Diffusion Equations on Polyhedral Meshes with Mixed Cells

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http://lacsi.rice.edu/review/slides_2006

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LACSI Project: 2005

Advanced Numerical Methods for Diffusion Equations in Heterogeneous Media on Distorted Polyhedral Meshes

LANL: M. Shashkov – PI
K. Lipnikov, D. Moulton, S. Runnels

UH: Y. Kuznetsov – PI
O. Boyarkin – PostDoc
V. Gvozdev, D. Svyatskiy – Graduate Students
S. Repin – Visiting Research Professor

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OUTLINE

- **Problem Formulation**
- **Meshes with Mixed Cells**
- **New Polyhedral Discretization**
- **Numerical Results**
- **Applications to Homogenization and AMR**
- **Project Activities**
- **Further Research Plans**

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Diffusion Equation

$$-\operatorname{div}(K \operatorname{grad} p) + cp = F \quad \text{in} \quad \Omega$$

$$(K \operatorname{grad} p) \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega$$

Here,

Ω	--	polyhedral computational domain
K	--	diffusion tensor
c	--	nonnegative coefficient
$\mathbf{n}$	--	outward normal
F	--	source function

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First Order System

- **Flux Equation (Darcy Law)**

$$\boldsymbol{u} = -K \text{ grad } p$$

or

$$K^{-1}\boldsymbol{u} + \text{grad } p = 0$$

- **Conservation Law Equation**

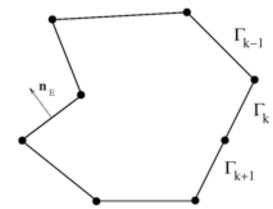
$$\text{div } \boldsymbol{u} + cp = F$$

Polyhedral H-mesh

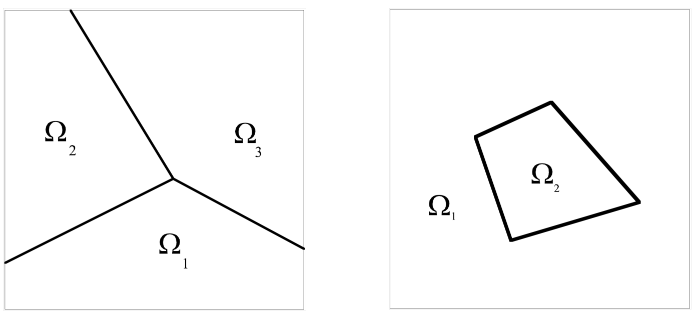
$$\grave{U}_H = \bigcup_i E_i$$

where $\{E_i\}$ – polyhedral cells

Polyhedral cell E



Mixed Cells



Discrete Conservation Law (1a)

By integration over a polyhedral cell E:

$$\int_E \text{div } \boldsymbol{u} + \int_E cp = \int_E F$$

we get the discrete equation

$$\sum_k u_{E,k}\, s_{E,k} + c_E\, p_E\, V_E = F_E\, V_E$$

where

V_E -- volume of E

$s_{E,k}$ -- area of $\tilde{A}_k$

$\boldsymbol{n}_E$ -- outward unit normal

Discrete Conservation Law (1b)

$$u_{E,k} = \frac{1}{s_{E,k}} \int_{\Gamma_k} \boldsymbol{u} \cdot \boldsymbol{n}_E \, \mathrm{ds}$$ -- mean value of the normal flux

$$c_E = \frac{1}{V_E} \int_E c \, \mathrm{dx}$$ -- mean value of c

$$p_E = \frac{\int_E cp \, \mathrm{dx}}{\int_E c \, \mathrm{dx}}$$ -- "c-weighted" mean value of p

$$F_E = \frac{1}{V_E} \int_E F \, \mathrm{dx}$$ -- mean value of F

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Discrete Conservation Law (2)

$$\mathrm{DIV}_H \, \boldsymbol{u}_H + c_H p_H = F_H \quad \text{in} \quad Ù$$

where *)

$$\mathrm{DIV}_H \boldsymbol{u}_H \equiv \frac{1}{V_E} \sum_k u_{E,k} \, s_{E,k} \quad \text{in} \quad E,$$

$$p_H \equiv p_E \quad \text{in} \quad E,$$

$$F_H \equiv F_E \quad \text{in} \quad E.$$

*) Ref. to M. Shashkov for Mimetic Finite Difference methods

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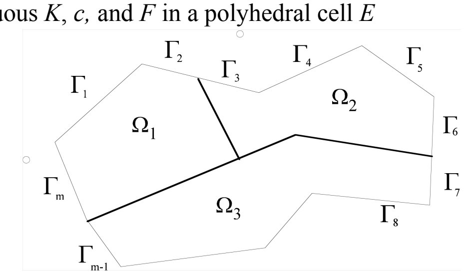
Major Target (1)

