Discontinuous Galerkin Finite Element Method for Multiscale Problems

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Outline

- Introduction of the discontinuous Galerkin (DG) method and the local DG (LDG) method
- Multiscale methods based on the DG scheme — three approaches
  - Heterogeneous multiscale method (HMM) + DG
  - Domain decomposition
  - DG method with multiscale basis
- Concluding remarks

Introduction to the DG method

DG method for hyperbolic equations

To solve a hyperbolic conservation law:

$$u_t + f(u)_x = 0 \tag{1}$$

Multiplying with a test function v, integrate over a cell $I_j = [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, and integrate by parts:

$$\int_{I_j} u_t v dx - \int_{I_j} f(u) v_x dx + f(u_{j+\frac{1}{2}}) v_{j+\frac{1}{2}} - f(u_{j-\frac{1}{2}}) v_{j-\frac{1}{2}} = 0$$

Now assume both the solution u and the test function v come from a finite dimensional approximation space V_h, which is usually taken as the space of piecewise polynomials of degree up to k:

$$V_h = \left\{ v : v|_{I_j} \in P^k(I_j),\ j = 1, \cdots, N \right\}$$

However, the boundary terms $f\left(u_{j+\frac{1}{2}}\right)$, $v_{j+\frac{1}{2}}$ etc. are not well defined when u and v are in this space, as they are discontinuous at the cell interfaces.

From the conservation and stability (upwinding) considerations, we take

- A single valued monotone numerical flux to replace $f\left(u_{j+\frac{1}{2}}\right)$:

$$\hat{f}_{j+\frac{1}{2}} = \hat{f}(u^-_{j+\frac{1}{2}}, u^+_{j+\frac{1}{2}})$$

  where $\hat{f}(u,u) = f(u)$ (consistency); $\hat{f}(\uparrow,\downarrow)$ (monotonicity) and $\hat{f}$ is Lipschitz continuous with respect to both arguments.

- Values from inside I_j for the test function v

$$v^-_{j+\frac{1}{2}}, \qquad v^+_{j-\frac{1}{2}}$$

Hence the DG scheme is: find $u \in V_h$ such that

$$\int_{I_j} u_t v dx - \int_{I_j} f(u) v_x dx + \hat{f}_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0 \qquad (2)$$

for all $v \in V_h$.

LDG method for parabolic and elliptic equations

Rewrite the heat equation $u_t = u_{xx}$ as

$$u_t - q_x = 0, \qquad q - u_x = 0,$$

and *formally* write out the DG scheme as: find $u, q \in V_h$ such that, for all test functions $v, w \in V_h$,

$$\begin{aligned} \int_{I_j} u_t v dx + \int_{I_j} q v_x dx - \hat{q}_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \hat{q}_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} &= 0 \qquad (3) \\ \int_{I_j} q w dx + \int_{I_j} u w_x dx - \hat{u}_{j+\frac{1}{2}} w^-_{j+\frac{1}{2}} + \hat{u}_{j-\frac{1}{2}} w^+_{j-\frac{1}{2}} &= 0, \end{aligned}$$

q can be locally (within cell I_j) solved and eliminated, hence local DG.

A key ingredient of the design of the LDG method is the choice of the numerical fluxes $\hat{u}$ and $\hat{q}$ (remember: no upwinding principle for guidance).

The best choice for the numerical fluxes is the following alternating flux

$$\hat{u}_{j+\frac{1}{2}} = u^-_{j+\frac{1}{2}}, \qquad \hat{q}_{j+\frac{1}{2}} = q^+_{j+\frac{1}{2}}. \tag{4}$$

The LDG method can be designed and analyzed for general nonlinear multi-dimensional convection diffusion equations

$$u_t + \sum_{i=1}^{d} f_i(u)_{x_i} - \sum_{i=1}^{d}\sum_{j=1}^{d} (a_{ij}(u)u_{x_j})_{x_i} = 0, \tag{5}$$

where $a_{ij}(u)$ are entries of a symmetric and semi-positive definite matrix.

Multiscale methods based on the DG scheme

Heterogeneous multiscale method (HMM) + DG

If we have a multiscale hyperbolic equation

$$u_t^\varepsilon + f^\varepsilon(u^\varepsilon, x)_x = 0$$

where ε is a small parameter and the solution u^ε involves the small scale ε. The usual DG scheme

$$\int_{I_j} (u_h)_t v dx - \int_{I_j} f(u_h) v_x dx + \hat{f}_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0$$

can be used to have the usual convergence if $h < \varepsilon$.

However, if $h \gg \varepsilon$ and we are interested only to approximate the homogenized solution $\bar{u}$ where

$$u^{\varepsilon} \longrightarrow \bar{u} \text{ weakly when } \varepsilon \longrightarrow 0,$$

we can design a HMM-DG method (heterogeneous multiscale method, E and Engquist) by obtaining the flux f through solving a local microscale problem wherever it is needed.

