxxxxy,Dxxxyy,Dxxyyy,Dxyyyy,Dyyyyy,
  Dxxxxxx,Dxxxxxy,Dxxxxyy,Dxxxyyy,Dxxyyyy,Dxyyyyy,Dyyyyyy,
  Dxxxxxxx,Dxxxxxxy,Dxxxxxyy,Dxxxxyyy,Dxxxyyyy,Dxxyyyyy,Dxyyyyyy,Dyyyyyyy];
```

```
 derivatives :=
[D[1,1,1,1,1,1,1](f)(0,0),D[1,1,1,1,1,1,2](f)(0,0),D[1,1,1,1,1,2,2](f)(0,0),
 D[1,1,1,1,2,2,2](f)(0,0),D[1,1,1,2,2,2,2](f)(0,0),D[1,1,2,2,2,2,2](f)(0,0),
 D[1,2,2,2,2,2,2](f)(0,0),D[2,2,2,2,2,2,2](f)(0,0),

 D[1,1,1,1,1,1](f)(0,0),D[1,1,1,1,1,2](f)(0,0),D[1,1,1,1,2,2](f)(0,0),
 D[1,1,1,2,2,2](f)(0,0),D[1,1,2,2,2,2](f)(0,0),D[1,2,2,2,2,2](f)(0,0),
 D[2,2,2,2,2,2](f)(0,0),

 D[1,1,1,1,1](f)(0,0),D[1,1,1,1,2](f)(0,0),D[1,1,1,2,2](f)(0,0),
 D[1,1,2,2,2](f)(0,0),D[1,2,2,2,2](f)(0,0),D[2,2,2,2,2](f)(0,0),

 D[1,1,1,1](f)(0,0),D[1,1,1,2](f)(0,0),D[1,1,2,2](f)(0,0),
 D[1,2,2,2](f)(0,0),D[2,2,2,2](f)(0,0),

 D[1,1,1](f)(0,0),D[1,1,2](f)(0,0),D[1,2,2](f)(0,0),
 D[2,2,2](f)(0,0),D[1,1](f)(0,0),D[1,2](f)(0,0),D[2,2](f)(0,0),
 D[1](f)(0,0),D[2](f)(0,0)]:

  nf := nops(rfinites):
  finites := [seq(rfinites[nf-i],i=0..nf-1)];
# Sometime the list must be reversed, particularily with polynominals

 sols := subs(sol,derivatives);
 sol := [seq(derivatives[i]=sols[i],i=1..nops(sols))];

 ff := a->sort(a,finites):
 gg := b->lhs(b)=ff(rhs(b)):
 sol := map(gg,sol):

# puts the solution into a sensible, consistent order in sol
#  from Dave R. Clark and Greg. J. Fee
```

```
#--------------------fix result
N := 5:
read 'result.ml':
expand(''):
tt := collect('',t);
for i from 0 to N do
 coeff(tt,t,i):
 collect( " ,finites,distributed):
 sort( " ,finites)*t^i:
 c[i] := collect( '',t):
 print('Terms of order '.i):
 print('');
 od;
#----------------------fix Cn
read 'Cn.m':
subs(x=t*hx,y=t*hy, " ):
expand(''):
tt := collect('',t):
for i from 0 to 5 do:
  fff := coeff(tt,t,i):
  ff := normal(fff):
#  if i <= 1 then aa := lcoeff('',t):
#   else aa := op(1,''): fi:
  fff := n*Co^n/Co^i:
  ffff := ff/fff:
#splits off the denominator term
  ffff := collect(ffff,Co);
  c[i] := fff*t^i*ffff:
  print('Terms of order '.i):
  print('');
  od;
#This routine has been changed variously and doesn't work well
quit;
#----------------------fix term
read 'term.ml':
subs(hx=x,hy=y, " ):
subs(x=t*hx,y=t*hy, " ):
expand(''):
tt := collect('',t):
for i from 0 to 5 do:
  coeff(tt,t,i):
  normal( " ):
  ff := n*Co^n/Co^i:
  ""/ff:
  collect( " ,Co);
  c[i] := ff*t^i*collect( " ,finites):
  print('Terms of order '.i):
  print('');
  od;
quit;
```

The program to organise the complete expression includes some special power substitutions to bring the large terms more in line.