To design a discretization for the diffusion equation with discontinuous K, c, and F in a polyhedral cell E



under the following conditions:

-- one DOF per Γ_k for the normal flux;

-- one DOF per cell E for the solution function.

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Major Target (2)

To design a discretization for the flux equation

$$K^{-1}\boldsymbol{u} + \mathrm{grad}\, p = 0$$

in the form

$$M_H \boldsymbol{u}_H + \mathrm{GRAD}_H \, p_H = G_H$$

where

$$\mathrm{GRAD}_H = (-\mathrm{DIV}_H)^*,$$

$$M_H = M_H^* > 0,$$

and G_H is an explicitly computed mesh function.

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Polyhedral Discretizations 2003/2004

Major assumptions:

$$c_E = \frac{1}{V_E}\int_E c \, \mathrm{dx} \approx c \quad \text{in} \quad E$$

$$F_E = \frac{1}{V_E}\int_E F \, \mathrm{dx} \approx F \quad \text{in} \quad E$$

Major advantages:

- Arbitrary diffusion tensor
- Arbitrary polyhedral meshes including meshes with nonconvex and degenerated cells
- Nonmatching and AMR polyhedral meshes

Impact on ASC Projects

LANL researchers M. Shashkov and K. Lipnikov in T7 group, and S. Runnels in X3 group have recently implemented the proposed polyhedral discretization scheme for the diffusion equations in FLAG code for SHAVANO project.

A parallel version of the code was developed by K. Lipnikov and S. Runnels in cooperation with other members of X3 group.

New Polyhedral Discretization on Mixed Cells (1)

Consider the diffusion equation on a polyhedral *H*-cell *E*:

$$K^{-1}\boldsymbol{u} + \operatorname{grad} p = 0$$
$$\operatorname{div} \boldsymbol{u} + cp = F$$

with the boundary conditions

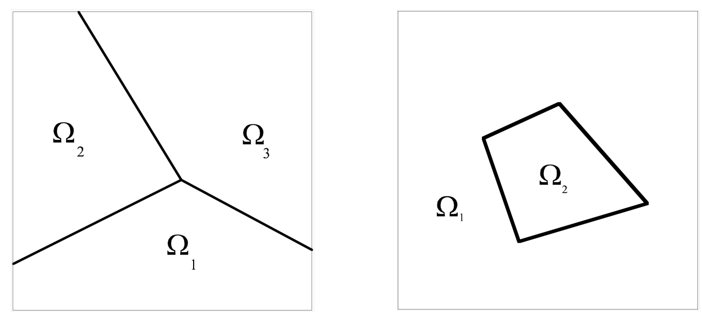
$$\boldsymbol{u}\cdot\boldsymbol{n}_E = u_{E,k} \quad \text{on} \quad \tilde{A}_k, \quad k = 1, 2, \ldots, m.$$

Polyhedral *h*-partitioning of *E*

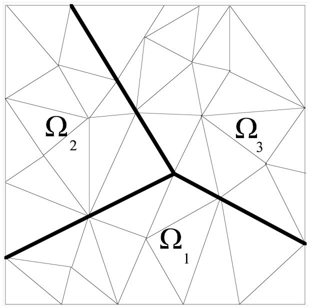
$$E_h = \bigcup_j e_j$$

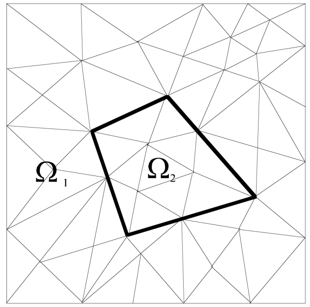
where $\{e_j\}$ are polyhedral *h*-cells.