DG method, because of its local conservation property and reliance on numerical fluxes, is well suited for the HMM framework:

- S. Chen, W. E and C.-W. Shu, *The heterogeneous multiscale method based on the discontinuous Galerkin method for hyperbolic and parabolic problems*, Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, v3 (2005), pp.871-894. Linear hyperbolic and parabolic equations, and nonlinear Euler equations; the micro solvers are kinetic equations
- W. Wang, X. Li and C.-W. Shu, *The discontinuous Galerkin method for the multiscale modeling of dynamics of crystalline solids*, Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, v7 (2008), pp.294-320. Solid mechanics; the micro solvers are molecular dynamics

An example: Euler equation of compressible gas dynamics

$$u_t^\varepsilon + f(u^\varepsilon)_x = 0, \tag{6}$$

where $u^\varepsilon = [\rho^\varepsilon, \rho^\varepsilon v^\varepsilon, E^\varepsilon]^T$,
$f(u^\varepsilon) = [\rho^\varepsilon v^\varepsilon, \rho^\varepsilon (v^\varepsilon)^2 + p^\varepsilon, v^\varepsilon (E^\varepsilon + p^\varepsilon)]^T$, and

$$p^\varepsilon = a^\varepsilon(x)[(E^\varepsilon - \frac{1}{2}\rho^\varepsilon (v^\varepsilon)^2)(\gamma - 1)] \tag{7}$$

where γ is a constant. This is clearly equivalent to having an oscillatory γ

$$\gamma^\varepsilon = 1 + (\gamma - 1)a^\varepsilon(x).$$

In the numerical test, we take

$$a^\varepsilon(x) = \frac{1}{1 + 0.1\sin(\frac{x}{\varepsilon}) + 0.1\sin(x)}. \tag{8}$$

We will use the following notations:

- u^ε: the solution of (6)-(7), with a^ε given by (8);
- $\bar{u}^\varepsilon$: the local average of u^ε, obtained by convolving u^ε with a mass-one local kernel of width $O(\varepsilon)$;
- $\tilde{u}$: the solution of (6)-(7) with $a^\varepsilon(x)$ in (7) replaced by a simple average

$$\tilde{a}(x) = \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{1+0.1\sin(y)+\sin(x)}dy.$$

- $\bar{u} = \lim_{\varepsilon\to 0} \bar{u}^\varepsilon$. This limit will serve as our "exact" solution of the homogenized Euler problem, which is not explicitly known.

