NOTATING STRATEGY FOR SYSTEMS OF PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. If one considers systems of partial differential equations in a multidimensional space, the notation becomes complicate and one may easily lose his or her consistency. In this note a notating strategy is suggested. The idea is to distinguish the effects of the dimensional variables and the state variables.

Having a better notation is helpful. It helps people to write things simpler and, more importantly, to think things clearer. Ever since I have learned systems of conservation laws in a multidimensional space, which was my graduate school years in Madison Wisconsin, I thought that there should be a more consistent way to denote things related to systems of partial differential equations in multidimension. Recently, I realized that the key is not better notations but to use them with a strategy.

My strategy is simple. Reserve row vectors for the vector fields related to the spacial dimension and column vectors for the ones related to the state variables. These two kinds of vector fields play different roles in the system and hence one may see that such a simple distinction makes notations systematic. If one is already doing that, there is probably nothing new in the rest of this note.

My notating goal is, if possible, to use the matrix multiplication as the only product with an exception of the inner product. We definitely want to avoid other products such as the tensor product. As a specific example we consider a reaction diffusion system which is from an imaginary wing disk modeling of Drosophila.

Example 1 (A typical derivation of conservation laws)**.** Let $\mathbf{y} = (y_1, y_2) \in \mathbb{R}^2$ be the spacial coordinates in two space dimension and $\mathbf{c}(\mathbf{y}, t)$ be the concentration vector of three kinds of proteins $\mathbf{c} = (c_1, c_2, c_3)\big(= (\mathrm{dpp}, \mathrm{wg}, \mathrm{Xvg})\big) \in \mathbb{R}^3$. Here we have chosen an example that the numbers of state variables and space dimension are different.

It seems reasonable to write the state vector $\mathbf{c}$ as a column vector due to the horizontal writing of equations. Let

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \in \mathbb{R}^{3\times 1}, \tag{1}$$

where $\mathbb{R}^{m\times n}$ is the collection of $m \times n$ real matrices. Other vector fields related to the state variables of the system will be considered as a column vector.

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There are several kinds of vector fields which are related to the space dimension. The velocity vector field $\mathbf{u}$, the gradient vector field ∇f of a functional, and the space variable $\mathbf{y}$ itself are also such vectors. We consider them as row vectors, i.e.,

$$\mathbf{y} = (y_1, y_2), \quad \mathbf{u} = (u_1, u_2), \quad \nabla f = (f_{y_1}, f_{y_2}) \quad \in \quad \mathbb{R}^{1\times 2}. \tag{2}$$

In fact it is natural to consider ∇f as a row vector since it is actually a linear transformation from $\mathbb{R}^2$ to $\mathbb{R}^1$. Let $F = (f_1, \cdots, f_k)$ be a vector field. Then its Jacobi matrix is denoted by DF and given by

$$D_{\mathbf{y}} F = \begin{pmatrix} (f_1)_{y_1} & (f_1)_{y_2} \\ \vdots & \vdots \\ (f_k)_{y_1} & (f_k)_{y_2} \end{pmatrix} = \begin{pmatrix} \nabla_{\mathbf{y}} f_1 \\ \vdots \\ \nabla_{\mathbf{y}} f_k \end{pmatrix}. \tag{3}$$

For a column vector field $\mathbf{c}$, $\nabla \mathbf{c}$ is the usual Jacobi matrix, i.e.,

$$\nabla \mathbf{c} = \nabla \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} \nabla c_1 \\ \nabla c_2 \\ \nabla c_3 \end{pmatrix} = D\mathbf{c} \in \mathbb{R}^{3\times 2}.$$

Notice that taking a gradient of a row vector field is not acceptable in our convention. For example

$$\nabla \mathbf{u} = \nabla(u_1, u_2) = (\nabla u_1, \nabla u_2) \in \mathbb{R}^{1\times 4}$$

is meaningless. If one wants to consider the Jacobi matrix of $\mathbf{u}$, then it should be written as $D\mathbf{u} = \nabla(\mathbf{u}^t) \in \mathbb{R}^{2\times 2}$, where the column vector $\mathbf{u}^t$ is the transpose of the row vector $\mathbf{u}$.