```
#Program to fix up the output of sf.ml
#  sf.ml is the version of the full phosphorus model
#  correct 28Jul92  William D. Scott
#   displays results properly
 printlevel := 0:
 words(0) : gc(0): #removes garbage collection
 N := 5:
 finites:= [Dx,Dy, Dxx,Dxy,Dyy, Dxxx,Dxxy,Dxyy,Dyyy,
  Dxxxx,Dxxxy,Dxxyy,Dxyyy,Dyyyy, Dxxxxx,Dxxxxy,Dxxxyy,Dxxyyy,Dxyyyy,Dyyyyy,
  Dxxxxxx,Dxxxxxy,Dxxxxyy,Dxxxyyy,Dxxyyyy,Dxyyyyy,Dyyyyyy,
  Dxxxxxxx,Dxxxxxxy,Dxxxxxyy,Dxxxxyyy,Dxxxyyyy,Dxxyyyyy,Dxyyyyyy,Dyyyyyyy];
 vars := [Rm1,Co,yo]:
 read 'F.m':
 F := convert(F,polynom):
 printlevel := 0:
 words(0) : gc(0): #removes garbage collection
 with(student):
 for i from 0 to 2 do;
  coeff(F,t,i):
  powsubs(Co^n=Co*(Rm1)/(n*k*yo^m), "):
# allows for the R form to be presented
  powsubs(hy/yo=hyyo, " ):
  collect( " ,vars):
  cc[i] := collect( " ,finites):
  if i=0 then powsubs(Dhy=Dy/hy,");
     collect(",Dhy):
     subs(Dhy=Dy/hy):
  fi;
  print('Terms of Order '.i):
  print(cc[i]):
 od;
# save cc, 'cc.m';
#quit;
```

6 Exploring the Terms

In the numerical solution of partial differential equations it is often not possible to assess the accuracy of the approximation. The present technique presents a general structure for such analysis and, perhaps, solution. The technique only depends on the validity of the expansion about the nodal point; it is a linear expansion that becomes more accurate with diminished time and space increments. Usually three criteria are used to assess the quality of the numerical technique; 'accuracy', 'convergence', and 'stability' (See Mickley et al [9]). Accuracy is determined by the size of increments used; the number of increments contributes to the error in round-off or storage of floating point numbers. The accuracy expected with smaller increments is disaffected by the number of calculations and the round-off error of each. There is a trade-off and an optimal increment size. This is especially so now that computer storage is in gigabytes and the speeds, in nanoseconds. The cost of computation has become insignificant.

With linear P.D.E.'s with constant coefficients, if the method is stable, convergence is likely but not guaranteed. Nothing really definite can be said about non-linear equations except that, with small increments, they become linear. There are a number of criteria that establish the stability of difference schemes with different numbers of terms [9],[14] but we won't dwell on them here. Instead we note that, if the differences are written in terms of functional values and in a matrix form of solution, stability is assured if the matrix is diagonally dominant. The same applies to the linear algebraic form for the different orders of differences. This relates to all the expressions here, with our new tools for analysis.

We consider the last expansion, Section 4.5, with order zero and order one terms being the best first attempt to improve the accuracy (and stability) of the calculation. Maple has produced algebraic codes without round-off error that, within the limits of the truncation of the terms, should emulate the the original P.D.E., equation2. The zero order terms, as an approximation of the original equation, are identical to the terms given by Notodarmojo et al [14]. As $\nabla_z = h_z \rightarrow 0$ or $\Delta_t = h_t \rightarrow 0$, the dependent differences in the 1^{st} and higher order terms all disappear. The finite, zero order expression converges on the infinitesimal form, equation2. That does not mean that the expanded form converges, as a series, when the calculation is stepped along to the next nodal point.

Here no attempt is made to look at all the possibilities of analysis but some ideas are presented. Maple offers an unlimited number of options. First we look at the usual method of adjusting the parameters (coefficients) in the equation. Then, consider the possibility of removal of terms by adjusting the values of hz or ht and the possibility of minimising the remaining error by increment adjustment. A alternative view is presented with the possibility of using an identity expression in Section 6.4.

6.1 Effective Coefficients

Following the ordinary approach, the coefficients in the zero order expansion are increased to include some of the linear terms. This procedure is hazardous because we immediately accept that the equation no longer converges to the same solution, with the possibility of increased instability with small changes (errors) in the values of the coefficients. Indeed, there are other first order terms that may be just as important as the selected, linear ones. The procedure uses Maple to collect terms in Dxx, Dx, Dy, and the constant expressions. The effective coefficients are:

		$0^{th} order$	$1^{st} order$
Effective dispersion coefficient	=	d	$-3 \cdot v \cdot hz/2$
Effective advection velocity	=	v	$+m(R-1) \cdot hz/to$
Effective Retardation coefficient	=	R	$+2m(R-1) \cdot ht/to$
Effective Sorption term	=	$-\frac{mCo(R-1)}{nto}$	$+\frac{(\frac{m}{n}-\frac{m^2}{n})Co(R-1)ht}{to^2}$

Remember that with all terms on the right of the equation (2), the retardation term is negative. If all the above terms are used in the calculation, the remaining error (to 1^{st} order) is

$$\begin{aligned} \text{Error} = & +\tfrac{(R-1)(1-n)}{Co \cdot ht} \cdot Dx \cdot Dy \quad +\tfrac{(R-1)(1-n)}{Co \cdot ht} \cdot Dy \cdot Dy \\ & -(\tfrac{v}{hx} + \tfrac{R}{ht}) \cdot Dxy \qquad -(\tfrac{R}{2 \cdot ht}) \cdot Dyy \\ & +(\tfrac{d}{hz^2}) \cdot Dxxx \qquad +(\tfrac{d}{hz^2}) \cdot Dxxy \end{aligned}$$

It appears that none of these terms may be removed by simply adjusting the values of hz or ht, the only really adjustable parameters. This contradicts

the procedures evolved by van Genucten and Wierenga??. However, noting that $R = 1 + n \cdot k \cdot to^m \cdot Co$ so that both R and $R - 1$ are greater than zero, the top two terms are removed if $n = 1$. This is unlikely in this case as we expect n to be around .5. The alternate possibility is to minimise the magnitude of the terms with increment adjustment. Perhaps the derivatives of the *Error* with respect to the two increments could be simply set to zero but this is a complex problem with unknown, dependent finite difference problems in the error expression. It is also possible that other types of differences, including divided differences would make it possible to gain an advantage either by making the coefficients zero or making the dependent terms respond to increment spacing.

6.2 Stability

Looking at the different orders and considering the mixed difference scheme, the stability of the calculation is difficult to assess. Two considerations come to mind, taking ratios of the terms of different order with the expectation that, say, the ratio $\frac{2^{nd}Order}{1^{st}Order}$ will be much less than one. Also, one needs to look at the expressions (sub-terms) within each order; these terms will take on a heirarchy of values with some terms dominating during one part of the calculation. It should happen, however, that the largest sub-term of one order is much less than the smallest term of the next higher order. Some experience with the break-up of the equations and these terms and sub-terms should allow a heuristic assessment of stability, with practical benefit.

6.3 Other Expansion Forms

If the expansion is simply considered as a function of x and y, there is no real reason why we need to settle on an form that is evaluated at the position (hx, hy) from the nodal point, as has been done so far. In fact, there is a continuum of possibilities here (see next section) though it is linked with considerstions of stability. In reality, the finite differences are approximations for the derivatives at the nodal point and, since the original Partial Differential Equation is valid over a large domain, the form should retain validity when the x and y values are evaluated at the nodal point and, say, $hx/2$ and $hy/2$, away. At the nodal point a simplier form obtains which doesn't contain as much information from the higher order differences:

Terms of Order 0

$$-\frac{m\,Co\,(R-1)}{n\,yo}+\frac{d\,Dxx}{2\,hx}+\left|-\frac{R-1}{hy}-\frac{1}{hy}\right|Dy-\frac{v\,Dx}{hx}$$

Terms of Order 1

$$\left|1/2\,\frac{R-1}{hy}+\frac{1}{2\,hy}\right|Dyy-1/2\,\frac{v\,Dxx}{hx}$$

Terms of Order 2

$$\left|\frac{1}{6\,hy}+1/6\,\frac{R-1}{hy}\right|Dyyy-1/12\,\frac{d\,Dxxxx}{2\,hx}+1/6\,\frac{v\,Dxxx}{hx}$$

Terms of Order 3

$$0$$

Terms of Order 4

$$-1/80\,\frac{v\,Dxxxxx}{hx}+\left|-\frac{1}{80\,hy}-1/80\,\frac{R-1}{hy}\right|Dyyyyy$$

It is interesting that the terms are limited. There is a entirely different set of effective coefficients, with only the dispersion coefficient d being different than the prescribed value.

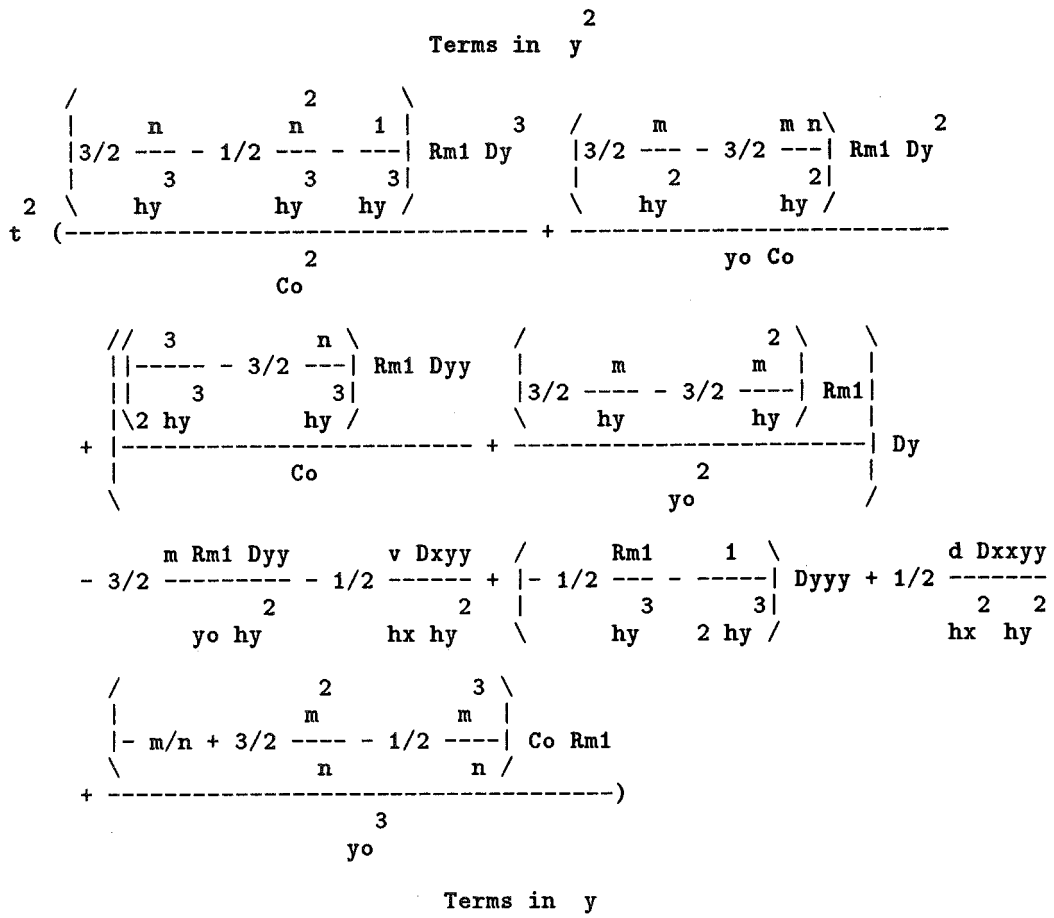
$$\begin{array}{rcll} & & 0^{th}order & 1^{st}order \\ \text{Effective dispersion coefficient} & = & d & -\cdot v\cdot hz/2 \end{array}$$

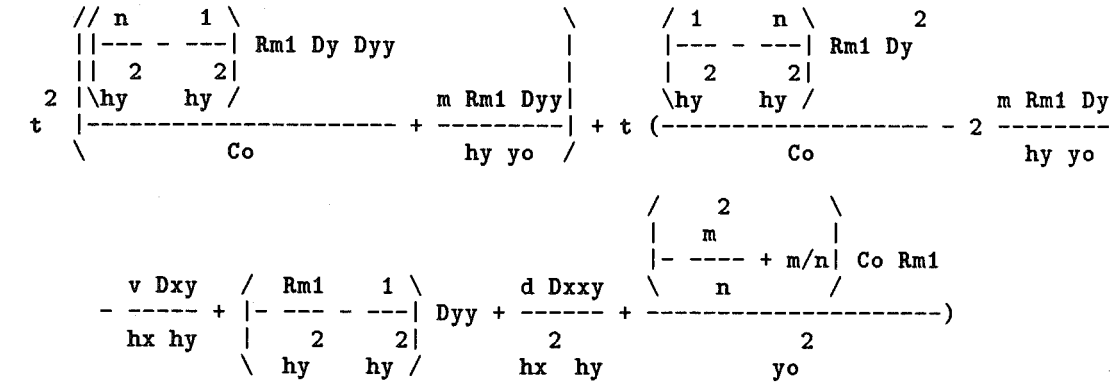
which still does not agree with Notodarmojo et al[14]. It is the same form used by van Genuchten and Wierenga[15] when sorption is ignored. The remaining error terms are as presented above, to fourth order.

6.4 An Identity Expansion

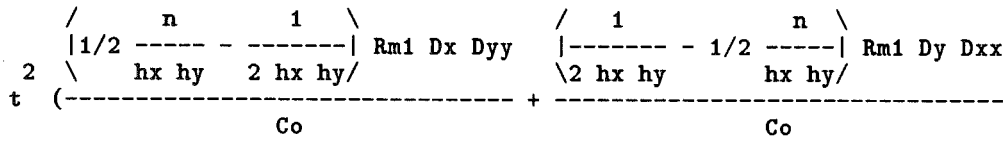
A different view of the equations is that they should be applicable not only at specified positions, but all along the path from one node to the next node, and perhaps, beyond. With Maple, this is a matter of simply arranging that

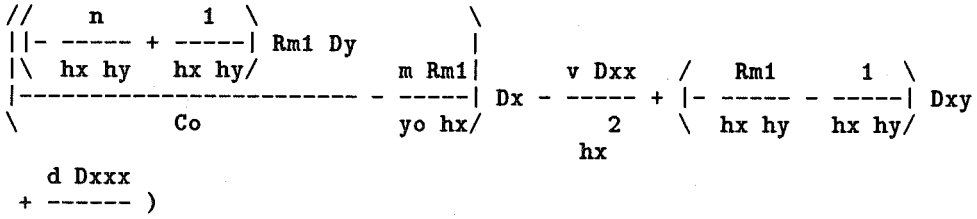
the interpolation formula contains x and y as arguments. The expansion is completed and the terms in powers of x or y are collected. If they are to apply over the entire step, all the coefficients must be zero. This gives an entirely different set of equations to solve, all of which are set to zero and, with the t-terms, associated with an order. Considering terms to 2^{th} order, the equations are given below. The constant terms are identical to those above, when both x and y are zero. That is, the above constant terms are an appropriate expansion at the first of the time step; the Newton/Everett parameters (p and q or $p1$ and $p2$, see Section 7.4) are zero.



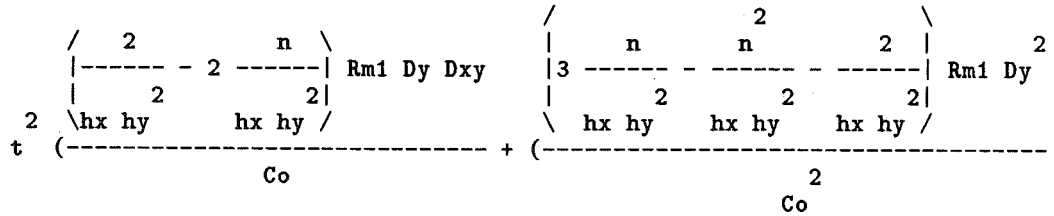


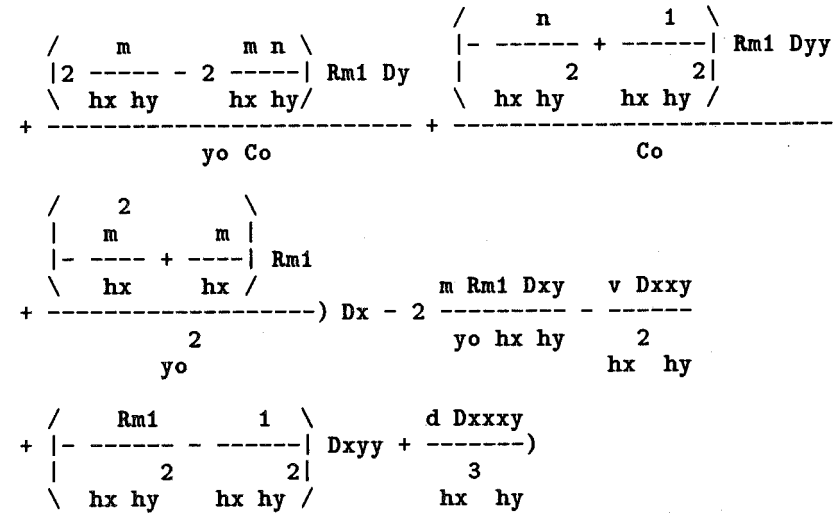
Terms in x



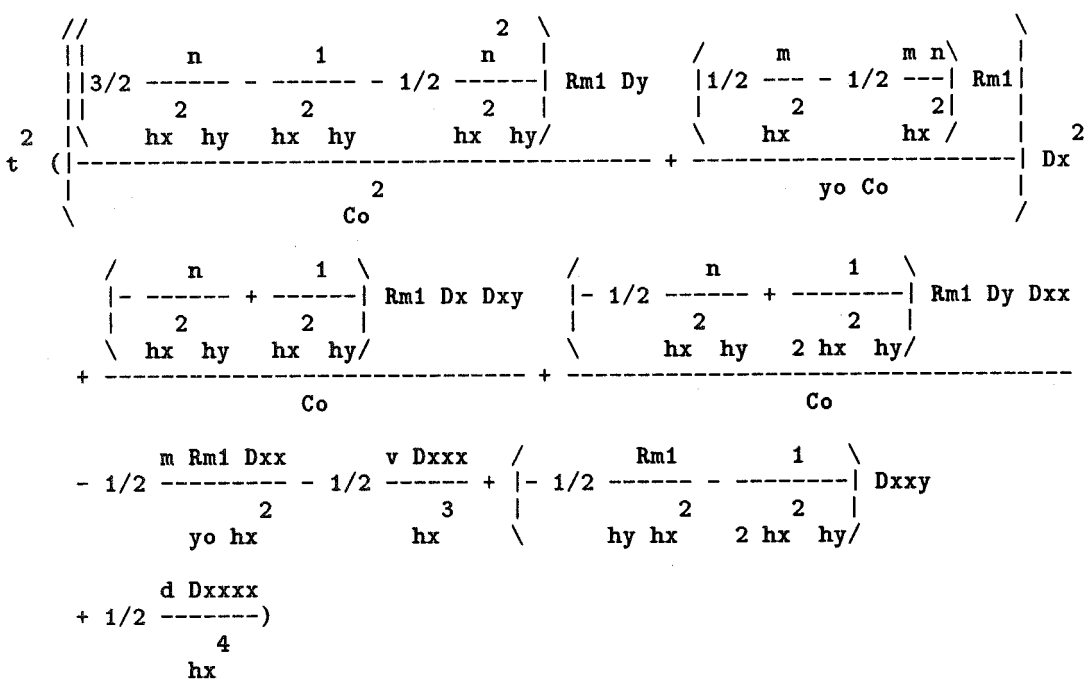


Terms in x y





Terms in x^2



Note that this is a variation of the approach in the next chapter, using p and q as measures of the number of increments, where they, generally, may be fractional or even larger than one.

6.5 Adding Linear Difference Equations

If all the terms of different order were linear, the problem/solution could be posed in a different way. We look at each series of sub-terms of a given order as a finite difference equation that has a solution. We find that solution for the appropriate finite differences, for instance, the value of Dtt as a function of Dx and $Dxxx$, etc and solve for Dtt. After Dt is calculated from the zero order approximation, the D's are added to give a better approximation. Of course, it doesn't work this way; a matrix solution is required. But the scheme, at least to some degree of approximation, should be able to correct for errors. Complex non-linear multivariate polynomials could even be handled by organising the equations using Grobner Bases, lists of easier-to-solve polynominal equations. Even when the equations are slightly out of linearity, one would expect some advantage. An example of this approach is presented in Section 7.5.

7 Future Developments

This document hopes to have laid down the foundation for a number of procedures for calculating the difference formulas and the use of them in analysis and solution of Partial Differential Equations. To be of general use they need to be more easily calculated[3] and extended to at least 3 dimensions. Knowing the values of the coefficients goes a long way toward producing more general formulas and has, as shown below, led to some general formulas.

7.1 A Simplier, Top-Down Approach

The approach presented forms a grid of functional values and proceeds to take every difference following certain rules. This builds up a difference pyramid. By trial and error, the initial sizes of the grid are chosen to produce just the right number of difference formulas to allow a solution. There are a number of problems with this bottom-up approach. One is the fact that the higher order terms may be truncated over the values they would have on an infinite grid. This is particularily so with complex, mixed order schemes for differencing and happens in any real problem at the edges. A well-structured analysis would always calculate the right number without ado. The logistics of location during differencing also gets out of hand. An alternative is to select a required difference and calculate it, extending the difference pyramid Top-Down. This approach is attractive since it automatically collects the right values of the functions when the subtractions are done at the bottom. It is recursive as well so it requires little code. Though it may repeat subtractions unnessarily, it also does not initially calculate any more differences or functional values than necessary. Also the look-up is different and combinations of terms at the function level may reduce the number of Taylor expansions. The program below has evolved from this concept.