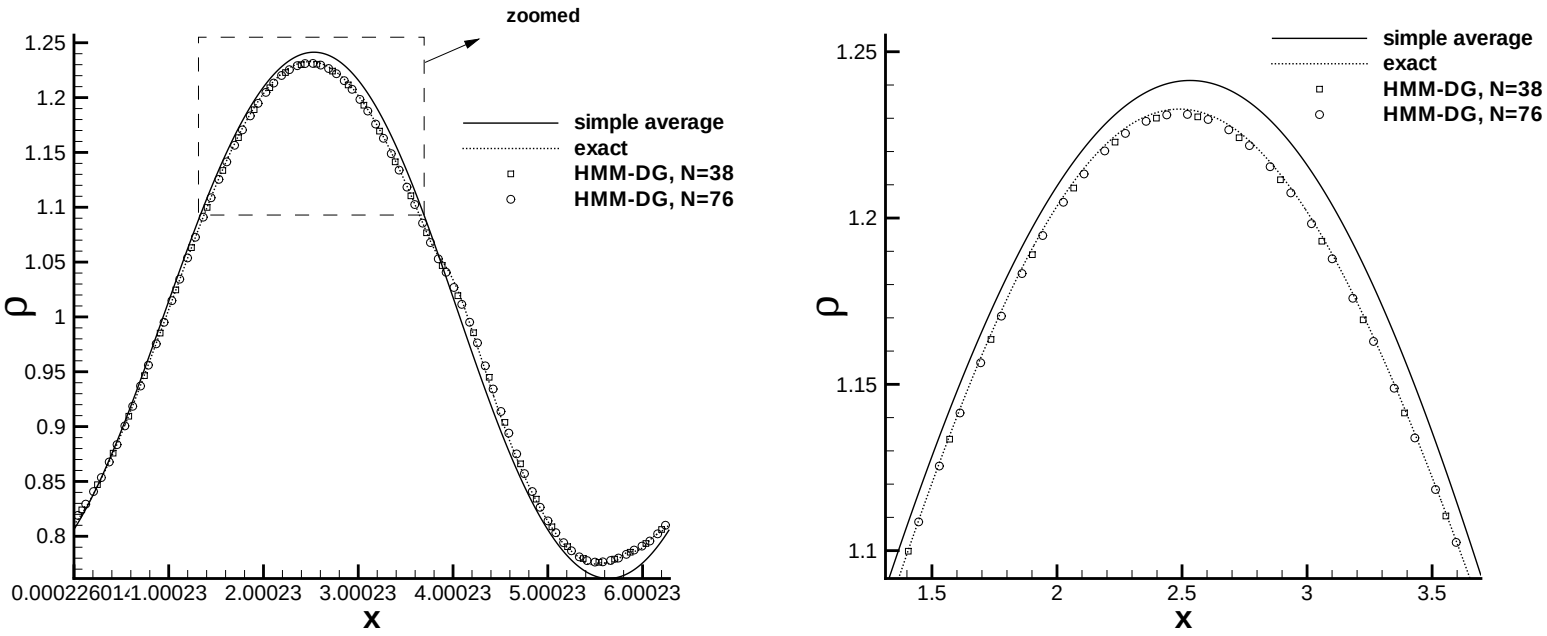

Figure 1: Density ρ. The HMM-DG solution with $N = 38$ and $N = 76$ uniform elements for $\varepsilon = 10^{-6}$, versus the "converged" local average solution $\bar{u}$ to the nonlinear oscillatory Euler equations (denoted by "exact" in the figures). The solution $\tilde{u}$ of the simply averaged Euler equations (denoted by "simple average" in the figures) is also plotted as a reference. Left: the solutions in the whole interval; right: zoomed around $x = 2.5$.

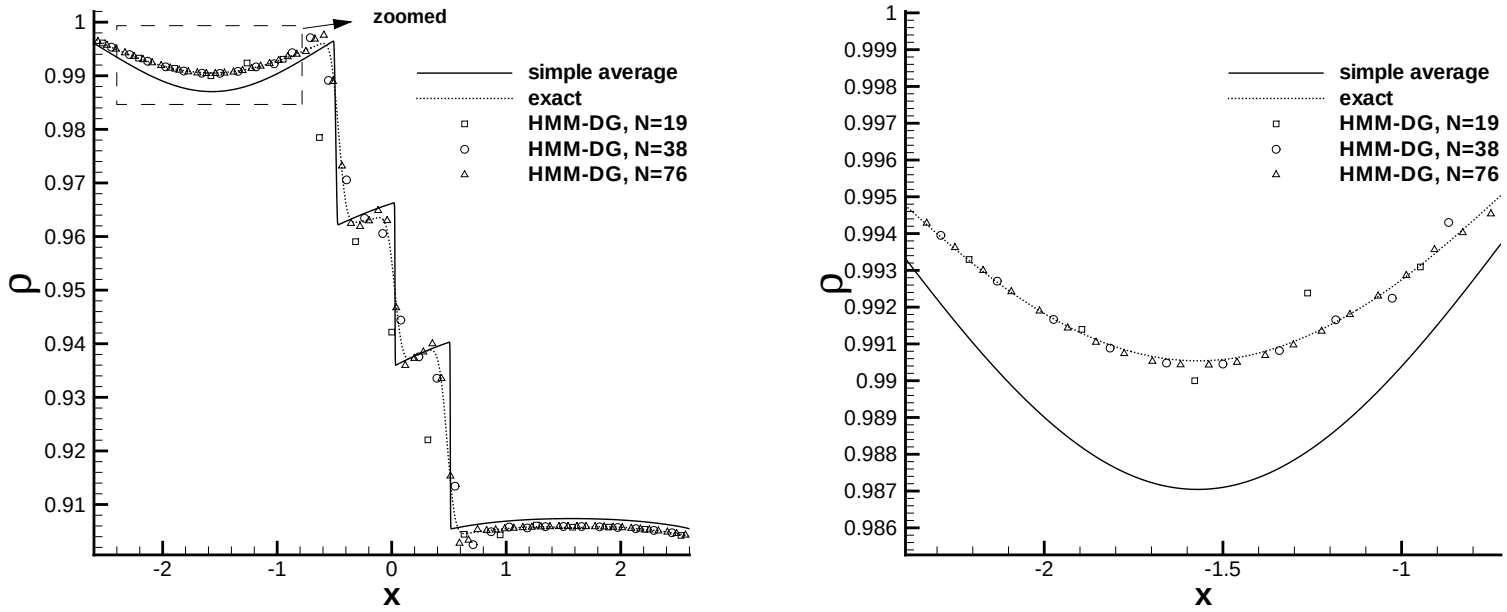

Figure 2: Sod's Shock tube problem. Density ρ. The HMM-DG solution with $N = 19$, 38 and 76 uniform elements for $\varepsilon = 10^{-6}$, versus the converged "exact" locally averaged solution $\bar{u}$ to the nonlinear oscillatory Euler equations. The solution $\tilde{u}$ of the simply averaged Euler equations (simple average) is also plotted as a reference. Left: the solutions in the whole interval; right: zoomed around $x = -1.5$.

