Non-conforming discretizations for diffusion equations

Yuri Kuznetsov

Dedicated to Prof. Guri Marchuk on the occation of his 90th anniversary
Department of Mathematics
University of Houston

April 2, 2015

Outline

- differential mixed formulation
- variational mixed formulations
- mixed hybrid formulations
- conforming and non-conforming discretization
- numerical example
- non-conforming / non-matching meshes

Diffusion Equation

$$\begin{aligned} -\mathrm{div}\left(D\,\mathrm{grad}\,p\right) + cp &= F \quad \text{in} \quad \Omega \\ (D\,\mathrm{grad}\,p)\cdot\mathbf{n} &= 0 \quad \text{on} \quad \partial\Omega \end{aligned}$$

Here,

Ω – polyhedral computational domain

$\mathbf{n}$ – unit normals

D – diffusion tensor

c – non-negative coefficient

F – source function

Mixed Formulation

Diffusion equation

$$
\begin{aligned}
D^{-1}\mathbf{u} \quad + \quad \nabla p \quad &= \quad 0 \quad \text{in} \quad \Omega \\
\nabla \cdot \mathbf{u} \quad + \quad cp \quad &= \quad F \quad \text{in} \quad \Omega \\
\mathbf{u} \cdot \mathbf{n} \quad &= \quad 0 \quad \text{on} \quad \partial\Omega
\end{aligned}
$$

Mixed Variational Formulation

Find $(\mathbf{u}, p) \in V \times Q$ such that

$$\int_\Omega D^{-1}\mathbf{u} \cdot \mathbf{v} \; dx - \int_\Omega p \cdot (\nabla \mathbf{v}) \; dx = 0$$

$$\int_\Omega (\nabla \mathbf{u}) \cdot q \; dx + \int_\Omega c \cdot p \cdot q \; dx = \int_\Omega F \cdot q \; dx$$

$$\forall \; (\mathbf{v}, q) \in V \times Q$$

Here

$$V = \{\mathbf{v} : \mathbf{v} \in H_{div}(\Omega), \; (\mathbf{v} \cdot \mathbf{n}) = 0 \; on \; \partial\Omega\}$$

$$Q = L_2(\Omega)$$

Constrained Mixed Variational Formulation

Here we assume that $c \equiv 0$ in Ω

Set of constrains

$$K = \{\mathbf{v} : \mathbf{v} \in V, \int_\Omega (\nabla \cdot \mathbf{v} - F)\; q\; dx = 0\; \forall q \in Q\}$$

Functional for minimization

$$\Phi(\mathbf{v}) = \int_\Omega D^{-1}\mathbf{v} \cdot \mathbf{v}\; dx$$

Constrained mixed Variational Problem: Find $\mathbf{u} \in K$ such that

$$\Phi(\mathbf{u}) = \min_{\mathbf{v} \in K} \Phi(\mathbf{v})$$

This formulation is equivalent to the previous mixed variational formulation.

Conforming Discretization

Let V_h and Q_h be subspaces V and Q, respectively
Then, the conforming mixed discretization is, as follows: Find $\mathbf{u}_h \in V_h$ and $p_h \in Q_h$ such that

$$\int_\Omega D^{-1}\mathbf{u}_h \cdot \mathbf{v}\ dx - \int_\Omega p_h \cdot (\nabla \mathbf{v})\ dx = 0$$

$$\int_\Omega (\nabla \mathbf{u}_h) \cdot q\ dx + \int_\Omega c \cdot p_h \cdot q\ dx = \int_\Omega F \cdot q\ dx$$

$$\forall\ (\mathbf{v}, q) \in V_h \times Q_h$$

Nonconforming Discretization

Important property of $\mathbf{v} \in H_{div}(\Omega)$:
Let γ be a curve/surface belonging to Ω and $\mathbf{n}$ be a normal to γ.
Then $\mathbf{v} \cdot \mathbf{n}$ is continuous almost everywhere on γ.

