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2015 J. Phys.: Conf. Ser. 633 012082

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A random field approach to the Lagrangian modeling of turbulent transport in vegetated canopies

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Abstract. We present an application of a Lagrangian Stochastic Model (LSM) to turbulent dispersion over complex terrain, where turbulent coherent structures are known to play a crucial role. We investigate the case of a vegetated canopy by using semi-empirical parameterizations of turbulence profiles in the region inside and above a canopy layer. The LSM is based on a 4-dimensional Fokker-Planck (4DFP) equation, which extends the standard Thomson87 Lagrangian approach. The 4DFP model is derived by means of a Random Field description of the turbulent velocity field. The main advantage of this approach is that not only the experimental Eulerian one-point statistics, but also the Eulerian two-point two-time covariance structure can be included explicitly in the LSM. At variance with the standard Thomson87 approach, the 4DFP model allows to consider explicit parameterizations of the turbulent coherent structures as it explicitly includes both spatial and temporal correlation functions. In order to investigate the effect of the turbulent geometrical structure on a scalar concentration profile, we performed numerical simulations with two different covariance parameterizations, the first one isotropic and the second anisotropic. We show that the accumulation of scalars near the ground is due to the anisotropic geometrical properties of the turbulent boundary layer.

1. Introduction

Lagrangian Stochastic Models (LSMs) provide a useful tool to describe turbulent dispersion. They are based on a (Markovian) Langevin Equation for the Lagrangian particle velocity [3], whose drift and noise terms are related through the *well-mixedness criterion* (WMC) stated in the 1987 milestone paper by Thomson (Th87) [2]. In the Th87 approach the 1-point 1-time Probability Density Function (PDF) of the Eulerian velocity is experimentally known. The noise term is described by the 2nd order structure function, whose scaling is linear when the time increments are limited to the inertial subrange scales: $\langle [u(t + \Delta t) - u(t)]^2 \rangle \simeq C_0 \epsilon \Delta t$, being ϵ the turbulent energy dissipation rate and C_0 a constant¹. Applying the WMC, the drift is

¹ This is assumed to be a constant in the original 1941 Kolmogorov similarity (K41) theory, but it is nowadays well-known that this assumption is not exactly true due to intermittency of the velocity field at the inertial scales and small higher-order corrections, related to the velocity statistics, are considered.



expressed as a function of ϵ and of the Eulerian PDF. Apart from the homogeneous isotropic Gaussian turbulence, the drift is not determined uniquely, but only up to a velocity curl [2, 9, 11]. The standard Th87 approach, based on the WMC, is a powerful technique extensively used in Lagrangian transport modeling. However, the spatio-temporal geometrical structure of the velocity field is given by the universal K41 theory, thus inserting a strong modeling constrain that does not allow to take into account the experimental knowledge about space-time correlations of the velocity field, but only that about the Eulerian PDF. Then, Th87 shows some limitations in highly structured velocity fields (e.g., wall turbulence [4]) and, in general, in conditions where the geometrical features of the velocity field play a crucial role. From the the first paper by Thomson [2], Th87 approach has since then been applied in attempts to overcome the limitations related to the geometrical structure and to other aspects such as the non-uniqueness problem (see, e.g., [10, 8, 7] for recent developments).

A different approach, with respect to the Th87, was proposed in Ref. [1]. These authors developed a mathematical formulation which explicitly relates a Random Velocity Field (RVF), describing the Eulerian statistics, to the associated Lagrangian Stochastic Model (LSM), describing the trajectory dynamics of a passive scalar. In this approach, the application of the Ito's lemma [3] to a 3-Dimensional RVF depending on a 4-Dimensional (4D) space-time vector allows to derive a sort of 4D Fokker-Planck (4DFP) equation for the PDF of the Eulerian velocity. Given a semi-empirical expression for the Eulerian PDF with experimentally known parameters, the WMC [2] is directly applied to the 4DFP equation describing the RVF and not at the level of the LSM. At variance with Th87, the noise term is not defined from the K41 theory. This freedom is exploited to explicitly include the 2-point 2-time velocity statistics by means of the 2-points 2-time covariance tensor, which describes the space-time RVF correlations. When the coefficients of the 4DFP equation are known from the Eulerian statistics (1-point Eulerian PDF and 2-points covariance tensor), the ordinary Fokker-Planck and Langevin equations describing the LSM are simply derived by applying the dynamical equation of the passive tracers: $\dot{\mathbf{x}} = \mathbf{v}$. The main advantage of 4DFP is that not only the experimental Eulerian one-point PDF, but also the space-time RVF correlation structure, can be explicitly included in the LSM, thus allowing to consider explicit parameterizations of the turbulent coherent structures.