Domain decomposition (DD)

DG method, because of its local nature with minimum communication with neighbors (only via numerical fluxes), is well suited for the DD framework:

- S. Chen, W. E, Y.-X. Liu and C.-W. Shu, *A discontinuous Galerkin implementation of a domain decomposition method for kinetic-hydrodynamic coupling multiscale problems in gas dynamics and device simulations*, Journal of Computational Physics, v225 (2007), pp.1314-1330. macro models and kinetic models in different parts of the domain; gas dynamics and semi-conductor device simulations

- W. Wang, X. Li and C.-W. Shu, *The discontinuous Galerkin method for the multiscale modeling of dynamics of crystalline solids*, Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, v7 (2008), pp.294-320. Solid mechanics; the numerical fluxes are based on constitutive laws or atomistic model in different domains

An example: Semiconductor device simulation. We apply the DDM-DG method to solve a GaAs diode problem

- The macro models are the hydrodynamic (HD) model where the electric current is small and and the high field (HF) model where the electric current is high
- The micro model is the kinetic (BGK) model for the intermediate regime
- The challenge is that we cannot and do not assume a Maxwellian distribution at the domain interface between the HF model and the kinetic model. We apply a novel approach of using the shape of the micro simulation at the boundary adjusted by the macro moment data to supply the boundary condition for the kinetic solver

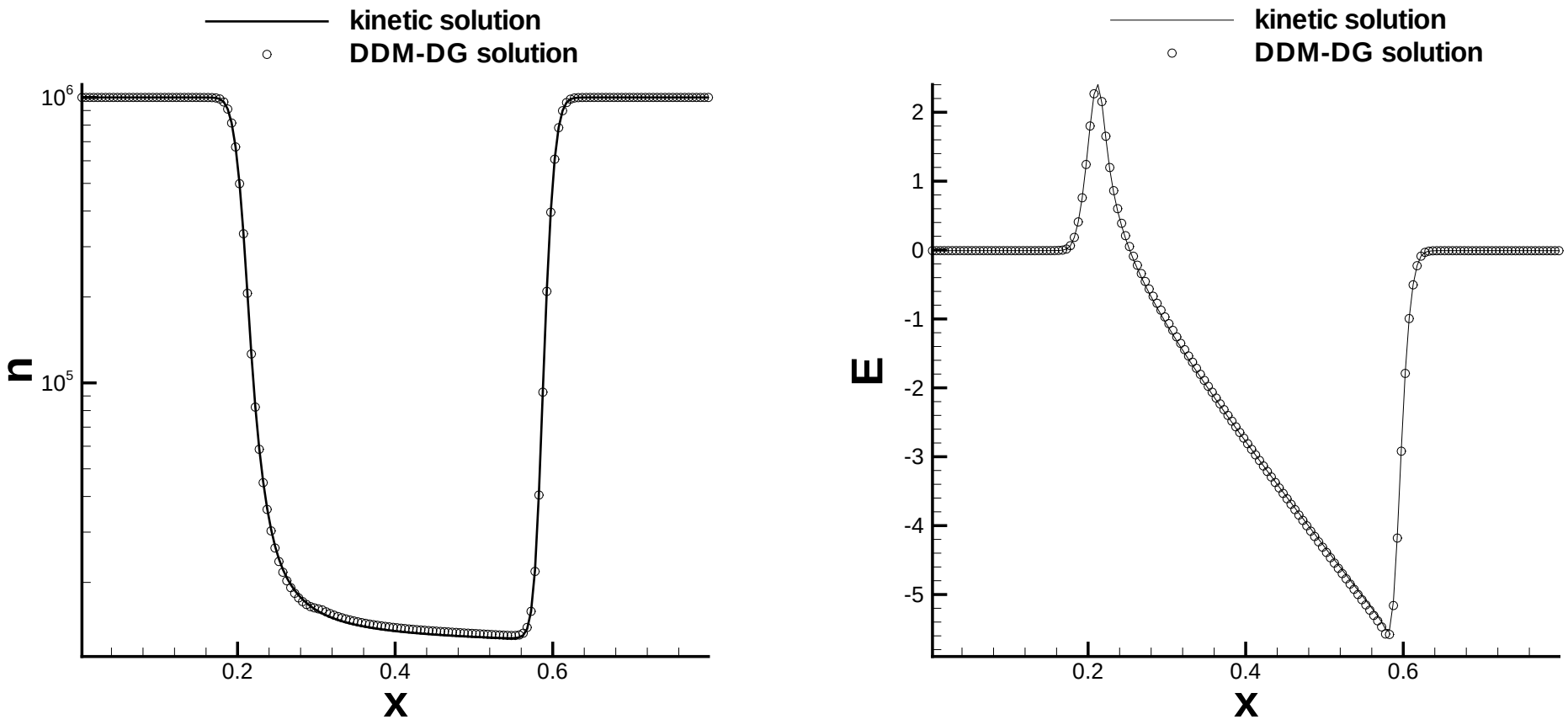

Figure 3: The global kinetic simulation (solid line) versus the DDM-DG solution (circles). Left: the concentration n; right: the electric field E.

