Application of symbolic algebra to the generation of coordinate transformations

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Abstract

In this paper we present tools for automatic generation of generalized (variable and terrain-following) coordinate transformations and its use in numerical models of atmospheric flows. Such methodology should be competitive with the more commonly employed nested grid schemes. We discuss the symbolic (computer) algebra program for analytical calculation of Christoffel symbols, metric tensor and other geometrical objects describing a transformation. An example, related to the numerical modeling of mesoscale flows, is given. This example shows how coupled terrain-following and stretching transformation can be easily created. The possible application of such methodology in numerical modeling of air pollution on cirrus clouds is briefly discussed.

1. Introduction

It is now common in many atmospheric mesoscale models to employ a terrain-following coordinate transformation. Starting with Gal-Chen and Somerville (1975) a number of researchers (Clark, 1977; Tripoli and Cotton, 1982; Pielke and Martin, 1981) used tensor procedures (Christoffel symbols, metric tensor) to describe the topography in this concise, mathematically elegant and simple way. Dutton (1976) and Pielke (1984) attempted to implement the well-known tensor algebra apparatus to the more general class of atmospheric problems namely those which employ *variable* as well as a terrain-following numerical grid. The variable grid, as opposed to the nested grid approach has not been yet fully exploited (Kitade, 1979). One of the problems is the extensive algebra arising in the calculation of the transformation tensors.

To ease the problem, a symbolic (computer) algebra program has been developed which is capable of easily generating the tensorial quantities important for the successful implementation of general coordinate transformations.

Recently, in atmospheric problems, symbolic algebra was applied in algebraic-extensive calculations (Flatau *et al.*, 1988; Flatau 1985) but this useful computer technique is not well-known in meteorology. The example which we present in this paper is applicable to the numerical modeling of pollutant dispersion in mountainous region but similar algebra is required to obtain high resolution in the upper-troposphere when simulating cirrus clouds. We want to have more resolution in a specific region (e.g., close to the stack) yet at the same time, to use a terrain following coordinate system. In Section 2 we illustrate the application of symbolic algebra to this specific problem.

2. Example: Terrain-Following and Locally Refined Transformation

In setting up a vertical and horizontal grid, grid increments can be kept constant, or allowed to stretch. The advantage of a constant grid is the relative ease of coding such a framework onto a computer as well as allowing a consistent computational treatment. For the simulation of air pollution in the framework of a three-dimensional large eddy simulation (LES) model, (e.g., Deardorff, 1974) one is faced with the need for local grid refinement close to a pollution source (e.g., a stack) yet to retain an adequate representation of large eddies in the atmospheric boundary layer and the dominant topographic features in the area. The need for high spatial resolution locally arises when modeling cirrus clouds imbedded within a large scale flow.

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The local refinement can be obtained in the way similar to that proposed by Anthes (1970). The slightly modified Anthes transformation is given by

$$\begin{aligned} x^1 &= (C_1 + R_2C_2)\,\bar{x}^1 \\ x^3 &= (C_1 + R_2C_2)\,\bar{x}^3, \end{aligned} \tag{1}$$

where

$$R_2 = \left[\left(\frac{x^1}{x^1_{\max}}\right)^2 + \left(\frac{x^3}{x^3_{\max}}\right)^2\right]^{\frac{1}{2}} \tag{2}$$

and C_1, C_2 are constants. Transformation (1) corresponds to coordinate stretching.

For simplicity we present the results in the two dimensional framework but the extension to three dimensions is straightforward. The $(x^1, x^3) \Leftrightarrow (\bar{x}^1\bar{x}^3)$ stretching transformation is performed first, followed by the terrain-following transformation defined by

$$\begin{aligned} \tilde{x}^1 &= x^1 & x^1 &= \tilde{x}^1 \\ \tilde{x}^3 &= \sigma\left(x^1, x^3\right) & x^3 &= h\left(\tilde{x}^1, \tilde{x}^3\right) \end{aligned} \tag{3}$$

with

$$\sigma = H\frac{x^3 - z_G}{H - z_G} \tag{4}$$

In these expressions H defines the flat top of the model atmosphere, and z_G defines the height of topography. For the example, the topographic shape is given by

$$z_G = \frac{ha^2}{x_1^2 + a^2} \tag{5}$$

where the mountain half-width is a and its maximum height is h.