Nonconforming disctretizations:

- discontinious Galerkin method
- mixed finite element methods with piecewise constant fluxes
- MORTAR element methods

Comforming Meshes

Let Ω be partitioned into m nonoverlapping (macro-)cells E_s, $s = \overline{1,m}$ i.e. $E_s \cap E_t = \emptyset$, $s \neq t$, and

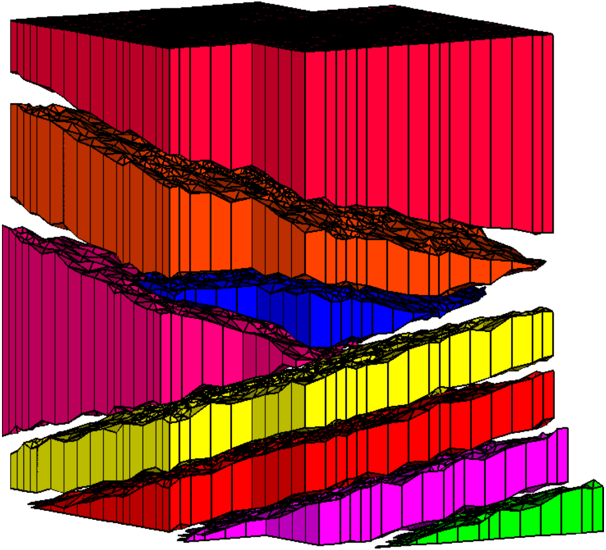
$$\overline{\Omega} = \Omega_H = \bigcup_{s=1}^{m} \overline{E_s}$$

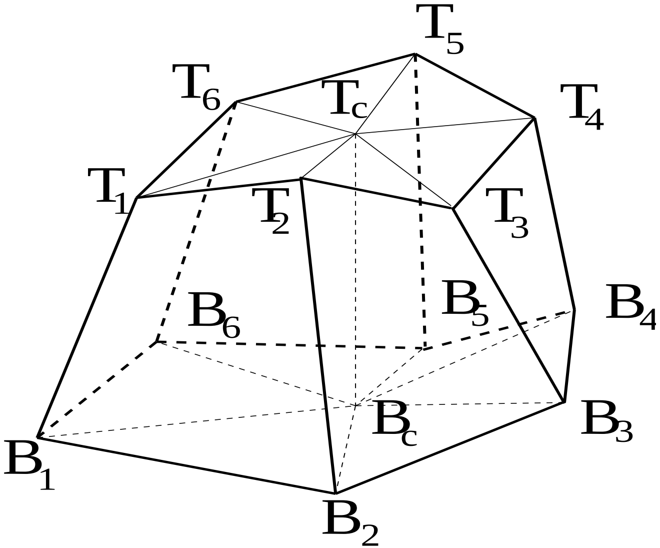
We denote by Γ_{st} the intefaces between Ω_s and Ω_t, i.e.

$$\Gamma_{st} = \partial E_s \cap \partial E_t \;\; s \neq t$$

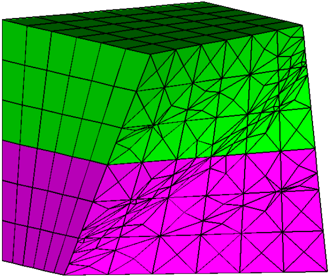
We call such mesh conforming.

Layered Polyhedral Mesh

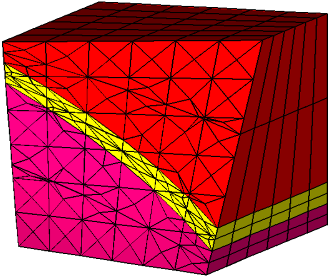



T5
T6
Tc
T4
T1
T2
T3
B5
B4
B6
Bc
B3
B1
B2

Non-Matching Meshes on Faults

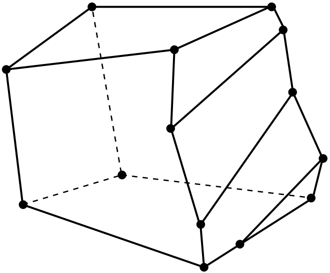


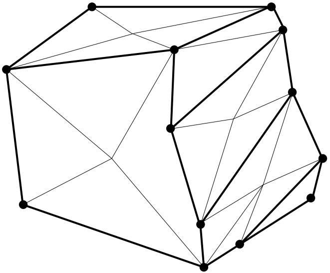
Left subdomain



Right subdomain

Example of a Distorted Hexahedral Mesh Cell on a Fault Surface: Nonmatching, or Nonconforming Polyhedral Meshes