DG method with multiscale basis

This approach is more aggressive, we aim for obtaining small errors $||u - u_h||$ in a strong norm (typically L^2 norm) where the exact solution u has a small scale ε and the mesh size $h \gg \varepsilon$.

- The idea is to use suitable multiscale basis specific to the application in the DG method. Such basis should have explicit expressions if at all possible, in order to reduce computational cost
- Advantage: The DG method is quite flexible in its local approximation space (for each cell), as there is no continuity requirement at the cell boundary

- Advantage: Stability properties for DG methods usually only depend on the choice of the numerical fluxes, not the local approximation spaces
- Challenge: We must carefully analyze the errors associated with these discontinuities across element interfaces, to obtain convergence and (high order) error estimates

Semiconductor devices: Schrödinger-Poisson system

W. Wang and C.-W. Shu, *The WKB local discontinuous Galerkin method for the simulation of Schrödinger equation in a resonant tunneling diode*, Journal of Scientific Computing, v40 (2009), pp.360-374.

B. Dong, C.-W. Shu and W. Wang, *A new multiscale discontinuous Galerkin method for one-dimensional stationary Schrödinger equation*, Journal of Scientific Computing, to appear.

- Resonant tunneling diode (RTD) involves the solution of a large number of Schrödinger equations to collect the resonances
- Ben Abdallah and Pinaud (JCP 06) proposed a WKB approach using traditional continuous finite element method for the 1D model
- The continuous finite element based WKB method cannot be easily generalized to 2D
- We have developed a DG/LDG WKB solver which has better potential for 2D generalization and for adaptive calculations (2D work ongoing, originally in collaboration with Ben Abdallah)

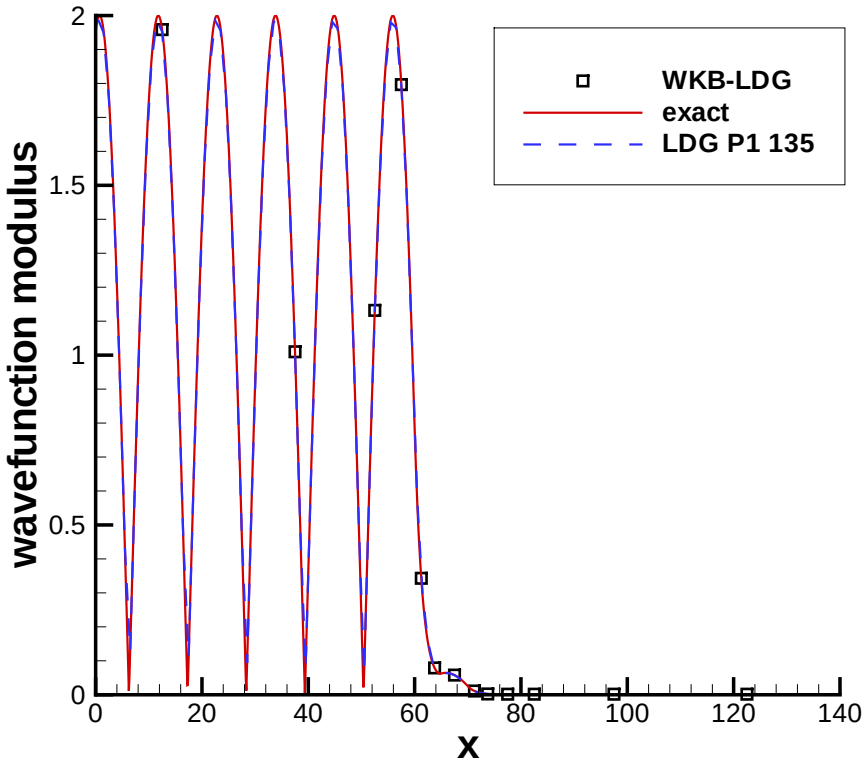

Figure 4: Comparison among the exact solution, the WKB-LDG solution and the LDG P^1 solution: non-resonant case with $E = 0.046072eV$. 13 cells are used in the WKB-LDG method. 135 cells are used in the LDG P^1 method.

