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Application of binomial coefficients in representing central difference solution to a class of PDE arising in chemistry

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The use of differential equations for modeling chemical systems and solving by numerical approaches (e.g. finite difference methods) are prevalent in chemistry-related problems. As an extension to the direct use of Pascal's Triangle to obtain the forward and backward difference equations to partial differentials by Lim [Mathematical Medley 31 (2004) 2], this paper proposes the use of binomial coefficient to generate central difference equations to odd-ordered partial differentials in a single-step operation. All finite difference equations to partial differentials shown herein display finite series of palindromic coefficients with alternating signs.

KEY WORDS: binomial coefficient, finite difference, partial differential, Pascal's triangle

AMS subject classification: 11B65, 35G99, 65N06, 92E99

1. Introduction

There is no doubt that mathematics has been playing an increasing role in the realm of chemistry [1–12]. Such phenomenon is not surprising since many chemical systems can be satisfactorily modeled as ordinary and partial differential equations (e.g. [13–28]). A few examples of partial differential equations that are of concern in chemical processes are listed in the Appendix A. Although analytical solutions exists for standard differential equations, the complexity of chemical systems demand numerical solutions, such as the finite difference method (e.g. [29–46] apply the finite difference equations). The use of seemingly "pure" mathematics has also found their way into chemistry – thereby broadening the applications aspect of mathematics and deepening the understanding for chemistry. A few such examples are given as follows:

(a) Hosoya [47,48] discussed the topological indices and Fibonacci numbers with relation to chemistry.

(b) El-Basil [49] showed how Fibonacci relations and Lucas sequence can be used to generate characteristic polynomials of a family of chemical graphs starting from smaller ones.

(c) Klein and Trinajstic [50] showed that the Kekule structures of benzenoid and coronoid hydrocarbons may be counted using the truncated Pascal's Triangle.

(d) Hosoya [51,52] demonstrated the use of symmetric and anti-symmetric Pascal's Triangles in the enumeration of $s, p, d, f, \ldots$ orbitals of the H-atom in D-dimensional hyperspace.

(e) Mandal et al. [53] showed the generation of characteristic polynomial coefficients of reciprocal chemical graphs from Pascal's Triangle.

(f) Mukherjee et al. [54] demonstrated how the characteristic polynomial coefficients of linear polyacene graphs are related to the Pascal's Triangle, and

(g) Hosoya [55] reviewed a list of chemico-physical problems which are related to Pascal's triangle and Pascal's asymmetrical triangle.

In this paper we show that the binomial coefficient

$$\binom{n}{r} = \frac{n!}{r!\,(n-r)!}, \tag{1}$$

(which is well-known to give the r-th element on the n-th row of the Pascal's Triangle and the number of ways to select r objects from a total of n objects) can be applied to generate the odd-ordered central difference equation to a class of partial differentials.

2. Analysis

Since the usual method of generating finite difference equation from a partial differential $\frac{\partial^n \phi_i}{\partial x^n}$ [56] can be time consuming for higher orders, recently Lim [57] proposed the use of Pascal's Triangle to obtain the forward and backward difference equations in a single step. As evident from figures 1 and 2, the forward and backward difference forms of the partial differential of order n can be written as

$$\frac{\partial^n \phi_i}{\partial x^n} = \frac{1}{(\delta x)^n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} \phi_{i-r+n} \tag{2}$$

and

$$\frac{\partial^n \phi_i}{\partial x^n} = \frac{1}{(\delta x)^n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} \phi_{i-r} \tag{3}$$

respectively, where ϕ is the quantity, δx is the grid interval, and the non-negative integer $r \in [0, n]$ is used for assigning the terms. The multiplier $(-1)^r$ was incorporated in order to reflect the alternating signs for each finite difference equation. Figure 3 shows the central difference equations derived in the same manner. However the so-called central difference representations to odd-ordered partial differentials displayed in figure 3 are invalid as the solution requires data at the intermediate points, that is, $i = \pm\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$ etc. Hence the partial differential's central difference equations

$$\frac{\partial^n \phi_i}{\partial x^n} = \frac{1}{(\delta x)^n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} \phi_{i-r+(\frac{n}{2})} \tag{4}$$

is applicable only for n = even. Kirsten [56] showed that the usual method to obtain the central difference equations of odd-ordered partial differentials can be obtained by splitting the zeroth-order quantity into two equal parts, each at an intermediate point

$$\phi_i = \frac{1}{2} \left(\phi_{i+\frac{1}{2}} + \phi_{1-\frac{1}{2}} \right). \tag{5}$$