Macro-Hybrid Mixed Formulation

The diffusion problem associated with a cell E_k in Ω_H can be written as follows:

$$\begin{aligned} D_k^{-1}\mathbf{u}_k + \operatorname{grad} p_k &= 0 \quad \text{in} \quad E_k\,, \\ -\operatorname{div} \mathbf{u}_k - c p_k &= -f_k \quad \text{in} \quad E_k\,, \\ \mathbf{u}_k \cdot \mathbf{n}_k &= 0 \quad \text{on} \quad \partial E_k \cap \partial\Omega\,, \\ \mathbf{u}_k \cdot \mathbf{n}_k &= -\psi_k \quad \text{on} \quad \partial E_k \setminus \partial\Omega\,, \end{aligned}$$

where ∂E_k is the boundary of E_k, and $\mathbf{n}_k$ is the outward unit normal to ∂E_k.
The function ψ_k denotes the incoming normal flux on the interfaces between E_k and neighboring mesh cells.
We also assume that the global function p ($p = p_k$ in E_k) is continuous in Ω.

Mixed Macro-Hybrid Formulation

Find $(\mathbf{u}_s, p_s) \in V_s \times Q_s,\ \lambda_{st} \in \Lambda_s t$ such that:

$$\int_{E_s} (D^{-1}\mathbf{u}_s)\cdot\mathbf{v}_s \, dx - \int_{E_s} p_s\cdot(\nabla\cdot\mathbf{v}_s)\, dx + \sum_{\substack{t=1\\ s\neq t}}^{m} \int_{\Gamma_{st}} \lambda_{st}(\mathbf{v}_s\cdot\mathbf{n}_s)\, dl \ = 0$$

$$\int_{E_s} (D\mathbf{u}_s)\cdot q_s \ dx + \int_{E_s} c\cdot p_s\cdot q_s \ dx = \int_{E_s} F\cdot q_s \ dx$$

$$\forall\ (\mathbf{v}_s, q_s) \in V_s \times Q_s$$

$$\int_{\Gamma_{st}} (\mathbf{u}_s, \mathbf{n}_s)\cdot\mu_{st} \ dl \ + \ \int_{\Gamma_{st}} (\mathbf{u}_t, \mathbf{n}_t)\cdot\mu_{st} \ dl = 0$$

$$\forall \mu_{st} \in \Lambda_{st} \equiv L_2(\Gamma_{s,t}),\ s < t,\ s,t = \overline{1,m}$$

Here $V_s = \{\mathbf{v} : \mathbf{v} \in H_{div}(E_s), (\mathbf{v}_s, \mathbf{n}) = 0 \ on \ \partial E_s \cap \partial\Omega\}$

$$Q_s = L_2(E_s),\ s = \overline{1,m}$$

Algebraic System

Conforming/non-conforming discretization results in an algebraic system $(c \equiv 0)$ in Ω:

$$M\overline{u} + B^T\overline{p} + C^T\overline{\lambda} = 0$$

$$B\overline{u} = \overline{F},$$

$$C\overline{u} = 0,$$

where

$$M = \operatorname{diag}\{M_1\,,\, M_2\,,\, \ldots\,,\, M_m\}$$

is a block diagonal symmetric positive definite matrix. Here, the first block equation comes from the discretization of the equation $\boldsymbol{u} = -a\nabla p$, the second represents the discrete conservation law, and the third one governs the continuity of the normal fluxes, or global flux on the interfaces between macrocells.

Constrained Variational Formulation

The variational formulation is as follows: find the vector $\overline{u} \in W_h$ such that

$$(M\,\overline{u},\ \overline{u}) \;=\; \min_{\overline{v} \in W_h} (M\,\overline{v},\ \overline{v})\,,$$

where

$$W_h \;=\; \left\{ \overline{v} \,:\, B\,\overline{v} = \overline{F}\,, \quad C\,\overline{v} = 0 \right\}\,.$$

Coarsening of Normal Fluxes

In non-conforming discretization, we may impose additional conditions on vectors $\overline{u}_s,\ s = \overline{1,m}$. Namely, we may assume that