Mixed Cells



Triangulated Mixed Cells





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New Polyhedral Discretization on Mixed Cells (2)

Discretization in E_h

$$(*) \qquad M_H \boldsymbol{u}_H + M^*_{h,H} \boldsymbol{u}_h + B^*_{h,H} p_h = -D_H \, p_{\tilde{A},H}$$

$$(**) \qquad M_{h,H} \boldsymbol{u}_H + M_h \boldsymbol{u}_h + B^*_h p_h = 0$$

$$(***) \qquad B_{h,H} \boldsymbol{u}_H + B_h \boldsymbol{u}_h - C_h p_h = F_h$$

where

(*) -- flux equations on the boundary Γ_H of E

(**) -- flux equations in the interior of E

(***) -- conservation law equations in E_h

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New Polyhedral Discretization on Mixed Cells (3)

The mesh operator

$$L_h = \begin{pmatrix} M_h & B^*_h \\ B_h & -C_h \end{pmatrix} = (L_h)^*$$

is nonsingular. Thus,

$$\begin{bmatrix} \boldsymbol{u}_h \\ p_h \end{bmatrix} = -(L_h)^{-1} \begin{bmatrix} M_{h,H} \\ B_{h,H} \end{bmatrix} \boldsymbol{u}_H + (L_h)^{-1} \begin{bmatrix} 0 \\ F_h \end{bmatrix}.$$

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New Polyhedral Discretization on Mixed Cells (4)

Substituting $\boldsymbol{u}_h$ and p_h in the flux equation on Γ_H we get the equation

$$A_{E,H} \boldsymbol{u}_H + D_H \, p_{\tilde{A},H} = \hat{G}_{E,H}$$

where

$$A_{E,H} = \begin{bmatrix} M^*_{h,H} & B^*_h \end{bmatrix} (L_h)^{-1} \begin{bmatrix} M_{h,H} \\ B_h \end{bmatrix} = (A_{E,H})^* > 0$$

and

$$p_{\tilde{A},H} = \frac{1}{s_{E,k}} \int_{\tilde{A}_k} p \, \mathrm{ds} \quad \text{on} \quad \tilde{A}_k, \quad k = 1, 2, \ldots, m.$$

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New Polyhedral Discretization on Mixed Cells (5)

Major Theoretical Result

$$A_{E,H} = M_{E,H} + \frac{1}{c_E} \mathrm{GRAD}_{E,H} \cdot \mathrm{DIV}_{E,H}$$

where

$$M_{E,H} = (M_{E,H})^{t} > 0, \qquad \mathrm{cond}\, M_{E,H} \leq \mathrm{const}$$

Reminder: The discrete conservation law in E

$$\mathrm{DIV}_{E,H}\, \boldsymbol{u}_H + c_E\, p_E = F_E$$

New Polyhedral Discretization on Mixed Cells (6)

Hybrid system in terms of $\boldsymbol{u}_H$, p_H, and $p_{\Gamma,H}$

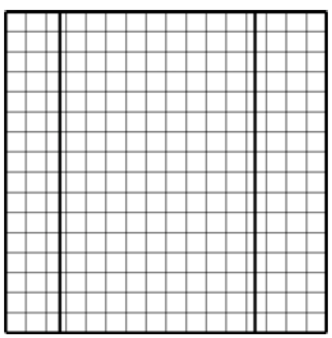
$$\begin{aligned} M_{E,H}\, \boldsymbol{u}_H + \mathrm{GRAD}_{E,H}\, p_E + D_{\tilde{A},H}\, p_{\tilde{A},H} &= G_{E,H} \\ \mathrm{DIV}_{E,H}\, \boldsymbol{u}_H + c_E\, p_E &= F_{E,H} \end{aligned}$$

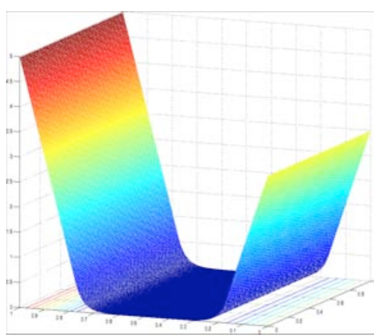
\+ interface conditions for the normal fluxes

