APPARENT CONDUCTIVITY OF RANDOM COMPOSITE FORMATIONS

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ABSTRACT

Permeability of most geologic formations varies erratically in space by orders of magnitude and is often modeled as a random space field. It is often computationally expedient to determine the mean values of state variables (pressure heads, velocity) by replacing spatially varying (random) local conductivities with their effective or apparent counterparts. We explore the concept of apparent parameters for formations with uncertain spatial arrangement of geological facies and hydraulic properties within each facies. Our analysis relies on the composite media theory, which employs random domain decomposition to explicitly account for the separate effects of material and geometric uncertainty on ensemble moments of head and flux. We present a general expression for the apparent conductivity of such media and analyze it in detail for one-dimensional steady flow in a bounded random medium composed of two materials of contrasting hydraulic conductivities. Location of the internal boundary between the two materials is random and normally distributed. The resulting apparent conductivity is compared with approximate perturbation solutions.

Keywords: composite media, random fields, moment equations, effective, equivalent.

INTRODUCTION AND PROBLEM FORMULATION

It has long been recognized that deterministic analyses of flow and transport in subsurface environment are rendered less than optimal by the lack of detailed site characterization of the kind required for most high-resolution numerical simulations. Uncertainty in hydraulic and transport parameters of geologic formations is conveniently accounted for by treating them as random fields. It is often computationally expedient to replace spatially varying (random) local conductivity, $K(\boldsymbol{x})$, with its effective counterpart, K_{eff} , which is defined as a coefficient of proportionality between the ensemble mean flux, $\langle \boldsymbol{q}(\boldsymbol{x})\rangle$, and ensemble mean hydraulic head gradient, $\nabla\langle h(\boldsymbol{x})\rangle$. For mean uniform flows (defined as flows with $\nabla\langle h(\boldsymbol{x})\rangle$ = const) in statistically homogeneous and isotropic infinite domains, effective conductivity K_{eff} is a characteristic of the medium only. It is given by the harmonic, K_h, and geometric, K_g, means of $K(\boldsymbol{x})$ in one and two dimensions, respectively (Dagan, 1989, and references therein). However, if flow is not uniform in the mean and/or a flow domain is bounded, K_{eff} depends not only on the medium properties, but also on the flow regime (Sánchez-Vila, 1997 and references therein). To make this distinction clear, it is usually referred to as 'equivalent' or 'apparent' conductivity, K_{app}, rather than 'effective'. Much of the existing literature on stochastic hydrogeology deals with effective (apparent) properties of mildly heterogeneous formations composed of a single material whose heterogeneous properties are treated as statistically homogeneous (stationary) random fields with small variances. One recent example of this approach is given by Tartakovsky et al. (2002), who explored the tensorial nature of the apparent transmissivity in a rectangular flow domain by localization and perturbation expansion of the nonlocal mean flow equations in the variance of log-transmissivity (conductivity), σ_Y^2. The requirement that variances, such as σ_Y^2, be small (i.e., $\sigma_Y^2 << 1$) is crucial for closing the moment differential equations or for making Monte Carlo simulations manageable. At the same time, it clearly limits the applicability of these analyses. Several approaches have emerged to deal with highly heterogeneous natural formations composed of multiple geological facies (Winter et al., 2002).

The recently proposed method (*Winter and Tartakovsky*, 2002) of random domain decomposition (RDD) provides a general framework for modelling flow and transport in heterogeneous composite porous media. It allows for uncertainty in both spatial arrangement of geological facies and hydraulic properties within each facies. Since perturbation expansions are carried out within each facies separately, their accuracy and robustness remain high for most geological settings. The main goal of this study is to use RDD to derive and analyze the effective (apparent) conductivity of geologic media composed of several materials with uncertain geometries and conductivities.

