Lecture Notes in Computational Science and Engineering

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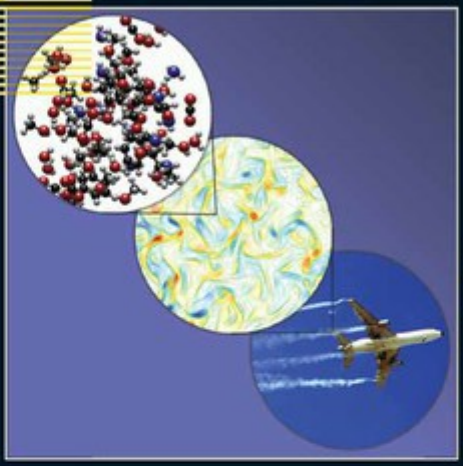



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Editors

# Multiscale Methods in Science and Engineering

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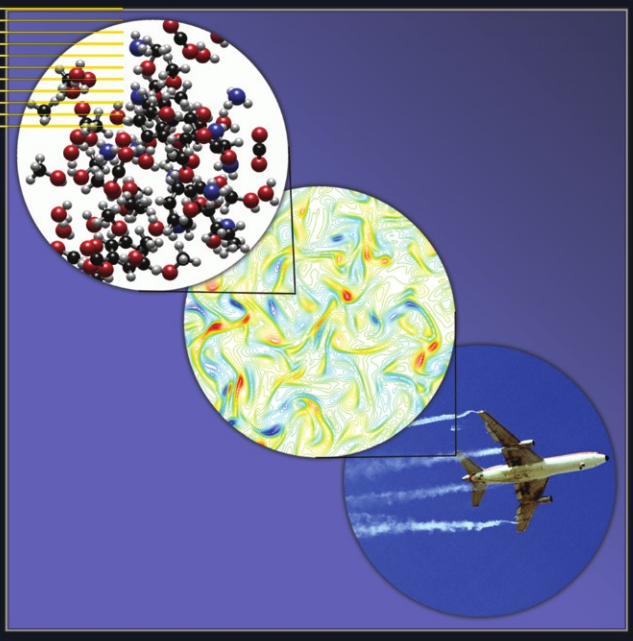



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# Multiscale Methods in Science and Engineering

With 85 Figures and 17 Tables

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*Editors*

Björn Engquist
Olof Runborg

Department of Numerical Analysis
and Computer Science
Royal Institute of Technology
SE-10044 Stockholm, Sweden

engquist@nada.kth.se
olofr@nada.kth.se

Per Lötstedt

Department of Information Technology
Uppsala University
Box 337
SE-75105 Uppsala, Sweden

perl@it.uu.se

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# Preface

Multiscale problems naturally pose severe challenges for computational science and engineering. The smaller scales must be well resolved over the range of the larger scales. Multiscale objects must therefore typically be described by a very large set of unknowns. The larger the ranges of scales, the more unknowns are needed and the higher the computational cost. It has been possible to meet many of these challenges by the recent progress in multiscale computational techniques coupled to the capability of the latest generation of computer systems.

This recent progress was presented at the conference *Multiscale Methods in Science and Engineering*, which was held in Uppsala, Sweden on January 26–28, 2004. More than 55 participants from six countries discussed the issues presented in the papers of this proceeding. The conference was sponsored by he Swedish Foundation for Strategic Research (SSF) and by the Swedish Agency for Innovation Systems, Vinnova via the Parallel and Scientific Computing Institute (PSCI).

Challenging multiscale problems are very common. One example can be average airflow, which typically depends on the details of small swirling eddies, which in turn depend on the interaction of molecules on much smaller scales in space and time. One can go further and see how the forces between the molecules depend on the electrons. Typically, a narrow range of scales is modeled by effective equations for that particular range. Turbulence models would then describe the coarsest scales of the phenomena mentioned above. The finer scales could be approximated by the Navies–Stokes equations, the Boltzmann equation and the Schrödinger equation respectively.