Now consider taking the divergence of a vector field. It is clear that the vector field should have two components which is the spacial dimension. Hence we think that the divergence should be applied to a row vector field. Hence $\mathrm{div}(\mathbf{u})$ and $\mathrm{div}(\nabla f)$ make sense. However, $\mathrm{div}(\mathbf{c})$ is definitely meaningless. (Notice that, even if the number of state variables are same as the dimension, there should be no such thing as $\mathrm{div}(\mathbf{c})$ in a meaningful equation.)

One can easily model the dynamics of the morphogen concentration. Let $\mathbf{u} = \mathbf{u}(\mathbf{y}, t), \mathbf{c} = \mathbf{c}(\mathbf{y}, t)$ be functions of space and time variables. Let $R_i(\mathbf{c}, \mathbf{y}, t)$ model the reaction, production and degradation of the i-th state variable c_i. Therefore the vector $\mathbf{R}$ that consists of R_i's should be considered as a column vector, i.e,

$$\mathbf{R}(\mathbf{c}, \mathbf{y}, t) = \begin{pmatrix} R_1(\mathbf{c}, \mathbf{y}, t) \\ R_2(\mathbf{c}, \mathbf{y}, t) \\ R_3(\mathbf{c}, \mathbf{y}, t) \end{pmatrix} \in \mathbb{R}^{3\times 1}. \tag{4}$$

Consider a fixed bounded domain E in the flow and let $\mathbf{n}$ be the outward unit normal vector at the boundary. The rate of change of the amount of the i-th protein in the region E is modelled by

$$\int_E \frac{\partial}{\partial t} c_i(\mathbf{y}, t) d\mathbf{y} = \int_E R_i(\mathbf{c}, \mathbf{y}, t) d\mathbf{y} - \int_{\partial E} \mathbf{j} \cdot \mathbf{n} ds, \tag{5}$$

where $\mathbf{j}$ is the flux of the morphogen c_i. This flux consists of two parts. The first one is due to the flux of the fluid flow and the second one is due to the gradient of the concentration. Let τ_i be the corresponding diffusion tensor. Then the flux is given as a row vector,

$$\mathbf{j} = c_i \mathbf{u} - \tau_i \nabla c_i.$$

After applying the divergence theorem, one obtains

$$(c_i)_t(\mathbf{y},t) + \operatorname{div}(c_i\mathbf{u}) = \operatorname{div}(\tau_i \nabla c_i) + R_i(\mathbf{c},\mathbf{y},t). \tag{6}$$

We consider the isotropic case. Then τ_i is actually a scalar and (6) can be rewritten in a vector form, which is

$$\mathbf{c}_t(\mathbf{y},t) + \operatorname{div}(\mathbf{c}\mathbf{u}) = \tau\Delta\mathbf{c} + \mathbf{R}(\mathbf{c},\mathbf{y},t), \tag{7}$$

where τ is the diagonal matrix with τ_i in the i-th diagonal element. Using earlier notations, one may easily see that the notations mean

$$\operatorname{div}(\mathbf{c}\mathbf{u}) = \operatorname{div}\begin{pmatrix} c_1\mathbf{u} \\ c_2\mathbf{u} \\ c_3\mathbf{u} \end{pmatrix} = \begin{pmatrix} \operatorname{div}(c_1\mathbf{u}) \\ \operatorname{div}(c_2\mathbf{u}) \\ \operatorname{div}(c_3\mathbf{u}) \end{pmatrix}, \quad \operatorname{div}(\nabla\mathbf{c}) = \begin{pmatrix} \operatorname{div}(\nabla c_1) \\ \operatorname{div}(\nabla c_2) \\ \operatorname{div}(\nabla c_3) \end{pmatrix} = \Delta\mathbf{c}.$$

Notice that $\mathbf{cu}$ is a 3×2 matrix obtained by the matrix multiplication. If both of $\mathbf{c}$ and $\mathbf{u}$ are considered as row or column vectors, then it should be replaced with a tensor product. Hence we have saved a tensor product by considering $\mathbf{u}$ as a row vector and $\mathbf{c}$ as a column one. Furthermore the meaning of $\operatorname{div}(\mathbf{cu})$ is more direct than the one using a tensor product. □