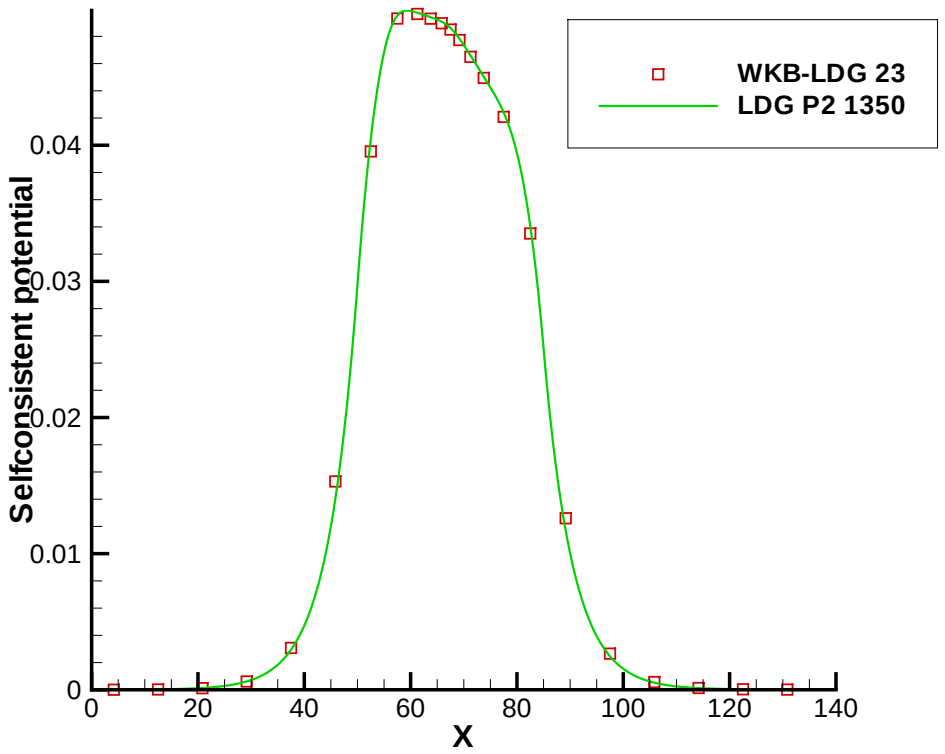

Figure 5: Comparison between the reference solution and the WKB-LDG solution: self-consistent potential for the full non-linear case. 23 cells are used in the WKB-LDG method.

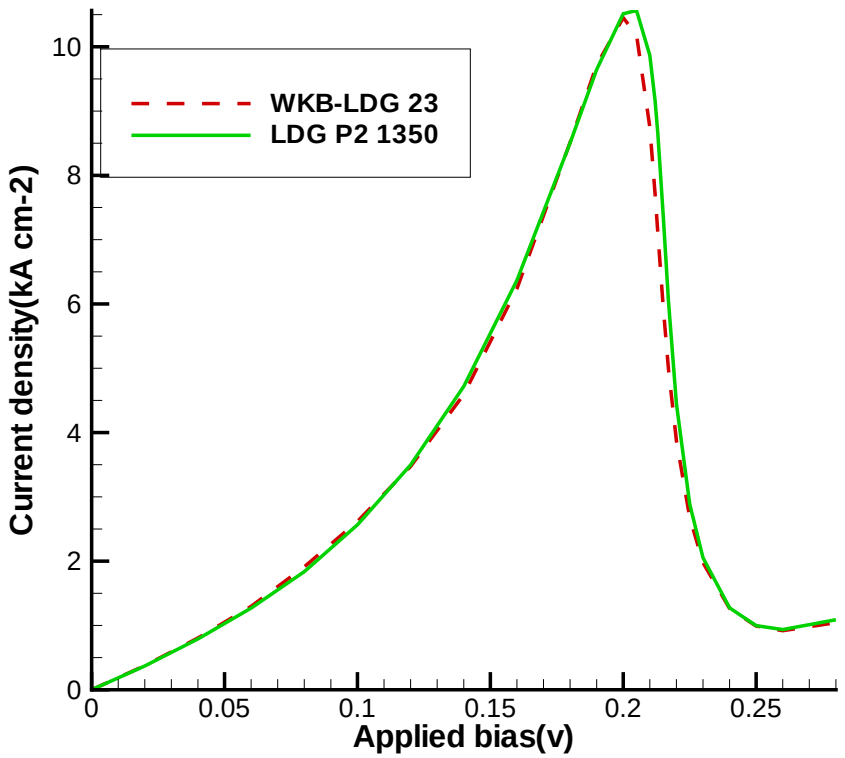

Figure 6: Comparison between the reference solution and the WKB-LDG solution: the I-V characteristics of a RTD. 23 cells are used in the WKB-LDG method.

Elliptic equations with oscillatory coefficients

L. Yuan and C.-W. Shu, *Discontinuous Galerkin method for a class of elliptic multi-scale problems*, International Journal for Numerical Methods in Fluids, v56 (2008), pp.1017-1032.

W. Wang, J. Guzmán and C.-W. Shu, *The multiscale discontinuous Galerkin method for solving a class of second order elliptic problems with rough coefficients*, International Journal of Numerical Analysis and Modeling, v8 (2011), pp.28-47.

Y. Zhang, W. Wang, J. Guzmán and C.-W. Shu, *Multi-scale discontinuous Galerkin method for solving elliptic problems with curvilinear unidirectional rough coefficients*, Journal of Scientific Computing, v61 (2014), pp.42-60.