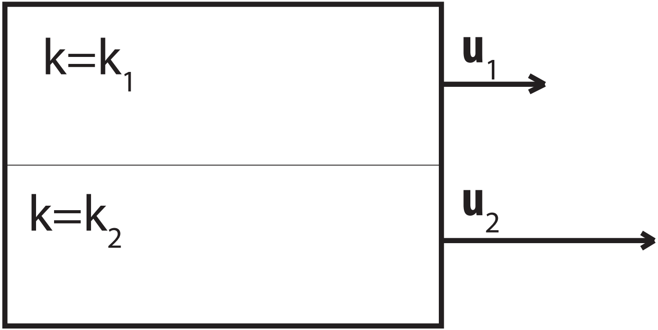
$$\overline{u}_s \ = \ R_s \cdot \overline{u}_{s,new}$$

with some matrices $R_s,\ s = \overline{1,m}$. Then we get $\overline{u} = R\overline{u}_s,\ s = \overline{1,m}$ with the block diagonal matrix

$$R = \begin{pmatrix} R_1 & & 0 \\ & \ddots & \\ 0 & & R_m \end{pmatrix}$$

Simplest Example for Flux Coarsening

Let $k_1 < k_2$



$$\frac{1}{k_1}\mathbf{u}_1 = \frac{1}{k_2}\mathbf{u}_2 \;\Rightarrow \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = R u_{new}, \;\; R = \begin{pmatrix} 1 \\ \frac{k_1}{k_2} \end{pmatrix}$$

Constrained Variational Formulation

Thus we get the following variational problem: find $\overline{u} \in \widehat{W}_h$ such that

$$(\widehat{M}\,\overline{u},\ \overline{u}) \;=\; \min_{\overline{v} \in \widehat{W}_h} (\widehat{M}\,\overline{v},\ \overline{v})\,,$$

where

$$\widehat{M} \;=\; R^T M R\,.$$

Algebraic System for Coarsened Fluxes

The latter variation problem results in the algebraic system

$$\widehat{M}\overline{u} + \widehat{B}^T\overline{p} + \widehat{C}^T\overline{\lambda} = 0$$

$$\widehat{B}\overline{u} = \overline{F}_{new} \equiv R\overline{F}$$

$$\widehat{C}\overline{u} = 0$$

where

$$\widehat{B} = BR, \quad \widehat{C} = CR.$$

Example: Adjacent Mesh Macrocells

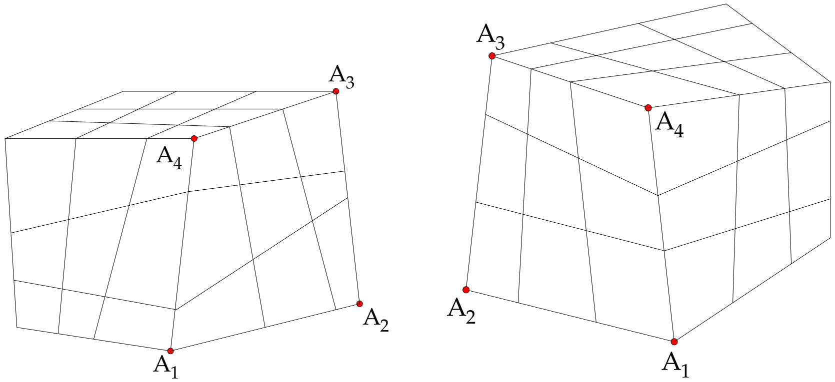


Figure: An example of two adjacent macrocells in Ω_h.

Example of Interface Meshes

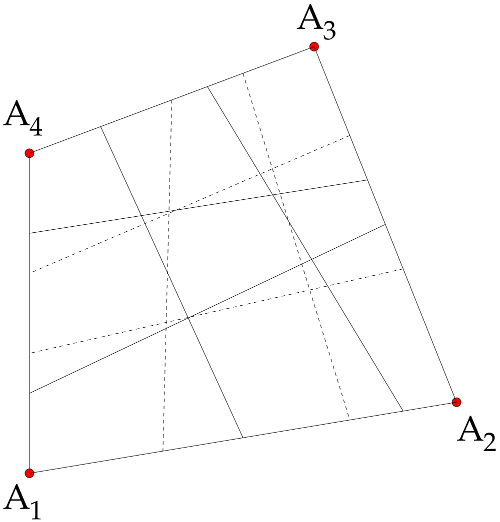


Figure: The traces of meshes on the interface between macrocells (left in solid, right in dashed)