One of the main features of the notation is in the multiplication $\mathbf{cu}$ in (7). Since the space dimension and the number of state variables are different and not one, matrix multiplications such as $\mathbf{uc}, \mathbf{uu}$ and $\mathbf{cc}$ are not defined. Hence, such terms should not appear anywhere. Even if the number of state variables is same as the space dimension, such terms are not physical and hence should not appear. However, if one includes tensor product, then tensor products of such combinations are possible. For the sake of remembering formulas or reducing possible mistakes, using a notation that exclude such nonphysical terms is helpful.

Example 2 (Change of variables using material coordinates)**.** In this example we will remind that taking the gradient as a row vector makes change of variables convenient. Consider Lagrangian coordinates which are also row vectors and denoted by $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^{1\times 2}$. We may implicitly consider the Eulerian coordinates $\mathbf{y}$ as a trajectory function of $\mathbf{x}$ or more explicitly introduce $\Gamma(\mathbf{x},t)$ which indicates the position of a particle $\mathbf{x}$ at time $t > 0$. In other words we may set

$$\mathbf{y} = \mathbf{y}(\mathbf{x},t) \quad \text{or} \quad \mathbf{y} = \Gamma(\mathbf{x},t), \quad \mathbf{x} = (x_1,x_2) \in \mathbb{R}^{1\times 2}. \tag{8}$$

The Lagrangian coordinate $\mathbf{x}$ actually denotes the particle which was placed at the point $\mathbf{x}$ initially and the trajectory $\Gamma(\mathbf{x},t)$ denoted the position of the particle at time $t \geq 0$. Therefore, one may set

$$\Gamma(\mathbf{x},0) = \mathbf{y}(\mathbf{x},0) = \mathbf{x}, \qquad \mathbf{u}(\mathbf{x},t) = \mathbf{u}(\mathbf{y}(\mathbf{x},t),t) = \frac{\partial\Gamma}{\partial t}(\mathbf{x},t), \tag{9}$$

where $\mathbf{u}$ is the velocity vector field introduced earlier. Note that we abuse our notation here. Using the same notation $\mathbf{u}$ for the velocity, $\mathbf{u}(\mathbf{x},t)$ denotes the velocity of the particle $\mathbf{x}$ at time $t > 0$ and $\mathbf{u}(\mathbf{y},t)$ denotes the velocity at the position $\mathbf{y}$ at time $t > 0$. We take the same convention for $\mathbf{c}$ and $\mathbf{R}$, too.

Let $D_{\mathbf{x}}\Gamma := \Gamma_{\mathbf{x}}$ be the Jacobi matrix of the trajectory, i.e.,

$$\Gamma_{\mathbf{x}} = D_{\mathbf{x}}\Gamma = \nabla_{\mathbf{x}}(\Gamma^t) = \begin{pmatrix} \nabla y_1(\mathbf{x},t) \\ \nabla y_2(\mathbf{x},t) \end{pmatrix} = \begin{pmatrix} (y_1)_{x_1} & (y_1)_{x_2} \\ (y_2)_{x_1} & (y_2)_{x_2} \end{pmatrix}.$$

Then, for a vector field F, we obtain the chain rule

$$D_{\mathbf{x}}F = (D_{\mathbf{y}}F)\Gamma_{\mathbf{x}} \quad \text{or} \quad D_{\mathbf{y}}F = (D_{\mathbf{x}}F)\Gamma_{\mathbf{x}}^{-1}. \tag{10}$$