The resulting transformation is presented in Fig. 1. Dots represent the grid points position in the $x - z$ plane. The mountain shape is clearly seen. To the east of the mountain ridge the grid is locally refined. The constant number of grid points in the vertical (for different x-values) cause the top of the model grid to exhibit "folding". In the (x^1, x^3) space the grid is rectangular with constant grid spacing. The transformation tensors for the σ-transformations are given in Pielke (1984) and are not repeated here. Part of the symbolic algebra program written in REDUCE (Hearn, 1984) is given in the Appendix A. A simple example of output for the spherical coordinates is included in Appendix B. More examples are available in Flatau *et al.*, (1988). Similar capabilities are coded in MACSYMA (Bogen, *et al.*, 1983) and SMP (Wolfram and Cole, 1983). Both transformations (1) and (3) can be treated together and the

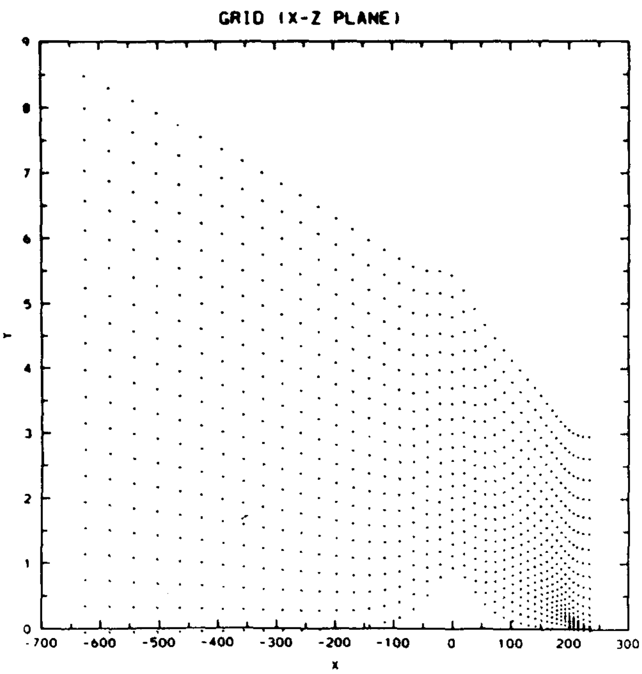

Figure 1: The grid in the $x - z$ plane. The terrain-following transformation is applied and the increased grid resolution can be observed for positive x-values on the ridge slope. Dots indicate grid points after transformation.

resulting Christoffel symbols, metric tensor, etc. can be calculated. For any general coordinate transformation which has a functional form, no matter how complex, the transformation can be calculated using symbolic algebra and stored for subsequent calculations.

3. Conclusions

A procedure is described in which symbolic algebra is applied to a coordinate transformation in order to obtain quick, accurate values for the transformation tensors. While the example presented here was for a stretched-grid in a terrain following coordinate system, the transformation tensors can be pre-calculated for any general coordinate transformation which has a functional form, using symbolic algebra and stored for subsequent calculations.

4. Acknowledgements

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5. References

[1] Gal-Chen, T. and R. C. J. Somerville, (1975): On the use of a coordinate transformation for the solution of the Navier-Stokes equations. *J. Comput. Phys.*, **17**, 276.

[2] Clark, T. L., (1977): A small-scale dynamic model using a terrain-following coordinate transformation. *J. Comput. Phys.*, **24**, 186-215.

[3] Tripoli, G. J. and W. R. Cotton, (1982): The Colorado State University three-dimensional cloud/mesoscale model-1982. Part I: General theoretical framework and sensitivity experiments. *J. Rech. Atmos.*, **16**, 185-219.

[4] Pielke, R. A. and C. L. Martin, (1981): The derivation of a terrain-following coordinate system for use in a hydrostatic model. *J. Atmos. Sci.*, **38**, 1703-1707.

[5] Dutton, J. A., (1976): *The Ceaseless Wind - An Introduction to the Theory of Atmospheric Motion*, New York, McGraw-Hill.

[6] Pielke, R.A., 1984: *Mesoscale Meteorological Modeling.* Academic Press, New York, N.Y., 612 pp.

[7] Kitade, T., 1979: A method of numerical time integration using a moving variable grid. *J. Meteor. Soc. Japan*, **57**, 576-586.

[8] Flatau, P. J., J. P. Boyd and W. R. Cotton, (1988): Symbolic algebra in applied mathematics and geophysical fluid dynamics. REDUCE Examples, Atmospheric Science Paper, Colorado State University, Department of Atmospheric Science, Fort Collins, CO 80523 (to be published).

[9] Flatau, P. J., (1985): Study of second-order turbulence closure technique and its application to atmospheric flows, Colorado State University Paper **393**. Colorado State University, Department of Atmospheric Science, Fort Collins, CO 80523.

