ANSTO/E722

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by
G. Pantelis

May 1995

ISBN0642 59960 2
ISSN 1030-7745

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DIFFERENTIAL EQUATIONS; FLUID FLOW; NONLINEAR PROBLEMS; NUMERICAL SOLUTIONS; POROUS MATERIALS; TRANSFORMATIONS; TURBULENT FLOW

DERIVATION OF A MACROSCALE FORMULATION FOR A CLASS OF NON-LINEAR PARTIAL DIFFERENTIAL EQUATIONS

Garry Pantelis
Australian Nuclear Science and Technology Organisation
PMB 1, Menai, NSW, 2234
Australia

ABSTRACT

A macroscale formulation is constructed from a system of partial differential equations which govern the microscale dependent variables. The construction is based upon the requirement that the solutions of the macroscale partial differential equations satisfy, in some approximate sense, the system of partial differential equations associated with the microscale. These results are resricted to the class of nonlinear partial differential equations which can be expressed as polynomials of the dependent variables and their partial derivatives up to second order. A linear approximation of transformations of second order contact manifolds is employed.

Introduction

Macroscale formulations are often derived from the partial differential equations which govern the microscale variables by three main procedures: (i) stochastic, (ii) asymptotic and (iii) space/time/mass averaging methods. By examining the heterogeneity of the porous medium Gelhar and Axness [1] adopted a stochastic approach to infer macrodispersion of species fluid transport. By assuming a periodic structure for porous media Ene and Sanchez-Palencia [2] employed asymptotic methods to derive macroscale balance equations for heat and mass transport through porous media. Nguyen et *al.* [3] started with the balance equations for the microscale dependent variables and applied space/time/mass averaging techniques to derive macroscale partial differential equations for multiphase flow through porous media.

The latter approach is similar to techniques used to derive fluid turbulent models. Here mean flows are sought by applying certain time or space averaging operators to the Navier-Stokes and continuity equations [4]. What results are time/space averaged nonlinear terms involving the microscale fluctuations of the velocities. Closure models are then obtained by assuming that these terms are some functions of the macroscale dependent variables and their partial derivatives.

The approach taken here is to start with a system of partial differential equations in a generalized form and examine the conditions under which the system is eligible to represent a macroscale formulation of some microscale system of partial differential equations. The criteria for this eligibility could be stated as follows:
(i) that solutions of the macroscale partial differential equations satisfy, in some approximate sense, the partial differential equations which govern the microscale variables.
(ii) that the macroscale partial differential equations are dissipative to microscale fluctuations in the solution (not necessarily dissipative to macroscale fluctuations) and
(iii) that the solutions of the macroscale partial differential equations, subject to appropriate boundary and initial conditions, are representative of the macroscale behaviour of the system under question.

Here we will concentrate on (i) to obtain the macroscale partial differential equations in the most general form involving a set of empirically based parameters. The constraints on these parameters which address (ii) and (iii) are application specific and will be investigated at a later stage.

The style here is one of construction by derivation but for brevity use is made of the notation of the theory of horizontal ideals as developed by Edelen [5]. Therefore familiarity with this work is assumed. The scope of this theory as employed here is condensed in the Appendix.

Macroscale/microscale contact manifolds

Let M and $\tilde{M}$ denote the spaces of the independent variables of the macroscale and microscale systems, respectively, with coordinates (x^i) and $(\tilde{x}^i)$, respectively. Here and throughout the indices i, j, k, l are to be assumed to range from 1 to n, where n is the dimension of the base manifold M and $\tilde{M}$. The Greek indices $\alpha, \beta, \gamma, \lambda, \eta$ are associated with the dependent variables and range from 1 to N (≥ 1).

The microscale and macroscale independent variables are related by the map $\Phi: M \to \tilde{M}$ such that $\Phi^* \tilde{x}^i = x^i/\varepsilon$ for some small parameter $\varepsilon > 0$. Let K_2 and $\tilde{K}_2$ denote the second order contact manifolds associated with the macroscale and microscale, respectively, with local coordinates $(x^i, q^\alpha, r_i^\alpha, r_{ij}^\alpha)$ and $(\tilde{x}^i, \tilde{q}^\alpha, \tilde{r}_i^\alpha, \tilde{r}_{ij}^\alpha)$, respectively.

Let $H[K_2]$ and $H[\tilde{K}_2]$ be the horizontal ideals on K_2 and $\tilde{K}_2$, respectively. The collection of regular solution maps $\phi: M \to K_2$ which annihilate the horizontal ideal $H[K_2]$ is denoted by $\Sigma[M, H[K_2]]$. Similarly, the collection of regular solution maps $\tilde{\phi}: \tilde{M} \to \tilde{K}_2$ which annihilate the horizontal ideal $H[\tilde{K}_2]$ is denoted by $\Sigma[\tilde{M}, H[\tilde{K}_2]]$.