Since $DF = \nabla F$ for any column vector field or a scalar function, the chain rule gives

$$\nabla c_i(\mathbf{y},t) = \nabla c_i(\mathbf{x},t)\Gamma_{\mathbf{x}}^{-1}, \tag{11}$$

$$\mathrm{div}(\mathbf{u}(\mathbf{y},t)) = Tr(D\mathbf{u}(\mathbf{y},t)) = Tr((D\mathbf{u}(\mathbf{x},t))\Gamma_{\mathbf{x}}^{-1}), \tag{12}$$

$$\Delta c_i(\mathbf{y},t) = Tr\big(D(\nabla c_i(\mathbf{y},t))\big) = Tr\big(D[\nabla c_i(\mathbf{x},t)(\Gamma_{\mathbf{x}}^{-1})]\Gamma_{\mathbf{x}}^{-1}\big), \tag{13}$$

where $Tr(A)$ is the trace of a square matrix A. Notice that, if the gradient is considered as a column vector, one should take a transpose of a gradient vector and, hence, the notation becomes messy, which is undesirable. (Independent variables of the differential operators in the previous calculations should be clear. For example in the writing $\nabla c_i(\mathbf{y},t)$ the independent variables are $\mathbf{y}$ and t and hence the gradient operator is with respect to $\mathbf{y}$. On the other hand, specifying independent variables of each term makes lengthy equations. Hence we specify only one of them for each side of equalities.)

Similar change of variables with respect to the time variable $t > 0$, we obtain

$$\mathbf{c}_t(\mathbf{y},t) + \mathrm{div}(\mathbf{cu}) = \mathbf{c}_t(\mathbf{y},t) + (\nabla\mathbf{c})\mathbf{u}^t + \mathbf{c}\mathrm{div}\mathbf{u} = \mathbf{c}_t(\mathbf{x},t) + \mathbf{c}Tr((D\mathbf{u})\Gamma_{\mathbf{x}}^{-1}). \tag{14}$$

Therefore, (7) is transformed to

$$(c_i)_t(\mathbf{x},t) = \tau_i Tr\big(D[(\nabla c_i)\Gamma_{\mathbf{x}}^{-1}]\Gamma_{\mathbf{x}}^{-1}\big) + R_i(\mathbf{c},\mathbf{x},t) - c_i Tr((D\mathbf{u})\Gamma_{\mathbf{x}}^{-1}), \quad i = 1,2,3. \tag{15}$$

Notice that the equation (15) is written in a scalar form since taking the Jacobian of $\nabla\mathbf{c}$ is not clearly defined. □

Remark 3. Consider the products between $\nabla\mathbf{c}$ and $\mathbf{u}$ or their transposes. Then there are eight possibilities. Since $\mathbf{u}$ is a row vector, the products such as $(\nabla\mathbf{c})\mathbf{u}$, $(\nabla\mathbf{c})^t\mathbf{u}$, $\mathbf{u}^t(\nabla\mathbf{c})$ and $\mathbf{u}^t(\nabla\mathbf{c})^t$ are not defined. Furthermore, $\mathbf{u}(\nabla\mathbf{c})$ and $\mathbf{u}^t(\nabla\mathbf{c})^t$ are defined only if the number of state variables is same as the space dimension, which is not of our case. Hence those six products should not appear in any case. Notice that, even if the dimension and the number of state variables are same, a product such as $\mathbf{u}(\nabla\mathbf{c})$ and $\mathbf{u}^t(\nabla\mathbf{c})^t$ has no physical meaning. The other two are $(\nabla\mathbf{c})\mathbf{u}^t$ and $\mathbf{u}(\nabla\mathbf{c})^t$, which are column and row vectors, respectively, and have identical components. Hence $(\nabla\mathbf{c})\mathbf{u}^t$ is the only possible case that may appear as in (14).

Consider the product rule used in (14) which is

$$\begin{pmatrix} \mathrm{div}(c_1\mathbf{u}) \\ \mathrm{div}(c_2\mathbf{u}) \\ \mathrm{div}(c_3\mathbf{u}) \end{pmatrix} - \begin{pmatrix} c_1\mathrm{div}\mathbf{u} \\ c_2\mathrm{div}\mathbf{u} \\ c_3\mathrm{div}\mathbf{u} \end{pmatrix} = \begin{pmatrix} \nabla c_1\cdot\mathbf{u} \\ \nabla c_2\cdot\mathbf{u} \\ \nabla c_3\cdot\mathbf{u} \end{pmatrix} = \begin{pmatrix} (\nabla c_1)\mathbf{u}^t \\ (\nabla c_2)\mathbf{u}^t \\ (\nabla c_3)\mathbf{u}^t \end{pmatrix} = (\nabla\mathbf{c})\mathbf{u}^t.$$

Hence $(\nabla\mathbf{c})\mathbf{u}^t$ is basically an inner (or dot) product and one may rewrite it as $\nabla\mathbf{c}\cdot\mathbf{u}$. Notice that the inner product is always between two vectors related to the space, not the state variables. Hence the inner product should be understood as

$$A\cdot B = AB^t,$$

where the dot product is meaningful or physical only if the numbers of columns of A and B are same as the space dimension. The inner product in (5) is also in this form.