```
# Program Fd.mpl
#  Must use Maple 5.2  wdscott/jsdevitt Aug92
#  Use a Top-Down calculation to produce equations for the finite differences
     ndif := 5: ndim := 3: NP := ndif + 1;
#  number of differences, number of dimensions, polynominal terms
```

[3]It takes, perhaps an hour to complete the calculations in two dimensions with 7^{th} degree polynominal expansions

```
# -A recursive process for a forward difference scheme:
#   computes the forward difference with a repeated subtraction,
#     ending in the functional difference
#         F(i1*h1,i2*h2,..,(ip+1)*hp,..,in*hn)
#            - F(i1*h1,i2*h2,...ip*hp....in*hn)
#   (Offset, nodal values are omitted here; they make no difference)
# -The F values are approximated using a multivariate taylor
#   expansion about (0,..0) of the function f.
# -The equation set is solved for the derivatives at (0,0,0) as a
#   function of the finite differences.

# The recursive, finite difference process FD
FD := proc(F:{procedure}) local i,p,idx,argv1,argv2;
   if not type(procname,indexed) then ERROR(`use indexed name`) fi;
   idx := [op(procname)];
   if idx = [] then
RETURN( F );
   else
i := nops(idx);
p := idx[i];
idx := op( subsop(i=NULL,idx) );
argv1 := arguments(F);
argv2 := op(subsop(p=argv1[p] + h.p,[argv1]));
unapply( FD[idx](F)(argv2) - FD[idx](F)(argv1), argv1 );
   fi;
end;

arguments := proc(g:procedure) local g;   #This collects the arguments
   op(1,eval(g));                         # from the procedure f
end:

 F := proc(x1,x2,x3) 'F'(args) end;       #Defines F as a process in the
                                          # selected variates x1,x2,x3

#> FD[1,1,2](F)(x,y,z);
#
#     F(x + 2 h1, y + h2, z) - 2 F(x + h1, y + h2, z) + F(x, y + h2, z)
#          - F(x + 2 h1, y, z) + 2 F(x + h1, y, z) - F(x, y, z)
#
#>

readlib(mtaylor);

# Find the names of the finite differences by analogy with D:
   argus := seq(t*x.i,i=1..ndim):
   taylor(f(argus),t,NP):
   partials := select(has,indets(",function),D):
# returns derivatives @ (0,..0)
   partial := map( proc(x) op(0,x) end , partials):
# scrapes off the argument list
   finite := subs(D=Fd,partial);
```

```
# Set up the equations containing the finite differences Fd
#  as a function of F
  eqns := NULL:
  finites := NULL:
for t in finite do
   fff := t(0,0,0);
   finites := finites, fff;
   eqns := eqns, fff = eval(subs(Fd=FD,f=F,fff));
 od:
# FD should recursively expand the finite differences in terms of
#  functional values.
 eqns := {eqns};
 whattype(eqns);
  nops(eqns);

#-------------------------------------
# Now we allow the program to make a Taylor series approximation to f

taym := proc(g:algebraic,X:list(name));
  # suggested args := seq(x.i*h.i,i=1..ndim);
    RETURN( unapply( mtaylor(g(op(X)),X,NP),op(X)) );
# note that NP is the number of terms and is a global variable
end;

    ans := eval(subs(F=taym(f,[x1,x2,x3]),eqns)):
#-------------------------------------

# Calculate the partials in terms of the finite differences
    solve(ans,partials);
    ans := collect(",finites);

# Some expansion and simplification needs to be done
 partials := [sort(partials,lexorder)]; #sorted partial derivative names
 finites := [sort(finites,lexorder)]; #sorted finite difference names
 ff := a->sort(a,finites):
 gg := b->lhs(b)=ff(rhs(b)):
 sol := map(gg,ans):
 sol := [sort(sol,lexorder)];
```

The recursive process FD breaks down the forward difference. That is[4]. Normally this form would be applied to a function f and be evaluated at a position, say $(x1, x2, x3)$; written $Fd[1,1,2,2,2](f)(x1,x2,x3)$. $Dxxyy$ at position (x, y) becomes $Dxxy$ at position (x, y) subtracted from $Dxxy$ at position (x,y+hy). In turn, Dxxy is broken into differences Dxx, etc., until the last x-difference is taken and the function F remains, finishing the

[4]We have now gone to a more general, operator notation, as used by Maple for derivatives; the names are derived using the analogy with the D operator, $Fd[1,1,2,2,2] \equiv Dxxyyy$

calculation[5]. This creates a difference pyramid with a 'progenator' at the top with 'generations' below that form the 'base'.

After the differences are all formed, a substitution is make for the F values with the taylor series expansion for f, minimising the number of substitutions. The equation set is solved for the derivatives (partials) at (0,0,0) in terms of the finite differences (finites). After a little ordering, the solution is complete. The program can produce a fifth-0rder expansion in about two hours.

7.2 Newton/Everett Difference Forms

Substitution of the difference equations for the derivatives in a Taylor expansion of the function yields a difference equation for the function. This is used in interpolation to positions less than ($p < 1$) or more than ($p > 1$) the increment hz. (The arguments are now z and t.) Also the forms can be used to derive expressions for the derivatives in terms of the differences by simply differentiating. In the case of a single argument, these latter forms are called the Markov formulas. Variations of the formulas are given in Abranowitz and Stegen [1] and the Mathematical Tables of the National Bureau of Standards [?]. However, in these standard tables the general expressions are not given for either the multivariate cases or are they given for the central difference form.

Maple program newton creates the series:

```
# Program newton
#  Substitutes the finite difference expansions back into the Taylor
#   series expansion, to interpolate to position p*hz and q*ht
#  uses arguments z and t.

N := 7; NP := N+1; a := 0: b:= 0:
readlib(mtaylor);
# usage:  tay(g(2*x,y),x,y);
tay := proc(g,x,y) local t1;
    t1 := mtaylor(g,[x=a,y=b],NP); t1 := convert(t1,polynom);
       end;

ffff := tay(f(z,t),z,t);=:
```

[5]It is important at this point that we have not evaluated the function F interms of a Taylor series–in fact it could be any function, even experimental values. The taylor series form of the function f is substituted later

```
read 'msol.m';
# Change statement to read the appropriate differencing solution as sol
sol := convert(sol,set):
new := subs(sol,ffff):
new := subs(z=p*hz,t=q*ht,new):

 finites:= [Dx,Dy, Dxx,Dxy,Dyy, Dxxx,Dxxy,Dxyy,Dyyy,
  Dxxxx,Dxxxy,Dxxyy,Dxyyy,Dyyyy, Dxxxxx,Dxxxxy,Dxxxyy,Dxxyyy,Dxyyyy,Dyyyyy,
  Dxxxxxx,Dxxxxxy,Dxxxxyy,Dxxxyyy,Dxxyyyy,Dxyyyyy,Dyyyyyy,
  Dxxxxxxx,Dxxxxxxy,Dxxxxxyy,Dxxxxyyy,Dxxxyyyy,Dxxyyyyy,Dxyyyyyy,Dyyyyyyy]:

new := collect(new,finites):
new := sort(new,finites);
quit;
```

7.2.1 Forward Differences, a multivariate case of Newton's Forward Difference Formula

```
  f(p hz, q ht) =
                                                  2                          2
   q Dt + p Dz + (- 1/2 q + 1/2 q ) Dtt + p q Dzt + (- 1/2 p + 1/2 p ) Dzz

                    3          2                    2
 + (1/3 q + 1/6 q  - 1/2 q ) Dttt + (1/2 p q  - 1/2 p q) Dztt

         2                                      2        3
 + (1/2 p  q - 1/2 p q) Dzzt + (1/3 p - 1/2 p  + 1/6 p ) Dzzz

   /       3                   4    11   2\
 + |- 1/4 q  - 1/4 q + 1/24 q  + ---- q | Dtttt
   \                             24    /

                       3          2
 + (1/3 p q + 1/6 p q  - 1/2 p q ) Dzttt

            2                        2  2          2
 + (- 1/4 p  q + 1/4 p q + 1/4 p  q  - 1/4 p q ) Dzztt

                      2          3
 + (1/3 p q - 1/2 p  q + 1/6 p  q) Dzzzt

   / 11   2                   4        3\
 + |---- p  - 1/4 p + 1/24 p  - 1/4 p | Dzzzz
   \ 24                               /

                     5          3         4         2
 + (1/5 q + 1/120 q  + 7/24 q  - 1/12 q  - 5/12 q ) Dttttt