Simplest Discretization

Conforming discretizaions:

$$\mathbf{u}_{s,h} \cdot \mathbf{n}_s \equiv const \ on \ \Gamma_{s,t} \ \ s,t = \overline{1,m}$$

$$\mathbf{u}_{s,h} \cdot \mathbf{n}_s \ + \ \mathbf{u}_{t,h} \cdot \mathbf{n}_t \equiv const \ on \ \Gamma_{s,t}, \ \ s < t, \ \ s,t = \overline{1,m}$$

Nonconforming discretizations:

- no special assumption for $\mathbf{u}_{s,h} \cdot \mathbf{n}_s$ on $\Gamma_{s,t}, \ \ s,t = \overline{1,m}$
- Conformity conditions for the total flux on $\Gamma_{s,t}$

$$\int_{\Gamma_{s,t}} \mathbf{u}_{s,h} \cdot \mathbf{n}_s \ + \ \int_{\Gamma_{s,t}} \mathbf{u}_{t,h} \cdot \mathbf{n}_t = 0, \ \ s < t, \ \ s,t = \overline{1,m}$$

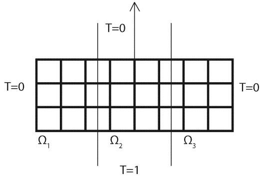
Numerical Example

Equations

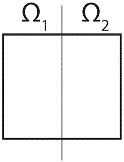
$$\frac{\partial T}{\partial t} = \nabla \mathbf{u} \ in \ \Omega$$

$$\mathbf{u} = -K \cdot T \ in \ \Omega$$

$$T(\mathbf{x}, 0) = 0 \ in \ \Omega, \ T(\mathbf{x}, t) = g(\mathbf{x}) \ on \ \partial\Omega$$



(a) Mesh Ω_H



(b) "Mixed" cells

Numerical Example

Parameters

Domain: $\Omega = (-1, 1) \times (0, 2)$
Mesh: Ω_h 20×20 cells $h_x = h_y = 0.1$
Time Step: $\delta t = 0.005$

Subdomains

$\Omega_1 = (-1, -0.25) \times (0, 2),\ \ k_1 = 10^{-12}$
$\Omega_2 = (-0.25, 0.25) \times (0, 2),\ \ k_2 = 1$
$\Omega_3 = (0.25, 1) \times (0, 2),\ \ k_3 = 10^{-12}$

Implicit FD scheme in time variable

- Conforming MFE with 4 DOFs for the normal flux on faces; continuity of the normal fluxes on the interfaces
- Nonconformity MFE with 6 DOFs for the normal fluxes in mixed cells; continuity of the total normal fluxes on interfaces.

Numerical Test Results 1

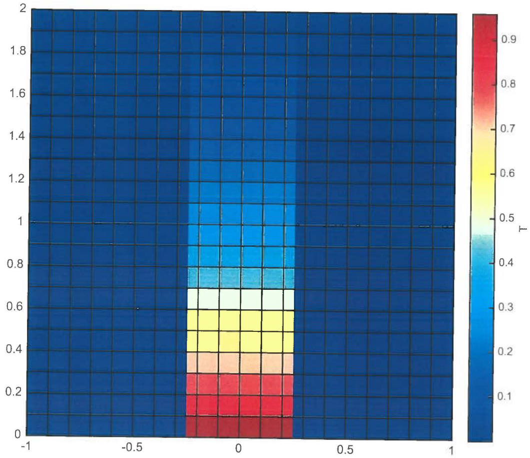


Figure 12: Alg.1: T distribution at $t = 0.455$.

Numerical Test Results 2

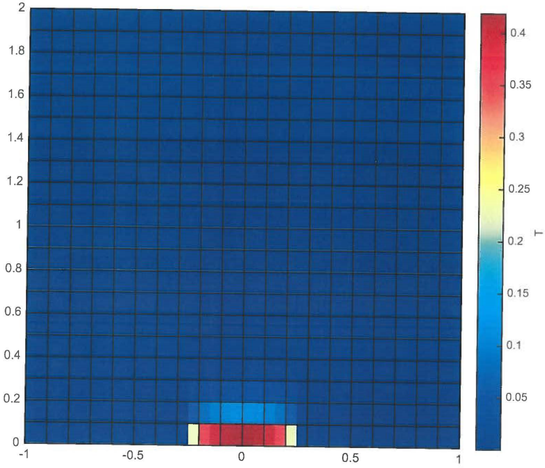


Figure 16: Alg.2: T distribution at $t = 0.005$.