The canonical basis $\{V_i \mid 1 \leq i \leq n\}$ for the module $H^*[K_2]$ of Cauchy characteristic vector fields of $H[K_2]$ are given by

$$(1) \qquad V_i = \frac{\partial}{\partial x^i} + r_i^\alpha \frac{\partial}{\partial q^\alpha} + r_{ij}^\alpha \frac{\partial}{\partial r_j^\alpha} + A_{ijk}^\alpha \frac{\partial}{\partial r_{jk}^\alpha}$$

where $A_{ijk}^\alpha \in \Lambda^0(K_2)$ satisfy the symmetry conditions (A3). Integrability of the horizontal ideal $H[K_2]$ requires that A_{ijk}^α satisfy the conditions (A8). Similar properties hold for $\tilde{A}_{ijk}^\alpha \in \Lambda^0(\tilde{K}_2)$ associated with the horizontal ideal $H[\tilde{K}_2]$.

Here the maps $\phi \in \Sigma[M, H[K_2]]$ and $\tilde{\phi} \in \Sigma[\tilde{M}, H[\tilde{K}_2]]$ are restricted to the case where the independent variables are unchanged, i.e. $\phi^* x^i = x^i$ and $\tilde{\phi}^* \tilde{x}^i = \tilde{x}^i$. The extensions of the following to general base manifold coordinate transformations should be immediate.

A map $\tilde{\phi} \in \tilde{M} \to \tilde{K}_2$, $\tilde{\phi} \in \Sigma[\tilde{M}, H[\tilde{K}_2]]$, yields an association with the coordinates of $\tilde{K}_2$ and some $\tilde{\phi}^\alpha \in \Lambda^0(\tilde{M})$ and their partial derivatives.

$$(2) \qquad \tilde{\phi}^* \tilde{q}^\alpha = \tilde{\phi}^\alpha(\tilde{x}^l), \quad \tilde{\phi}^* \tilde{r}_i^\alpha = \frac{\partial \tilde{\phi}^\alpha(\tilde{x}^l)}{\partial \tilde{x}^i}, \quad \tilde{\phi}^* \tilde{r}_{ij}^\alpha = \frac{\partial^2 \tilde{\phi}^\alpha(\tilde{x}^l)}{\partial \tilde{x}^i \partial \tilde{x}^j}$$

Hence if such a map also annihilates some $\tilde{F}^\alpha \in \Lambda^0(\tilde{K}_2)$, the expression

$$(3) \qquad \tilde{\phi}^* \tilde{F}^\alpha(\tilde{x}^l, \tilde{q}^\alpha, \tilde{r}_i^\alpha, \tilde{r}_{ij}^\alpha) = \tilde{F}^\alpha\left(\tilde{x}^i, \tilde{\phi}^\alpha(\tilde{x}^l), \frac{\partial \tilde{\phi}^\alpha(\tilde{x}^l)}{\partial \tilde{x}^i}, \frac{\partial^2 \tilde{\phi}^\alpha(\tilde{x}^l)}{\partial \tilde{x}^i \partial \tilde{x}^j}\right) = 0$$

represents a system of N second order partial differential equations with respect to the coordinates $(\tilde{x}^l)$ of $\tilde{M}$.

Here we have in mind the situation where $\tilde{\phi}^\alpha(\tilde{x}^l)$ admits the decomposition

$$(4) \quad \tilde{\phi}^{\alpha}(\tilde{x}^{i}) = \bar{\phi}^{\alpha}(\tilde{x}^{i}) + \hat{\phi}^{\alpha}(\tilde{x}^{i})$$

where $\hat{\phi}^{\alpha}(\tilde{x}^{i})$ and $\bar{\phi}^{\alpha}(\tilde{x}^{i})$ represent the fluctuating and nonfluctuating components, respectively, of $\tilde{\phi}^{\alpha}(\tilde{x}^{i})$.

The class of partial differential equations to be considered here are obtained from $\tilde{F}^{\alpha} \in \Lambda^{0}(\tilde{K}_2)$ which can be expressed as polynomials of the coordinates of $\tilde{K}_2$. The procedure that follows could be generalized to include polynomials of the coordinates of $\tilde{K}_2$ to any degree. For demonstration purposes and also because it includes many important applications, e.g. fluid equations of motion, convection-diffusion, heat conduction, etc., we consider the expression

$$(5) \quad \tilde{F}^{\alpha} = \lambda_{\beta}^{\alpha i}\tilde{r}_{i}^{\beta} + \eta_{\beta\gamma}^{\alpha i}\tilde{q}^{\beta}\tilde{r}_{i}^{\gamma} + \nu_{\beta}^{\alpha ij}\tilde{r}_{ij}^{\beta}$$

where the λ, η, ν's are prescribed constants. In applications the dissipation terms ($\nu_{\beta}^{\alpha ij}\tilde{r}_{ij}^{\beta}$) are, for example, associated with diffusion/conduction or fluid viscosity.

The interest here is in applications where it is difficult to obtain solutions of (3) as explicit functions of the independent coordinates ($\tilde{x}^{i}$) and where some kind of numerical approximate solution is sought. It is often the case that solutions are sought on a domain which is relatively large in $\tilde{M}$ and hence macroscale independent coordinates (x^{i}) are introduced. From the composite map $\tilde{\phi} \circ \Phi : M \rightarrow \tilde{K}_2$ we obtain the pullback of $\tilde{F}^{\alpha} \in \Lambda^{0}(\tilde{K}_2)$ to the partial differential equations

$$(6) \quad (\tilde{\phi} \circ \Phi)^{*}\tilde{F}^{\alpha} = 0$$

on the manifold M. Note that $\tilde{\phi} \circ \Phi \in \Sigma[M, H[\tilde{K}_2]]$.

