counterFlowFlame2Dレビュー

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はじめに

・counterFlowFlame2DはOpenFOAMの燃焼チュートリアルの一つであり、非予混合燃焼を対象としたreactingFoamをソルバーとして用いている。

・当初はPaSRをベースとした乱流燃焼モデルを用いていたが、最近は層流モデルとなった。

・OpenFOAM　ver.5.0では派生したtutorialとしてcounterFlowFlame2DLTS、counterFlowFlame2D_GRI,counterFlowFlame2D_GRI_TDAC,counterFlow2DLTS_GRI_TDACが追加された。

・reactingFoamは以前からGRIメカニズムなどの素反応燃焼モデルの利用もできるが、Local Time Stepping(LTS)やTabulation of Dynamic Adaptation Chemistry(TDAC)などの機能を使ったチュートリアルがver.5に追加されて、計算量を軽減する手法が使えるようになった。

LTS:定常問題について計算領域によって時間刻み幅を変化させる

TDAC:化学反応速度を定義式で計算するのではなく補間表を用いて計算

OpenFOAM 5.0

Combustion

TDAC/ISAT: new *TDACChemistryModel* chemistry model providing Tabulation of Dynamic Adaptive Chemistry (TDAC) **[commit f2c26]**; new Eddy Dissipation Concept (EDC) turbulent combustion model, including support for TDAC/ISAT for efficient chemistry **[commit ad825]**; added variable time-step and local time stepping (LTS) in ISAT for TDAC chemistry **[commit 92335]**

Other: new limiting of local time step (for solving steady-state) to specie reaction rate in *reactingFoam* **[commit d36d8]**; support for isothermal, compressible flow in *reactingEulerFoam* **[commit 77ade]**; reactions can optionally be enabled only in a specified list of *cellZones*. **[commit 5d503]**

支配方程式

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0$$

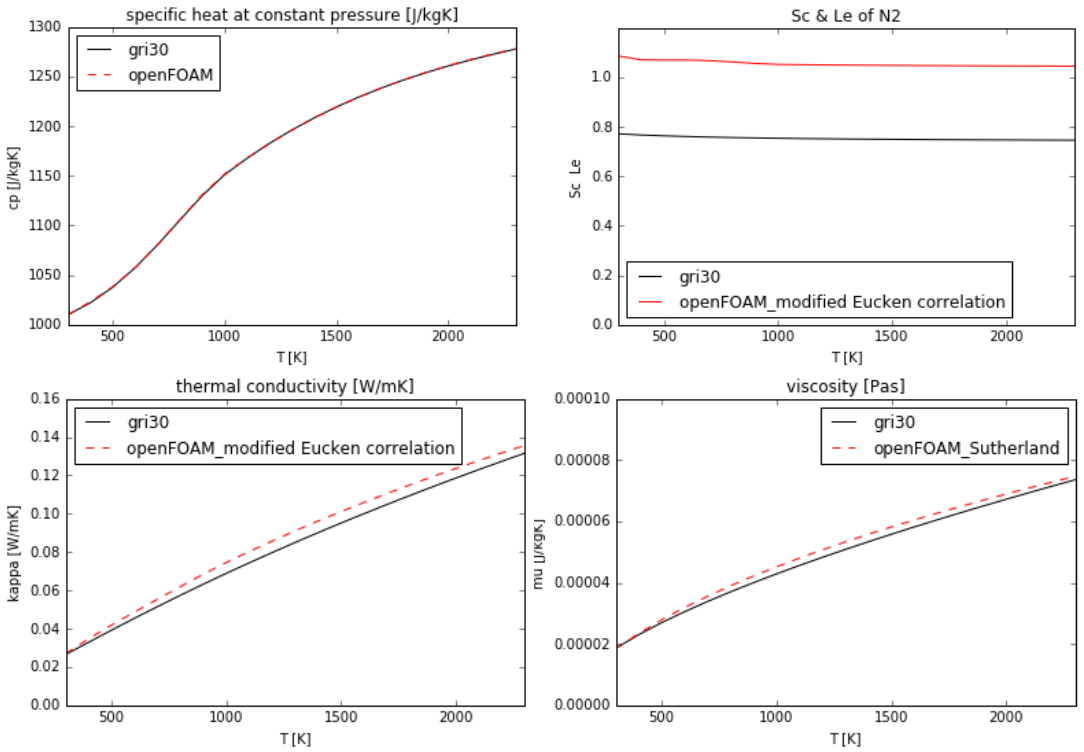
$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \left\{ \mu (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) - \frac{2}{3} \mu \nabla \cdot \boldsymbol{v} I \right\}$$

$$\frac{\partial \left(\rho h_s + \frac{\rho v^2}{2} \right)}{\partial t} + \nabla \cdot \left(\rho \boldsymbol{v} h_s + \rho \boldsymbol{v} \frac{v^2}{2} \right) - \frac{\partial p}{\partial t} = \nabla \left(\frac{\lambda}{C_p} \nabla h_s \right) + \nabla \cdot \boldsymbol{q}_r - \sum_k h_k^0 R_i$$