Since the starting equation falls on intermediate points, it follows that subsequent result for even-orders would similarly fall on intermediate points – thereby enabling the odd-orders to fall on the grid points. See figure 4. As before, obtaining the finite difference solution from the starting point as described in equation (5) can be cumbersome for higher orders. To generate the central difference equation of odd-orders differential in a single step, we note that each term in equation (4) can be separated into two terms such that each intermediate point (for n =odd) is split into two halves that fall onto the grid points,

$$\frac{\partial^n \phi_i}{\partial x^n} = \frac{1}{2(\delta x)} \sum_{r=0}^{n} (-1)^r \binom{n}{r} \left[\phi_{i-r+\frac{(n+1)}{2}} - \phi_{i-r+\frac{(n-1)}{2}} \right]. \tag{6}$$

It is easy to see that, unlike equation (4), equation (6) enables the central difference coefficients to fall on grid points for n = odd. However, equation (6) does not provide a direct solution since the terms in the square parenthesis refers to two neighboring grid points. An equivalent form to equation (6) that displays specific terms to the grid points can be obtained by firstly expanding and rearranging equation (6) as

$$2\frac{\partial^n \phi_i}{\partial x^n}(\delta x)^n = (-1)^0 \binom{n}{0} \phi_{i+\frac{(n+1)}{2}} + \left\{ \sum_{r=1}^{n} \left[(-1)^r \binom{n}{r} + (-1)^{r-1} \binom{n}{r-1} \right] \phi_{i-r+\frac{(n+1)}{2}} \right\} + (-1)^n \binom{n}{n} \phi_{i-\frac{(n+1)}{2}}. \quad (7)$$

Substituting

$$(-1)^0 = -(-1)^n = 1 \quad (8)$$

for $n =$ odd, and

$$\binom{n}{0} = \binom{n}{n} = 1 \quad (9)$$

into the first and third terms on the RHS of equation (7), with

$$(-1)^{r-1} = -(-1)^r \quad (10)$$

and

$$\binom{n}{r-1} = \left(\frac{r}{n-r+1} \right) \binom{n}{r} \quad (11)$$

into the second term on the RHS of equation (7) leads to

$$\frac{\partial^n \phi_i}{\partial x^n} = \frac{1}{2(\delta x)^n} \left[\phi_{1+\frac{(n+1)}{2}} - \phi_{1-\frac{(n+1)}{2}} \right] + \frac{1}{2(\delta x)^n} \sum_{r=1}^{n} (-1)^r \binom{n}{r} \left(\frac{n+1-2r}{n+1-r} \right) \phi_{i-r+\frac{(n+1)}{2}}. \quad (12)$$

Since

$$\left[(-1)^r \binom{n}{r} \left(\frac{n+1-2r}{n+1-r} \right) \phi_{i-r+\frac{(n+1)}{2}} \right]_{r=0} = \phi_{i+\frac{(n+1)}{2}}, \quad (13)$$

then equation (12) can be contracted to

$$\frac{\partial^n \phi_i}{\partial x^n} = \frac{1}{2(\delta x)^n} \left\{ \sum_{r=0}^{n} \left[(-1)^r \left(\frac{n+1-2r}{n+1-r} \right) \binom{n}{r} \phi_{i-r+\frac{(n+1)}{2}} \right] - \phi_{i-\frac{(n+1)}{2}} \right\}. \quad (14)$$