Assembled system in terms of $\boldsymbol{u}_H$ and p_H

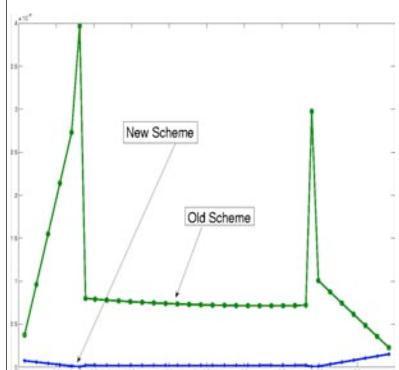
$$\begin{aligned} M_H\, \boldsymbol{u}_H + \mathrm{GRAD}_H\, p_H &= G_H \\ \mathrm{DIV}_H\, \boldsymbol{u}_H + c_H\, p_H &= F_H \end{aligned}$$

Test1



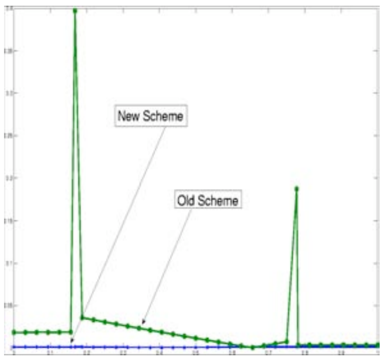


Error for Solution Function



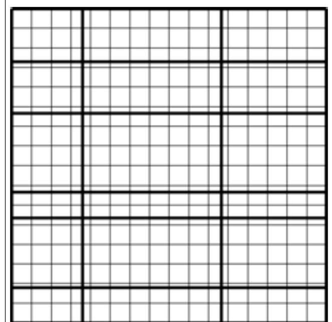
	New Scheme	Old Scheme
	$\Vert p_h - p_{exact} \Vert_{\max}$	$\Vert p_h - p_{exact} \Vert_{\max}$
16x16	**0.0011**	**0.026**
32x32	**0.0003**	**0.0038**
64x64	**0.000078**	**0.0012**
128x128	**0.000019**	**0.00036**

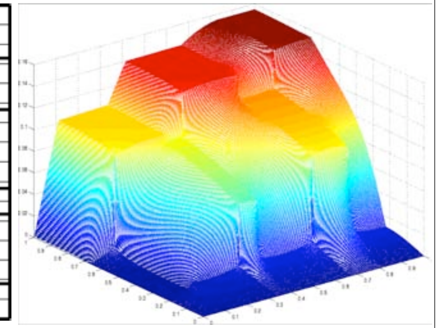
Error for Flux



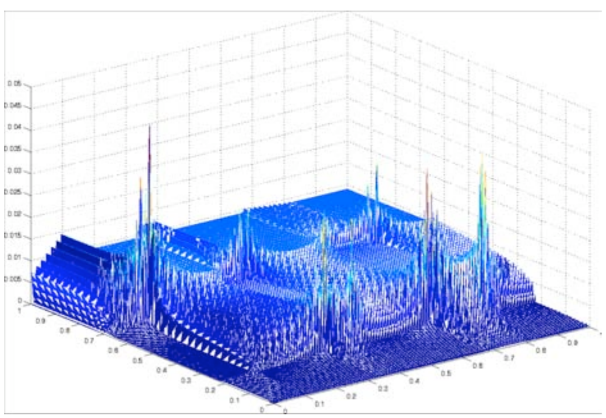
	New Scheme	Old Scheme
	$\|\| \boldsymbol{u}_h - \boldsymbol{u}_{exact} \|\|_{H_{div}}$	$\|\| \boldsymbol{u}_h - \boldsymbol{u}_{exact} \|\|_{H_{div}}$
16x16	0.76	9.40
32x32	0.38	5.57
64x64	0.19	4.11
128x128	0.096	3.35