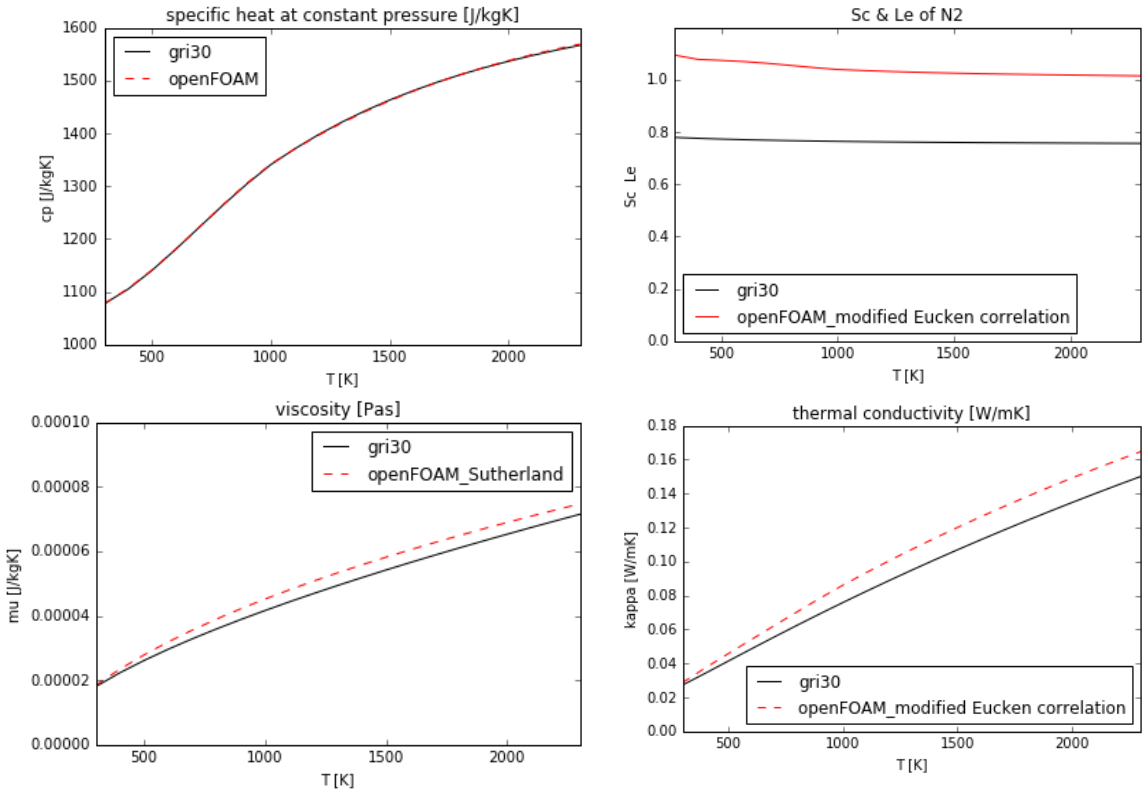
$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} Y_i) = \nabla \cdot (\mu \nabla Y_i) + R_i$$

Dufour効果無視,Sore効果無視,$D_{ij} = D$, $Le = \frac{\lambda}{\rho D C_p} = 1$, $\mathrm{Sc} = \frac{\mu}{\rho D} = 1$

GRIMECH3.0との物性値の比較



空気（P=101.325kPa)



メタン空気予混合気
（ストイキ、P=101.325kPa）

GRIMECH3.0

```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2     H      O      O2     OH     H2O    HO2    H2O2
C      CH     CH2    CH2(S) CH3    CH4    CO     CO2
HCO    CH2O   CH2OH  CH3O   CH3OH  C2H    C2H2   C2H3
C2H4   C2H5   C2H6   HCCO   CH2CO  HCCOH  N      NH
NH2    NH3    NNH    NO     NO2    N2O    HNO    CN
HCN    H2CN   HCNN   HCNO   HOCN   HNCO   NCO    N2
AR     C3H7   C3H8   CH2CHO CH3CHO
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                    1.200E+17   -1.000      .00
M= H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
```