We consider solving the second order elliptic equation

$$-\nabla \cdot (a^{\varepsilon}(x)\nabla u) = f \qquad \text{in } \Omega \tag{9}$$

with the boundary condition

$$u = 0 \qquad \text{on } \partial\Omega, \tag{10}$$

where the coefficient $a^{\varepsilon}(x)$ is an oscillatory function involving a small scale ε. For example, $a^{\varepsilon}(x) = a(x, \frac{x}{\varepsilon})$. However, scale separation is not required in this framework.

Multi-Scale Approximation Spaces

The new approximation spaces are constructed as below:

$$S^1 = \{\phi : \nabla \cdot (a^\varepsilon(x)\nabla\phi)|_K = 0\} \tag{11}$$

and

$$S^k = \{\phi : \nabla \cdot (a^\varepsilon(x)\nabla\phi)|_K \in P^{k-2}(K)\} \qquad \text{for } k \geq 2 \tag{12}$$

where K denotes the cell in space discretization.

Note: no continuity requirement along element boundary, hence easy to construct in 2D.

1-D case

Now consider the 1-D elliptic problem

$$-(a^{\varepsilon}(x)u_x)_x = f, \qquad 0 \le x \le 1 \tag{13}$$

with boundary condition

$$u(0) = u(1) = 0, \tag{14}$$

where

$$0 < \alpha \le a^{\varepsilon}(x) \le \beta < +\infty. \tag{15}$$

1-D multi-scale approximation space:

$$S^k = \left\{ v : v|_{I_j} \in span\left\{ 1, \int_{x_j}^{x} \frac{1}{a^{\varepsilon}(x)} d\xi, \int_{x_j}^{x} \frac{\xi - x_j}{a^{\varepsilon}(x)} d\xi, \cdots, \int_{x_j}^{x} \frac{(\xi - x_j)^{k-1}}{a^{\varepsilon}(x)} d\xi \right\} \right\}.$$

For the IP-DG method, we have the following error estimate:

Theorem (Error Estimates) Let $u(x)$ be the exact solution of the PDE and u_h be the numerical solution of the IP-DG method. There exists a constant C independent of ε such that

$$||u - u_h||_{L^2(0,1)} \leq Ch^{k+1}|f|_{H^{k-1}(0,1)}. \tag{16}$$

2-D case, oscillation in coordinate directions

Now consider the 2-D elliptic problem

$$-(a^{\varepsilon}(x)u_x)_x - (b^{\varepsilon}(y)u_y)_y = f(x,y), \tag{17}$$

where

$$0 < \alpha \leq a^{\varepsilon}(x),\ b^{\varepsilon}(y) \leq \beta < +\infty. \tag{18}$$

Sample 2-D multi-scale approximation space:

$$S_2^2 = \left\{ v : v|_K \in \text{span}\left\{ 1, \int_{x_K}^{x} \frac{1}{a(\xi)} d\xi, \int_{y_K}^{y} \frac{1}{b(\eta)} d\eta, \right.\right.$$
$$\left.\left. \int_{x_K}^{x} \frac{\xi - x_K}{a(\xi)} d\xi, \int_{x_K}^{x} \frac{1}{a(\xi)} d\xi \int_{y_K}^{y} \frac{1}{b(\eta)} d\eta, \int_{y_K}^{y} \frac{\eta - y_K}{b(\eta)} d\eta \right\} \right\}.$$

For the IP-DG method, we have the following error estimate:

Theorem (Error Estimates) Let u be the exact solution of the PDE and u_h be the numerical solution of the IP-DG method with $V_h = S_2^1$. There exists a constant C independent of ε such that

$$||u - u_h||_{L^2(0,1)} \leq Ch^2 |f|_{L^2(0,1)}. \tag{19}$$

Note: Numerical experiments indicate that the convergence rate holds for k higher than 1 (higher than second order), however we do not have a proof for this yet.

2-D case, curvilinear unidirectional rough coefficients

We consider the 2-D elliptic problem

$$-(a^{\varepsilon}(x,y)u_x)_x - (b^{\varepsilon}(x,y)u_y)_y = f(x,y), \tag{20}$$

where there is a smooth (independent of ε) change of variables (can be locally defined) such that the equation becomes

$$-(\tilde{a}^{\varepsilon}(\xi)u_\xi)_\xi - (\tilde{b}(\xi,\eta)u_\eta)_\eta = \tilde{f}(\xi,\eta),$$

locally, where $\tilde{b}(\xi,\eta)$ does not depend on ε. The challenge is that the oscillation direction ξ changes with the spatial location (x,y), although this change is smooth (does not depend on ε).

The multiscale DG method can be designed for this problem with the following two advantages:

1. The basis functions can be analytically given, thus saving a lot of computational cost over methods which would need to obtain such “multiscale basis” numerically;

2. There is no continuity requirement across element interfaces, hence the construction of DG spaces in each element can be done independently.

We prove a similar convergence result with error estimates as in the previous case of oscillation in coordinate directions.

We advocate an “easy” implementation of DG basis with the oscillation direction frozen at the center of each element. We observe second order accuracy in L^2 norm with this implementation.