   /         3    11     2           4          \
 + |- 1/4 p q  + ---- p q  + 1/24 p q  - 1/4 p q| Dztttt +
   \              24                             /
```

$$(-\tfrac{1}{12} p q^3 - \tfrac{1}{6} p q - \tfrac{1}{4} p^2 q^2 + \tfrac{1}{12} p^2 q^3 + \tfrac{1}{4} p q^2 + \tfrac{1}{6} p^2 q)\, Dzzttt$$

$$+$$

$$(-\tfrac{1}{12} p^3 q + \tfrac{1}{4} p^2 q + \tfrac{1}{12} p^3 q^2 - \tfrac{1}{4} p^2 q^2 - \tfrac{1}{6} p q + \tfrac{1}{6} p q^2)\, Dzzztt$$

$$+ \left(\tfrac{1}{24} p^4 q - \tfrac{1}{4} p^3 q + \tfrac{11}{24} p^2 q - \tfrac{1}{4} p q\right) Dzzzzt$$

$$+ (\tfrac{7}{24} p^3 + \tfrac{1}{5} p - \tfrac{1}{12} p^4 - \tfrac{5}{12} p^2 + \tfrac{1}{120} p^5)\, Dzzzzz$$

$$+ \left(\tfrac{1}{720} q^6 - \tfrac{1}{48} q^5 + \tfrac{17}{144} q^4 - \tfrac{1}{6} q + \tfrac{137}{360} q^2 - \tfrac{5}{16} q^3\right) Dttttt$$

$$+ (\tfrac{1}{120} p q^5 - \tfrac{5}{12} p q^2 + \tfrac{7}{24} p q^3 + \tfrac{1}{5} p q - \tfrac{1}{12} p q^4)\, Dtttttt +$$

$$(-\tfrac{1}{48} p q^4 + \tfrac{11}{48} p^2 q^2 - \tfrac{1}{8} p^2 q - \tfrac{1}{8} p^2 q^3 + \tfrac{1}{48} p^2 q^4 + \tfrac{1}{8} p q$$

$$+ \tfrac{1}{8} p q^3 - \tfrac{11}{48} p q^2)\, Dzttttt + (\tfrac{1}{18} p^3 q - \tfrac{1}{6} p^2 q + \tfrac{1}{36} p^3 q^3$$

$$+ \tfrac{1}{4} p^2 q^2 + \tfrac{1}{18} p q^3 - \tfrac{1}{12} p^2 q^3 + \tfrac{1}{9} p q - \tfrac{1}{12} p^3 q^2 - \tfrac{1}{6} p q^2)$$

$$Dzzzttt + (\tfrac{1}{8} p^3 q - \tfrac{1}{8} p^3 q^2 - \tfrac{11}{48} p^2 q + \tfrac{1}{48} p^4 q^2 + \tfrac{11}{48} p^2 q^2$$

$$+ \tfrac{1}{8} p q - \tfrac{1}{48} p^4 q - \tfrac{1}{8} p q^2)\, Dzzzztt$$

$$+ (-\tfrac{1}{12} p^4 q + \tfrac{7}{24} p^3 q - \tfrac{5}{12} p^2 q + \tfrac{1}{5} p q + \tfrac{1}{120} p^5 q)\, Dzzzzzt$$

$$+ \left(-\tfrac{1}{48} p^5 - \tfrac{1}{6} p - \tfrac{5}{16} p^3 + \tfrac{137}{360} p^2 + \tfrac{17}{144} p^4 + \tfrac{1}{720} p^6\right) Dzzzzzz +$$

$$\left(\tfrac{29}{90} q^3 - \tfrac{7}{48} q^4 + \tfrac{5}{144} q^5 + \tfrac{1}{7} q + \tfrac{1}{5040} q^7 - \tfrac{1}{240} q^6 - \tfrac{7}{20} q^2\right)$$

$$Dtttttttt +$$

```
/137    2          5    17    4          3                      6\
|--- p q  - 1/48 p q  + --- p q  - 5/16 p q  - 1/6 p q + 1/720 p q | Dzttttt
\360                     144                                      /

              5         2             4         2  3         2  4          3
 + (- 1/240 p q  + 1/10 p  q + 1/24 p q  + 7/48 p  q  - 1/24 p  q  - 7/48 p q

         2  2          2         2  5                                  3  3
 - 5/24 p  q  + 5/24 p q  + 1/240 p  q  - 1/10 p q) Dzttttt + (- 1/24 p  q

         2  4         3          2  3    11   2  2    11  3  2          3
 - 1/48 p  q  - 1/24 p  q + 1/8 p  q  - ---- p  q  + --- p  q  - 1/12 p q
                                        48           144

        2          3  4    11     2          4
 + 1/8 p  q + 1/144 p  q  + ---- p q  + 1/72 p q  - 1/12 p q) Dzzztttt + (
                            72

        3      11  2  3         4  2          4  3          2         4
- 1/12 p  q + --- p  q  - 1/48 p  q  + 1/144 p  q  + 1/8 p q  + 1/72 p  q
              144

          3    11   2  2        3  2    11   2           3  3
 - 1/24 p q  - ---- p  q  + 1/8 p  q  + ---- p  q - 1/24 p  q  - 1/12 p q)
               48                      72

                    4  2          2         3  2         4          2  2
Dzzzzttt + (- 1/24 p  q  + 1/10 p q  + 7/48 p  q  + 1/24 p  q - 5/24 p  q

          5          3          2          5  2
 - 1/240 p  q - 7/48 p  q + 5/24 p  q + 1/240 p  q  - 1/10 p q) Dzzzzztt +

/        3      17  4          5               137  2           6  \
|- 5/16 p  q + --- p  q - 1/48 p  q - 1/6 p q + --- p  q + 1/720 p  q| Dzzzzzzt
\              144                              360                /

  /        2    29   3                    6          5         4          7\
 + |- 7/20 p  + ---- p  + 1/7 p - 1/240 p  + 5/144 p  - 7/48 p  + 1/5040 p |
  \             90                                                        /

Dzzzzzzz + f(0, 0)
```

7.2.2 Backward Differences, Newton's Backward Difference Formula

These terms are identical in magnitude to the terms in the forward case, only they are all of positive sign. For example:

```
f(p hz, q ht) =
                                  2                                  2
 q Dt + p Dz + (1/2 q  + 1/2 q) Dtt + p q Dzt + (1/2 p + 1/2 p ) Dzz
```

$$+ (1/3\ q + 1/6\ q^3 + 1/2\ q^2)\ Dttt + (1/2\ p\ q^2 + 1/2\ p\ q)\ Dztt + \text{etc.}$$

7.2.3 Central Differences, a variation of Everett's Interpolation Formula

$$f(p\ hz,\ q\ ht) =$$

$$q\ Dt + p\ Dz + 1/2\ q^2\ Dtt + p\ q\ Dzt + 1/2\ p^2\ Dzz + (1/6\ q^3 - 1/6\ q)\ Dttt$$

$$+ 1/2\ p\ q^2\ Dztt + 1/2\ p^2\ q\ Dzzt + (-1/6\ p + 1/6\ p^3)\ Dzzz$$

$$+ (-1/6\ q^2 + 1/24\ q^4)\ Dtttt + (-1/6\ p\ q + 1/6\ p\ q^3)\ Dzttt$$

$$+ 1/4\ p^2\ q^2\ Dzztt + (1/6\ p^3\ q - 1/6\ p\ q)\ Dzzzt + (1/24\ p^4 - 1/6\ p^2)\ Dzzzz$$

$$+ (1/120\ q^5 - 1/12\ q^3 + 3/40\ q)\ Dttttt + (1/24\ p\ q^4 - 1/6\ p\ q^2)\ Dzttttt$$

$$+ (-1/12\ p^2\ q + 1/12\ p^2\ q^3)\ Dzzttt + (1/12\ p^3\ q^2 - 1/12\ p\ q^2)\ Dzzztt$$

$$+ (-1/6\ p^2\ q + 1/24\ p^4\ q)\ Dzzzzt + (1/120\ p^5 - 1/12\ p^3 + 3/40\ p)\ Dzzzzz$$

$$+ (1/720\ q^6 - 1/36\ q^4 + 4/45\ q^2)\ Dtttttt$$

$$+ (1/120\ p\ q^5 + 3/40\ p\ q - 1/12\ p\ q^3)\ Dzttttt$$

$$+ (-1/12\ p^2\ q^2 + 1/48\ p^2\ q^4)\ Dzzttttt$$

$$+ (-1/36\ p^3\ q + 1/36\ p^3\ q^3 - 1/36\ p\ q^3 + 1/36\ p\ q)\ Dzzzttt$$

$$+ (1/48\ p^4\ q^2 - 1/12\ p^2\ q^2)\ Dzzzztt$$

$$+ (1/120\ p^5\ q + 3/40\ p\ q - 1/12\ p^3\ q)\ Dzzzzzt$$

$$+ (1/720\ p^6 - 1/36\ p^4 + 4/45\ p^2)\ Dzzzzzz$$

```
  / 37  3                      7          5\
+ |--- q  - 5/112 q + 1/5040 q  - 1/144 q | Dttttttt
  \720                                     /

             4          2           6
+ (- 1/36 p q  + 4/45 p q  + 1/720 p q ) Dtttttt

          2  5        2          2  3
+ (1/240 p  q  + 3/80 p  q - 1/24 p  q ) Dzttttt

           2          4        3  2         3  4
+ (1/36 p q  - 1/144 p q  - 1/36 p  q  + 1/144 p  q ) Dzzttttt

          4  3        4          2  3        2
+ (1/144 p  q  - 1/144 p  q - 1/36 p  q  + 1/36 p  q) Dzzzttt

          3  2        5  2          2
+ (- 1/24 p  q  + 1/240 p  q  + 3/80 p q ) Dzzzztt

          6          2          4
+ (1/720 p  q + 4/45 p  q - 1/36 p  q) Dzzzzzt

  / 37  3          5          7          \
+ |--- p  - 1/144 p  + 1/5040 p  - 5/112 p| Dzzzzzzz + f(0, 0)
  \720                                     /
```

7.2.4 Mixed Differences, a corruption of the central difference formula

```
f(p hz, q ht) =
                    2                                        2
 q Dt + p Dz + (1/2 q  - 1/2 q) Dtt + p q Dzt + (1/2 p + 1/2 p ) Dzz

                   3                  2           2
   + (- 1/6 q + 1/6 q ) Dttt + 1/2 p q  Dztt + 1/2 p  q Dzzt

         3                          2         4
   + (1/6 p  - 1/6 p) Dzzz + (- 1/24 q  + 1/24 q ) Dtttt

                        3              2  2
   + (- 1/24 p q + 1/6 p q ) Dzttt + 1/4 p  q  Dzztt

         3                                2         4
   + (1/6 p  q - 1/24 p q) Dzzzt + (- 1/24 p  + 1/24 p ) Dzzzz

          5         3                                2          4
   + (1/120 q  - 1/48 q  + 1/80 q) Dttttt + (- 1/24 p q  + 1/24 p q ) Dzttttt