Let us consider steady-state saturated flow in a flow domain $\Omega = \Omega_1 \cup \Omega_2$, which is composed of two disjoint sub-domains, Ω_1 and Ω_2, separated by a contact surface $\Gamma_{12} = \Omega_1 \cap \Omega_2$. It is described by Darcy's law, $\boldsymbol{q} = -K\,\nabla h$, and mass conservation, $-\nabla \cdot \boldsymbol{q} + f = 0$, where f is a (generally random) forcing term. The (random) hydraulic conductivity field belongs to two distinct populations,

$$K(\boldsymbol{x}) = \begin{cases} K_1(\boldsymbol{x}) & \boldsymbol{x} \in \Omega_1 \\ K_2(\boldsymbol{x}) & \boldsymbol{x} \in \Omega_2 \end{cases} \tag{1}$$

Then, the flow problem can be rewritten as

$$\nabla \cdot [K_i(\boldsymbol{x})\,\nabla h] + f(\boldsymbol{x}) = 0 \qquad \boldsymbol{x} \in \Omega_i \tag{2}$$

subject to the boundary

$$h(\boldsymbol{x}) = H(\boldsymbol{x}) \qquad \boldsymbol{x} \in \Gamma_D = \Gamma_{D_1} \cup \Gamma_{D_2} \tag{3}$$

$$K_i(\boldsymbol{x})\,\nabla h \cdot \mathbf{n}(\boldsymbol{x}) = Q(\boldsymbol{x}) \qquad \boldsymbol{x} \in \Gamma_N = \Gamma_{N_1} \cup \Gamma_{N_2} \tag{4}$$

and contact surface conditions

$$h(\boldsymbol{x}^-) = h(\boldsymbol{x}^+) \qquad \boldsymbol{x} \in \Gamma_{12} \tag{5}$$

$$K(\boldsymbol{x}^-)\,\nabla h(\boldsymbol{x}^-) \cdot \mathbf{n}(\boldsymbol{x}^-) = K(\boldsymbol{x}^+)\,\nabla h(\boldsymbol{x}^+) \cdot \mathbf{n}(\boldsymbol{x}^+) \qquad \boldsymbol{x} \in \Gamma_{12} \tag{6}$$

Here the superscripts –/+ denote the portions of the domain characterized by conductivities K_1 and K_2, respectively, Γ_{D_i} and Γ_{N_i} (i = 1, 2) are the Dirichlet and Neumann outer boundaries of i-th material, Γ_D and Γ_D are the Dirichlet and Neumann boundaries of domain Ω, and $\mathbf{n}$ is the unit vector normal to the bounding surfaces.

To derive an expression for the apparent conductivity K_{app} of such media, we localize the mean fluxes, along the lines of *Tartakovsky et al*. (2002). The resulting approximations are then solved for the special case of one-dimensional flow in a bounded domain. An exact solution of the mean flow equation is derived for the same flow regime and the nature of K_{app} for the composite formation is discussed.

LOCALIZATION OF MEAN FLUXES

The mean Darcy's law,

$$\langle \boldsymbol{q}(\boldsymbol{x})\rangle = -\langle K_i(\boldsymbol{x})\rangle \nabla\langle h(\boldsymbol{x})\rangle + \mathbf{r}_i(\boldsymbol{x}) \qquad \boldsymbol{x} \in \Omega_i \tag{7}$$

is derived by applying the Reynolds decomposition to represent random fields $\Re = \langle \Re \rangle + \Re'$ as the sum of their ensemble means $\langle \Re \rangle$ and zero-mean fluctuations $\Re'$ and then averaging over the ensemble of realizations. In (7) $\langle K_i(\boldsymbol{x})\rangle$ denotes the (ensemble) mean hydraulic conductivity of the material i, and $\mathbf{r}_i = -\langle K'_i \nabla h'\rangle$ is the residual flux, representing the cross-covariance between hydraulic head gradient and conductivity fluctuations. The latter can be found as the solution of an integral equation

$$\mathbf{r}_i(\boldsymbol{x}) = \int_{\Omega_i} \mathbf{a}_i(\boldsymbol{y}, \boldsymbol{x}) \nabla\langle h(\boldsymbol{y})\rangle \, d\boldsymbol{y} + \int_{\Omega_i} \mathbf{b}_i(\boldsymbol{y}, \boldsymbol{x}) \, \mathbf{r}_i(\boldsymbol{y}) \, d\boldsymbol{y} \tag{8}$$

where $\mathbf{a}_i$ and $\mathbf{b}_i$ are symmetric positive-semidefinite and non-symmetric dyadic. It follows from (7) and (8) that the mean Darcy's flux $\langle \boldsymbol{q}(\boldsymbol{x})\rangle$ is nonlocal, i.e., depends on the mean head gradient $\nabla\langle h\rangle$ at points other than $\boldsymbol{x}$. Hence the effective (apparent) conductivity generally does not exist.