[10] Deardorff, T.W., (1974): Three dimensional numerical study of the height and mean structure of a heated planetary boundary layer. *Bound.-Layer Meteor.*, **7**, 81-106.

[11] Anthes, R. A., (1970): Numerical experiments with a two-dimensional horizontal variable grid. *Mon. Wea. Rev.*, **98**, 810-822.

[12] Hearn, A. C., (1984): *REDUCE User's Manual, Ver. 3.0,* The RAND Corp., Santa Monica, Rand Publ. CP78(4/83).

[13] Bogen, R., J. Golden, M. Genesereth, R. Pavelle, M. Wester, R. Fateman and A. Doohovsky, (1983): *MACSYMA Reference Manual, Ver. 10.* Technical Report, The Mathlab Group Laboratory for Computer Science, MIT.

[14] Wolfram, S. and C. Cole, (1983): *A symbolic manipulation program SMP.* Reference Manual. Technical Report, Inference Corp.

6. Appendix A

The Christoffel symbol ($CS1, CS2, CS3$) are defined as

$$\tilde{\Gamma}^{s}_{ml} = \frac{1}{2}\tilde{G}^{sj}\left(\frac{\partial \tilde{G}_{lj}}{\partial \tilde{x}^{m}} + \frac{\partial \tilde{G}_{mj}}{\partial \tilde{x}^{l}} - \frac{\partial \tilde{G}_{lm}}{\partial \tilde{x}^{j}}\right)$$

(See Pielke, 1984, p. 108, Eq. (6.14).)

```
% + ----------------------------------------------------+
% ! Coordinate transformations                          !
% !                                                     !
% ! REDUCE 3.3 Program. Calculates metrics and Christoffel !
% ! symbols for generalized coordinate transformations.  !
% !                                                     !
% ! Based on:                                           !
% ! R. A. Pielke, 1984, Mesoscale Meteorological Modeling, !
% ! Academic Press.                                     !
% !                                                     !
% ! Written by P. J. Flatau                             !
% + ----------------------------------------------------+
```

```
PROCEDURE TRANSF(XX);
BEGIN;
 ARRAY TAU1(3), TAU2(3),TAU3(3);
 ARRAY ETA1(3), ETA2(3),ETA3(3);
 MATRIX DXDXT(3,3), DXTDX(3,3);
 FOR I:=1:3 DO
      BEGIN;
      TAU1(I):=DF(XX(I),XTT(1));
      TAU2(I):=DF(XX(I),XTT(2));
      TAU3(I):=DF(XX(I),XTT(3));
      DXDXT(I,1):=TAU1(I);
      DXDXT(I,2):=TAU2(I);
      DXDXT(I,3):=TAU3(I);
    END;
 WRITE " Tau vectors calculated ";
  DXTDX:=TP(DXDXT**(-1)) ;
 FOR I:=1:3 DO
    BEGIN;
     ETA1(I):=DXTDX(I,1);
     ETA2(I):=DXTDX(I,2);
     ETA3(I):=DXTDX(I,3);
    END;
 WRITE " Eta vectors calculated ";
MATRIX G(3,3),GI(3,3);
FOR J:=1:3 DO FOR M:=1:3 DO G(J,M):= FOR I:=1:3
     SUM DF(XX(I),XTT(M))*DF(XX(I),XTT(J));
WRITE " G - metric tensor calculated ";
GI:=TP (    G**(-1)   ) ;
WRITE " GI- metric tensor calculated ";
GTILDA:=DET(G);
WRITE " Det(G)           calculated ";
%Calculate G in different way;
  MATRIX G1(3,3),GI1(3,3);
  FOR J:=1:3 DO FOR M:=1:3 DO
    G1(J,M):= FOR I:=1:3 SUM DXDXT(I,J)*DXDXT(I,M);
GI1 := TP ( G1**(-1)  );
WRITE " G1 AND GI1        calculated ";
FOR N:=1:3 DO FOR M:=1:3 DO FOR L:=1:3 DO
  BEGIN;
  CS1:= FOR J:=1:3 SUM GI(N,J)*DF(G(L,J),XTT(M))   ;
  CS2:= FOR J:=1:3 SUM GI(N,J)*DF(G(M,J),XTT(L))   ;
  CS3:= FOR J:=1:3 SUM GI(N,J)*DF(G(L,M),XTT(J))   ;
  CS(N,M,L):=(1/2)*(CS1+CS2-CS3);
  END;
 WRITE " Christoffel symbols calculated ";
 ARRAY VEL(3); VEL(1):=U; VEL(2):=V; VEL(3):=W;
 FACTOR U,V,W;
 UT1 :=  FOR I:=1:3  SUM TAU1(I)*VEL(I);
 VT1 :=  FOR I:=1:3  SUM TAU2(I)*VEL(I);
 WT1 :=  FOR I:=1:3  SUM TAU3(I)*VEL(I);
 UT2 :=  FOR I:=1:3  SUM ETA1(I)*VEL(I);
 VT2 :=  FOR I:=1:3  SUM ETA2(I)*VEL(I);
 WT2 :=  FOR I:=1:3  SUM ETA3(I)*VEL(I);
WRITE " end of transformation routine " ;
END;
```