It is often impractical to solve the system of partial differential equations (6) numerically if dissipative terms are small (i.e. $\nu_{\beta}^{\alpha ij}$ are small) since grid sizes need to be extremely refined to resolve the fluctuations in the solution, if they exist. One then attempts to replace this system of partial differential equations with a new set of partial differential equations whose solutions are somehow representative of the macroscale behaviour of the physical variables. Often apparent physical processes are introduced at the macroscale which are manifestations of these microscale fluctuations. An example of this can be found in the process of dispersion of solute transport through fluids.

In fluid flow the macroscale dependent variables are often thought of as being representative of some mean flow. In time/space/mass average approaches this association is immediate. Here we shall regard the macroscale dependent variables in a more general sense. The eligibilty of some $F^{\alpha} \in \Lambda^{0}(K_2)$ as being a representation of a macroscale formulation of some $\tilde{F}^{\alpha} \in \Lambda^{0}(\tilde{K}_2)$ is made only on the basis that the solution maps of the F^{α} are approximate solution maps of the microscale system $\tilde{F}^{\alpha}$ through some pullback to the base manifold M. If the microscale partial differential equations are statements of balance or conservation of some physical variables then the criterion of eligibility of a macroscale formulation used here is equivalent to the statement that the macroscale physical variables do not violate the microscale conservation laws (at least by approximation).

Contact Manifold Transformations

Let $S: K_2 \rightarrow \tilde{K}_2$ such that $S^* H[\tilde{K}_2] \subset H[K_2]$. In this study there is no requirement that S^{-1} exists. If S^{-1} does not exist then the set of solution maps of the horizontal ideal $H[K_2]$ is mapped to only a subset of the set of solution maps of $H[\tilde{K}_2]$.

We consider the map S such that

$$(7) \qquad s^i = S^* \tilde{x}^i = x^i/\varepsilon, \quad s^\alpha = S^* \tilde{q}^\alpha = q^\alpha + \varepsilon\zeta^\alpha$$

for some $\zeta^\alpha \in \Lambda^0(K_2)$. Noting the properties of S (see Appendix)

$$(8) \qquad V_i < s^j >= \delta_i^j/\varepsilon, \quad s_i^\alpha = S^* \tilde{r}_i^\alpha = \varepsilon(r_i^\alpha + \varepsilon V_i < \zeta^\alpha >),$$

$$s_{ij}^\alpha = S^* \tilde{r}_{ji}^\alpha = \varepsilon^2(r_{ij}^\alpha + \varepsilon V_j < V_i < \zeta^\alpha \gg)$$

The pullback of $\tilde{F}^\alpha$ under the action of S is given by

$$(9) \qquad S^* \tilde{F}^\alpha = \varepsilon\left(\Psi^\alpha + \varepsilon\Omega^\alpha + \varepsilon^2\Theta^\alpha\right)$$

where $\Psi^\alpha, \Omega^\alpha, \Theta^\alpha \in \Lambda^0(K_2)$ are given by

$$(10) \qquad \Psi^\alpha = \lambda_\beta^{\alpha i} r_i^\beta + \eta_{\beta\gamma}^{\alpha i} q^\beta r_i^\gamma$$

$$(11) \qquad \Omega^\alpha = \nu_\beta^{\alpha ji} r_{ij}^\beta + \lambda_\beta^{\alpha i} V_i < \zeta^\beta > + \eta_{\beta\gamma}^{\alpha i} q^\beta V_i < \zeta^\gamma > + \eta_{\beta\gamma}^{\alpha i} \zeta^\beta r_i^\gamma$$

and

$$(12) \qquad \Theta^\alpha = \eta_{\beta\gamma}^{\alpha i} \zeta^\beta V_i < \zeta^\gamma > + \nu_\beta^{\alpha ij} V_j < V_i < \zeta^\beta \gg$$

Let $F^\alpha \in \Lambda^0(K_2)$ represent the macroscale equations on K_2. We assume the closure of the ideal $\Upsilon[K_2, F^\alpha]$ which is guaranteed if the identity (A12) holds for some choice of $L_{\beta i}^\alpha \in \Lambda^0(K_2)$. We associate F^α with the pullback of $\tilde{F}^\alpha$ through the identity

$$(13) \qquad S^* \tilde{F}^\alpha = s_\beta^\alpha F^\beta + t_\beta^{\alpha i} V_i < F^\beta > + u_\beta^{\alpha ij} V_j < V_i < F^\beta \gg + E^\alpha$$

where $s_\beta^\alpha, t_\beta^{\alpha i}, u_\beta^{\alpha ij} \in \Lambda^0(K_2)$ are yet to be determined and $E^\alpha \in \Lambda^0(K_2)$ is included as some remainder term. If (A12) and (A13) hold then for any $\phi \in \Sigma[D \subset M, \Upsilon[K_2, F^\alpha]]$ we have

(14) $\quad (So\phi)^* \tilde{F}^\alpha = \phi^* E^\alpha$

This suggests that we seek an $F^\alpha \in \Lambda^0(K_2)$ and $s^\alpha_\beta, t^{\alpha i}_\beta, u^{\alpha ij}_\beta \in \Lambda^0(K_2)$ such that $\phi^* E^\alpha$ is either identically zero or at least sufficiently small. At first glance the presence of the terms $V_i < F^\beta >$ and $V_j < V_i < F^\beta \gg$ in (13) appear to be superfluous given the identities (A12) and (A13). However, it will be seen later that their presence will enable us to write F^α in a more desired form.