ELEMENTS
使用する原子の指定（5原子）

SPECIES
使用する原子の指定（53種）

REACTIONS
使用する化学反応の指定
（正逆反応の合計　325反応）
化学反応式　A_i　β_i　E_i

3体反応促進係数

化学反応速度

量論係数　化学式

化学反応式

$$\sum_{k=1}^{K} \upsilon'_{ki} \chi_k \Leftrightarrow \sum_{k=1}^{K} \upsilon''_{ki} \chi_k \ (i = 1, \ldots, I)$$

例

$CH_4 + 2O_2 \Leftrightarrow CO_2 + 2H_2O$

k種の化学反応速度

$$R_k = \sum_{i=1}^{I} \upsilon_{ki} q_i \ (k = 1, \ldots, K)$$

$$\upsilon_{ki} = \upsilon''_{ki} - \upsilon'_{ki}$$

モル分率

$$q_i = k_{fi} \prod_{k=1}^{K} [X_k]^{\upsilon'_{ki}} - k_{ri} \prod_{k=1}^{K} [X_k]^{\upsilon''_{ki}}$$

頻度因子　温度指数　活性化エネルギー

k種の正反応定数

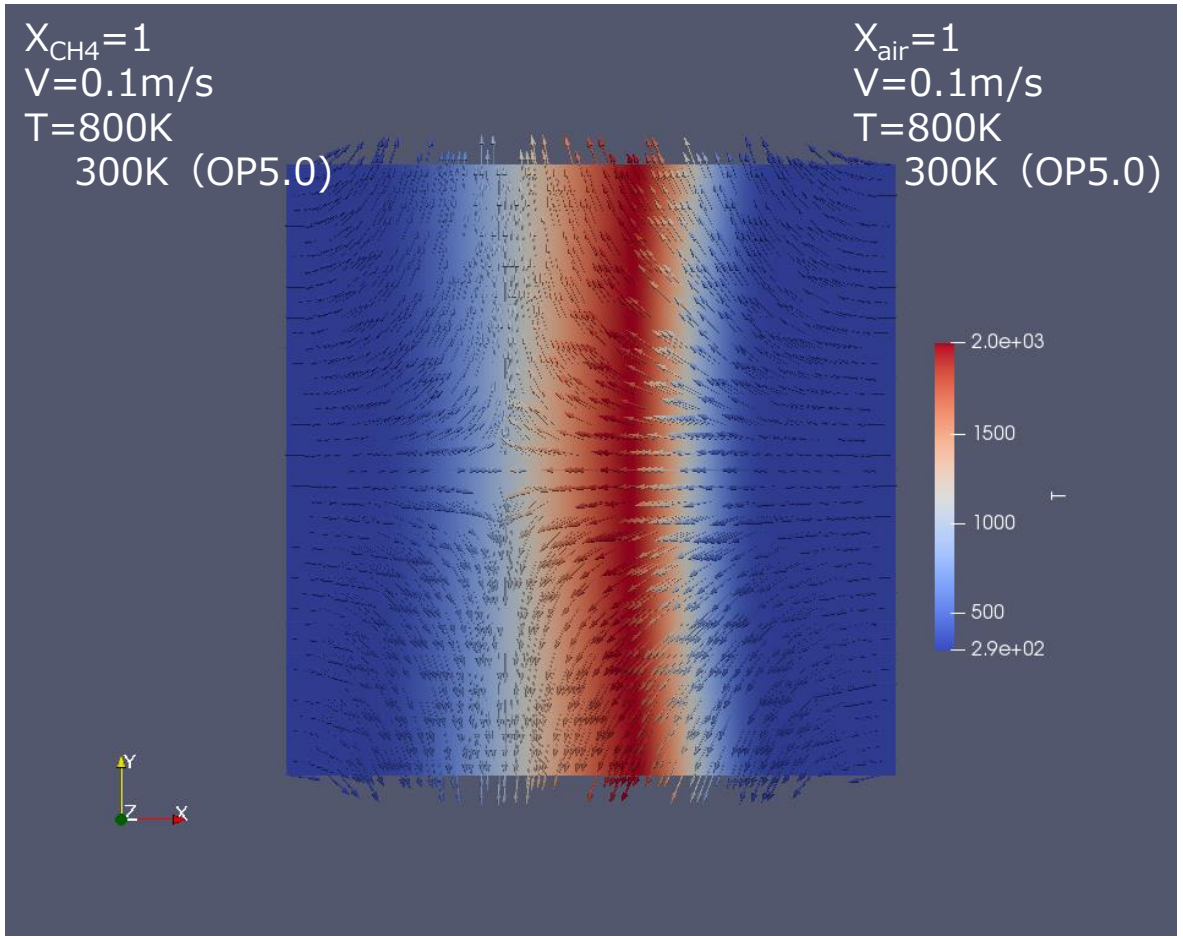
$$k_{f\,i} = A_i T^{\beta_i} \exp\left(\frac{-E_i}{R_c T} \right)$$