7. Appendix B

Output from the program provided in Appendix A for the transformation

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

```
%        EXAMPLES               = = = = = = = = = = = = = =$
WRITE" SPHERICAL COORDINATES "$
% = = = = = = = = = = = = = = = = = = = = = = = = = = = = =$
XX(1):=XTT(3)*SIN(XTT(1))*COS(XTT(2))$
XX(2):=XTT(3)*SIN(XTT(1))*SIN(XTT(2))$
XX(3):=XTT(3)*COS(XTT(1))$
```

```
TRANSF(XX)$
 Tau vectors calculated
 Eta vectors calculated
 G - metric tensor calculated
 GI- metric tensor calculated
 Det(G)            calculated
 G1 AND GI1        calculated
 Christoffel symbols calculated
 end of transformation routine

FOR ALL YY LET COS(YY)**2=1-SIN(YY)**2$
PRINTT(THETA,PHI,R)$
                                            2  4
GT - DETERMINANT OF METRICS      SIN(THETA) *R
C ======= TAU vectors ==========================
TAU1(1)=COS(THETA)*COS(PHI)*R
TAU1(2)=SIN(PHI)*COS(THETA)*R
TAU1(3)= - SIN(THETA)*R

TAU2(1)= - SIN(THETA)*SIN(PHI)*R
TAU2(2)=SIN(THETA)*COS(PHI)*R
TAU2(3)=0

TAU3(1)=SIN(THETA)*COS(PHI)
TAU3(2)=SIN(THETA)*SIN(PHI)
TAU3(3)=COS(THETA)

C ======= ETA vectors ===========================

        COS(THETA)*COS(PHI)
ETA1(1)=----------------------
                 R

        SIN(PHI)*COS(THETA)
ETA1(2)=----------------------
                 R

           SIN(THETA)
ETA1(3)= - ------------
               R

             SIN(PHI)
ETA2(1)= - --------------
           SIN(THETA)*R

          COS(PHI)
ETA2(2)=--------------
        SIN(THETA)*R

ETA2(3)=0

ETA3(1)=SIN(THETA)*COS(PHI)

ETA3(2)=SIN(THETA)*SIN(PHI)

ETA3(3)=COS(THETA)

C ======= UT,VT,WT COMPONENTS====================

UT CO = - ( - U*COS(THETA)*COS(PHI)*R - V*SIN(PHI)
*COS(THETA)*R + W*SIN(THETA)*R)

VT CO= - (U*SIN(THETA)*SIN(PHI)*R
      - V*SIN(THETA)*COS(PHI)*R)

WT CO=U*SIN(THETA)*COS(PHI) + V*SIN(THETA)*SIN(PHI)
      + W*COS(THETA)

UT CN = - ( - U*COS(THETA)*COS(PHI) - V*SIN(PHI)*COS(THETA)
       + W*SIN(THETA))/R
```

```
         U*SIN(PHI) - V*COS(PHI)
VT CN= - -------------------------
              SIN(THETA)*R

WT CN=U*SIN(THETA)*COS(PHI) + V*SIN(THETA)*SIN(PHI)
      + W*COS(THETA)

C ======= G metric tensor (0 elements not printed) =====

        2
 G(1,1)=R

                 2  2
 G(2,2)=SIN(THETA) *R

 G(3,3)=1

C ======= Gamma - Christoffel symbols =================

            1
 GAM(1,1,3)=---
            R

 GAM(1,2,2)= - SIN(THETA)*COS(THETA)

            1
 GAM(1,3,1)=---
            R

            COS(THETA)
 GAM(2,1,2)=------------
            SIN(THETA)

            COS(THETA)
 GAM(2,2,1)=------------
            SIN(THETA)

            1
 GAM(2,2,3)=---
            R

            1
 GAM(2,3,2)=---
            R

 GAM(3,1,1)= - R

                         2
 GAM(3,2,2)= - SIN(THETA) *R
```