Consider the expression

(15) $\quad F^\alpha = \Psi^\alpha + \varepsilon R^\alpha$

where Ψ^α is given by (10) and $R^\alpha \in \Lambda^0(K_2)$.

If we set

(16) $\quad s^\alpha_\beta = \varepsilon \delta^\alpha_\beta, \quad t^{\alpha i}_\beta = \varepsilon^2 e^{\alpha i}_\beta, \quad u^{\alpha ij}_\beta = \varepsilon^2 f^{\alpha ij}_\beta$

for some $e^{\alpha i}_\beta, f^{\alpha i}_\beta \in \Lambda^0(K_2)$ we obtain from (13)

(17) $\quad E^\alpha = \varepsilon^2[\Omega^\alpha - R^\alpha - e^{\alpha i}_\beta V_i < \Psi^\beta > - f^{\alpha ij}_\beta V_j < V_i < \Psi^\beta \gg] + \varepsilon^3 T^\alpha$

where $T^\alpha \in \Lambda^0(K_2)$ is given by

(18) $\quad T^\alpha = \Theta^\alpha - e^{\alpha i}_\beta V_i < R^\beta > - f^{\alpha ij}_\beta V_j < V_i < R^\beta \gg$

To minimize E^α a suitable choice for R^α is given by

(19) $\quad R^\alpha = \Omega^\alpha - e^{\alpha i}_\beta V_i < \Psi^\beta > - f^{\alpha ij}_\beta V_j < V_i < \Psi^\beta \gg$

It should be pointed out that the assumptions (16) do not exhaust all the possibilities of F^α and have been made in order to obtain an identity for R^α explicitely in known quantities.

In applications where it is practical to obtain solutions to partial differential equations through approximation by the employment of numerical schemes, e.g. finite difference or finite element methods, the accuracy of the solution is dependent on the mesh or element size of the discretization used. For computational speed one aims to maximize the mesh or element sizes such that sufficient accuracy is maintained. It is often the case that for practical computational reasons the mesh or element sizes are too large to resolve the microscale fluctuations in the solution. Here we address this by replacing the original system of partial differential equations (6) by a new system based on (15) which describes the macroscale behaviour of the solution over each mesh or element of this discretization. Each mesh or element should be thought of as a representative elemenatry volume (REV) over which the macroscale behaviour is of interest. Since solution by numerical methods is one of approximation it would be sufficient also to consider the macroscale behaviour over each REV in an approximate sense. The proviso here is that the error introduced by the latter does not overwhelm the error introduced by the numerical scheme.

We shall examine the macroscale behaviour locally over some small open subdomain $D \subset M$ which we associate with some REV. The small scaling parameter ε is associated with this REV and the macroscale formulation is dependent on ε and hence is scale dependent.

If $\phi^{\alpha}(x^{i}) \equiv \phi^{*}q^{\alpha}$, where $\phi \in \Sigma[D \subset M, \Upsilon[K_2, F^{\alpha}]]$, are regarded as the macroscale dependent variables then the macroscale partial differential equations are given by

$$(20) \qquad \phi^{*}F^{\alpha} = 0$$

where F^{α} is given by (15). We have on each open subdomain $D \subset M$

$$(21) \qquad (S o \phi)^{*}\tilde{q}^{\alpha} = \phi^{*}(S^{*}\tilde{q}^{\alpha}) = \phi^{\alpha} + \varepsilon\phi^{*}\zeta^{\alpha}$$

Since $\zeta^{\alpha} \in \Lambda^{0}(K_2)$ the term $\varepsilon\phi^{*}\zeta^{\alpha}$ will be small relative to the order of magnitude of ϕ^{α} if ϕ^{α} is sufficiently smooth and does not exhibit microscale fluctuations with respect to the macroscale base manifold coordinates (x^{i}). Thus on the subdomain $D \subset M$, $(S o \phi)^{*}\tilde{q}^{\alpha}$ are, for sufficiently small ε, approximations of the macroscale dependent variables $\phi^{\alpha}(x^{i})$. The next step is to examine whether $S o \phi$ is an approximation to an anninilator of $\tilde{F}^{\alpha}$.