3. Conclusion

The importance of differential equations for modeling chemical systems and the usefulness of the finite difference solution to these chemistry-related differential equations is evident from recent examples (e.g. [13–46]). By using the binomial coefficient, central difference equations corresponding to odd-ordered partial differentials can be obtained in a single step. This is not surprising because the coefficients of finite difference equations (figures 1–3) reflect the elements in the Pascal's Triangle. Although the Pascal's Triangle is not reflected in the central difference equation of the odd-ordered partial differentials, the central difference equations (odd-orders) shown in figure 4 nevertheless display palindromic patterns with alternating signs in similar manner as those of the forward, backward and central (even-orders) differences equations furnished in figures 1–3. Since the generation of finite difference equations can be attained in a single step, the proposed models are useful particularly when dealing with high order partial differentials.

n	**Partial differential**	**Forward difference equations**
0	$\phi_i =$	$\dfrac{\mathbf{1}\phi_i}{(\delta x)^{\mathbf{0}}}$
1	$\dfrac{\partial \phi_i}{\partial x} =$	$\dfrac{\mathbf{1}\phi_{i+1} - \mathbf{1}\phi_i}{(\delta x)^{\mathbf{1}}}$
2	$\dfrac{\partial^2 \phi_i}{\partial x^2} =$	$\dfrac{\mathbf{1}\phi_{i+2} - \mathbf{2}\phi_{i+1} + \mathbf{1}\phi_i}{(\delta x)^{\mathbf{2}}}$
3	$\dfrac{\partial^3 \phi_i}{\partial x^3} =$	$\dfrac{\mathbf{1}\phi_{i+3} - \mathbf{3}\phi_{i+2} + \mathbf{3}\phi_{i+1} - \mathbf{1}\phi_i}{(\delta x)^{\mathbf{3}}}$
4	$\dfrac{\partial^4 \phi_i}{\partial x^4} =$	$\dfrac{\mathbf{1}\phi_{i+4} - \mathbf{4}\phi_{i+3} + \mathbf{6}\phi_{i+2} - \mathbf{4}\phi_{i+1} + \mathbf{1}\phi_i}{(\delta x)^{\mathbf{4}}}$
5	$\dfrac{\partial^5 \phi_i}{\partial x^5} =$	$\dfrac{\mathbf{1}\phi_{i+5} - \mathbf{5}\phi_{i+4} + \mathbf{10}\phi_{i+3} - \mathbf{10}\phi_{i+2} + \mathbf{5}\phi_{i+1} - \mathbf{1}\phi_i}{(\delta x)^{\mathbf{5}}}$

Figure 1. Forward difference equations displaying Pascal's Triangle.

n	Partial differential	Backward difference equations
0	$\phi_i =$	$\frac{1\phi_i}{(\delta x)^0}$
1	$\frac{\partial \phi_i}{\partial x} =$	$\frac{1\phi_i - 1\phi_{i-1}}{(\delta x)^1}$
2	$\frac{\partial^2 \phi_i}{\partial x^2} =$	$\frac{1\phi_i - 2\phi_{i-1} + 1\phi_{i-2}}{(\delta x)^2}$
3	$\frac{\partial^3 \phi_i}{\partial x^3} =$	$\frac{1\phi_i - 3\phi_{i-1} + 3\phi_{i-2} - 1\phi_{i-3}}{(\delta x)^3}$
4	$\frac{\partial^4 \phi_i}{\partial x^4} =$	$\frac{1\phi_i - 4\phi_{i-1} + 6\phi_{i-2} - 4\phi_{i-3} + 1\phi_{i-4}}{(\delta x)^4}$
5	$\frac{\partial^5 \phi_i}{\partial x^5} =$	$\frac{1\phi_i - 5\phi_{i-1} + 10\phi_{i-2} - 10\phi_{i-3} + 5\phi_{i-4} - 1\phi_{i-5}}{(\delta x)^5}$

Figure 2. Backward difference equations displaying Pascal's Triangle.