In this work, a particular version of the 4DFP-LSM, introduced in Ref. [1], is derived and applied to the case of the turbulent transport of passive scalars in vegetated canopies, thus allowing to get some information about the role of coherent structures. In particular, two different modeling choices, one with isotropic and the other with anisotropic motion structures, are compared.

The paper is organized as follows. In Section 2 we introduce the the 4DFP-LSM, in Section 3 we discuss the RVF statistics, both the Eulerian PDF and the covariance tensor, in Section 4 we show the numerical simulations and, finally, in Section 5 we draw some conclusions. In Appendix A the expression for the noise covariance tensor is introduced.

2. The 4DFP Lagrangian model

We recall here the main definitions and equations of the 4DFP Lagrangian model (see Ref. [1] for details). A RVF is formally defined through the assignment of n -point statistics for every n . The theoretical treatment of the general case is much involved and, actually, it is not really interesting for many applications, as n -point statistics is hardly obtained with the currently available instrumental technology. Then, the Lagrangian properties of the RVF are defined only in terms of 1-point 1-time Eulerian PDF and of 2-point 2-time covariance tensor, this being related to the 2nd order space-time structure function.

Now, we can define a zero-mean, incompressible RVF $\mathbf{u}(\mathbf{x}, t)$, with 2nd order space-time structure function scaling linearly in the increments $|\mathrm{d}\mathbf{x}|$ and dt at small space-time separations. We introduce 4-vector notation: $x^\mu = \{x^0, x^i\} \equiv \{t, \mathbf{x}\}$, $\partial_\mu \equiv \frac{\partial}{\partial x^\mu}$ and we stick rigorously to the Einstein convention of summation over covariant-contravariant repeated indices. We have the

following equation for the velocity increment:

$$du^i \equiv dx^\mu \partial_\mu u^i = A_\mu^i(\mathbf{u}, x^\mu) dx^\mu + dw^i; \quad A_\mu^i(\mathbf{u}, x^\mu) = \langle \partial_\mu u^i(\mathbf{x}, t) | \mathbf{u}(\mathbf{x}, t) \rangle \quad (1)$$

and $\langle d\mathbf{w} | \mathbf{u} \rangle = 0$. A possible expression for the noise correlation structure $\langle dw^i dw^j | \mathbf{u}(\mathbf{x}, t) \rangle$ is given in Appendix A. In the case of Gaussian Eulerian PDF, we have:

$$\rho_E(\mathbf{u}, x^\mu) \equiv \rho_G(\mathbf{u}, x^\mu) = (8\pi^3 ||R||)^{-\frac{1}{2}} \exp(-\frac{1}{2} S_{ij} u^i u^j) \quad (2)$$

where $S_{ij} = (R^{-1})_{ij}$ is the inverse of the Reynolds covariance tensor $R_{ij} = \langle u'_i u'_j \rangle$, being u'_i the components of the fluctuating velocity. In this case, the coefficients in Eq. (1) are given by the following expressions:

$$A_\mu^i = \bar{A}_\mu^i + \frac{1}{\rho_E} \Phi_\mu^i + \frac{1}{\rho_E} \Psi_\mu^i; \quad \bar{A}_\mu^i dx^\mu = -\frac{1}{2} \langle dw^i dw^j \rangle S_{jk} u^k \quad (3)$$

$$\Phi_\mu^i = \frac{1}{2} (\partial_\mu R^{ik}) S_{kl} u^l \rho_E; \quad \Psi_j^i = \frac{1}{4} [-\delta_j^i (\partial_l R^{lk}) S_{km} + (\partial_l R^{li}) S_{jm}] u^m \rho_E \quad (4)$$