If both the mean head gradient and the residual flux vary slowly in space, then (8) can be localized, leading to an approximate expression

$$\mathbf{r}_i(\boldsymbol{x}) \approx \mathbf{A}_i(\boldsymbol{x}) \nabla\langle h(\boldsymbol{x})\rangle + \mathbf{B}_i(\boldsymbol{x}) \, \mathbf{r}_i(\boldsymbol{x}) \tag{9}$$

where

$$\mathbf{A}_i(\boldsymbol{x}) = \int_{\Omega_i} \mathbf{a}_i(\boldsymbol{y}, \boldsymbol{x}) \, d\boldsymbol{y}\,; \qquad \mathbf{B}_i(\boldsymbol{x}) = \int_{\Omega_i} \mathbf{b}_i(\boldsymbol{y}, \boldsymbol{x}) \, d\boldsymbol{y} \tag{10}$$

This gives an approximate (localized) form of the mean Darcy's law

$$\langle \boldsymbol{q}(\boldsymbol{x})\rangle \approx -\mathbf{K}_{app_i}(\boldsymbol{x}) \nabla\langle h(\boldsymbol{x})\rangle \qquad \boldsymbol{x} \in \Omega_i \tag{11}$$

The spatially varying apparent conductivity tensor is given by

$$\mathbf{K}_{app_i}(\boldsymbol{x}) = \langle K_i(\boldsymbol{x})\rangle \, \mathbf{I} + \mathbf{k}_i(\boldsymbol{x}); \qquad \mathbf{k}_i(\boldsymbol{x}) = [\mathbf{I} - \mathbf{B}_i(\boldsymbol{x})]^{-1} \, \mathbf{A}_i(\boldsymbol{x}) \tag{12}$$

where $\mathbf{I}$ is the identity tensor. Evaluation of the apparent conductivity in general requires some closure approximation of (9). One of the most popular approaches is to use perturbation expansion in σ_Y^2, variance of log-hydraulic conductivity, $Y = \ln K$. The first order (in σ_Y^2) approximation of the apparent hydraulic conductivity tensor is

$$\mathbf{K}_{app_i}^{[1]} = K_{gi}(\boldsymbol{x})\mathbf{I} + K_{gi}(\boldsymbol{x})\frac{\sigma_{Y_i}^2}{2}\mathbf{I} - \int_{\Omega_j} K_{gi}(\boldsymbol{x})\, K_{gi}(\boldsymbol{y})\, \sigma_{Y_i}^2\ \rho_{Yii}(\boldsymbol{y},\boldsymbol{x})\, \nabla_y\ \nabla_x^T G_i(\boldsymbol{y},\boldsymbol{x})\, d\boldsymbol{y} \qquad (13)$$

where $K_{gi}(\boldsymbol{x})$ and $\sigma_{Y_i}^2$ are geometric mean and variance of local conductivities in the i-th material, $\rho_{Yii}(\boldsymbol{y}, \boldsymbol{x})$ is log-hydraulic conductivity correlation function between the points $\boldsymbol{y}$ and $\boldsymbol{x}$ within Ω_i, and G_i is the deterministic Green's function for the Laplace equation in Ω subject to the appropriate homogeneous boundary conditions. It is important to note that (13) represents the *conditional* apparent conductivity, since it corresponds to a *realization* of the random sub-domains Ω_i. The final step in obtaining the apparent conductivity consists of the ensemble averaging over the contact surface Γ_{12}.

The perturbation approximation in (13) is carried out in terms of the variances within the materials, $\sigma_{Y_i}^2$, which are small in most natural formations. However, if they are not small enough for (13) to remain accurate, one can generalize this expression by means of the Landau-Matheron conjecture (e.g., Paleologos *et al*., 1996).

COMPUTATIONAL EXAMPLE: ONE-DIMENSIONAL FLOW

To analize our general expression for the apparent conductivity of composite media in detail, we consider one-dimensional flow in a bounded domain. In this particular situation, the mean flow equation is also amenable to an exact solution, from which we derive an exact expression of the apparent conductivity, to contrast with the first-order approximation (13). This makes it possible to ascertain the accuracy of our general perturbation approximation.