n	Partial differential	Central difference equations
0	$\phi_i =$	$\frac{1\phi_i}{(\delta x)^0}$
1	$\frac{\partial \phi_i}{\partial x} =$	$\frac{1\phi_{i+\frac{1}{2}} - 1\phi_{i-\frac{1}{2}}}{(\delta x)^1}$
2	$\frac{\partial^2 \phi_i}{\partial x^2} =$	$\frac{1\phi_{i+1} - 2\phi_i + 1\phi_{i-1}}{(\delta x)^2}$
3	$\frac{\partial^3 \phi_i}{\partial x^3} =$	$\frac{1\phi_{i+\frac{3}{2}} - 3\phi_{i+\frac{1}{2}} + 3\phi_{i-\frac{1}{2}} - 1\phi_{i-\frac{3}{2}}}{(\delta x)^3}$
4	$\frac{\partial^4 \phi_i}{\partial x^4} =$	$\frac{1\phi_{i+2} - 4\phi_{i+1} + 6\phi_i - 4\phi_{i-1} + 1\phi_{i-2}}{(\delta x)^4}$
5	$\frac{\partial^5 \phi_i}{\partial x^5} =$	$\frac{1\phi_{i+\frac{5}{2}} - 5\phi_{i+\frac{3}{2}} + 10\phi_{i+\frac{1}{2}} - 10\phi_{i-\frac{1}{2}} + 5\phi_{i-\frac{3}{2}} - 1\phi_{i-\frac{5}{2}}}{(\delta x)^5}$

Figure 3. Central difference equations displaying Pascal's Triangle (valid for n =even).

n	Partial differential	Central difference equations
1	$\frac{\partial \phi_i}{\partial x} =$	$\frac{1}{2}\left[\frac{\phi_{i+1} - \phi_{i-1}}{(\delta x)^1}\right]$
3	$\frac{\partial^3 \phi_i}{\partial x^3} =$	$\frac{1}{2}\left[\frac{\phi_{i+2} - 2\phi_{i+1} + 2\phi_{i-1} - \phi_{i-2}}{(\delta x)^3}\right]$
5	$\frac{\partial^5 \phi_i}{\partial x^5} =$	$\frac{1}{2}\left[\frac{\phi_{i+3} - 4\phi_{i+2} + 5\phi_{i+1} - 5\phi_{i-1} + 4\phi_{i-2} - \phi_{i-3}}{(\delta x)^5}\right]$

Figure 4. Central difference equation for n =odd.

Appendix A.

Various partial differential equations appear in chemical processes that involve flow and diffusion. The irrotational motion of a perfect fluid

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = \nabla^2 \phi = 0 \tag{A1}$$

is a Laplace equation whereby the scalar function $\phi = \phi(x, y, z, t)$ of position and time is defined as

$$\begin{Bmatrix} u \\ v \\ w \end{Bmatrix} = - \begin{Bmatrix} \partial \phi / \partial x \\ \partial \phi / \partial y \\ \partial \phi / \partial z \end{Bmatrix} \tag{A2}$$

whilst the free surface motion along a horizontal (y-axis) is described as

$$\frac{\partial^2 \phi}{\partial t^2} + g \frac{\partial \phi}{\partial y} = 0 \tag{A3}$$

under a gravitational influence g. For a flow near a suddenly accelerated wall, as encountered by a fluid particle adjacent to a turbine blade surface, the velocity along x-direction, u, is

$$\frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial y^2}, \tag{A4}$$

where μ is the kinematic viscosity of the fluid. Equation (A4) corresponds to the general form of the diffusion equation

$$\nabla^2 u = \frac{1}{D}\frac{\partial u}{\partial t}, \tag{A5}$$

where D is a property that is dependent on the fluid medium. The mass diffusion as a result of concentration gradient and liquid flow is

$$\frac{\partial C}{\partial t} + \left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} \right) = D\,\nabla^2 C, \tag{A6}$$

