March, Nathan G.; **Carr, Elliot J.**; **Turner, Ian W.**

A fast algorithm for semi-analytically solving the homogenization boundary value problem for block locally-isotropic heterogeneous media. (English) Zbl 1481.74636

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Summary: Direct numerical simulation of diffusion through heterogeneous media can be difficult due to the computational cost of resolving fine-scale heterogeneities. One method to overcome this difficulty is to homogenize the model by replacing the spatially-varying fine-scale diffusivity with an effective diffusivity calculated from the solution of an appropriate boundary value problem. In this paper, we present a new semi-analytical method for solving this boundary value problem and computing the effective diffusivity for pixellated, locally-isotropic, heterogeneous media. We compare our new solution method to a standard finite volume method and show that equivalent accuracy can be achieved in less computational time for several standard test cases. We also demonstrate how the new solution method can be applied to complex heterogeneous geometries represented by a two-dimensional grid of rectangular blocks. These results indicate that our new semi-analytical method has the potential to significantly speed up simulations of diffusion in heterogeneous media.

MSC:

74Q05 Homogenization in equilibrium problems of solid mechanics
35B27 Homogenization in context of PDEs; PDEs in media with periodic structure
35Q74 PDEs in connection with mechanics of deformable solids

Keywords:

effective diffusivity; homogenization; semi-analytical solution; heterogeneous media; steady-state diffusion equation

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References:

[1] Davit, Y.; Bell, C. G.; Byrne, H. M.; Chapman, L. A.C.; Kimpton, L. S.; Lang, G. E.; Leonard, K. H.L.; Oliver, J. M.; Pearson, N. C.; Shipley, R. J.; Waters, S. L.; Whiteley, J. P.; Wood, B. D.; Quintard, M., Homogenization via formal multiscale asymptotics and volume averaging: how do the two techniques compare?, Adv. Water. Resour., 62, 178-206 (2013)

[2] Carr, E. J.; Turner, I. W.; Perré, P., Macroscale modelling of multilayer diffusion: using volume averaging to correct the boundary conditions, Appl. Math. Model., 47, 600-618 (2017) · Zbl 1446.74011

[3] Zhou, Z.; Su, Y.; Wang, W.; Yan, Y., Application of the fractal geometry theory on fracture network simulation, J. Petrol Explor. Prod. Technol., 7, 2, 487-496 (2017)

[4] Carr, E. J.; Turner, I. W.; Perré, P., A dual-scale modelling approach for drying hygroscopic porous media, Multiscale Model Sim., 11, 1, 362-384 (2013) · Zbl 1267.76106

[5] Torquato, S., Random heterogeneous media: microstructure and improved bounds on effective properties, Appl. Mech. Rev., 44, 2, 37-76 (1991)

[6] Dykaar, B. B.; Kitanidis, P. K., Determination of the effective hydraulic conductivity for heterogeneous porous media using a numerical spectral approach: 1. method, Water Resour. Res., 28, 4, 1155-1166 (1992)

[7] Szymkiewicz, A., Modelling Water Flow in Unsaturated Porous Media (2013), Springer

[8] Szymkiewicz, A., Calculating effective conductivity of heterogeneous soils by homogenization, Arch. Hydro-Eng. Environ. Mech., 52, 2, 111-130 (2005)

[9] Carr, E. J.; Turner, I. W., Two-scale computational modelling of water flow in unsaturated soils containing irregular-shaped inclusions, Int. J. Numer. Meth. Eng., 98, 3, 157-173 (2014) · Zbl 1352.76110

[10] Ray, N.; Rupp, A.; Schulz, R.; Knabner, P., Old and new approaches predicting the diffusion in porous media, Transp. Porous Med., 124, 3, 803-824 (2018)

[11] Carr, E. J.; Turner, I. W., A semi-analytical solution for multilayer diffusion in a composite medium consisting of a large number of layers, Appl. Math. Model., 40, 7034-7050 (2016) · Zbl 1471.74014

[12] Hornung, U., Homogenization and Porous Media (1997), Springer-Verlag · Zbl 0872.35002

[13] Herrera, I., Trefftz method: a general theory, Numer. Meth. Part D E, 16, 6, 561-580 (2000) · Zbl 0978.65114

[14] Plawsky, J. L., Transport Phenomena Fundamentals. Transport Phenomena Fundamentals, Chemical Industries (2009), CRC Press

[15] Carr, E. J.; March, N. G., Semi-analytical solution of multilayer diffusion problems with time-varying boundary conditions and general interface conditions, Appl. Math. Comput., 333, 286-303 (2018) · Zbl 1427.35106

[16] Polyanin, A. D., Handbook of Linear Partial Differential Equations for Engineers and Scientists (2002), Chapman and Hall · Zbl 1027.35001

[17] Domínguez, V., FIlon-Clenshaw-Curtis rules for a class of highly-oscillatory integrals with logarithmic singularities, J. Comput. Appl. Math., 261, 299-319 (2014) · Zbl 1280.65026

[18] Filon, L. N.G., On a quadrature formula for trigonometric integrals, Proc. R. Soc. Edin A-Ma, 49, 38-47 (1928) · Zbl 55.0946.02

[19] Levin, D., Fast integration of rapidly oscillatory functions, J. Comput. Math., 67, 95-101 (1996) · Zbl 0858.65017

[20] Deaño, A.; Huybrechs, D.; Iserles, A., Computing Highly Oscillatory Integrals (2018), SIAM: SIAM Philadelphia · Zbl 1400.65004

[21] S. Potticary, Efficient evaluation of highly oscillatory integrals, 2005. Master's Thesis, University of Reading.

[22] Sviercoski, R. F.; Winter, C. L.; Warrick, A., An analytical effective tensor and its approximation properties for upscaling flows through generalized composites, Adv. Water Resour., 33, 7, 728-739 (2010)

[23] Ray, N.; Rupp, A.; Prechtel, A., Discrete-continuum multiscale model for transport, biomass development and solid restructuring in porous media, Adv. Water Resour., 107, 393-404 (2017)

[24] Perumal, D. A.; Dass, A. K., A review on the development of lattice Boltzmann computation of macro fluid flows and heat transfer, Alex. Eng. J., 54, 4, 955-971 (2015)

[25] Amaziane, B.; Hontans, T.; Koebbe, J. V., Equivalent permeability and simulation of two-phase flow in heterogenous porous media, Comput. Geosci., 5, 279-300 (2001) · Zbl 1169.74535

[26] Sohn, D., Periodic mesh generation and homogenization of inclusion-reinforced composites using an element-carving technique with local mesh refinement, Compos. Struct., 185, 65-80 (2018)

[27] Amanbek, Y.; Singh, G.; Wheeler, M. F.; van Duijn, H., Adaptive numerical homogenization for upscaling single phase flow and transport, J. Comput. Phys., 387, 117-133 (2019)

[28] Vondřejc, J.; Zeman, J.; Marek, I., An FFT-based Galerkin method for homogenization of periodic media, Comput. Math. Appl., 68, 3, 156-173 (2014) · Zbl 1369.65151