For any $\phi: D \subset M \to K_2$, $\phi \in \Sigma[D \subset M, H[K_2]]$ consider the composite map $S o \phi: D \subset M \to \tilde{K}_2$. It follows that $S o \phi \in \Sigma[D \subset M, H[\tilde{K}_2]]$ by simply noting that $(S o \phi)^{*}H[\tilde{K}_2] = \phi^{*}(S^{*}H[\tilde{K}_2])$ and $S^{*}H[\tilde{K}_2] \subset H[K_2]$. Furthermore, if $\phi \in \Sigma[D \subset M, \Upsilon[K_2, F^{\alpha}]]$ then it follows from (14)-(19) that on the open subdomain $D \subset M$

$$(22) \qquad \frac{1}{\varepsilon}(S o \phi)^{*}\tilde{F}^{\alpha} = \varepsilon^{2}\phi^{*}T^{\alpha}$$

The term $1/\varepsilon$ has been introduced in (22) to remove the common factor of ε which arises from the scaling of independent coordinates. Since $T^{\alpha} \in \Lambda^{0}(K_2)$ the error term $\varepsilon^{2}\phi^{*}T^{\alpha}$ will be small if the macroscale solution $\phi^{*}q^{\alpha} = \phi^{\alpha}(x^{i})$ is sufficiently smooth and free of microscale fluctuations with respect to the macroscale coordinates (x^{i}).

Linear transformation

Since local approximations are of interest it would make sense to consider $\zeta^{\alpha} \in \Lambda^0(K_2)$ as a polynomial of the coordinates of K_2. The order of these polynomials may be arbitrary. To reduce the calculations we shall consider here the linear case

$$(23) \qquad \zeta^{\beta} = a^{\beta} + b^{\beta}_{\gamma} q^{\gamma} + c^{\beta j}_{\gamma} r^{\gamma}_{j} + d^{\beta jk}_{\gamma} r^{\gamma}_{jk}$$

where the a, b, c, d's are arbitrary constants. We simplify matters even further by assuming that $e^{\alpha i}_{\beta}$ and $f^{\alpha ij}_{\beta}$ are constants rather than functions of the coordinates of K_2.

From (11) and (23) a calculation yields

$$(24) \qquad \Omega^{\alpha} = (\lambda^{\alpha i}_{\beta} b^{\beta}_{\gamma} + \eta^{\alpha i}_{\beta\gamma} a^{\beta}) r^{\gamma}_{i} + (\lambda^{\alpha i}_{\beta} c^{\beta j}_{\gamma} + \nu^{\alpha ji}_{\gamma}) r^{\gamma}_{ij} + (\eta^{\alpha i}_{\beta\lambda} b^{\lambda}_{\gamma} + \eta^{\alpha i}_{\lambda\gamma} b^{\lambda}_{\beta}) q^{\beta} r^{\gamma}_{i} + \eta^{\alpha i}_{\lambda\gamma} c^{\lambda j}_{\beta} r^{\beta}_{j} r^{\gamma}_{i} +$$
$$\eta^{\alpha i}_{\beta\lambda} c^{\lambda j}_{\gamma} q^{\beta} r^{\gamma}_{ij} + \eta^{\alpha k}_{\lambda\beta} d^{\lambda ij}_{\gamma} r^{\beta}_{k} r^{\gamma}_{ij} + \lambda^{\alpha i}_{\gamma} d^{\gamma jk}_{\beta} A^{\beta}_{ijk} + \eta^{\alpha i}_{\beta\lambda} d^{\lambda jk}_{\gamma} q^{\beta} A^{\gamma}_{ijk}$$

If we wish to apply the constraint that the macroscale partial differential equations be second order we must remove the terms A_{jki} in (19). The terms $V_i < F^{\beta} >$ and $V_j < V_i < F^{\beta} \gg$ in (13) become useful here. We set

$$(25) \qquad f^{\alpha ji}_{\beta} = d^{\alpha ij}_{\beta} = \delta^{\alpha}_{\beta} g^{ij}$$

for some constants g^{ij}, to obtain

$$(26) \qquad R^{\alpha} = (\lambda^{\alpha i}_{\beta} b^{\beta}_{\gamma} + \eta^{\alpha i}_{\beta\gamma} a^{\beta}) r^{\gamma}_{i} + (\lambda^{\alpha i}_{\gamma} c^{\gamma j}_{\beta} - e^{\alpha i}_{\gamma} \lambda^{\gamma j}_{\beta} + \nu^{\alpha ji}_{\beta}) r^{\beta}_{ij} + (\eta^{\alpha i}_{\beta\lambda} b^{\lambda}_{\gamma} + \eta^{\alpha i}_{\lambda\gamma} b^{\lambda}_{\beta}) q^{\beta} r^{\gamma}_{i} +$$
$$(\eta^{\alpha i}_{\lambda\gamma} c^{\lambda j}_{\beta} - e^{\alpha j}_{\lambda} \eta^{\lambda i}_{\beta\gamma}) r^{\beta}_{j} r^{\gamma}_{i} + (\eta^{\alpha i}_{\beta\lambda} c^{\lambda j}_{\gamma} - e^{\alpha i}_{\lambda} \eta^{\lambda j}_{\beta\gamma}) q^{\beta} r^{\gamma}_{ij} - (g^{ki} + g^{ik}) \eta^{\alpha j}_{\beta\gamma} r^{\beta}_{k} r^{\gamma}_{ij}$$

where repeated use is made of the symmetry of r^{α}_{ij} and A^{α}_{ijk}.