Numerical Test Results 3

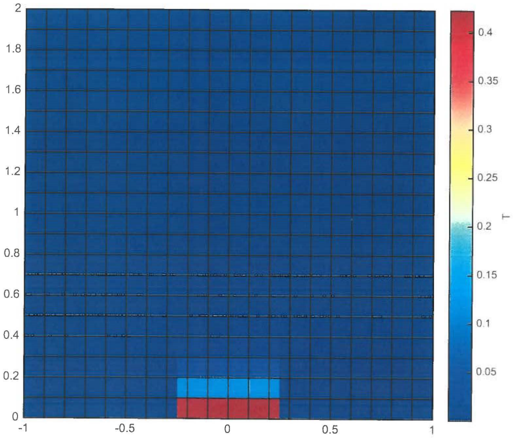


Figure 3: Alg.1: T distribution at $t = 0.005$.

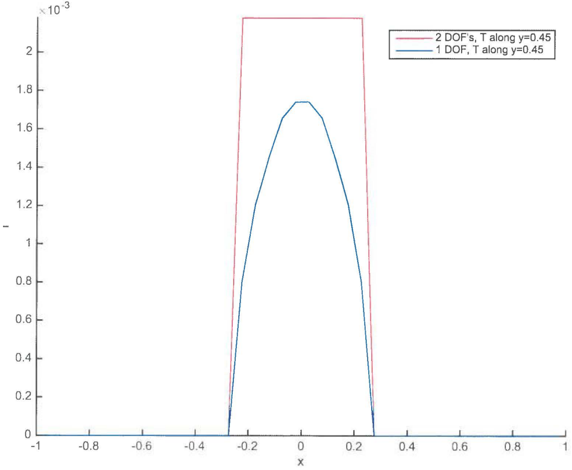


Figure 6: T at $t = 0.005$ along the fifth horizontal row of subcells.

Numerical Test Results 5

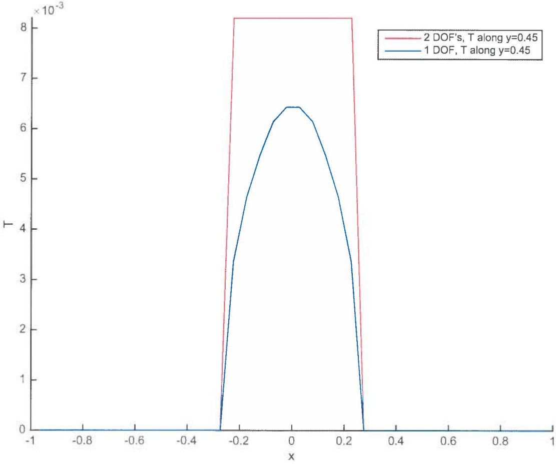


Figure 12: T at $t = 0.01$ along the fifth horizontal row of subcells.

Numerical test 2

Parameters

Domain: $\Omega = (-1, 1) \times (0, 2)$
Mesh: Ω_h 25×25 cells $h_x = h_y = 0.8$
Time Step: $\delta t = 0.005$

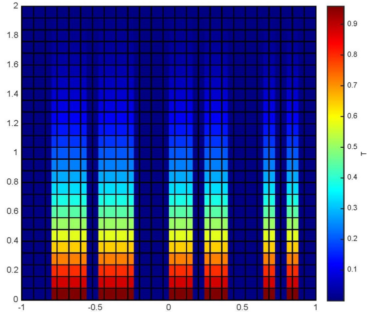
Subdomains: interleaving strips with $k_1 = 10^{-12}$ and $k_2 = 1$
Problem:

$$-\nabla(K\nabla T^k) + \frac{T^k}{\triangle t} = \frac{T^{k-1}}{\triangle t}$$

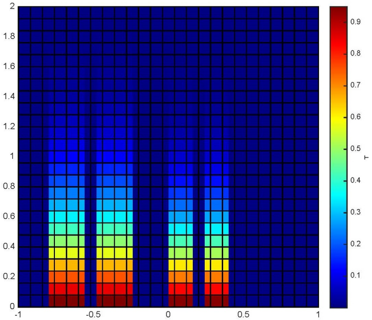
$$\begin{aligned} T &= 1 \; on \; \partial\Omega \cap (y = 0) \\ T &= 0 \; on \; \partial\Omega \cap (y = 2) \\ (K\nabla T) \cdot \mathbf{n} &= 1 \; on \; \partial\Omega \cap (x = -1), \; \partial\Omega \cap (x = 1) \\ T^0 &= 0 \; on \; \Omega \end{aligned}$$