which can be reduced to equation (A5) in the absence of flow. The following diffusion of vorticity

$$u\frac{\partial \zeta}{\partial x} + v\frac{\partial \zeta}{\partial y} + w\frac{\partial \zeta}{\partial t} = \mu\left(\frac{\partial^2 \zeta}{\partial x^2} + \frac{\partial^2 \zeta}{\partial y^2}\right), \tag{A7}$$

in which the vorticity component in the $x - y$ plane is

$$\zeta = \frac{1}{2}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right), \tag{A8}$$

can be expressed as a fourth order non-linear partial differential equation

$$\frac{\partial \nabla^2 \psi}{\partial t} + \frac{\partial \psi}{\partial y}\left(\frac{\partial \nabla^2 \psi}{\partial x}\right) - \frac{\partial \psi}{\partial x}\left(\frac{\partial \nabla^2 \psi}{\partial y}\right) = \mu\,\nabla^4 \psi \tag{A9}$$

where the stream function in 2-dimension $\psi = \psi(x, y)$ is defined as

$$\begin{Bmatrix} u \\ v \end{Bmatrix} = \begin{Bmatrix} -\partial\psi/\partial y \\ +\partial\psi/\partial x \end{Bmatrix}. \tag{A10}$$

For cases when the viscous forces predominate, equation (A9) simplifies to the biharmonic equation

$$\frac{\partial^4 \psi}{\partial x^4} + 2\frac{\partial^4 \psi}{\partial x^2 \partial y^2} + \frac{\partial^4 \psi}{\partial y^4} = \nabla^4 \psi = 0. \tag{A11}$$

References

[1] A. Kerber, MATCH Commun. Math. Comput. Chem. 39 (1999) 127.
[2] J. Andraos, J. Chem. Educ. 76 (1999) 258.
[3] G.W.A. Milne, J. Chem. Inf. Comput. Chem. 37 (1997) 639.
[4] J. Karle, J. Chem. Inf. Comput. Sci. 34 (1994) 381.
[5] J. Meija and J. Bisenieks, J. Chem. Educ. 81 (2004) 995.
[6] N. Trinajstic and I. Gutman, Croat. Chem. Acta. 75 (2002) 329.
[7] B. Gruber, J. Chem. Inf. Comput. Sci. 40 (2000) 580.
[8] T. Wieland, MATCH Commun. Math. Comput. Chem. 34 (1996) 179.