          2  3        2                          2         3  2
   + (1/12 p  q  - 1/48 p  q) Dzzttt + (- 1/48 p q  + 1/12 p  q ) Dzzztt
```

$$+ \left(\frac{1}{24} p^4 q - \frac{1}{24} p^2 q\right) Dzzzzt + \left(\frac{1}{120} p^5 + \frac{1}{80} p - \frac{1}{48} p^3\right) Dzzzzz$$

$$+ \left(\frac{1}{720} q^6 + \frac{1}{180} q^2 - \frac{1}{144} q^4\right) Dttttt$$

$$+ \left(\frac{3}{640} p q - \frac{1}{48} p q^3 + \frac{1}{120} p q^5\right) Dtttttt$$

$$+ \left(-\frac{1}{48} p^2 q^2 + \frac{1}{48} p^2 q^4\right) Dzttttt$$

$$+ \left(-\frac{1}{144} p q^3 + \frac{1}{36} p^3 q^3 + \frac{1}{576} p q - \frac{1}{144} p^3 q\right) Dzzzttt$$

$$+ \left(\frac{1}{48} p^4 q^2 - \frac{1}{48} p^2 q^2\right) Dzzzztt$$

$$+ \left(\frac{1}{120} p^5 q - \frac{1}{48} p^3 q + \frac{3}{640} p q\right) Dzzzzzt$$

$$+ \left(\frac{1}{180} p^2 + \frac{1}{720} p^6 - \frac{1}{144} p^4\right) Dzzzzzz$$

$$+ \left(-\frac{3}{1792} q + \frac{37}{11520} q^3 + \frac{1}{5040} q^7 - \frac{1}{576} q^5\right) Ttttttt$$

$$+ \left(\frac{1}{180} p q^2 + \frac{1}{720} p q^6 - \frac{1}{144} p q^4\right) Dtttttt$$

$$+ \left(\frac{3}{1280} p^2 q - \frac{1}{96} p^2 q^3 + \frac{1}{240} p^2 q^5\right) Dzttttt$$

$$+ \left(-\frac{1}{576} p q^4 + \frac{1}{576} p q^2 - \frac{1}{144} p^3 q^2 + \frac{1}{144} p^3 q^4\right) Dzzttttt$$

$$+ \left(-\frac{1}{144} p^2 q^3 + \frac{1}{144} p^4 q^3 - \frac{1}{576} p^4 q + \frac{1}{576} p^2 q\right) Dzzzttt$$

$$+ \left(\frac{3}{1280} p q^2 + \frac{1}{240} p^5 q^2 - \frac{1}{96} p^3 q^2\right) Dzzzztt$$

$$+ \left(-\frac{1}{144} p^4 q + \frac{1}{180} p^2 q + \frac{1}{720} p^6 q\right) Dzzzzzt$$

$$+ \left(\frac{1}{5040} p^7 + \frac{37}{11520} p^3 - \frac{1}{576} p^5 - \frac{3}{1792} p\right) Dzzzzzz + f(0, 0)$$

This form is asymmetric because the first differences are forward in t and backward in z.

7.3 Formulas for the Terms

The forward and backward forms are easily converted into a general term. If we take the term with $D\underbrace{zz\cdot\cdot zt}_{n}\underbrace{t\cdot\cdot t}_{m}$ where n is the number of differences with respect to z and m is the number of differences with respect to t[6], the formula for this term is

$$\binom{p}{n}\binom{q}{m}\cdot D\underbrace{zz\cdot\cdot z}_{n}\underbrace{tt\cdot\cdot t}_{m}$$

and the entire forward difference series is

$$f(z_o+ph_z,t_o+qh_t)=f(z_o,t_o)+pDz+qDt+\sum_{i=1}^{n}\sum_{j=1}^{m}\binom{p}{i}\binom{q}{j}\cdot D\underbrace{zz\cdot\cdot z}_{i}\underbrace{tt\cdot\cdot t}_{j}$$

The backward difference is the same series except all terms are positive. This is equivalent to replacing the binominal product with

$$(p+i)(q+j)\binom{p+i-1}{i}\binom{q+j-1}{j}$$

The central difference form is a product of series of the form

$i=1,$	$i=2,$	$i=3,$	$i=4,$	$i=5,$
p	p^2	$(p-1)p(p+1)/6$	$(p-2)p^2(p+2)\ /24$	$(p-3)(p-1)p(p+1)(p+3)/120$

divided by $i!$. This series is emulated by the maple process

```
pp := proc (p,m)

        p^(2-m mod 2)*product (p + (2 - m mod 2) + 2 * k, k=0..floor (m/2)-1)
        *product (p - (2 - m mod 2) - 2 * k, k=0..floor (m/2)-1)
end:
# Created by Lianxiang Wang, Aug92
```

[6]The n and m apply to the last term selected

No doubt there is an elegant way of writing this in a binomial or multinomial form. It is, however, the factorial quotient

$$2^{i-1} \cdot \frac{p(p/2+i/2-1)!}{(p/2-i/2)! \cdot i!}$$

which does not yield an appropriate binomial form when $i = 1$; the combined factor of i and $j$terms becomes 1 when both i and j are zero. This suggests that a most appropriate central difference expansion form is

$$f(z_o + ph_z, t_o + qh_t) = \mathbf{D}(f(z,t))$$

where $\mathbf{D}$ is the combined difference operator

$$\mathbf{D} = \sum_{i=0}^{n}\sum_{j=0}^{m} 2^{i+j-2} \cdot \frac{pq(p/2+i/2-1)! \cdot (q/2+j/2-1)!}{i! \cdot j! \cdot (p/2-i/2)! \cdot (q/2-j/2)!} \cdot D \underbrace{zz\cdot\cdot z}_{i} \underbrace{tt\cdot\cdot t}_{j}$$

and the final evaluation is at the position (z_o, t_o), the nodal point.

7.3.1 Creating the Derivatives from the Newton/Everett forms

The whole difference expansion is obtained by differentiating this form with respect to z and t the number of times required to produce the appropriate derivative. Then, if the nodal derivative is wanted, $p = 0$ and $q = 0$ are substituted into the differentiated form. Since $\frac{\partial f}{\partial z} = \frac{\partial f}{\partial p} \cdot \frac{dp}{dz} = \frac{\partial f}{\partial p} \cdot \frac{1}{hz}$ and $\frac{\partial f}{\partial t} = \frac{\partial f}{\partial q} \cdot \frac{dq}{dt} = \frac{\partial f}{\partial q} \cdot \frac{1}{ht}$, each differentiation will divide the factor by either hz or ht. For example, the result of differentiating the general term with respect to p is

$$2^{i+j-2} \frac{\Gamma(q/2+j/2) \cdot \Gamma(p/2+i/2+1) \cdot (p^2-ip) \cdot [(\Psi(p/2+i/2) - \Psi(p/2-i/2) - 2i]}{\Gamma(j+1) \cdot \Gamma(q/2-j/2+1) \cdot (p^2-i^2) \cdot \Gamma(p/2-i/2+1) \cdot \Gamma(i+1)}$$

We divide this by hz , sum and add the difference forms and have the approximation to the derivative. If we want the value at the nodal point, (z_o, t_o) this becomes a little less daunting.[7].

[7]The limiting form is tricky. In Maple one has to first establish the number of terms required and set the i and j values within a written-out sum, then assign 0 to p and q or take the limits as p and q go to zero. The general term, with i and j not defined and 0 for p ands q always evaluates to 0 for all i and j.

Difference formulas other than these are also important, including the mixed form used in the present, Phosphorus problem, Section 7.2.4. A future extension of the present work is to evolve such a form to remove the tedium of the present calculations when it is extended to multiple dimensions and more terms.

7.4 Three Dimensions and More

The Top-Down approach lends itself to multiple dimensions and a Newton-Everett form in three dimensions should be easily extendable to more dimensions. The formula from Section 7.3 is already set up to be extended to three dimensions and the improved program of Section 7.1 allows the three dimensional terms to be calculated. The basis for the the three dimensional problem is the three variate Taylor Series expansion with coefficients

$$\frac{1}{n!} \cdot \sum_{j=0}^{n} \sum_{i=0}^{n} B(n,i,j) D_{\$(1,i),\$(2,j),\$(3,n-i-j)}(f)(0,0,0) x^i y^j z^{n-i-j} \qquad (4)$$

Which are the powers with a combined sum of n. B is the multinominal, best calculated with the program

```
#Program taylorxyz.mpl
#  calculates the 3D taylor expansion as a general form
with(combinat):
oldmultinomial := eval(multinomial);

multinomial := proc(n) local a;
 if not type([args],list(nonneg)) then RETURN( 'procname(args)' ) fi;
  a := convert( [args[2..nargs]],'+');
  if a > n then 0
  elif a = n then oldmultinomial(args);
 else oldmultinomial(args,n-a);
fi;
end;
alias(B=multinomial);