When such effective equations for a narrow range of scales can be derived the numerical approximations can be greatly facilitated. These equations should include the influence from other scales in the original multiscale problem. Techniques of this type are presented in this proceeding. In the contributions by Berlyand et al. and Svanstedt and Wellander, new variants of the homogenization technique are described and analyzed. Stochastic differential equations are increasingly common models for multiscale phenomena. New adaptive techniques for stochastic equations are developed by Dzougoutov et al. Stochastic models are also part of the systems studied by Jourdain et al. Sometimes there exist well performing equations for most

of the computational domain but a small subdomain contains microscales that are difficult to represent by the numerical method. Special subgrid models need to be developed. Edelvik derives such models for thin wires and slots in electromagnetic simulations. Thin filaments or fibers in fluids are approximated in the contribution by Tornberg. The latter simulations can also be seen as a way of numerically deriving effective equations for suspensions of filaments in fluids. The multiscale discontinuous Galerkin method studied by Aarnes and Heimsund uses multiscale basis functions and is based on homogenization theory.

An important preprocessing step for all numerical multiscale computations is the choice of unknowns. The number of these unknowns should be kept to a minimum. In the two contributions by Larson and collaborators this is achieved by adaptive grid generation based on realistic a posteriori estimates. Runborg uses a wavelet like technique that allows for a hierarchical and efficient representation of geometrical structures.

Computational multiscale methods are of two types. In the more established class of methods the full multiscale problem is discretized and highly efficient numerical methods are then applied to accurately compute the full range of scales. Multigrid, and the fast multipole method are very successful examples of such technique. These algorithms rely on special properties of the solution operator in order to achieve their optimal computational complexity. The smoothing by elliptic operators is one such example. Eberhard and Wittum presents a multigrid method for flow in heterogeneous porous media and a multipole method for electromagnetic scattering is described by Nilsson and Lötstedt.

In the second and more recent class of computational multiscale methods only a fraction of the microscale space is included in order to reduce the number of unknowns. The microscales and the macroscales are coupled in the same simulation exploiting special properties in the original problem, for example, scale separation. The simulation over a wide range of scales can be based on first principles even if effective equations are not known. The techniques discussed by E and Engquist, Jourdain et al., Samaey et al. and Sharp et al. in this proceeding are examples of this type of methods.

There are several active areas of development at the present time for tackling the multiscale challenge and many of the important ones were presented at this conference. The progress will have importance on the whole field of computational science and engineering. Multiscale modeling is emerging as a new computational paradigm.

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April 2005

*Björn Engquist*
*Per Lötstedt*
*Olof Runborg*

# Contents

# List of Contributors

**Jørg Aarnes**
SINTEF Applied Mathematics
PB 124, N-0314 Oslo, Norway
Jorg.Aarnes@sintef.no

**Fredrik Bengzon**
Department of Mathematics
Umeå University
90187 Umeå, Sweden
fredrik.bengzon@math.umu.se

**Leonid Berlyand**
Department of Mathematics and
Materials Research Institute
Pennsylvania State University,
McAllister Bld.
University Park, PA 16802, USA
berlyand@math.psu.edu

**Anna Dzougoutov**
Department of Numerical Analysis and
Computer Science
KTH
SE-100 44 Stockholm, Sweden
annadz@kth.se

**Weinan E**
Department of Mathematics
Princeton University
Princeton, NJ 08544, USA
weinan@math.princeton.edu

**Jens Eberhard**
Simulation in Technology
University of Heidelberg
Im Neuenheimer Feld 368
D-69120 Heidelberg, Germany
eberhard@uni-hd.de

**Fredrik Edelvik**
Division of Scientific Computing
Department of Information Technology
Uppsala University
SE-75105 Uppsala, Sweden
fredrik.edelvik@it.uu.se

**Björn Engquist**
Department of Numerical Analysis and
Computer Science
KTH
SE-100 44 Stockholm, Sweden
engquist@nada.kth.se

**Yuliya Gorb**
Department of Mathematics and
Materials Research Institute
Pennsylvania State University,
McAllister Bld.
University Park, PA 16802, USA
gorb@math.psu.edu