[9] R.B. King, Coord. Chem. Rev. 122 (1993) 91.
[10] R.B. King, Acc. Chem. Res. 25 (1992) 247.
[11] A.B. Klonskii, J. Appl. Chem. USSR 63 (1990) 1194.
[12] J. Koca, Collect. Czech. Chem. Commun. 53 (1988) 3108.
[13] G. Terrones and A.J. Pearlstein, J. Am. Chem. Soc. 113 (1991) 2132.
[14] B.A. Luty, M.E. Davis and J.A. McCammon, J. Comput. Chem. 13 (1992) 1114.
[15] T. Aoyama and H. Ichikawa, J. Chem. Inf. Comput. Sci. 32 (1992) 492.
[16] Z.X. Xiang, Y.Y. Shi and Y.W. Xu, J. Comput. Chem. 16 (1995) 200.
[17] I. Lengyel, J. Li, K. Kustin and I.R. Epstein, J. Am. Chem. Soc. 118 (1996) 3708.
[18] E.B. Krissinel and N. Agmon, J. Comput. Chem. 17 (1996) 1085.
[19] K.T. Balinska, H. Galina, L.V. Quintas and J. Szymanski, J. Chem. Inf. Comput. Sci. 36 (1996) 347.
[20] L.K. Bieniasz, Comput. Chem. 20 (1996) 403.
[21] L.K. Bieniasz, Comput. Chem. 21 (1997) 1.
[22] J.M. Salvador, K. Hernandez, A. Beltran, R. Duran and A. Mactutis, J. Chem. Inf. Comput. Sci. 38 (1998) 1105.
[23] P.C. McKinney, J. Math. Chem. 32 (2002) 381.
[24] P.C. McKinney, J. Math. Chem. 32 (2002) 405.
[25] H. Taseli, I.M. Erhan and O. Ugur, J. Math. Chem. 32 (2002) 323.
[26] F. Aluffi-Pentini, V. De Fonzo and V. Parisi, J. Math. Chem. 33 (2003) 1.
[27] S.V. Zelentsov, S.K. Aranson and L.A. Belyakov, J. Math. Chem. 33 (2003) 39.
[28] L. Delle Site, J. Math. Chem. 35 (2004) 289.
[29] T.C. Richards and W.E. Geiger, J. Am. Chem. Soc. 116 (1994) 2028.
[30] E. Rajasekaran, B. Jayaram and B. Honig, J. Am. Chem. Soc. 116 (1994) 8238.
[31] J.P. Ma, S.H. Huo and J.E. Straub, J. Am. Chem. Soc. 119 (1997) 2541.
[32] M.M. Pariona and I.L. Muller, Comput. Chem. 22 (1998) 377.
[33] F. Fogolari, G. Esposito, P. Viglino, J.M. Briggs and J.A. McCammon, J. Am. Chem. Soc. 120 (1998) 3735.
[34] J. Srinivasan, T.E. Cheatham, P. Cieplak, P.A. Kollman and D.A. Case, J. Am. Chem. Soc. 120 (1998) 9401.
[35] T.E. Simos and P.S. Williams, Comput. Chem. 23 (1999) 513.
[36] R. Baronas, F. Ivanauskas and J. Kulys, J. Math. Chem. 32 (2002) 225.
[37] G. Avdelas, E. Kefalidis and T.E. Simos, J. Math. Chem. 31 (2002) 371.
[38] W. Rocchia, S. Sridharan, A. Nicholls, E. Alexov, A. Chiabrera and B. Honig, J. Comput. Chem. 23 (2002) 128.
[39] D. Britz, O. Osterby, J. Strutwolf and T.K. Svennesen, Comput. Chem. 26 (2002) 97.
[40] L.K. Bieniasz, Comput. Chem. 26 (2002) 633.
[41] R. Baronas, F. Ivanauskas, J. Kulys and M. Sapagovas, J. Math. Chem. 34 (2003) 227.
[42] W.P. Im, M.S. Lee and C.L. Brooks, J. Comput. Chem. 24 (2003) 1691.
[43] R. Schmid, J. Comput. Chem. 25 (2004) 799.
[44] R. Baronas, F. Ivanauskas, F. Ivanauskas and J. Kulys, J. Math. Chem. 35 (2004) 199.
[45] M.V. Putz, N. Russo and E. Sicilia, J. Comput. Chem. 25 (2004) 994.
[46] L.K. Bieniasz, J. Comput. Chem. 25 (2004) 1515.
[47] H. Hosoya, Fibonacci Quart. 11 (1973) 255.
[48] H. Hosoya, Bull. Chem. Soc. Jpn. 44 (1971) 2332.
[49] S. El-Basil, Theor. Chim. Acta 65 (1984) 199.
[50] D.J. Klein and N. Trinajstic, J. Mol. Struct. THEOCHEM 206 (1990) 153.
[51] H. Hosoya, J. Phys. Chem. A 101 (1997) 418.
[52] H. Hosoya, Int. J. Quantum Chem. 64 (1997) 35.
[53] B. Mandal, K. Datta, A.K. Mukherjee and M. Banerjee, Mol. Phys. 96 (1999) 1069.

[54] G. Mukherjee, K. Datta and A.K. Mukherjee, Proc. Indian Acad. Sci. Chem. Sci. 112 (2000) 27.
[55] H. Hosoya, J. Math. Chem. 23 (1998) 169.
[56] R.D. Kersten, *Engineering Differential Systems* (McGraw-Hill, New York, 1969).
[57] T.C. Lim, Math. Medley 31 (2004) 2.