Algorithm 1:$B \in \Re^{7\times 7}, \; B \in \Re^{2\times 7}, C \in \Re^{4\times 7}$
Algorithm 2:$B \in \Re^{5\times 5}, \; B \in \Re^{2\times 5}, C \in \Re^{4\times 5}$

Numerical Test Results for Numerical Example 2



(a) Alg.1: T distribution at t = 0.305.



(b) Alg.2: T distribution at t = 0.305.

Numerical Test Results for Numerical Example 2

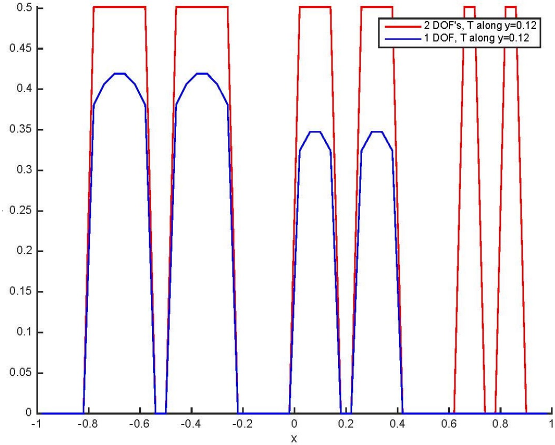


Figure: T at t = 0.02 along the second horizontal row of subcells.

Non-conforming meshes

In theoretical research, a mesh is said to be conforming if any two adjacent mesh cells satisfy the condition:

- "vertex-to-vertex"
- "edge-to-edge"
- "face-to-face"

Otherwise, the meshes are said to be non-conforming. For instance, non-matching meshes,generally speaking, are non-conforming ones. In practice, very often we have to use non-conforming meshes $\Omega_H = \cup_{s=1}^{m} \overline{E}_s$ such that either $|E_s \cap E_t| \neq 0$ for some $s \neq t$ or $\Omega_H \neq \overline{\Omega}$, or both.

An Example of the Initial Conforming Mesh

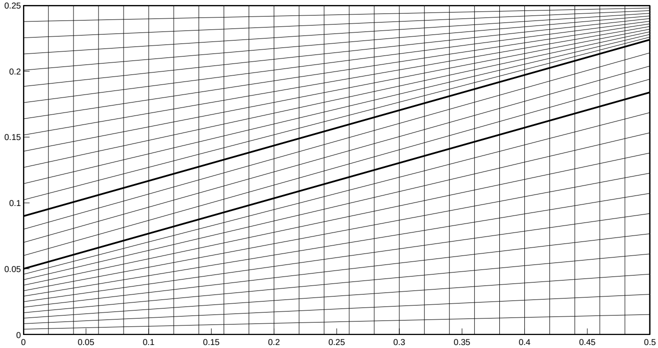


Figure: An example of the initial conforming mesh

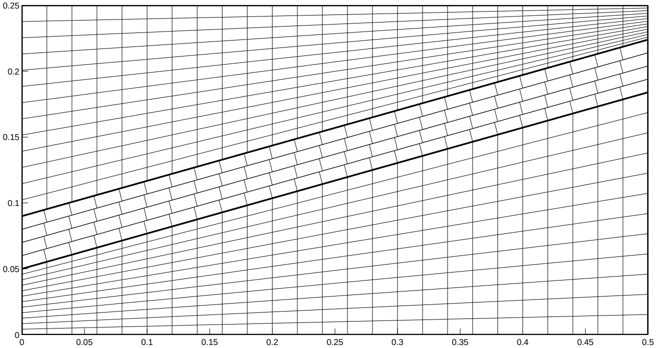
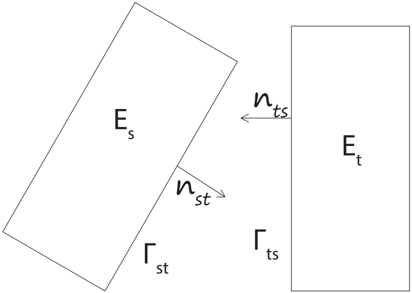