tp := proc(n) local i,j;
   Sum(Sum(multinomial(n,i,j)*D[1$i,2$j,3$(n-i-j)](f)\
   (0,0,0)*x^i*y^j*z^(n-i-j),i=0..n),j=0..n)
end;
```

It rather appears that this may be extended to multi-dimensionial situations just using the multinominal. The extended Newton/Everett formulas (as a function of $p_1, p_1, p_3, \cdots, p_n$) are not so clear, however. Such a form should allow a fast and simple calculation of the terms in the finite difference formulas.

The outputs from the Up-Down program (Section 6.1) for three dimensions are in the tables below. The 4^{th} and 5^{th} derivative formulas are approximated by the appropriate difference divided by the appropriate interval values to the level for the 5^{th} power expansions used (6 Taylor series terms).

7.4.1 Forward Difference formulas for the Derivatives

$$
\begin{aligned}
\text{[D[1](f)(0, 0, 0)} = {} & \frac{\text{Fd[1](f)(0, 0, 0)}}{\text{h1}} - 1/2\ \frac{\text{Fd[1, 1](f)(0, 0, 0)}}{\text{h1}} \\
& - 1/4\ \frac{\text{Fd[1, 1, 1, 1](f)(0, 0, 0)}}{\text{h1}} + 1/5\ \frac{\text{Fd[1, 1, 1, 1, 1](f)(0, 0, 0)}}{\text{h1}} \\
& + 1/3\ \frac{\text{Fd[1, 1, 1](f)(0, 0, 0)}}{\text{h1}},
\end{aligned}
$$

$$
\begin{aligned}
\text{D[2](f)(0, 0, 0)} = {} & \frac{\text{Fd[2](f)(0, 0, 0)}}{\text{h2}} - 1/4\ \frac{\text{Fd[2, 2, 2, 2](f)(0, 0, 0)}}{\text{h2}} \\
& + 1/5\ \frac{\text{Fd[2, 2, 2, 2, 2](f)(0, 0, 0)}}{\text{h2}} - 1/2\ \frac{\text{Fd[2, 2](f)(0, 0, 0)}}{\text{h2}} \\
& + 1/3\ \frac{\text{Fd[2, 2, 2](f)(0, 0, 0)}}{\text{h2}},
\end{aligned}
$$

$$
\begin{aligned}
\text{D[3](f)(0, 0, 0)} = {} & \frac{\text{Fd[3](f)(0, 0, 0)}}{\text{h3}} - 1/4\ \frac{\text{Fd[3, 3, 3, 3](f)(0, 0, 0)}}{\text{h3}} \\
& + 1/5\ \frac{\text{Fd[3, 3, 3, 3, 3](f)(0, 0, 0)}}{\text{h3}} - 1/2\ \frac{\text{Fd[3, 3](f)(0, 0, 0)}}{\text{h3}} \\
& + 1/3\ \frac{\text{Fd[3, 3, 3](f)(0, 0, 0)}}{\text{h3}},
\end{aligned}
$$

$$D[1,\ 1](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1](f)(0,\ 0,\ 0)}{h1^2} + \frac{11}{12}\,\frac{Fd[1,\ 1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^2} - 5/6\,\frac{Fd[1,\ 1,\ 1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^2} - \frac{Fd[1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^2},$$

$$D[1,\ 2](f)(0,0,0) = \frac{Fd[1,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} - 1/4\,\frac{Fd[1,\ 2,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} - 1/6\,\frac{Fd[1,\ 1,\ 1,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} - 1/4\,\frac{Fd[1,\ 1,\ 1,\ 1,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} - 1/2\,\frac{Fd[1,\ 1,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} - 1/6\,\frac{Fd[1,\ 1,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} + 1/4\,\frac{Fd[1,\ 1,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} + 1/3\,\frac{Fd[1,\ 1,\ 1,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} - 1/2\,\frac{Fd[1,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1\ h2} + 1/3\,\frac{Fd[1,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1\ h2},$$

$$D[1,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} - 1/2\,\frac{Fd[1,\ 1,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} - 1/6\,\frac{Fd[1,\ 1,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} + 1/3\,\frac{Fd[1,\ 1,\ 1,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} - 1/4\,\frac{Fd[1,\ 1,\ 1,\ 1,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} + 1/3\,\frac{Fd[1,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} - 1/4\,\frac{Fd[1,\ 3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} - 1/2\,\frac{Fd[1,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} + 1/4\,\frac{Fd[1,\ 1,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1\ h3} - 1/6\,\frac{Fd[1,\ 1,\ 1,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1\ h3},$$

$$D[2,\ 2](f)(0,\ 0,\ 0) = \frac{Fd[2,\ 2](f)(0,\ 0,\ 0)}{h2^2} + \frac{11}{12}\,\frac{Fd[2,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h2^2}$$

$$- 5/6\,\frac{Fd[2,\ 2,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h2^2} - \frac{Fd[2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h2^2},$$

$$D[2,\ 3](f)(0,0,0) = \frac{Fd[2,\ 3](f)(0,\ 0,\ 0)}{h2\ h3} - 1/4\,\frac{Fd[2,\ 2,\ 2,\ 2,\ 3](f)(0,\ 0,\ 0)}{h2\ h3}$$

$$- 1/6\,\frac{Fd[2,\ 2,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3} - 1/4\,\frac{Fd[2,\ 3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3}$$

$$- 1/2\,\frac{Fd[2,\ 2,\ 3](f)(0,\ 0,\ 0)}{h2\ h3} + 1/3\,\frac{Fd[2,\ 2,\ 2,\ 3](f)(0,\ 0,\ 0)}{h2\ h3}$$

$$- 1/2\,\frac{Fd[2,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3} - 1/6\,\frac{Fd[2,\ 2,\ 2,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3}$$

$$+ 1/4\,\frac{Fd[2,\ 2,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3} + 1/3\,\frac{Fd[2,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3},$$

$$D[3,\ 3](f)(0,0,0) = \frac{Fd[3,\ 3](f)(0,\ 0,\ 0)}{h3^2} + \frac{11}{12}\,\frac{Fd[3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h3^2}$$

$$- 5/6\,\frac{Fd[3,\ 3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h3^2} - \frac{Fd[3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h3^2},$$

$$D[1,\ 1,\ 1](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^3}$$

$$- 3/2\,\frac{Fd[1,\ 1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^3} + 7/4\,\frac{Fd[1,\ 1,\ 1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^3},$$

$$D[1,1,2](f)(0,0,0) = \frac{Fd[1,1,2](f)(0,0,0)}{h1\ h2^2}$$

$$+ 1/3\ \frac{Fd[1,1,2,2,2](f)(0,0,0)}{h1\ h2^2} + \frac{11}{12}\ \frac{Fd[1,1,1,1,2](f)(0,0,0)}{h1\ h2^2}$$

$$- 1/2\ \frac{Fd[1,1,2,2](f)(0,0,0)}{h1\ h2^2} - \frac{Fd[1,1,1,2](f)(0,0,0)}{h1\ h2^2}$$

$$+ 1/2\ \frac{Fd[1,1,1,2,2](f)(0,0,0)}{h1\ h2^2},$$

$$D[1,1,3](f)(0,0,0) = \frac{Fd[1,1,3](f)(0,0,0)}{h1\ h3^2}$$

$$- 1/2\ \frac{Fd[1,1,3,3](f)(0,0,0)}{h1\ h3^2} + 1/3\ \frac{Fd[1,1,3,3,3](f)(0,0,0)}{h1\ h3^2}$$

$$- \frac{Fd[1,1,1,3](f)(0,0,0)}{h1\ h3^2} + \frac{11}{12}\ \frac{Fd[1,1,1,1,3](f)(0,0,0)}{h1\ h3^2}$$

$$+ 1/2\ \frac{Fd[1,1,1,3,3](f)(0,0,0)}{h1\ h3^2},$$

$$D[1,2,2](f)(0,0,0) = \frac{Fd[1,2,2](f)(0,0,0)}{h1\ h2^2}$$

$$+ \frac{11}{12}\ \frac{Fd[1,2,2,2,2](f)(0,0,0)}{h1\ h2^2} + \frac{1}{3}\ \frac{Fd[1,1,1,2,2](f)(0,0,0)}{h1\ h2^2}$$

$$- 1/2 \frac{Fd[1, 1, 2, 2](f)(0, 0, 0)}{h1\ h2^2} - \frac{Fd[1, 2, 2, 2](f)(0, 0, 0)}{h1\ h2^2}$$

$$+ 1/2 \frac{Fd[1, 1, 2, 2, 2](f)(0, 0, 0)}{h1\ h2^2},$$

$$D[1, 2, 3](f)(0, 0, 0) = \frac{Fd[1, 2, 3](f)(0, 0, 0)}{h1\ h2\ h3}$$

$$- 1/2 \frac{Fd[1, 2, 3, 3](f)(0, 0, 0)}{h1\ h2\ h3} + 1/4 \frac{Fd[1, 1, 2, 3, 3](f)(0, 0, 0)}{h1\ h2\ h3}$$

$$+ 1/4 \frac{Fd[1, 2, 2, 3, 3](f)(0,0,0)}{h1\ h2\ h3} + 1/3 \frac{Fd[1, 2, 3, 3, 3](f)(0, 0, 0)}{h1\ h2\ h3}$$

$$- 1/2 \frac{Fd[1, 1, 2, 3](f)(0, 0, 0)}{h1\ h2\ h3} + 1/3 \frac{Fd[1, 1, 1, 2, 3](f)(0, 0, 0)}{h1\ h2\ h3}$$

$$- 1/2 \frac{Fd[1, 2, 2, 3](f)(0, 0, 0)}{h1\ h2\ h3} + 1/4 \frac{Fd[1, 1, 2, 2, 3](f)(0, 0, 0)}{h1\ h2\ h3}$$

$$+ 1/3 \frac{Fd[1, 2, 2, 2, 3](f)(0, 0, 0)}{h1\ h2\ h3},$$

$$D[1, 3, 3](f)(0, 0, 0) = \frac{Fd[1, 3, 3](f)(0, 0, 0)}{h1\ h3^2} - \frac{Fd[1, 3, 3, 3](f)(0,0,0)}{h1\ h3^2}$$

$$+ \frac{11}{12} \frac{Fd[1, 3, 3, 3, 3](f)(0, 0, 0)}{h1\ h3^2} + 1/2 \frac{Fd[1, 1, 3, 3, 3](f)(0,0,0)}{h1\ h3^2}$$

$$- 1/2 \frac{Fd[1, 1, 3, 3](f)(0, 0, 0)}{h1\ h3^2} + 1/3 \frac{Fd[1, 1, 1, 3, 3](f)(0, 0, 0)}{h1\ h3^2},$$

$$D[2, 2, 2](f)(0, 0, 0) = \frac{Fd[2, 2, 2](f)(0, 0, 0)}{h2^3}$$

$$- 3/2 \frac{Fd[2, 2, 2, 2](f)(0, 0, 0)}{h2^3} + 7/4 \frac{Fd[2, 2, 2, 2, 2](f)(0, 0, 0)}{h2^3},$$

$$D[2, 2, 3](f)(0, 0, 0) = \frac{Fd[2, 2, 3](f)(0, 0, 0)}{h2^2\ h3}$$

$$+ \frac{11}{12} \frac{Fd[2, 2, 2, 2, 3](f)(0, 0, 0)}{h2^2\ h3} + 1/3 \frac{Fd[2, 2, 3, 3, 3](f)(0,0,0)}{h2^2\ h3}$$

$$- \frac{Fd[2, 2, 2, 3](f)(0, 0, 0)}{h2^2\ h3} + 1/2 \frac{Fd[2, 2, 2, 3, 3](f)(0, 0, 0)}{h2^2\ h3}$$

$$- 1/2 \frac{Fd[2, 2, 3, 3](f)(0, 0, 0)}{h2^2\ h3},$$

$$D[2, 2, 2, 2, 3](f)(0, 0, 0) = \frac{Fd[2, 2, 2, 2, 3](f)(0, 0, 0)}{h2^4\ h3},$$

$$D[3, 3, 3](f)(0, 0, 0) = \frac{Fd[3, 3, 3](f)(0, 0, 0)}{h3^3}$$

$$- 3/2 \frac{Fd[3, 3, 3, 3](f)(0, 0, 0)}{h3^3} + 7/4 \frac{Fd[3, 3, 3, 3, 3](f)(0, 0, 0)}{h3^3},$$

$$D[1, 1, 1, 1](f)(0, 0, 0) =$$

$$\frac{Fd[1, 1, 1, 1](f)(0, 0, 0)}{h1^4} - 2 \frac{Fd[1, 1, 1, 1, 1](f)(0, 0, 0)}{h1^4},$$

$$D[1, 1, 1, 2](f)(0, 0, 0) = \frac{Fd[1, 1, 1, 2](f)(0, 0, 0)}{h1^3\ h2}$$

$$- 1/2\ \frac{Fd[1,\ 1,\ 1,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1^{3}\ h2} - 3/2\ \frac{Fd[1,\ 1,\ 1,\ 1,\ 2](f)(0,0,0)}{h1^{3}\ h2},$$

$$D[1,\ 1,\ 1,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 1,\ 3](f)(0,\ 0,\ 0)}{h1^{3}\ h3}$$

$$- 3/2\ \frac{Fd[1,\ 1,\ 1,\ 1,\ 3](f)(0,\ 0,\ 0)}{h1^{3}\ h3} - 1/2\ \frac{Fd[1,\ 1,\ 1,\ 3,\ 3](f)(0,0,0)}{h1^{3}\ h3},$$

$$D[1,\ 1,\ 2,\ 2](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1^{2}\ h2^{2}}$$

$$- \frac{Fd[1,\ 1,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1^{2}\ h2^{2}} - \frac{Fd[1,\ 1,\ 1,\ 2,\ 2](f)(0,\ 0,\ 0)}{h1^{2}\ h2^{2}},$$

$$D[1,\ 1,\ 2,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 2,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h2\ h3}$$

$$- 1/2\ \frac{Fd[1,\ 1,\ 2,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h2\ h3} - \frac{Fd[1,\ 1,\ 1,\ 2,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h2\ h3}$$

$$- 1/2\ \frac{Fd[1,\ 1,\ 2,\ 2,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h2\ h3},$$

$$D[1,\ 1,\ 3,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h3^{2}}$$