**Bjørn-Ove Heimsund**
University of Bergen
Allégaten 41, N-5007 Bergen, Norway
Bjorn-Ove.Heimsund@uib.no

**August Johansson**
Department of Mathematics
Umeå University
90187 Umeå, Sweden
august.johansson@math.umu.se

**Benjamin Jourdain**
CERMICS
Ecole Nationale des Ponts et Chaussées
6 & 8 Av. Pascal, F–77455 Champs-sur-Marne, France
jourdain@cermics.enpc.fr

**Ioannis G. Kevrekidis**
Department of Chemical Engineering
PACM and Department of Mathematics
Princeton University
Princeton, NJ 08544, USA
yannis@princeton.edu

**Mats G. Larson**
Department of Mathematics
Umeå University
90187 Umeå, Sweden
mats.larson@math.umu.se

**Claude Le Bris**
CERMICS
Ecole Nationale des Ponts et Chaussées
6 & 8 Av. Pascal, F–77455 Champs-sur-Marne, France
lebris@cermics.enpc.fr

**Tony Lelièvre**
CERMICS
Ecole Nationale des Ponts et Chaussées
6 & 8 Av. Pascal, F–77455 Champs-sur-Marne, France
lelievre@cermics.enpc.fr

**Per Lötstedt**
Department of Information Technology
Division of Scientific Computing
Uppsala University, SE-75105 Uppsala, Sweden
per.lotstedt@it.uu.se

**Axel Målqvist**
Department of Mathematics
Chalmers University of Technology
SE-412 96, Göteborg, Sweden
axel@math.chalmers.se

**Kyoung-Sook Moon**
Department of Mathematics
University of Maryland
College Park, MD 20742, USA
moon@math.umd.edu

**Martin Nilsson**
Department of Information Technology
Division of Scientific Computing
Uppsala University, SE-75105 Uppsala, Sweden
martin.nilsson@it.uu.se

**Alexei Novikov**
Department of Mathematics and
Materials Research Institute
Pennsylvania State University,
McAllister Bld.
University Park, PA 16802, USA
anovikov@math.psu.edu

**Dirk Roose**
Department of Computer Science
K.U. Leuven
Celestijnenlaan 200A, B-3000 Leuven, Belgium
dirk.roose@cs.kuleuven.ac.be

**Olof Runborg**
Department of Numerical Analysis and Computer Science
KTH
SE-100 44 Stockholm, Sweden
olofr@nada.kth.se

**Giovanni Samaey**
Department of Computer Science
K.U. Leuven
Celestijnenlaan 200A, B-3000 Leuven, Belgium
giovanni.samaey@cs.kuleuven.ac.be

**Erik von Schwerin**
Department of Numerical Analysis and Computer Science
KTH
SE-100 44 Stockholm, Sweden
schwerin@nada.kth.se

**Richard Sharp**
Program in Applied and Computational Mathematics
Princeton University
Princeton, NJ 08544, USA
rsharp@math.princeton.edu

**Nils Svanstedt**
Department of Mathematics
Chalmers University of Technology and Göteborg University,
SE-412 96 Göteborg, Sweden
nilss@math.chalmers.se

**Anders Szepessy**
Department of Numerical Analysis and Computer Science
KTH
SE-100 44 Stockholm, Sweden
szepessy@nada.kth.se

**Raúl Tempone**
ICES
University of Texas at Austin,
1 Texas Longhorns,
Austin, Texas 78712, USA
rtempone@ices.utexas.edu

**Anna-Karin Tornberg**
Courant Institute of Mathematical Sciences
New York University
251 Mercer Street, New York, NY 10012-1185, USA
tornberg@cims.nyu.edu

**Yen-Hsi Tsai**
Department of Mathematics
University of Texas at Austin
1 University Station C1200
Austin, Texas 78712, USA
ytsai@math.utexas.edu

**Niklas Wellander**
Swedish Defence Research Agency, FOI
SE-581 11 Linköping, Sweden
niklas@foi.se

**Gabriel Wittum**
Simulation in Technology
University of Heidelberg
Im Neuenheimer Feld 368
D-69120 Heidelberg, Germany
wittum@uni-hd.de