In physical applications such as fluid flow the parameters $a^{\alpha}, b^{\alpha}_{\beta}, c^{\alpha i}_{\beta}, e^{\alpha i}_{\beta}, g^{ij}$ can be regarded as empirically defined parameters based on properties of the fluid and possibly the geometry of the domain and boundary/initial conditions. It must be stressed that it is the choice of these empirical parameters which will ultimately dictate whether the resulting solutions of (20) adequately describe the macroscale behaviour of a specific application. One may impose constraints on these parameters which originate from physical arguments. These may include conditions which will require that the terms R^{α} are dissipative to perturbations in the solution with frequencies above some cutoff value. This will ensure that the macroscale solutions are free of microscale fluctuations.

Example: Incompressible Turbulent Fluid Flow.

Let the coordinates of $\tilde{M}$ be $(\tilde{x}^1, \tilde{x}^2, \tilde{x}^3, \tilde{x}^4) \equiv (\tilde{x}, \tilde{y}, \tilde{z}, \tilde{t})$ (n=4), where $(\tilde{x}, \tilde{y}, \tilde{z})$ are the space coordinates and $\tilde{t}$ is the time. If $(\tilde{x}^i)$ are nondimensional coordinates then the Navier-Stokes and the continuity equations can be written in the nondimensional form

(27) $$\tilde{F}^a = \tilde{r}^a_4 + \sum_{b=1}^{3} \tilde{q}^b \tilde{r}^a_b + \tilde{r}^4_a - \mu \sum_{b=1}^{3} \tilde{r}^a_{bb}, \qquad 1 \le a \le 3$$

(28) $$\tilde{F}^4 = \sum_{b=1}^{3} \tilde{r}^b_b$$

where $(\tilde{q}^1, \tilde{q}^2, \tilde{q}^3, \tilde{q}^4) \equiv (\tilde{v}_x, \tilde{v}_y, \tilde{v}_z, \tilde{p})$ and $\mu = 1/\mathrm{Re}$ and Re is the Reynolds number. Here $(\tilde{v}_x, \tilde{v}_y, \tilde{v}_z)$ are the nondimensional velocity components and $\tilde{p}$ is the nondimensional fluid pressure. $\tilde{F}^\alpha$ can be written in the form given by (5) if

$$\lambda^{a4}_a = \lambda^{aa}_4 = \lambda^{4a}_a = 1, \qquad 1 \le a \le 3$$

(29) $$\eta^{ab}_{ba} = 1, \qquad 1 \le a, b \le 3$$

$$\nu^{abb}_a = -\mu, \qquad 1 \le a, b \le 3$$

and the λ, η, ν's are zero otherwise (in (29) the summation convention on repeated indicies does not hold). It can be shown that (27)-(28) can be obtained from balance n-forms through the identity (A18) and hence are balance or conservation equations.

We recall the transformation of coordinates $\Phi: M \to \tilde{M}$, $\Phi^* \tilde{x}^i = x^i/\varepsilon$. The simplest macroscale equations can be obtained from the identity map for the dependent variables

(30) $$s^i = S^* \tilde{x}^i = x^i/\varepsilon, \qquad s^\alpha = S^* \tilde{q}^\alpha = q^\alpha$$

$(\zeta^\alpha = 0)$, and setting $F^\alpha = (S^* \tilde{F}^\alpha)/\varepsilon$ to obtain

(31) $$F^a = r^a_4 + \sum_{b=1}^{3} q^b r^a_b + r^4_a - \varepsilon\mu \sum_{b=1}^{3} r^a_{bb}, \qquad 1 \le a \le 3$$

(32) $$F^4 = \sum_{b=1}^{3} r^b_b$$

Note that in this case the error term $\varepsilon^2 T^\alpha$ is identically zero and the pullback of (31)-(32) by some $\phi \in \Sigma[M, \Upsilon[K_2, F^\alpha]]$ is equivalent to (6). For high Reynolds number flow the parameter μ is typically small and the viscous term in (31) is of the order $\varepsilon\mu$. For high Reynolds number which results in turbulent flow the system (31) is inappropriate for numerical solution since it is often the case that grid sizes would have to be too small for practical computation. As a result closure models for turbulent flow have been proposed which attempt to describe the flow only at scales larger than some cutoff length. In the *large-eddy simulation model* one applies a Gaussian filter to the flow equations which introduces a Reynolds stress for small-scale turbulence below the cutoff length [6]. A brief and concise review of some turbulent closure models may be found in [4].

A closure model for turbulent flow similar to the large-eddy simulation model can be obtained by the approach outlined in the previous sections by the appropriate selection of the empirically based parameters $a^{\alpha}, b^{\alpha}_{\beta}, c^{\alpha i}_{\beta}, e^{\alpha i}_{\beta}, g^{ij}$. To ensure that mass conservation at the macroscale is maintained to an error of $\varepsilon^2 T^4$, i.e.

$$(33) \qquad R^4 = 0$$

we introduce the linear constraints on the parameters $b^{\alpha}_{\beta}, c^{\alpha i}_{\beta}, e^{\alpha ij}_{\beta}$

$$(34) \qquad \lambda^{4i}_{\beta} b^{\beta}_{\gamma} = 0, \quad \lambda^{4i}_{\gamma} c^{\gamma j}_{\beta} - e^{4i}_{\gamma} \lambda^{\gamma j}_{\beta} = 0, \quad e^{4j}_{\lambda} \eta^{\lambda i}_{\beta\gamma} = 0$$