FIRST-ORDER SOLUTION

We consider the one-dimensional version of (2) in the absence of sources

$$\frac{d}{dx}\left[K(x)\,\frac{dh(x)}{dx}\right] = 0 \qquad x \in (0,\,1) \qquad (14)$$

subject to the boundary conditions:

$$K(x)\,\frac{dh(x)}{dx} = -Q\,; \quad x = 0; \qquad h(x) = 0; \quad x = 1 \qquad (15)$$

The porous medium is composed of two materials with randomly varying hydraulic conductivities $K_1(x)$ and $K_2(x)$. The random internal boundary is at $x = \beta$, so that $\Omega_1 = (0, \beta)$ and $\Omega_2 = (\beta, 1)$,

$$K(\boldsymbol{x}) = \begin{cases} K_1(\boldsymbol{x}) & 0 < \boldsymbol{x} < \beta \\ K_2(\boldsymbol{x}) & \beta < \boldsymbol{x} < 1 \end{cases} \qquad (15)$$

and

$$h(\beta^-) = h(\beta^+) \qquad K_1(\beta^-)\,\frac{dh(x=\beta^-)}{dx} = K_2(\beta^+)\,\frac{dh(x=\beta^+)}{dx} \qquad (16)$$

We treat hydraulic conductivities K_1 and K_2 as two uncorrelated, lognormal, statistically homogeneous random fields. Each is characterized by the corresponding geometric mean $K_{gi} = \exp(\langle Y_i \rangle)$ (where $Y_i = ln\ K_i$, $i = 1, 2$), variance $\sigma^2_{Y_i}$ and correlation function $\rho(y, x)$. The Green's function, $G(y, x)$, is now

$$G(\boldsymbol{y}, x < \beta) = \begin{cases} \dfrac{x-y}{K_{g1}} H(y-x) + \dfrac{\beta - x}{K_{g1}} + \dfrac{1-\beta}{K_{g2}} & 0 < \boldsymbol{y} < \beta \\ \dfrac{1-y}{K_{g2}} & \beta < \boldsymbol{y} < 1 \end{cases} \tag{17}$$

and

$$G(\boldsymbol{y}, x > \beta) = \begin{cases} \dfrac{1-x}{K_{g2}} & 0 < \boldsymbol{y} < \beta \\ \dfrac{x-y}{K_{g2}} H(y-x) + \dfrac{1-x}{K_{g2}} & \beta < \boldsymbol{y} < 1 \end{cases} \tag{18}$$

where $H(z)$ is the Heaviside function. On this basis, the first-order approximation of medium's conditional apparent conductivity is

$$K_{app}^{[1]}(x) = K_{g1}\left(1 - \frac{\sigma^2_{Y1}}{2}\right) H(\beta - x) + K_{g2}\left(1 - \frac{\sigma^2_{Y2}}{2}\right) H(\beta - x) \tag{19}$$

Note that the conditional apparent conductivity (19) is independent of the conductivity correlation function $\rho(y, x)$.

EXACT SOLUTION

The exact solution of the mean flow equation is obtained by integrating (14) once while considering (15)

$$\frac{dh(x)}{dx} = -Q\left(\frac{H(\beta - x)}{K_1(x)} + \frac{H(x-\beta)}{K_2(x)}\right) \tag{20}$$

Taking conditional mean yields

$$\frac{d\langle h(x)\rangle}{dx} = -Q\left(\frac{H(\beta - x)}{K_{h1}(x)} + \frac{H(x-\beta)}{K_{h2}(x)}\right) \tag{21}$$

where $K_{hi} = K_{gi} \exp(-\sigma^2_{Y_i}/2)$, $i = 1, 2$, are the harmonic means of $K_i(x)$. It then follows that the expression for apparent conductivity, conditional on the location, β, of the point of contact between the two materials, is

$$K_{app}^{-1}(x|\beta) = \frac{H(\beta - x)}{K_{h1}} + \frac{H(x-\beta)}{K_{h2}} \tag{22}$$

where the symbol | implies conditioning. Recalling the definition of the harmonic mean shows that (19) is indeed the first-order approximation of the exact expression (22).