# Multiscale Discontinuous Galerkin Methods for Elliptic Problems with Multiple Scales

Jørg Aarnes[1] and Bjørn–Ove Heimsund[2]

[1] SINTEF Applied Mathematics, PB. 124, 0314 Oslo, Norway.
Jorg.Aarnes@sintef.no
[2] University of Bergen, Allégaten 41, 5007 Bergen, Norway.
Bjorn-Ove.Heimsund@cipr.uib.no

**Summary.** We introduce a new class of discontinuous Galerkin (DG) methods for solving elliptic problems with multiple scales arising from e.g., composite materials and flows in porous media. The proposed methods may be seen as a generalization of the multiscale finite element (FE) methods. In fact, the proposed DG methods are derived by combining the approximation spaces for the multiscale FE methods and relaxing the continuity constraints at the inter-element interfaces. We demonstrate the performance of the proposed DG methods through numerical comparisons with the multiscale FE methods for elliptic problems in two dimensions.

**Key words:** multiscale methods, discontinuous Galerkin methods, elliptic partial differential equations

## 1 Introduction

We consider solving the second-order elliptic equation

$$\begin{cases} -\nabla \cdot (a(x)\nabla u) = f, & \text{in } \Omega \subset \mathcal{R}^{\mathrm{d}}, \\ u = 0, & \text{on } \Gamma_{\mathrm{D}} \subset \partial\Omega, \\ -a(x)\nabla u \cdot n = 0, & \text{on } \Gamma_{\mathrm{N}} = \partial\Omega \backslash \Gamma_{\mathrm{D}}, \end{cases} \tag{1}$$

where $\Omega$ is bounded, $\partial\Omega$ is Lipschitz, $n$ is the outward unit normal on $\partial\Omega$ and $a(x) = (a_{ij}(x))$ is a symmetric positive definite tensor with uniform upper and lower bounds:

$$0 < \alpha|y|^2 \leq y^T a(x) y \leq \beta|y|^2 < \infty, \quad \forall x \in \Omega,\ \forall y \in \mathcal{R}^d,\ y \neq 0.$$

We will interpret the variable $u$ as the (flow) potential and $q$ as the (flow) velocity. The homogeneous boundary conditions are chosen for presentational brevity. General boundary conditions can be handled without difficulty.

Equation (1) may represent incompressible single-phase porous media flow or steady state heat conduction through a composite material. In single-phase flow, $u$

is the flow potential, $q = -a(x)\nabla u$ is the Darcy filtration velocity and $a(x)$ is the (rock) permeability of the porous medium. For heat conduction in composite materials, $u$, $q$ and $a(x)$ represents temperature, heat flow density, and thermal conductivity respectively. These are typical examples of problems where $a(x)$ can be highly oscillatory and the solution of (1) displays a multiscale structure. This leads to some fundamental difficulties in the development of robust and reliable numerical models.

In this paper we introduce a new class of DG methods for solving this particular type of multiscale elliptic problems. Until recently, DG methods have been used mainly for solving partial differential equations of hyperbolic type, see e.g. [10] for a comprehensive survey of DG methods for convection dominated problems. Indeed, whereas DG methods for hyperbolic problems have been subject to active research since the early seventies, it is only during the last decade or so that DG methods have been applied to purely elliptic problems, cf. [5] and the references therein. The primary motivation for applying DG methods to elliptic problems is perhaps their flexibility in approximating rough solutions that may occur in elliptic problems arising from heterogeneous and anisotropic materials. However, to our knowledge, previous research on DG methods for elliptic problems has been confined to solving elliptic partial differential equations with smooth coefficients.