The Langevin and Fokker-Planck equations associated with 4DFP-LSM are derived by substituting the dynamical equations of the passive tracer $dx^\mu = \{dt, \mathbf{u}dt\}$:

$$du^i \equiv \dot{u}^i dt = (\mathbf{u} \cdot \mathbf{A}^i + A_0^i) dt + dw^i \quad (5)$$

$$(\partial_t + \mathbf{u} \cdot \nabla) \rho_L + \partial_{u^i} [(\mathbf{u} \cdot \mathbf{A}^i + A_0^i) \rho_L] = \frac{1}{2} \partial_{u^i} \partial_{u^j} (\mathcal{B}^{ij} \rho_L) \quad (6)$$

where $\mathcal{B}^{ij}(x^\mu, \mathbf{u}) = \frac{d}{d\Delta^0} \langle \Delta w^i \Delta w^j \rangle = \frac{u_T^2}{\tau_E} [B_t^{ij}(1) + B^{ij}(\mathbf{u})]$ [see Eqn. (A.1)]. We used the notation $A_\mu^i = \{A_0^i, \mathbf{A}^i\}$.

3. RVF statistics in a vegetated canopy

We limit ourselves to consider a 2D version of the 4DFP-LSM and the Gaussian Eulerian PDF, Eq. (2), as a 2D PDF. We consider only the streamwise and vertical directions $x_1 \equiv x$ and $x_3 \equiv z$ and the corresponding velocity components $u_1 \equiv u$ and $u_3 \equiv w$. In order to define the 1-point statistics in Eq. (2), the Reynolds covariance tensor and the mean velocity must be given. Firstly, it results $R_{12} = R_{22} = R_{23} = 0$. Then, the mean vertical velocity W is zero, as such as the spanwise component V . The vertical profiles of the 1-point statistics (mean wind $U(x_3)$, Reynolds covariance tensor and Eulerian time) are taken from [5]. Let us indicate the mean canopy height with h and the friction velocity with u_* . Then, we have:

$$U(z) = \begin{cases} \frac{u_*}{k} \log\left(\frac{z-d}{z_0}\right); & z \geq h \\ U(h) \exp\left(a_1\left(1 - \frac{z}{h}\right)\right); & z < h \end{cases} \quad R_{11} = \langle uu \rangle = \begin{cases} (a_4 u_*^2); & z \geq h \\ (a_4 u_*^2) \exp\left(2a_5\left(1 - \frac{z}{h}\right)\right); & z < h \end{cases} \quad (7)$$

$$R_{33} = \langle ww \rangle = \begin{cases} (a_6 u_*^2); & z \geq h \\ (a_6 u_*^2) [0.5(a_7 + a_6) + 0.5(a_7 - a_6) \cos(\pi z/h)]^2; & z < h \end{cases} \quad (8)$$

$$R_{13} = \langle uw \rangle = \begin{cases} u_*^2; & z \geq h \\ u_*^2 \max(a_3 - a_2 z/h; a_3 - 0.45a_2); & z < h \end{cases} \quad (9)$$

$$\tau_E = \max(a_8 h / u_*; k(z-d) u_* / R_{33}) \quad (10)$$

where $k = 0.4$ is the Von Karman constant, d the displacement height and z_0 the aerodynamic roughness. These formulations are partially derived from Boundary Layer similarity theory

and from turbulence measurements. More specifically, the parameters used in Ref. [5] for the turbulent transport of CO₂ are the following:

$$a_1 = -3; a_2 = 1.79; a_3 = 0.79; a_4 = 2.0; a_5 = -2; a_6 = 1.2; a_7 = 0.07; a_8 = 0.3 . \quad (11)$$

Furthermore, following [5], we set $\frac{d}{h} = \frac{2}{3}$ and $z_0 = 0.1$.

Regarding the 2-point covariance tensor, we restrict ourselves to coherent structures with axial symmetry around the vertical axis. As shown in Appendix A, only three coefficients need to be estimated. In order to do this we should know the behavior of at least three components of the tensor β_l^{ij} defined in Eq. (A.10). Alternatively, we need to know only two components as we can estimate the isotropic coefficient a in Eqs. (A.11) as a rate between the eddy life-time (given approximately by τ_E) and the eddy rotation time. This last one is estimated by means of the rate between a sort of isotropic scale L_{iso} and u_T (see Appendix A). Then, we have:

$$a = C \frac{u_T \tau_E}{L_{iso}} ; \quad \frac{L_{iso}}{h} = \max(h - d; k(z - d)) \quad (12)$$

where C is a free adimensional model parameter, which is set $C = 1$ in our simulations. Then, b^{33} and c^{33} are given by Eq. (A.12). The normalized structure function can be evaluated in the following way:

$$\beta_l^{ij} = \frac{\tau_E R^{ij}}{u_T L_l^{ij}} \quad (13)$$

where L_l^{ij} is the correlation length of the velocity components u^i and u^j along the direction x_l . In Finnigan [6] it is possible to find some experimental results about the behavior of L_1^{11} and L_1^{33} . According to these data, we can propose the following interpolation formulas:

$$\frac{L_1^{11}}{h} = \begin{cases} f_1 \left(\frac{z}{h}\right)^3 + f_2 \left(\frac{z}{h}\right)^2 + f_3 ; & z \leq z_1 \\ f_4 \left(\frac{z}{h}\right)^2 + f_5 \left(\frac{z}{h}\right) + f_6 ; & z_1 \leq z \leq z_2 \\ k \left(\frac{z-d}{h}\right) ; & z > z_2 \end{cases} ; \quad \frac{L_1^{33}}{h} = \begin{cases} f_7 \left(\frac{z-z_3}{h}\right)^2 + f_8 ; & z \leq z_3 \\ f_9 \left(\frac{z-z_3}{h}\right)^3 + f_{10} \left(\frac{z-z_3}{h}\right)^2 + f_8 ; & z_3 \leq z \leq z_4 \\ k \left(\frac{z-d}{h}\right) & z > z_4 \end{cases} \quad (14)$$

where: $f_1 = -0.3$; $f_2 = 0.9$; $f_3 = 2$; $f_4 = 0.033136$; $f_5 = -0.32817$; $f_6 = 3.7337$; $f_7 = -0.03$; $f_8 = 0.85$; $f_9 = -0.22083$; $f_{10} = 0.7625$; $z_1 = 2.1h$; $z_2 = 10.987h$; $z_3 = 4h$; $z_4 = 6h$. Note that far from the canopy the correlation lengths are required to satisfy a isotropy condition. For this reason they are equal to each other and equal to L_{iso} (see Appendix A).

4. Numerical simulations

Simulations have been performed for CO₂ dispersion in a Neutral Boundary Layer. The source is placed at the bottom ($z = 0$), while the top boundary condition at $z/h = 20$ is an absorbing one. Two different versions of 4DFP model have been considered. The first one is a isotropic version, with the coefficients b^{33} and c^{33} set to zero, while the second one is the version with axisymmetric coherent structures described in the previous section. In this way, in the isotropic version the role of anisotropy (related to coherent structures) is neglected. The comparison between the isotropic and anisotropic versions of the model are reported in Fig. 4. It is evident that the inclusion of coherent structures in the anisotropic version substantially modify the concentration profiles and, in particular, it determines an accumulation of tracers at a given height. It follows that the role of coherent structures cannot be neglected in 4DFP model and, in particular, the accumulation is related to the presence of anisotropic motion structures. This result is in qualitative agreement with experimental and modeling studies on the subject [8].

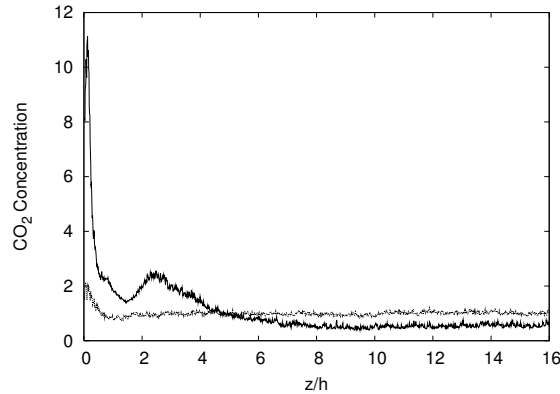


Figure 1. Numerical results for the CO₂ vertical profile. The isotropic (dotted line) and anisotropic (continuous line) models are compared.

5. Conclusions

We have shown that 4DFP-LSM can explicitly include the geometrical properties of the turbulent structures. Numerical simulations have been performed in the case of vegetated canopies, comparing a isotropic version of the model with a version including coherent structures with rotational symmetry around vertical axis. Far from being a complete treatment of turbulent transport in vegetated canopies, the results suggest that the role of geometrical structure should be explicitly included. Even if limited to time scales comparable to or larger than the Eulerian/Lagrangian time scales, 4DFP model can explicitly include experimental information about space-time correlation structure of the velocity field. This is a crucial aspect in many situations such as wall turbulence and the motion of solid particles on time and space scales where the trajectory crossing effect is important [1]. In particular, the application to turbulent transport in vegetated canopies prove that accumulation features are associated with anisotropic motion structures in the fluid flow.