It is important to contrast our expression for the (conditional) apparent conductivity with the apparent conductivity obtained via a homogeneous approximation. This approximation seeks to replace the composite medium with a homogeneous medium, whose conductivity (as one can readily verify) is given by the weighted sum of the sub-domains' harmonic means:

$$K_{app}^{\text{hom}} = \frac{\beta}{K_{h1}} + \frac{1-\beta}{K_{h2}} \tag{23}$$

The final step is to average the conditional apparent conductivity (22), or its first-order approximation (19), in the probability space of β. Let β be a truncated Gaussian variable with mean ⟨β⟩ and standard deviation σ_β, so that its probability density function is

$$p(\beta) = \frac{1}{W} \exp\left[-\frac{1}{2} \left(\frac{\beta - \langle \beta \rangle}{\sigma_\beta} \right)^2 \right] \qquad W(\langle \beta \rangle, \sigma_\beta) = \int_0^1 \exp\left[-\frac{1}{2} \left(\frac{\beta - \langle \beta \rangle}{\sigma_\beta} \right)^2 \right] d\beta \tag{24}$$

It is also shown in Figure 1 for several values ⟨*β*⟩ and σ_β.

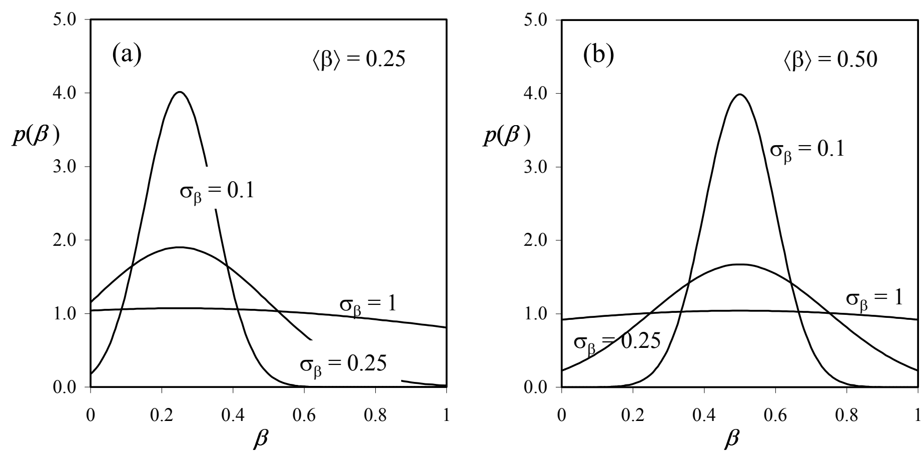

Figure 1. Probability density function for the internal boundary, *β*, with ⟨*β*⟩ = 0.25 (a), and = 0.50 (b) and various degrees of uncertainty, σ_β.

Then the apparent conductivity of the random composite medium is given

$$K_{app}^{-1}(x) = \frac{erf(u) - erf(u_0)}{erf(u_1) - erf(u_0)} \left[\frac{1}{K_{h1}} - \frac{1}{K_{h2}} \right] + \frac{1}{K_{h1}} \tag{25}$$

where

$$u = \left(\frac{x - \langle \beta \rangle}{\sqrt{2}\, \sigma_\beta} \right) \qquad u_0 = -\frac{\langle \beta \rangle}{\sqrt{2}\, \sigma_\beta} \qquad u_1 = \frac{1 - \langle \beta \rangle}{\sqrt{2}\, \sigma_\beta} \tag{26}$$

If β is deterministic, i.e., $\sigma_\beta = 0$, (25) reduces to (22), as it should. Figures 2 and 3 demonstrate the spatial distributions of $K_{app}(x)$ for $\langle Y_1 \rangle = 3.5$, $\langle Y_2 \rangle = 7.0$, $\sigma_{Y1}^2 = \sigma_{Y2}^2 = 1$, and the values of $\langle \beta \rangle$ and σ_β corresponding to Figures 1(a) and 1(b), respectively. These are contrasted with the homogeneous approximation of K_{app} given by (23).