DG methods approximate the solution to partial differential equations in finite dimensional spaces spanned by piecewise polynomial base functions. As such, they resemble the FE methods, but, unlike the FE methods, no continuity constraints are explicitly imposed at the inter-element interfaces. This implies that the weak formulation subject to discretization must include jump terms across interfaces and that some artificial penalty terms must be added to control the jump terms. On the other hand, the weak continuity constraints give DG methods a flexibility which allows a simple treatment of, e.g., unstructured meshes, curved boundaries and $h$- and $p$-adaptivity. Another key feature with DG methods is their natural ability to impose mass conservation locally. Moreover, the "local" formulation of the discrete equations allows us us to use grid cells of arbitrary shapes without difficulty. We may therefore choose the gridlines to be aligned with sharp contrasts in, for instance, underlying heterogeneous materials.

The multiscale FE methods (MsFEMs) introduced in [9, 12] have been successfully applied to multiscale elliptic problems, but their accuracy is to some degree sensitive to the selection of the boundary conditions that determine the FE base functions. If, for instance, strong heterogeneous features penetrate the inter-cell interfaces, then simple, e.g. linear, boundary conditions may be inadequate. In such situations, oversampling strategies or other techniques for the generation of adaptive boundary conditions must be used to recover the desired order of accuracy. This sensitivity to the selection of boundary conditions is partly due to the strong continuity requirements at the inter-element interfaces implicit in the FE methods.

Here we propose a class of multiscale DG methods (MsDGMs) for solving elliptic problems with multiple scales. One of the primary motives for developing MsDGMs is to generate multiscale methods that are less sensitive to the selection of boundary conditions for the base functions than is the case for the MsFEMs. Another nice feature with MsDGMs is that they produce solutions for both the potential

variable (e.g. pressure or temperature) and the velocity variable (e.g. phase velocity or thermal flux density) that reflect important subgrid variations in the elliptic coefficients. We will demonstrate the benefit of using multiscale methods in comparison with ordinary monoscale numerical methods and perform numerical experiments to display the performance of the MsDGMs relative to the original and mixed MsFEMs. We therefore attempt to reveal that there is a need for multiscale methods, and to demonstrate under what circumstances it may be advantageous to relax the inter-element continuity assumptions implicit in the MsFEMs.

The paper is organized as follows. We give the general mathematical setting for the DG methods in Sect. 2 and show how they are related to the more familiar FE methods. In particular we show that both standard and mixed FE methods may be viewed as special DG methods. This observation allows us to extend this type of FE methods to corresponding DG methods. In Sect. 3 we outline the MsFEMs introduced in [12] and [9] and exploit the relationship between FE methods and DG methods to derive a corresponding class of MsDGMs. Finally, Sect. 4 contains the numerical experiments and we conclude with a discussion of the results in Sect. 5.

## 2 Mathematical Formulations

In Sect. 2.1 we give the mathematical formulation of the DG methods for (1) and discuss the selection of the so-called numerical fluxes that are used to force weak continuity of the solution across inter-element interfaces. In Sect. 2.2 we show how the conforming and mixed FE methods may be viewed as special DG methods, and describe how such FE methods can be extended to corresponding DG methods.

### 2.1 Discontinuous Galerkin Methods

To define the DG methods we split (1) into the first order system,

$$\begin{aligned} q &= -a(x)\nabla u, && \text{in } \Omega, \\ \nabla \cdot q &= f, && \text{in } \Omega, \\ u &= 0, && \text{on } \Gamma_{\mathrm{D}}, \\ q \cdot n &= 0, && \text{on } \Gamma_{\mathrm{N}}. \end{aligned}$$

Furthermore, define the following approximation spaces:

$$\begin{aligned} Q_N &= \{p \in (H^1(\Omega))^d : p \cdot n = 0 \text{ on } \Gamma_N\}, \\ U_D &= \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D\}. \end{aligned}$$

Upon integration by parts, we now deduce the weak formulation: Find $q \in Q_N$ and $u \in U_D$ such that

$$\int_\Omega a^{-1} q \cdot p \,\mathrm{d}x = \int_\Omega u \nabla \cdot p \,\mathrm{d}x \qquad \forall p \in Q_N,$$

$$\int_\Omega q \cdot \nabla v \,\mathrm{d}x = -\int_\Omega f v \,\mathrm{d}x \qquad \forall v \in U_D.$$