Appendix A. The model for the noise covariance tensor

A general form for the noise tensor, satisfying the incompressibility condition $\partial \langle \Delta w^i \Delta w^j \rangle / \partial \Delta^i = 0$, is a superposition of terms in the form:

$$\langle \Delta w^i \Delta w^j \rangle = \frac{2u_T^2}{\tau_E} [B_t^{ij}(\Delta^0) + B^{ij}(\mathbf{\Delta} - \bar{\mathbf{u}}\Delta^0)]; \quad \partial_i B^{ij}(\mathbf{\Delta}) = 0. \quad (\text{A.1})$$

where $\Delta^0 = \Delta t$ and $\mathbf{\Delta} = \Delta \mathbf{x}$, τ_E is the time scale of fluctuations, given by the Eulerian correlation time in the Gaussian case, $u_T^2 = \frac{1}{3} R_i^i$, and $B_t^{ij} = |\Delta^0| \delta^{ij} + \hat{B}_t^{ij}$, with \hat{B}_t^{ij} symmetric and traceless².

In moderately anisotropic situations, it may be expedient to expand the space component B^{ij} in spherical tensors, following the SO(3) decomposition technique [12]: $B^{ij}(\mathbf{\Delta}) = \sum_{J=0} B_J^{ij}(\mathbf{\Delta})$, where B_J^{ij} indicates a combination of J -th order spherical tensors. A symmetric two-index tensor function can be decomposed in spherical tensors in the form

$$\begin{aligned} & \delta^{ij} Y_J(\mathbf{x}), \quad \partial^i \partial^j Y_J(\mathbf{x}), \quad x^i x^j Y_J(\mathbf{x}), \quad (x^i \partial^j + x^j \partial^i) Y_J(\mathbf{x}), \\ & x_n (\epsilon^{jnm} x^i + \epsilon^{inm} x^j) \partial_m Y_J(\mathbf{x}) \quad \text{and} \quad x_n (\epsilon^{jnm} \partial^i + \epsilon^{inm} \partial^j) \partial_m Y_J(\mathbf{x}) \end{aligned} \quad (\text{A.2})$$

² For lighter notation we leave in this section the dependence from the space-time position unindicated.

where $Y_J(\mathbf{x})$ is a J -order polynomial in the components x_i :

$$Y_J(\mathbf{x}) = y^{i_1 i_2 \dots i_J} x_{i_1} x_{i_2} \dots x_{i_J} \quad (\text{A.3})$$

and $y^{i_1 i_2 \dots i_J}$ is traceless with respect to any pair of indices. In consequence of this, the spherical tensors in Eq. (A.3) will be polynomials of order $L = J, J - 2, J + 2, J, J + 1$ and $J - 1$ respectively. In the case of the noise tensor $\langle \Delta w^i \Delta w^j \rangle$, we have the additional symmetry with respect to spatial inversion, which imposes the condition that L be even. This implies J even for the first four spherical tensors and J odd for the last two. Limiting the analysis to $J \leq 2$, we notice immediately that the last spherical tensor in Eq. (A.2) disappears. Similarly the $J = 1$ contribution from $x_n (\epsilon^{jnm} x^i + \epsilon^{inm} x^j) \partial_m Y_J(\mathbf{x})$ is absent due to incompressibility. Writing $Y_1(\mathbf{x}) = y_m x^m$ it results:

$$\partial_i x_n (\epsilon^{jnm} x^i + \epsilon^{inm} x^j) \partial_m Y_1(\mathbf{x}) = 5 \epsilon^{jnm} x_n y_m = 0,$$

which imposes $y_m = 0$. We are thus left only with the $J = 0$ and $J = 2$ contributions. From the SO(3) decomposition introduced above, the $J = 0$ and $J = 2$ contributions to B^{ij} will have the form:

$$u_T B_0^{ij}(\mathbf{x}) = a |\mathbf{x}| \delta^{ij} + \hat{a} \frac{x^i x^j}{|\mathbf{x}|} \quad (\text{A.4})$$

$$\begin{aligned} u_t B_2^{ij}(\mathbf{x}) = & \frac{4b^{lm}}{|\mathbf{x}|} x_l x_m \delta^{ij} + 2c^{lm} |\mathbf{x}| \partial_i \partial_j x_l x_m + \frac{d^{lm}}{|\mathbf{x}|^3} x_l x_m x^i x^j \\ & + \frac{e^{lm}}{2|\mathbf{x}|} (x^j \partial^i + x^i \partial^j) x_l x_m \end{aligned} \quad (\text{A.5})$$