Example 4 (a uniform wing disk growth)**.** For an imaginary wing disk modeling with a growth we consider a circular domain for simplicity. The domain in the

Lagrangian coordinate is simply a unit disk. The domain in Eulerian coordinate is growing in time and we set the domain as

$$\mathbf{x} \in B_\varepsilon(0), \qquad \mathbf{y} \in \mathcal{D}(t), \tag{16}$$

where $B_\varepsilon(0)$ is the disk of radius $\varepsilon > 0$ centered at the origin and $\mathcal{D}(t)$ is an expanding domain in Eulerian space. We assume a uniform growth and hence set the trajectory function as

$$\Gamma(\mathbf{x}, t) = \mathbf{x}e^{a(t)}, \quad 0 \le t \le T, \tag{17}$$

where $a(0) = 0$ and $a(t)$ is increasing as $t \to T$. Then $\mathbf{u} = \Gamma_t = a'(t)\mathbf{x}e^{a(t)}$, $\mathrm{div}(\mathbf{u}) = 2a'(t)e^{a(t)}$ and $\Gamma_\mathbf{x} = e^{a(t)}I$, where I is the identity matrix. Therefore, (15) is transformed to

$$\mathbf{c}_t(\mathbf{x}, t) = e^{-2a(t)}\tau\Delta\mathbf{c}(\mathbf{x}, t) + \mathbf{R}(\mathbf{c}, \mathbf{x}, t) - 2a'(t)\mathbf{c}. \tag{18}$$

□

Example 5 (Setting the details)**.** To complete the model we should have reasonably correct dimensions. We could not find appropriate quantitative data from the literature. Collecting data needed seems important. However, in the computation, it is more important to know what kind of factors make essential differences and what others do not.

The time length of the event is about 4 days. Hence lets take days for the time unit and

$$T = 3(days).$$

For the diffusion constant the range is about

$$10^{-11}m^2/day \le \tau_1, \tau_2 \le 10^{-9}m^2/day$$

and the initial radius of the disk is about

$$\varepsilon = 4 \times 10^{-5}m = 40\mu m$$

and grows upto $200\mu m$. The diffusion constant τ_3 for Xvg should be much smaller than others and we may set

$$\tau_3 = \tau_1/10.$$

The setup for the reaction part $\mathbf{R}(\mathbf{c}, \mathbf{x}, t)$ is more tricky and should be considered in a physically meaningful way. $\mathbf{R}$ consists of two part

$$\mathbf{R} := \mathbf{R_p} - \mathbf{R_d},$$

production and degradation, respectively. We assume simple degradation,

$$\mathbf{R_d} = \mathbf{R_d}(\mathbf{c}) = d\mathbf{c}, \qquad d > 0.$$

Morphogens $c_1 =$ dpp and $c_2 =$ wg are produced in specified regions. Let P_i be the i-th component of the production $\mathbf{R_p}$ and set

$$P_1(\mathbf{x}, t) := \begin{cases} k_1(t), & |x_1| < b(t), \\ 0\ , & \text{otherwise}, \end{cases} \quad P_2(\mathbf{x}, t) := \begin{cases} k_2(t), & |x_2| < b(t), \\ 0\ , & \text{otherwise}, \end{cases}$$

where $k_i(t)$ controls the strength of the source and $b(t)$ the region. Since the spacial domain increases, the fixed material domain gives exponential growth. Hence, $b(t)$ should be a decreasing function. We may take k_i's be proportional to the area of the source in spacial domain.