Test2

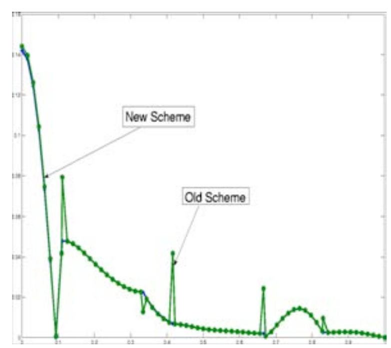




Error for Solution Function

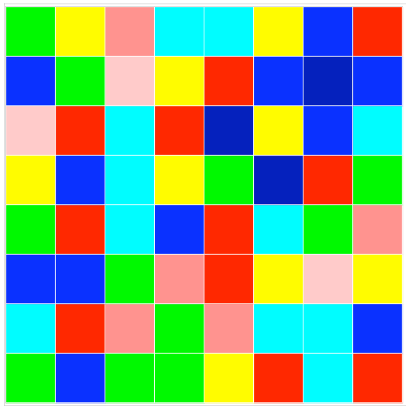


Error for Flux

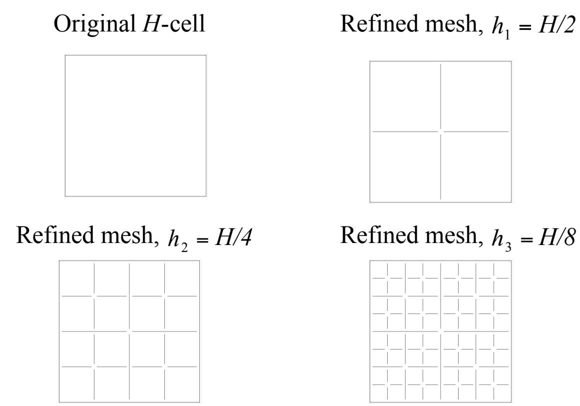


	New Scheme	Old Scheme
	$\|\| \boldsymbol{u}_h - \boldsymbol{u}_{exact} \|\|_{H_{div}}$	$\|\| \boldsymbol{u}_h - \boldsymbol{u}_{exact} \|\|_{H_{div}}$
16x16	2.6	16.31
32x32	1.35	8.49
64x64	0.6	4.32
128x128	0.29	3.1

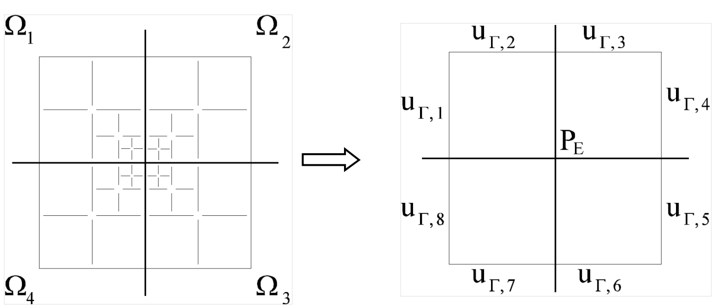
Heterogeneous *H*-cell



Multilevel Homogenization



Multilevel AMR Mesh



LANL -- UH Communication

- LACSI Symposium, Santa Fe 2005:
  Workshop on advanced numerical methods for PDEs

  LANL presentations:
  - K. Lipnikov, T7
  - D. Moulton, T7
  - S. Runnels, X3
  - M. Shashkov, T7
  - J. Warsa, CCS4

  UH presentations:
  - V. Gvozdev – Ph.D. student
  - Y. Kuznetsov
  - D. Svyatskiy – Ph.D. student

- Meeting at UH, January 11—14, 2006

  Attendees: LANL: M. Shashkov
  UH: Y. Kuznetsov, O. Boyarkin, D. Svyatskiy

Education Issues (1)

Konstantin Lipnikov:

2001 & 2002: -- summer semesters at LANL (Ph.D. Thesis – 2002)
2002 -- 2004: -- PostDoc at T7 group, LANL
since January 2005: -- limited term staff member at T7 group, LANL

Vadim Dyadechko:

2002 & 2003: -- summer semesters at LANL (Ph.D. Thesis – 2003)
since September 2003: -- PostDoc at T7 group, LANL

Education Issues (2)

Oleg Boyarkin:

2001—2004: -- Graduate Student at UH supported by LACSI
2004: -- Ph.D. Thesis
since January 2005: -- PostDoc at Department of Mathematics, UH

Daniil Svyatskiy:

2004 & 2005: -- summer semesters at LANL
Plan: -- Ph.D. Thesis – April 2006
-- PostDoc at T7 group, LANL – from June 2006

Further Research Plans

- **3D evaluation of new polyhedral discretizations**
- **Applications to AMR**
- **Multilevel preconditioners based on polyhedral discretizations**
- **Discretizations on anisotropic polyhedral meshes**