Numerical Examples

Example 1. 1-D elliptic problem with

$$a^{\varepsilon}(x,\varepsilon) = \frac{1}{2 + x + \sin\left(\frac{\sin x}{\varepsilon}\cos x\right)}, \quad f = -\cos x, \quad x \in [0,1]. \tag{21}$$

Note: No scale separation.

Table 1: L^2 errors and orders of accuracy by the multiscale IP-DG method: one-dimensional example. S^1

	$\varepsilon = 0.01$				$\varepsilon = 0.001$			
S^1	$u - u_h$		$q - q_h$		$u - u_h$		$q - q_h$	
N	error	order	error	order	error	order	error	order
10	1.50E-03	–	6.36E-02	–	1.44E-03	–	6.18E-02	–
20	3.51E-04	2.09	2.92E-02	1.12	3.67E-04	1.97	3.09E-02	1.00
40	8.95E-05	1.97	1.50E-02	0.96	9.26E-05	1.99	1.54E-02	1.00
80	2.33E-05	1.94	7.68E-03	0.97	2.33E-05	1.99	7.61E-03	1.02
160	5.93E-06	1.97	3.87E-03	0.99	5.55E-06	2.07	3.59E-03	1.08

Table 2: L^2 errors and orders of accuracy by the multiscale IP-DG method: one-dimensional example. S^2

	$\varepsilon = 0.01$				$\varepsilon = 0.001$			
S^2	$u - u_h$		$q - q_h$		$u - u_h$		$q - q_h$	
N	error	order	error	order	error	order	error	order
10	8.39E-06	–	5.74E-04	–	7.87E-06	–	5.60E-04	–
20	1.10E-06	2.94	1.38E-04	2.05	9.75E-07	3.01	1.40E-04	2.00
40	1.41E-07	2.97	3.50E-05	1.98	1.27E-07	2.94	3.49E-05	2.00
80	1.77E-08	3.00	8.80E-06	1.99	1.59E-08	2.99	8.51E-06	2.04
160	2.21E-09	3.00	2.20E-06	2.00	1.96E-09	3.02	2.14E-06	1.99

Example 2. 2-D elliptic problem with

$$a(x) = a^{\varepsilon}(x, \varepsilon) = \frac{1}{4 + x + \sin\left(\frac{\sin x}{\varepsilon} \cos x\right)},$$

$$b(y) = b^{\varepsilon}(y, \varepsilon) = \frac{1}{4 + y + \sin\left(\frac{\sin y}{\varepsilon} \cos y\right)}, \qquad f = x + y.$$

An explicit formula for the exact solution is unavailable, and we are using the numerically obtained reference solution.

Note: Again there is no scale separation.

Table 3: L^2 errors and orders of accuracy by the multiscale IP-DG method: two-dimensional example. S_2^1.

	$\varepsilon = 0.01$		$\varepsilon = 0.005$	
S_2^1				
N	error	order	error	order
10	4.00E-02	–	6.45E-02	–
20	1.26E-02	1.67	1.80E-02	1.84
40	3.54E-03	1.83	4.83E-03	1.90
80	9.34E-04	1.92	1.22E-03	1.98

Table 4: L^2 errors and orders of accuracy by the multiscale IP-DG method: two-dimensional example. S_2^2.

	$\varepsilon = 0.01$		$\varepsilon = 0.005$	
S_2^2				
N	error	order	error	order
10	1.23E-03	–	1.34E-03	–
20	1.81E-04	2.76	1.84E-04	2.87
40	2.64E-05	2.78	2.57E-05	2.84
80	3.69E-06	2.84	3.55E-06	2.85

Example 3. 2-D elliptic problem with

$$a^\epsilon(x,y) = b^\epsilon(x,y) = \frac{1}{4+\sin(\frac{\cos(x^2+y^2)}{\epsilon})},$$

$$f = 2$$

with Dirichlet boundary conditions. An explicit formula for the exact solution is again unavailable, and we are using the numerically obtained reference solution.

We use the “easy implementation” basis functions.

Table 5: L^2 errors and orders of accuracy obtained by the easy implementation

	$\epsilon = 0.01$		$\epsilon = 0.005$	
N	error	order	error	order
10	4.71E-01	–	5.41E-01	–
20	1.72E-01	1.45	1.83E-01	1.56
40	5.12E-02	1.75	5.12E-02	1.84
80	1.39E-02	1.88	1.36E-02	1.91
160	3.60E-03	1.95	3.66E-03	1.93

Concluding remarks

- DG methods are suitable for multiscale problems in three different frameworks: HMM; domain decomposition; and multiscale basis.
- DG methods have the advantage in their compact form (minimum communication with neighbors) and in their freedom of complete discontinuity across element interfaces.
- The challenge is to design suitable numerical fluxes and then estimate the terms from the element interfaces to obtain stability and error estimates.

The End

THANK YOU!