For the fluid momentum equations (F^a, $1 \le a \le 3$) the terms obtained from (26) for R^a, $1 \le a \le 3$ subject to the algebraic constraints (34) are the most general that can be obtained from the linear transformation (23) under the assumptions based on (16) and the constraint (25) which restrict the flow equations to second order partial differential equations. One of course could seek more complex turbulent closure models by replacing ζ^{α} in (23) with a higher order polynomial of the coordinates of K_2. As it stands the expressions on the right hand side of (26) still involve time derivatives of the dependent flow variables. If desired these may be removed in a number of ways, the most direct being the introduction of additional algebraic constraints on the parameters $a^{\alpha}, b^{\alpha}_{\beta}, c^{\alpha i}_{\beta}, e^{\alpha i}_{\beta}, g^{ij}$.

For specific applications it is likely that one could continue by adding algebraic constraints on these parameters based on sound physical arguments. These may include constraints which require that R^a, $1 \le a \le 3$ are dissipative to microscale fluctuations in the solution. In the end one expects that there will remain several unknowns in the set of parameters which will be determined empirically. Specific applications addressing these issues are left open for future investigations.

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APPENDIX

K_2 is the second order contact manifold with coordinates $(x^i, q^\alpha, r_i^\alpha, r_{ij}^\alpha)$, $1 \le i,j \le n$; $1 \le \alpha \le N$ where it can be assumed that $r_{ij}^\alpha = r_{ji}^\alpha$. M is the base manifold of the independent coordinates (x^i). The horizontal ideal $H[K_2]$ on K_2 is given by

(A1) $\quad H[K_2] = I\{C^\alpha, C_i^\alpha, H_{ij}^\alpha\}$

generated by the differential 1-forms

(A2) $\quad C^\alpha = dq^\alpha - r_i^\alpha dx^i, \quad C_i^\alpha = dr_i^\alpha - r_{ij}^\alpha dx^j, \quad H_{ij}^\alpha = dr_{ij}^\alpha - A_{ijk}^\alpha dx^k$

where $A_{ijk}^\alpha \in \Lambda^0(K_2)$ satisfy the symmetry conditions

(A3) $\quad A_{ijk}^\alpha = A_{jik}^\alpha = A_{jki}^\alpha$

The set of regular maps $\phi: M \to K_2$ which annihilate any ideal $\Upsilon[K_2]$ on K_2 is denoted by

(A4) $\quad \Sigma[M, \Upsilon[K_2]] = \{\phi: M \to K_2 \mid \phi^* \mu \neq 0, \phi^* \Upsilon[K_2] = 0\}$

where $\mu = dx^1 \wedge dx^2 \wedge \cdots \wedge dx^n$ is the volume n-form on M. A map $\phi \in \Sigma[M, H[K_2]]$ yields the pullback identities to the base manifold

(A5) $\quad \phi^* q^\alpha = \phi^\alpha(x^l), \quad \phi^* r_i^\alpha = \dfrac{\partial \phi^\alpha(x^l)}{\partial x^i}, \quad \phi^* r_{ij}^\alpha = \dfrac{\partial^2 \phi^\alpha(x^l)}{\partial x^i \partial x^j}, \quad \phi^* A_{ijk}^\alpha = \dfrac{\partial^3 \phi^\alpha(x^l)}{\partial x^i \partial x^j \partial x^k}$

Associated with $H[K_2]$ is the module of Cauchy Characteristic vector fields

(A6) $\quad H^*[K_2] = \{U \in T(K_2) \mid U \rfloor H[K_2] \subset H[K_2]\}$

$H^*[K_2]$ admits the basis of canonical vector fields $\{V_i \mid 1 \le i \le n\}$ where

(A7) $\quad V_i = \dfrac{\partial}{\partial x^i} + r_i^\alpha \dfrac{\partial}{\partial q^\alpha} + r_{ij}^\alpha \dfrac{\partial}{\partial r_j^\alpha} + A_{ijk}^\alpha \dfrac{\partial}{\partial r_{jk}^\alpha}$

$H[K_2]$ is closed, i.e. $dH[K_2] \subset H[K_2]$, if and only if

(A8) $\quad V_i < A_{jkl}^\alpha > = V_j < A_{ikl}^\alpha >$

For any $F \in \Lambda^0(K_2)$ ($\Lambda^0(K_2)$ is the collection of differential 0-forms or continuously differentiable functions on K_2), (A9) $dF = V_i < F > dx^i \bmod\{H[K_2]\}$

For any $\phi \in \Sigma[M, H[K_2]]$ such that $\phi^* F^\alpha = 0$, $(1 \le \alpha \le N)$ for some $F^\alpha \in \Lambda^0(K_2)$ defines a system of N second order partial differential equations

$$(A10)) \quad F^\alpha\left(x^i, \phi^\alpha(x^l), \frac{\partial \phi^\alpha(x^l)}{\partial x^i}, \frac{\partial^2 \phi^\alpha(x^l)}{\partial x^i \partial x^j}\right) = 0$$

The horizontal ideal $H[K_2]$ is a subideal of the ideal

$$(A11) \quad \Upsilon[K_2; F^\alpha] = I\{C^\alpha, C_i^\alpha, H_{ij}^\alpha, F^\alpha\}$$

which contains the 0-forms F^α as generators. Thus, we can say that a map $\phi \in \Sigma[M, H[K_2]]$ which annihilates F^α belongs to the set $\phi \in \Sigma[M, \Upsilon[K_2; F^\alpha]]$.