$$- \frac{Fd[1,\ 1,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h3^{2}} - \frac{Fd[1,\ 1,\ 1,\ 3,\ 3](f)(0,\ 0,\ 0)}{h1^{2}\ h3^{2}},$$

$$D[1,2,2,2](f)(0,0,0) = \frac{Fd[1,2,2,2](f)(0,0,0)}{h1\,h2^{3}}$$

$$- 3/2\,\frac{Fd[1,2,2,2,2](f)(0,0,0)}{h1\,h2^{3}} - 1/2\,\frac{Fd[1,1,2,2,2](f)(0,0,0)}{h1\,h2^{3}},$$

$$D[1,2,2,3](f)(0,0,0) = \frac{Fd[1,2,2,3](f)(0,0,0)}{h1\,h2^{2}\,h3}$$

$$- 1/2\,\frac{Fd[1,2,2,3,3](f)(0,0,0)}{h1\,h2^{2}\,h3} - 1/2\,\frac{Fd[1,1,2,2,3](f)(0,0,0)}{h1\,h2^{2}\,h3}$$

$$- \frac{Fd[1,2,2,2,3](f)(0,0,0)}{h1\,h2^{2}\,h3},$$

$$D[1,2,3,3](f)(0,0,0) = \frac{Fd[1,2,3,3](f)(0,0,0)}{h1\,h2\,h3^{2}}$$

$$- 1/2\,\frac{Fd[1,1,2,3,3](f)(0,0,0)}{h1\,h2\,h3^{2}} - 1/2\,\frac{Fd[1,2,2,3,3](f)(0,0,0)}{h1\,h2\,h3^{2}}$$

$$- \frac{Fd[1,2,3,3,3](f)(0,0,0)}{h1\,h2\,h3^{2}},$$

$$D[1,3,3,3](f)(0,0,0) = \frac{Fd[1,3,3,3](f)(0,0,0)}{h1\,h3^{3}}$$

$$- 3/2\,\frac{Fd[1,3,3,3,3](f)(0,0,0)}{h1\,h3^{3}} - 1/2\,\frac{Fd[1,1,3,3,3](f)(0,0,0)}{h1\,h3^{3}},$$

$$D[2,2,2,2](f)(0,0,0) =$$

$$\frac{Fd[2,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h2^4} - 2\,\frac{Fd[2,\ 2,\ 2,\ 2,\ 2](f)(0,\ 0,\ 0)}{h2^4},$$

$$D[2,\ 2,\ 2,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[2,\ 2,\ 2,\ 3](f)(0,\ 0,\ 0)}{h2^3\ h3}$$

$$- 3/2\,\frac{Fd[2,\ 2,\ 2,\ 2,\ 3](f)(0,\ 0,\ 0)}{h2^3\ h3} - 1/2\,\frac{Fd[2,\ 2,\ 2,\ 3,\ 3](f)(0,0,0)}{h2^3\ h3},$$

$$D[2,\ 2,\ 3,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[2,\ 2,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2^2\ h3^2}$$

$$- \frac{Fd[2,\ 2,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2^2\ h3^2} - \frac{Fd[2,\ 2,\ 2,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2^2\ h3^2},$$

$$D[2,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0) = \frac{Fd[2,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3^3}$$

$$- 1/2\,\frac{Fd[2,\ 2,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3^3} - 3/2\,\frac{Fd[2,\ 3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h2\ h3^3},$$

$$D[3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0) =$$

$$\frac{Fd[3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h3^4} - 2\,\frac{Fd[3,\ 3,\ 3,\ 3,\ 3](f)(0,\ 0,\ 0)}{h3^4},$$

$$D[1,\ 1,\ 1,\ 1,\ 1](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 1,\ 1,\ 1](f)(0,\ 0,\ 0)}{h1^5},$$

$$D[1,\ 1,\ 1,\ 1,\ 2](f)(0,\ 0,\ 0) = \frac{Fd[1,\ 1,\ 1,\ 1,\ 2](f)(0,\ 0,\ 0)}{h1^4\ h2},$$

$$
\begin{aligned}
D[2, 3, 3](f)(0, 0, 0) = {} & \frac{Fd[2, 3, 3](f)(0, 0, 0)}{h2\ h3^{2}} \\
& + \frac{11}{12}\ \frac{Fd[2, 3, 3, 3, 3](f)(0, 0, 0)}{h2\ h3^{2}} + 1/3\ \frac{Fd[2, 2, 2, 3, 3](f)(0,0,0)}{h2\ h3^{2}} \\
& - 1/2\ \frac{Fd[2, 2, 3, 3](f)(0, 0, 0)}{h2\ h3^{2}} - \frac{Fd[2, 3, 3, 3](f)(0, 0, 0)}{h2\ h3^{2}} \\
& + 1/2\ \frac{Fd[2, 2, 3, 3, 3](f)(0, 0, 0)}{h2\ h3^{2}},
\end{aligned}
$$

7.4.2 Newton's Forward Difference Formula in Three Dimensions

Note that the finite difference forms have been now been written with $Fd[1,1,2,2,2] \equiv Dxxyyy$ for sorting purposes and to conserve space. This is a simple extension of the difference form used in Sections 2, 3, and 4, $(Dzt \equiv Dxy \equiv Fd11)$ to allow for multiple dimensions and avoid confusion with the D operator.

$$
\begin{aligned}
& f(p1\ h1,\ p2\ h1,\ p3\ h3) := \\
& \quad p1\ Fd1 + p2\ Fd2 + p3\ Fd3 + (-\ 1/2\ p1 + 1/2\ p1^{2})\ Fd11 + p1\ p2\ Fd12 + \\
& (1/2\ p2^{2} - 1/2\ p2)\ Fd22 + p2\ p3\ Fd23 + (-\ 1/2\ p3 + 1/2\ p3^{2})\ Fd33 + \\
& (1/3\ p1 - 1/2\ p1^{2} + 1/6\ p1^{3})\ Fd111 + (-\ 1/2\ p1\ p2 + 1/2\ p1^{2}\ p2)\ Fd112 + \\
& (1/2\ p1\ p2^{2} - 1/2\ p1\ p2)\ Fd122 + (-\ 1/2\ p2^{2} + 1/3\ p2 + 1/6\ p2^{3})\ Fd222 + \\
& (-\ 1/2\ p2\ p3 + 1/2\ p2^{2}\ p3)\ Fd223 + (-\ 1/2\ p2\ p3 + 1/2\ p2\ p3^{2})\ Fd233 + \\
& (1/3\ p3 - 1/2\ p3^{2} + 1/6\ p3^{3})\ Fd333 + \\
& \left(-\ 1/4\ p1 + \frac{11}{24}\ p1^{2} + 1/24\ p1^{4} - 1/4\ p1^{3}\right) Fd1111 +
\end{aligned}
$$

$$(-1/2\ p1^2\ p2 + 1/6\ p1^3\ p2 + 1/3\ p1\ p2)\ Fd1112 +$$

$$(-1/4\ p1^2\ p2 + 1/4\ p1^2\ p2^2 - 1/4\ p1\ p2^2 + 1/4\ p1\ p2)\ Fd1122 +$$

$$(-1/2\ p1\ p2^2 + 1/6\ p1\ p2^3 + 1/3\ p1\ p2)\ Fd1222 +$$

$$\left(-1/4\ p2^3 - 1/4\ p2 + 1/24\ p2^4 + \frac{11}{24}\ p2^2\right)\ Fd2222 +$$

$$(1/3\ p2\ p3 + 1/6\ p2^3\ p3 - 1/2\ p2^2\ p3)\ Fd2223 +$$

$$(1/4\ p2\ p3 + 1/4\ p2^2\ p3^2 - 1/4\ p2^2\ p3 - 1/4\ p2\ p3^2)\ Fd2233 +$$

$$(1/3\ p2\ p3 + 1/6\ p2\ p3^3 - 1/2\ p2\ p3^2)\ Fd2333 +$$

$$\left(1/24\ p3^4 + \frac{11}{24}\ p3^2 - 1/4\ p3^3 - 1/4\ p3\right)\ Fd3333 +$$

$$(-5/12\ p1^2 - 1/12\ p1^4 + 1/120\ p1^5 + 7/24\ p1^3 + 1/5\ p1)\ Fd11111 +$$

$$\left(\frac{11}{24}\ p1^2\ p2 - 1/4\ p1^3\ p2 + 1/24\ p1^4\ p2 - 1/4\ p1\ p2\right)\ Fd11112 +$$

$$(1/4\ p1^2\ p2 - 1/12\ p1^3\ p2 - 1/4\ p1^2\ p2^2 + 1/12\ p1^3\ p2^2 + 1/6\ p1\ p2^2 - 1/6\ p1\ p2)\ Fd11122 +$$

$$(1/6\ p1^2\ p2 - 1/4\ p1^2\ p2^2 + 1/4\ p1\ p2^2 + 1/12\ p1^2\ p2^3 - 1/12\ p1\ p2^3 - 1/6\ p1\ p2)\ Fd11222 +$$

$$\left(1/24\ p1\ p2^4 + \frac{11}{24}\ p1\ p2^2 - 1/4\ p1\ p2 - 1/4\ p1\ p2^3\right)\ Fd12222 +$$

$$(1/5\ p2 + 7/24\ p2^3 + 1/120\ p2^5 - 5/12\ p2^2 - 1/12\ p2^4)\ Fd22222 +$$

$$\left(-1/4\ p2\ p3 + 1/24\ p2^4\ p3 - 1/4\ p2^3\ p3 + \frac{11}{24}\ p2^2\ p3\right)\ Fd22223 +$$

$$(-\tfrac{1}{6}\,p2\,p3 + \tfrac{1}{12}\,p2^3\,p3^2 - \tfrac{1}{12}\,p2^3\,p3 + \tfrac{1}{4}\,p2^2\,p3 + \tfrac{1}{6}\,p2\,p3^2 - \tfrac{1}{4}\,p2^2\,p3^2)\,Fd22233 +$$

$$(\tfrac{1}{4}\,p2\,p3^2 - \tfrac{1}{6}\,p2\,p3 + \tfrac{1}{12}\,p2^2\,p3^3 - \tfrac{1}{12}\,p2\,p3^3 - \tfrac{1}{4}\,p2^2\,p3^2 + \tfrac{1}{6}\,p2^2\,p3)\,Fd22333 +$$

$$\left(\frac{11}{24}\,p2\,p3^2 - \tfrac{1}{4}\,p2\,p3 + \tfrac{1}{24}\,p2\,p3^4 - \tfrac{1}{4}\,p2\,p3^3\right)Fd23333 +$$

$$(\tfrac{1}{5}\,p3 + \tfrac{1}{120}\,p3^5 + \tfrac{7}{24}\,p3^3 - \tfrac{5}{12}\,p3^2 - \tfrac{1}{12}\,p3^4)\,Fd33333$$

7.4.3 Central Differences-Derivative Formulas

$$[D[1](f)(0,0,0) = \frac{Fd[1](f)(0,0,0)}{h1} + 3/640\,\frac{Fd[1,1,1,1,1](f)(0,0,0)}{h1} - 1/24\,\frac{Fd[1,1,1](f)(0,0,0)}{h1},$$

$$D[2](f)(0,0,0) = \frac{Fd[2](f)(0,0,0)}{h2} + 3/640\,\frac{Fd[2,2,2,2,2](f)(0,0,0)}{h2} - 1/24\,\frac{Fd[2,2,2](f)(0,0,0)}{h2},$$

$$D[3](f)(0,0,0) = \frac{Fd[3](f)(0,0,0)}{h3} + 3/640\,\frac{Fd[3,3,3,3,3](f)(0,0,0)}{h3} - 1/24\,\frac{Fd[3,3,3](f)(0,0,0)}{h3},$$

$$D[1,1](f)(0,0,0) = \frac{Fd[1,1](f)(0,0,0)}{h1^2} - 1/12\,\frac{Fd[1,1,1,1](f)(0,0,0)}{h1^2},$$

$$D[1, 2](f)(0, 0, 0) = \frac{Fd[1, 2](f)(0, 0, 0)}{h1\ h2} - 1/24\ \frac{Fd[1, 2, 2, 2](f)(0, 0, 0)}{h1\ h2}$$

$$- 1/24\ \frac{Fd[1, 1, 1, 2](f)(0, 0, 0)}{h1\ h2},$$

$$D[1, 3](f)(0, 0, 0) = \frac{Fd[1, 3](f)(0, 0, 0)}{h1\ h3} - 1/24\ \frac{Fd[1, 3, 3, 3](f)(0, 0, 0)}{h1\ h3}$$

$$- 1/24\ \frac{Fd[1, 1, 1, 3](f)(0, 0, 0)}{h1\ h3},$$

$$D[2, 2](f)(0, 0, 0) = \frac{Fd[2, 2](f)(0, 0, 0)}{h2^2} - 1/12\ \frac{Fd[2, 2, 2, 2](f)(0, 0, 0)}{h2^2},$$

$$D[2, 3](f)(0, 0, 0) = \frac{Fd[2, 3](f)(0, 0, 0)}{h2\ h3} - 1/24\ \frac{Fd[2, 2, 2, 3](f)(0, 0, 0)}{h2\ h3}$$

$$- 1/24\ \frac{Fd[2, 3, 3, 3](f)(0, 0, 0)}{h2\ h3},$$

$$D[3, 3](f)(0, 0, 0) = \frac{Fd[3, 3](f)(0, 0, 0)}{h3^2} - 1/12\ \frac{Fd[3, 3, 3, 3](f)(0, 0, 0)}{h3^2},$$

$$D[1, 1, 1](f)(0, 0, 0) =$$

$$\frac{Fd[1, 1, 1](f)(0, 0, 0)}{h1^3} - 1/8\ \frac{Fd[1, 1, 1, 1, 1](f)(0, 0, 0)}{h1^3},$$

$$D[1, 1, 2](f)(0, 0, 0) = \frac{Fd[1, 1, 2](f)(0, 0, 0)}{h1^2\ h2}$$

$$- 1/24\ \frac{Fd[1, 1, 2, 2, 2](f)(0, 0, 0)}{h1^2\ h2} - 1/12\ \frac{Fd[1, 1, 1, 1, 2](f)(0, 0, 0)}{h1^2\ h2},$$

$$D[1, 1, 3](f)(0, 0, 0) = \frac{Fd[1, 1, 3](f)(0, 0, 0)}{h1^2\, h3} - 1/24\, \frac{Fd[1, 1, 3, 3, 3](f)(0, 0, 0)}{h1^2\, h3} - 1/12\, \frac{Fd[1, 1, 1, 1, 3](f)(0, 0, 0)}{h1^2\, h3},$$

$$D[1, 2, 2](f)(0, 0, 0) = \frac{Fd[1, 2, 2](f)(0, 0, 0)}{h1\, h2^2} - 1/24\, \frac{Fd[1, 1, 1, 2, 2](f)(0, 0, 0)}{h1\, h2^2} - 1/12\, \frac{Fd[1, 2, 2, 2, 2](f)(0, 0, 0)}{h1\, h2^2},$$

$$D[1, 2, 3](f)(0, 0, 0) = \frac{Fd[1, 2, 3](f)(0, 0, 0)}{h1\, h2\, h3} - 1/24\, \frac{Fd[1, 2, 2, 2, 3](f)(0, 0, 0)}{h1\, h2\, h3} - 1/24\, \frac{Fd[1, 2, 3, 3, 3](f)(0, 0, 0)}{h1\, h2\, h3} - 1/24\, \frac{Fd[1, 1, 1, 2, 3](f)(0, 0, 0)}{h1\, h2\, h3},$$

$$D[1, 3, 3](f)(0, 0, 0) = \frac{Fd[1, 3, 3](f)(0, 0, 0)}{h1\, h3^2} - 1/24\, \frac{Fd[1, 1, 1, 3, 3](f)(0, 0, 0)}{h1\, h3^2} - 1/12\, \frac{Fd[1, 3, 3, 3, 3](f)(0, 0, 0)}{h1\, h3^2},$$

$$D[2, 2, 2](f)(0, 0, 0) = \frac{Fd[2, 2, 2](f)(0, 0, 0)}{h2^3} - 1/8\, \frac{Fd[2, 2, 2, 2, 2](f)(0, 0, 0)}{h2^3},$$

$$D[2, 2, 3](f)(0, 0, 0) = \frac{Fd[2, 2, 3](f)(0, 0, 0)}{h2^2\ h3} - 1/24\ \frac{Fd[2, 2, 3, 3, 3](f)(0, 0, 0)}{h2^2\ h3} - 1/12\ \frac{Fd[2, 2, 2, 2, 3](f)(0, 0, 0)}{h2^2\ h3},$$

$$D[2, 3, 3](f)(0, 0, 0) = \frac{Fd[2, 3, 3](f)(0, 0, 0)}{h2\ h3^2} - 1/24\ \frac{Fd[2, 2, 2, 3, 3](f)(0, 0, 0)}{h2\ h3^2} - 1/12\ \frac{Fd[2, 3, 3, 3, 3](f)(0, 0, 0)}{h2\ h3^2},$$

$$D[3, 3, 3](f)(0, 0, 0) = \frac{Fd[3, 3, 3](f)(0, 0, 0)}{h3^3} - 1/8\ \frac{Fd[3, 3, 3, 3, 3](f)(0, 0, 0)}{h3^3}$$

7.4.4 Newton/Everett Formula for Three Dimensions

$$\begin{aligned} f(p1\ h1, p2\ h1, p3\ h3) := \\ & p1\ Fd1 + p2\ Fd2 + p3\ Fd3 + 1/2\ p1\ Fd11 + p1\ p2\ Fd12 + 1/2\ p2\ Fd22 \\ & + p2\ p3\ Fd23 + 1/2\ p3^2\ Fd33 + (1/6\ p1^3 - 1/24\ p1)Fd111 + 1/2\ p1\ p2^2\ Fd112 \\ & + 1/2\ p1\ p2^2\ Fd122 + (1/6\ p2^3 - 1/24\ p2)\ Fd222 + 1/2\ p2^2\ p3\ Fd223 \\ & + 1/2\ p2\ p3^2\ Fd233 + (1/6\ p3^3 - 1/24\ p3)\ Fd333 + (1/24\ p1^4 - 1/24\ p1^2)\ Fd1111 \\ & + (-1/24\ p1\ p2 + 1/6\ p1^3\ p2)\ Fd1112 + 1/4\ p1^2\ p2^2\ Fd1122 \\ & + (-1/24\ p1\ p2 + 1/6\ p1\ p2^3)\ Fd1222 + (-1/24\ p2^2 + 1/24\ p2^4)\ Fd2222 \end{aligned}$$