Figure: An example of the resulting non-conforming mesh

"Logically" Conforming Meshes

An example



Flux matching conditions

$$\int_{\Gamma_{st}} (\nabla \mathbf{u}_s) \cdot \mathbf{n}_{st}\ dl + \int_{\Gamma_{ts}} (\nabla \mathbf{u}_t) \cdot \mathbf{n}_{ts}\ dl \ = \ 0$$

Relative Errors

Table: Relative error in PWC discrete solution $\boldsymbol{w}_h^{PWC}$, %, for angle $\alpha = 45^\circ$, conforming mesh

	G_1	G_2	G_3
$4\boldsymbol{h}$	6.47516	5.9941	5.98602
$2\boldsymbol{h}$	3.23569	2.02823	2.98601
$\boldsymbol{h}$	1.61761	0.842736	1.49213

Table: Relative error in PWC discrete solution $\boldsymbol{w}_h^{PWC}$, %, for angle $\alpha = 45^\circ$, non-conforming mesh

	G_1	G_2	G_3
$4\boldsymbol{h}$	6.47512	5.9229	5.98567
$2\boldsymbol{h}$	3.23567	1.96789	2.98584
$\boldsymbol{h}$	1.6176	0.812716	1.49205

Domain G and Mesh G_h for Mesh Step Size $4\boldsymbol{h}$, $(x_C,\ y_C) = (-1.475,\ 0.05)$

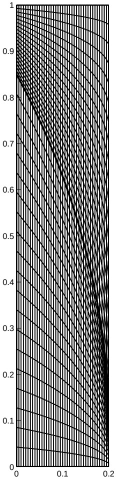


Figure: Domain G and mesh G_h for mesh step size $4\boldsymbol{h}$, $(x_C,\ y_C) = (-1.475,\ 0.05)$

Mesh Cell Inside $G_{h,2}$ for Angle $\alpha = 85^\circ$ and Mesh Step Size $2h$, Non-Conforming Mesh

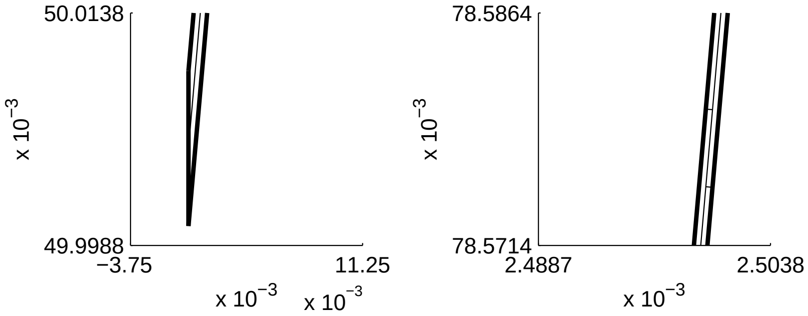


Figure: Mesh cell inside $G_{h,2}$ for angle $\alpha = 85^\circ$ and mesh step size $2h$, non-conforming mesh

Table: Relative error in PWC discrete solution $\boldsymbol{w}_h^{PWC}$, %, for angle $\alpha = 85^\circ$, conforming mesh

	G_1	G_2	G_3
$4\boldsymbol{h}$	5.11235	9.58808	4.74141
$2\boldsymbol{h}$	2.54404	2.98806	2.35079
$\boldsymbol{h}$	1.27059	1.06517	1.17285

Table: Relative error in PWC discrete solution $\boldsymbol{w}_h^{PWC}$, %, for angle $\alpha = 85^\circ$, non-conforming mesh

	G_1	G_2	G_3
$4\boldsymbol{h}$	5.11111	8.61626	4.73696
$2\boldsymbol{h}$	2.54334	2.02273	2.34864
$\boldsymbol{h}$	1.27043	0.905955	1.1724

Acknowledgements

This research was supported by:

- Exxon Mobil Upstream Research Company;
- The Department of Energy

The author is grateful to E.Kikinzon and V.Kramarenko for the assistance in the preparation of this talk.