The closure of $\Upsilon[K_2; F^\alpha]$, i.e. $d\Upsilon[K_2; F^\alpha] \subset \Upsilon[K_2; F^\alpha]$ is guaranteed if $H[K_2]$ is closed and (noting (A9))

$$(A12) \quad V_i < F^\alpha >= L^\alpha_{\beta i} F^\beta$$

for some $L^\alpha_{\beta i} \in \Lambda^0(K_2)$. It follows that

$$(A13) \quad V_j < V_i < F^\alpha \gg = \Gamma^\alpha_{\beta ij} F^\beta$$

where $\Gamma^\alpha_{\beta ij} \in \Lambda^0(K_2)$ is given by

$$(A14) \quad \Gamma^\alpha_{\beta ij} = V_j < L^\alpha_{\beta i} > + L^\alpha_{\gamma i} L^\gamma_{\beta j}$$

Let

$$(A15) \quad \Xi[K_2, F^\alpha] = \{P \in K_2 \mid F|_P = 0, F^\alpha \in \Lambda^0(K_2), \quad 1 \le \alpha \le N\}$$

be the point set of K_2 on which F^α vanishes. The image of some domain $D \subset M$ of a map $\phi \in \Sigma[M, H[K_2]]$ which intersects the point set $\Xi[K_2, F^\alpha]$ defines a solution map of the ideal $\Upsilon[K_2; F^\alpha]$ restricted to the domain $D \subset M$. Also, restricted to the point set $\Xi[K_2, F^\alpha]$, we have the identities which follow from (A12) and (A13)

$$(A16) \quad V_i < F^\alpha > |_P = 0, \quad V_j < V_i < F^\alpha >> |_P = 0 \qquad P \in \Xi[K_2, F^\alpha]$$

Alternatively one could consider the ideal $I\{C^\alpha, C_i^\alpha, H_{ij}^\alpha, B^\alpha\}$ which contain the balance n-forms

$$(A17) \quad B^\alpha = h^\alpha \mu - dW^{\alpha i} \wedge \mu_i$$

where $\mu_i = \partial / \partial x^i \rfloor \mu$, and h^α, $W^{\alpha i}$ are functions of $(x^i, q^\alpha, r_i^\alpha)$. The functions F^α can be obtained from the identity

(A18) $\quad F^\alpha = h^\alpha - V_i < W^{\alpha i} >$

The balance ideal is appropriate for applications where the partial differential equations $\phi^* F^\alpha = 0$ are statements of balance or conservation. The identities (A12) and (A13) above follow from the requirement that the canonical basis vector fields $\{V_i \mid 1 \le i \le n\}$ are also isovectors of the Balance ideal.

For our purposes it will be sufficient to allow $\Upsilon[K_2, F^\alpha]$ to denote the ideal generated by the generators of $H[K_2]$ and the 0-forms F^α or the balance n-forms B^α. There will be a need to employ the identities (A12) and (A13) which hold for both ideals with the properties stated above assumed.

Let $\tilde{K}_2$ be another second order contact manifold with coordinates $(\tilde{x}^i, \tilde{q}^\alpha, \tilde{r}_i^\alpha, \tilde{r}_{ij}^\alpha)$ and let $\tilde{M}$ be the associated base manifold with coordinates $(\tilde{x}^i)$. Associated with $\tilde{K}_2$ is the horizontal ideal $H[\tilde{K}_2] = I\{\tilde{C}^\alpha, \tilde{C}_i^\alpha, \tilde{H}_{ij}^\alpha\}$ with symmetry conditions (A3) and (A8) for $\tilde{A}_{ijk}^\alpha \in \Lambda^0(\tilde{K}_2)$.

A map $S: K_2 \rightarrow \tilde{K}_2$ such that $S^* H[\tilde{K}_2] \subset H[K_2]$ has the properties

(A19) $\quad V_i < s^j > \neq 0, \quad V_i < s^j > s_j^\alpha = V_i < s^\alpha >, \quad V_i < s^k > s_{jk}^\alpha = V_i < s_j^\alpha >,$

$$V_k < s^l > S^* A_{ijl}^\alpha = V_k < s_{ij}^\alpha >$$

where s^i, s^α, s_i^α, $s_{ij}^\alpha \in \Lambda^0(K_2)$ are defined by

(A20) $\quad s^i = S^* \tilde{x}^i, \quad s^\alpha = S^* \tilde{q}^\alpha, \quad s_i^\alpha = S^* \tilde{r}_i^\alpha, \quad s_{ij}^\alpha = S^* \tilde{r}_{ij}^\alpha$

The generators of S are s^i and s^α. If S is a diffeomorphism then S is referred to as an *extended precanonical transformation*. In the present application the existence of S^{-1} is not assumed.