```
          3                                    2   2
  + (1/6 p2  p3 - 1/24 p2 p3) Fd2223 + 1/4 p2  p3  Fd2233

          3                                   2          4
  + (1/6 p2 p3  - 1/24 p2 p3) Fd2333 + (- 1/24 p3  + 1/24 p3 ) Fd3333

                        3           5
  + (3/640 p1 - 1/48 p1  + 1/120 p1 ) Fd11111

         4              2                        3   2              2
+ (1/24 p1  p2 - 1/24 p1  p2) Fd11112 + (1/12 p1  p2  - 1/48 p1 p2 ) Fd11122

         2   3          2                       4              2
+ (1/12 p1  p2  - 1/48 p1  p2) Fd11222 + (1/24 p1 p2  - 1/24 p1 p2 ) Fd12222

          3           5
  + (- 1/48 p2  + 1/120 p2  + 3/640 p2) Fd22222

          4           2
  + (1/24 p2  p3 - 1/24 p2  p3) Fd22223

                2          3   2
  + (- 1/48 p2 p3  + 1/12 p2  p3 ) Fd22233

         2   3          2                       4              2
+ (1/12 p2  p3  - 1/48 p2  p3) Fd22333 + (1/24 p2 p3  - 1/24 p2 p3 ) Fd23333

          5          3
  + (1/120 p3  - 1/48 p3  + 3/640 p3) Fd33333
```

Note that this form, again, has far fewer terms then the forward difference form.

7.5 Navier-Stokes Equations

Of course, this general expansion analysis has broad application. One intended use involves the Navier-Stokes Equations. In their usual form, they are highly non-linear but, by collecting terms, they can be organised into a linear set of first order partial derivatives with complex dependent variables. Here we write the set vertically and presume that we are interested in calculating the time dependence of the flows. With three dimensions, there are four simultaneous equations to be solved, including the equation of continuity. Here we display one of the equations vertically.

$$
\begin{array}{ccccccccc}
Equation & & t^0 & & t^2 & & t^4 & & t^6 \\
\left\{\begin{array}{c} \frac{\partial A}{\partial t} \\ \| \\ \frac{\partial B}{\partial x} \\ + \\ \frac{\partial C}{\partial y} \\ + \\ \frac{\partial D}{\partial z} \end{array}\right\} & = & \left\{\begin{array}{c} \frac{D_t}{ht} \\ \| \\ \frac{D_x}{hx} \\ + \\ \frac{D_y}{hy} \\ + \\ \frac{D_z}{hz} \end{array}\right\} & -\frac{1}{6}\cdot & \left\{\begin{array}{c} \frac{D_{ttt}}{\cdot ht} \\ \| \\ \frac{D_{xxx}}{hx} \\ + \\ \frac{D_{yyy}}{hy} \\ + \\ \frac{D_{zzz}}{hz} \end{array}\right\} & +\frac{3}{40}\cdot & \left\{\begin{array}{c} \frac{D_{ttttt}}{\cdot ht} \\ \| \\ \frac{D_{xxxxx}}{hx} \\ + \\ \frac{D_{yyyyy}}{hy} \\ + \\ \frac{D_{zzzzz}}{hz} \end{array}\right\} & -\frac{5}{112}\cdot & \left\{\begin{array}{c} \frac{D_{ttttttt}}{\cdot ht} \\ \| \\ \frac{D_{xxxxxxx}}{hx} \\ + \\ \frac{D_{yyyyyyy}}{hy} \\ + \\ \frac{D_{zzzzzzz}}{hz} \end{array}\right\} & etc.
\end{array}
$$

Note that in these equations we have used the fact that the expansions have no cross terms and the differences of any one dependent variable (A, B, C, or D) are only with respect to one argument, respectively, (t, x, y or z). The concept is this: The finite difference equations shown to the right of the equal sign are solutions to linear problems that have no direct relevence to the problem. However, they are linear equations; this is a linear system. When added together (and weighted following the given coefficients, above) they produce the desired solution. We obtain the spatial differences (D_x, D_y, D_z and D_{xx}, etc.), add them appropriately, and obtain the time differences (D_t, D_{ttt}, D_{ttttt} and $D_{ttttttt}$, etc.). These are weighted with the above coefficents and added. Of course, the dependent variables are complex functions of velocity(squared), pressure, and shear stresses, but the A variables can always be organised so they are something like the momentum. This being so, it is also possible to allow that the last terms (or any terms) are closed with some sort of turbulence closure scheme. One of the usual forms, the eddy K scheme, however, might introduce non-linear forms. It might even be appropriate to allow that the last order determines the averaging required in this turbulent, stochastic flow problem.

8 Closing

Presented is a general technique for handling differential equations applied to the specialised non-linear problem of phosphorus movement in soils. The technique is not new and was mostly worked out by Newton and others[4]. The size of terms that can be considered is now almost unlimited. General extensions are possible without the drugery of hand calculations. This has lead to equations for the n^{th} term in an expansion and calculations in more than one dimension. The symbolic manipulator allows a number of unique opportunities for analysis and solution of partial differential equations. This document is offered as a working example for further exploitation of the technique.

9 Acknowledgements

The authors would like to thank all the members of the Symbolic Computation Group, Computer Science Department, University of Waterloo and Maple Waterloo Software, Inc. for their support. Special thanks go to David Clark, Lee Qiao, Greg Fee, Walter Neuenschwander, George Labahn, Benton Leong and David Hare, for their ever-present helping hands, through Maple.

10 References

References

[1] M. Abramowitz and I. A. Stegen, *Handbook of Mathematical Functions, with Formulas, Graphs, and Mathematical Tables*, Dover Publications, 1046 pgs, (see 877-883), (1972).

[2] N. J. Barrow, The reaction of plant nutrients and pollutants with soil, Australian J. Soil Research, 27, 475-492 (1989,).

[3] A. Binh, Neutralization of acid wastewater by limestone-bearing sand, Ph. D. thesis, Murdoch University, Western Australia (1981).

[4] G. Boole, *A Treatise on the Calculus of Finite Differences, 2nd Ed.*, (originally published in 1880 by Macmillian), Dover Publications, N. Y. (1960).

[5] A. D. Booth, *Numerical Methods, 3rd Ed.*, Buttterworths, London, 213 pgs. (1966).

[6] R. Butler and E. Kerr, *An Introduction to Numerical Methods*, Sir Isaac Pittman and Sons, London, 386pgs (1962).

[7] S. H. Chien and W. R. Clayton, Application of the Elovich Equation to the Kinetics of Phosphate Release and Sorption in Soils, J. Soil Sci. Soc. Am., 44, 265-268 (1990).

[8] P. M. Gresho and R. L. Lee, Don't suppress the wiggles- they're telling you something!, Computers and Fluids, 9, 223-253 (1981).

[9] H. S. Mickley, T. K. Sherwood, and C. E. Reed, *Applied Mathematics in Chemical Engineering, 2nd Ed.*, McGraw-Hill, N. Y., 413 pages (see pages 320-400) (1957).

[10] W. E. Milne, *Numerical Calculus*, Princeton University Press, 393 pgs. (1949).

[11] D. N. Munns and R. L. Fox, The slow reaction which continues after phosphate absorption: kinetics and equilibrium in in some tropical soils, Soil Science Society of America, 28, 585-595 (1976).

[12] National Bureau of Standards, U. S. Department of Commerce, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Applied Mathemathics Series 55, Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402 (1964).

[13] K. A. Redish, *An Introduction to Computational Methods*, English Universities Press, Richard Clay and Co., 211pgs. (1961).

[14] Supri Notodarmojo, G. E. Ho, W. D. Scott, and G. B. Davis, Modelling phosphorus transport in soils and groundwater with two-consecutive reactions, Water Research, 25, 1205-1216 (1991).

[15] M. Th. van Genucten and P. J. Wierenga, Simulation of one-dimensional solute transfer in porous media, New Mexico Agricultural Experimental Station, Bulletin 628 (1974).

[16] M. Th. van Genucten and P. J. Wierenga, Numerical solution of the convective-dispersion equation with intra-aggregate diffusion and non-linear adsorption. In *System Simulation in Water Resources* Edited by G. C. Vansteenkiste, North-Holland, N. Y., pages 275-292, (1976).