The main part of the model is to simulate the source domain of Xvg. Let

$$P_3(\mathbf{x},t) := \begin{cases} k_3(t), & \mathbf{x} \in \Omega(t) \\ 0\ , & \text{otherwise.} \end{cases}$$

We start with $\Omega(0) = \{\mathbf{x} : |x_2| < b(0)\}$ which is the support of the source function of wg. $\Omega(t)$ is a growing domain and we assume that a point $\mathbf{x}$ belongs to the domain $\Omega(t)$ if the following value

$$K(\mathbf{x}) = |\mathrm{Xvg}| \frac{|\nabla \mathrm{wg}|}{\mathrm{wg}} \frac{|\nabla \mathrm{dpp}|}{\mathrm{dpp}} \tag{19}$$

larger than certain critical point for certain amount of time. After setting up the scale of the coefficients we will do the non-dimensionalization. □

Remark 6 (Explanation of the third component Xvg). We want to see the pattern of cells such that vg is activated. vg is not a morphogen. It stays inside the cell. However, it activates vg of neighbor cells somehow. The process is now known. Let's assume that it makes certain protein, say Xvg, even if we do not know what it is. The effects is clearly different from the one of morphogen. The morphogen controls a larger region which is a little far from the source. However, the influence of Xvg seems of a short range. That is why we assumed that τ_3 is smaller than other diffusion constants. Our goal is to observe the dynamics of domain $\Omega(t)$ from the simulation based on quantities such as (19).

Example 7. The Euler's equations for inviscid fluid are usually written as

$$\rho_t + \mathrm{div}(\rho\mathbf{u}) = 0, \tag{20}$$

$$(\rho\mathbf{u})_t + \mathrm{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p = 0, \tag{21}$$

$$E_t + \mathrm{div}((E+p)\mathbf{u}) = 0, \tag{22}$$

where $\mathbf{y} \in \mathbb{R}^{1\times 2}$ and $\rho \geq 0, \mathbf{u}, p$ and E are density, velocity, pressure and total energy of the gas, respectively. If the internal energy e is considered, then E, e, p are related by

$$E = e + \frac{1}{2}|\mathbf{u}|^2, \qquad p = p(\rho, e).$$

One should notice that the components of the velocity $\mathbf{u}$ also play as state variables and makes the system closed. The gradient 'column' vector $\nabla_{\mathbf{y}} p$ in (21) appears due to the similar reason. This is why many people consider a gradient as a column vector, which is not our case here. We may easily rewrite the system under our strategy. Set $m_i := \rho u_i$ and

$$\mathbf{c} := \begin{pmatrix} \rho \\ m_1 \\ m_2 \\ E \end{pmatrix},\ \mathbf{R}(p, \nabla p) := -\begin{pmatrix} 0 \\ p_{y_1} \\ p_{y_2} \\ \mathrm{div}(p\mathbf{u}) \end{pmatrix} \in \mathbb{R}^{4\times 1}. \tag{23}$$

Then the Euler equations are written as

$$\mathbf{c}_t + \mathrm{div}(\mathbf{c}\mathbf{u}) = \mathbf{R}(p, \nabla p), \tag{24}$$

which is in the same form as (7) with a different reaction part $\mathbf{R}$ and zero viscosity $\tau = 0$. Hence the structure that characterizes the Euler equation is in the reaction part $\mathbf{R}(p, \nabla p)$ given by the pressure. □

Remark 8. Notations of this note are like followings.

(1) $\mathbf{v}^t$: transpose of the vector $\mathbf{v}$.
(2) $\mathbf{u}$: velocity row vector.
(3) $\mathbf{c}$: state column vector.
(4) ∇c: gradient row vector. $\nabla \mathbf{c}$: Jacobi matrix of the vector field $\mathbf{c}$.
(5) τ: (diagonal) diffusion matrix.
(6) $D\mathbf{f}$: Jacobi matrix of a vector field $\mathbf{f}$. If $\mathbf{f}$ is a column vector, then $D\mathbf{f} = \nabla \mathbf{f}$. If $\mathbf{f}$ is a row vector, then $D\mathbf{f} = \nabla(\mathbf{f}^t)$.

References

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