Applying the incompressibility condition $\partial_i B^{ij} = 0$ leads to the equations:

$$\begin{cases} \hat{a} = -\frac{a}{3} \\ 8b^{lm} + 4c^{lm} + 8e^{lm} = 0 \\ 3d^{lm} - 4b^{lm} - e^{lm} = 0 \end{cases} \quad (\text{A.6})$$

Substituting the solution to Eq. (A.6) into Eqs. (A.4-A.5) leads to:

$$\begin{aligned} B^{ij}(\Delta) = & \frac{|\Delta|}{u_T} [(a + 4b^{lm} \hat{\Delta}_l \hat{\Delta}_m) \delta^{ij} + \frac{1}{3} (-a + (2b^{lm} - c^{lm}) \hat{\Delta}_l \hat{\Delta}_m) \hat{\Delta}^i \hat{\Delta}^j \\ & - \hat{\Delta}_l [(2b^{li} + c^{li}) \hat{\Delta}^j + (2b^{lj} + c^{lj}) \hat{\Delta}^i] + 4c^{ij}] \end{aligned} \quad (\text{A.7})$$

where a gives the $J = 0$ part, while the tensors b^{ij} and c^{ij} , which are symmetric and traceless, account for the the $J = 2$ part.

We consider next some relevant limit cases. In the isotropic case, the $J = 2$ contribution disappears and we are left with the simple expression:

$$\langle \Delta w^i \Delta w^j \rangle = \frac{2u_T^2}{\tau_E} [|\Delta^0| \delta^{ij} + \frac{a|\Delta|}{u_T} (\delta^{ij} - \frac{1}{3} \hat{\Delta}^i \hat{\Delta}^j)] \quad (\text{A.8})$$

The parameter a identifies a length-scale $l_u = u_T \tau_E / a$ for the fluctuations and has therefore the meaning of a ratio between the eddy life-time τ_E and the eddy rotation time l_u / u_T .

In the axisymmetric case, taking the symmetry axis along x^3 , we have that only spherical harmonics with azimuthal quantum number $m = 0$ can contribute, i.e. Y_{00} and Y_{20} , the last one

depending only on $(\hat{\Delta}_3)^2$. This means that all coefficients b^{ij} and c^{ij} with $i \neq j$ are zero and we have, remembering also the zero trace condition $b_i^i = c_i^i = 0$:

$$b^{11} = b^{22} = -\frac{1}{2}b^{33}, \quad c^{11} = c^{22} = -\frac{1}{2}c^{33}. \quad (\text{A.9})$$

So, in this case, there are only three unknown: a , b^{33} and c^{33} . Let us denote with Δ_l the spatial increment in the direction x_l . Then, we define:

$$\beta_l^{ij} = \frac{u_T B^{ij}(\Delta_l)}{|\Delta_l|} \quad (\text{A.10})$$

as the normalized structure function relative to the velocity u^i and u^j along the direction x_l . If we know at least three components of the tensor β_l^{ij} , we can take the corresponding equations given in (A.7) and derive a solution for the coefficients a , b^{33} and c^{33} . If only two components are known, then it is possible to close the linear system by considering that a still represents the ratio of the eddy lifetime to the eddy rotation time.

For example, let us suppose that only information along x_1 is known and consider Eqn. (A.7) for the velocity components u_1 and u_3 in the direction x_1 :

$$\begin{cases} \frac{1}{3}(2a - b^{33} - \frac{5}{2}c^{33}) = \beta_1^{11}, \\ a + 4b^{33} - 2c^{33} = \beta_1^{33}, \end{cases} \quad (\text{A.11})$$

Taking the coefficient a as given and solving with respect to b^{33} and c^{33} , we find immediately the result:

$$\begin{cases} b^{33} = \frac{1}{8}a - \frac{1}{2}\beta_1^{11} + \frac{5}{24}\beta_1^{33} \\ c^{33} = \frac{3}{4}a - \beta_1^{11} - \frac{1}{12}\beta_1^{33} \end{cases} \quad (\text{A.12})$$

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