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Laplace-Transform Finite Element Solution of Nonlocal and Localized Stochastic Moment Equations of Transport

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Abstract. Morales-Casique et al. (Adv. Water Res., 29 (2006), pp. 1238-1255) developed exact first and second nonlocal moment equations for advective-dispersive transport in finite, randomly heterogeneous geologic media. The velocity and concentration in these equations are generally nonstationary due to trends in heterogeneity, conditioning on site data and the influence of forcing terms. Morales-Casique et al. (Adv. Water Res., 29 (2006), pp. 1399-1418) solved the Laplace transformed versions of these equations recursively to second order in the standard deviation $\sigma_{\rm Y}$ of (natural) log hydraulic conductivity, and iteratively to higher-order, by finite elements followed by numerical inversion of the Laplace transform. They did the same for a space-localized version of the mean transport equation. Here we recount briefly their theory and algorithms; compare the numerical performance of the Laplace-transform finite element scheme with that of a high-accuracy ULTIMATE-QUICKEST algorithm coupled with an alternating split operator approach; and review some computational results due to Morales-Casique et al. (Adv. Water Res., 29 (2006), pp. 1399-1418) to shed light on the accuracy and computational efficiency of their recursive and iterative solutions in comparison to conditional Monte Carlo simulations in two spatial dimensions.

AMS subject classifications: 65Z05, 65Z05, 68U20, 76S05 **Key words**: Geologic media, porous media, random heterogeneity, conditioning, stochastic transport, moment equations, nonlocality, localization, Laplace transform, finite elements, ultimatequickest.

1 Introduction

It has become increasingly common to describe the spatial variability of geologic medium properties geostatistically and to analyze subsurface fluid flow and solute transport in

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such media stochastically [11,44,55]. The most common and straightforward method of stochastic analysis is computational Monte Carlo simulation that produces a large number of equally likely results. These results are summarized statistically in terms of their sample averages, second (variance-covariance) or higher moments, or probability distributions. Results that honor measured values of medium properties and/or state variable are said to be conditioned on these data. One thus obtains (among others) conditional mean flow and transport variables that constitute optimum unbiased predictors of these random quantities, and conditional second moments that provide a measure of the associated prediction errors. An alternative is to compute these statistics directly on the basis of corresponding conditional moment equations. Commonly, the moment equations are derived *a priori* in an approximate manner which renders them local in space-time. We focus instead on exact forms of these equations, which are generally nonlocal in space-time, and their subsequent solution by approximation.

Exact space-time nonlocal first and second conditional moment equations have been developed for steady state [40,41] and transient [48-50] flow in bounded saturated media as well as advective [23, 39] and advective-dispersive [56] transport in infinite domains; related but somewhat different unconditional formulations of nonlocal transport in such domains are found in [10, 15, 30]. We concentrate here on exact first and second nonlocal moment equations for advective-dispersive transport in bounded media developed recently by Morales-Casique et al. [37]. Morales-Casique et al. [38] solved Laplace transformed versions of these equations recursively to second order in the standard deviation σ_Y of (natural) log hydraulic conductivity, and iteratively to higher-order, by finite elements followed by numerical inversion of the Laplace transform. They did the same for a space-localized version of the mean transport equation. Following a summary of their theory and algorithmic approach, we compare below the numerical performance of the Laplace-transform finite element scheme with that of a high-accuracy ULTIMATE-QUICKEST algorithm coupled with an alternating split operator approach. We then review some computational results due to Morales-Casique et al. [38] to shed light on the accuracy and computational efficiency of their recursive and iterative solutions in comparison to conditional and unconditional Monte Carlo simulations in two spatial dimensions.

2 Exact conditional moment equations for bounded media

Morales-Casique et al. [37] express advective-dispersive solute mass flux at some local support scale ω , centered about point **x** in a Cartesian coordinate system, as

$$\mathbf{J}(\mathbf{x},t) = \mathbf{v}(\mathbf{x},t)c(\mathbf{x},t) - \mathbf{D}_d \nabla c(\mathbf{x},t), \qquad (2.1)$$

where *c* is concentration, **v** is velocity, \mathbf{D}_d is a constant local dispersion tensor and *t* is time. The velocity is given by Darcy's law

$$\mathbf{v}(\mathbf{x},t) = -K(\mathbf{x})\nabla h(\mathbf{x},t)/\phi,$$