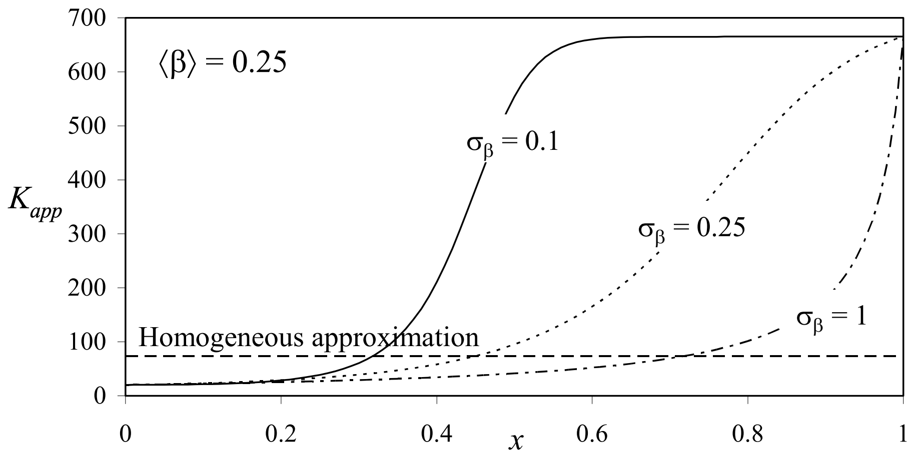

Figure 2. Spatial distribution of $K_{app}(x)$ for the internal structure of materials of Figure 1(a).

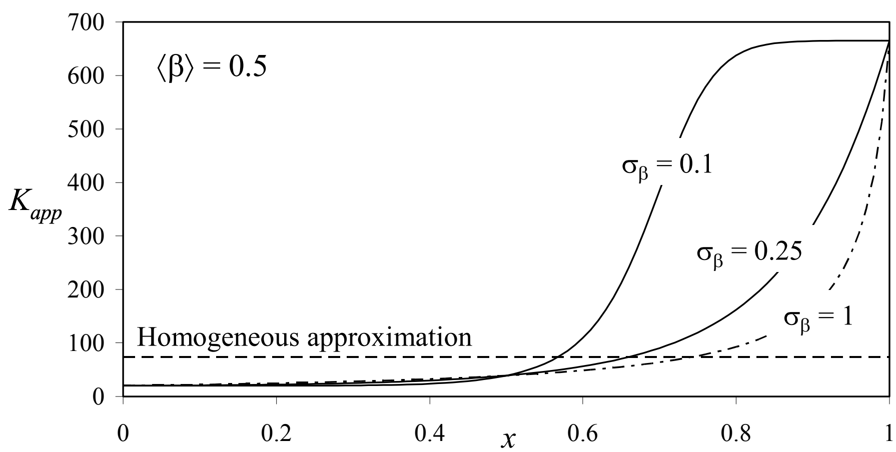

Figure 3. Spatial distribution of $K_{app}(x)$ for the internal structure of materials of Figure 1(b).

A simple analysis of the analytical expression for the apparent conductivity (25), as well as Figures 2 and 3, demonstrate that $K_{app}(x) = K_{h1}$ when x is deep within material 1 and $K_{app}(x) = K_{h2}$ when x is deep within material 2. Width of the transitional zone between the two harmonic means increases with the geometric uncertainty, i.e., with σ_β. If the geometry is deterministic ($\sigma_\beta = 0$), $K_{app}(x)$ becomes a step function.

CONCLUSIONS

We presented an expression for apparent (effective) hydraulic conductivity of porous media composed of different materials (geologic facies) whose internal geometries and conductivities are uncertain. Our work leads to the following major conclusions:

1. Apparent conductivity of the composite porous media should preserve their internal structure whenever possible. This is crucial for probabilistic analyses of preferential flow paths.
2. For steady-state flow in bounded heterogeneous composite media, we derived a general expression for the apparent conductivity by means of the perturbation expansion in variances of materials' log-conductivities. Since conductivity of each material is more uniform than that of the composite as a whole, this expression is more accurate and robust than its homogeneous counterpart.
3. The general perturbation expression for apparent conductivity is analyzed in detail for one-dimensional steady flow in the bounded porous medium composed of two materials. Both materials' log-conductivities and the internal boundary between materials are assumed to be Gaussian. Apparent conductivity is given by the harmonic means of the corresponding conductivities of each material for points away from the internal boundary, and varies smoothly from one harmonic mean to the other in the transitional zone around the boundary. Width of the transitional zone increases with the degree of uncertainty about the internal boundary.

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