k種の逆反応定数

$$k_{ri} = \frac{k_{f\,i}}{K_{ci}}$$

平衡定数

計算モデル

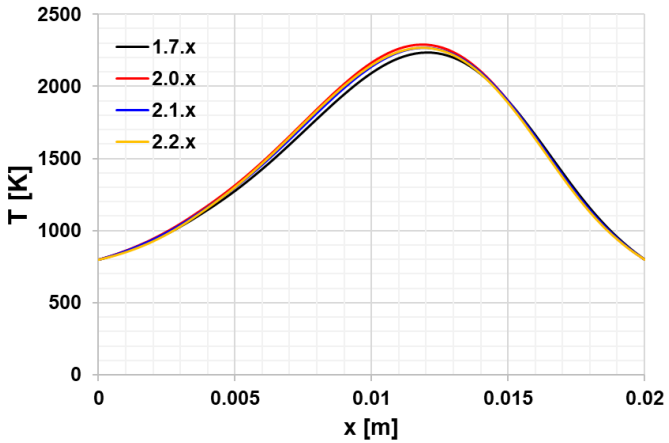

X_{CH4}=1
V=0.1m/s
T=800K
300K（OP5.0）
X_{air}=1
V=0.1m/s
T=800K
300K（OP5.0）
2.0e+03
1500
1000
500
2.9e+02
T
Y
Z
X

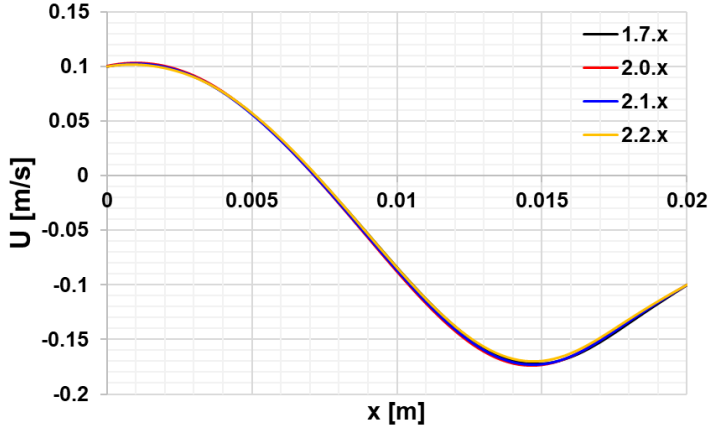
計算条件と時間

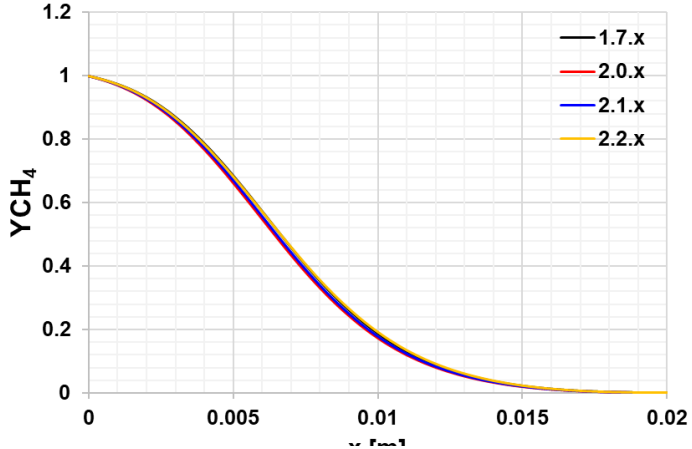
Environment	Ver.	End Time[s]	Flow	Turbulent Combustion	ODE	Execution Time[s]
DEXCS2010	1.7.x	1.0	kEpsilon	PaSR	Ode	120.6
DEXCS2011	2.0.x	0.3	kEpsilon	PaSR	Ode	56.2
DEXCS2012	2.1.x	0.3	kEpsilon	PaSR	Ode	50.8
DEXCS2013	2.2.x	0.3	kEpsilon	PaSR	Ode	47.9
DEXCS2014	2.3.x	0.5	laminar	-	Euler Implicit	68.5
DEXCS2015	2.4.x	0.5	laminar	-	Euler Implicit	68.1
DEXCS2016	4.x	0.5	laminar	-	Euler Implicit	57.0
Ubuntu14	5.0	0.5	laminar	-	Euler Implicit	57.0

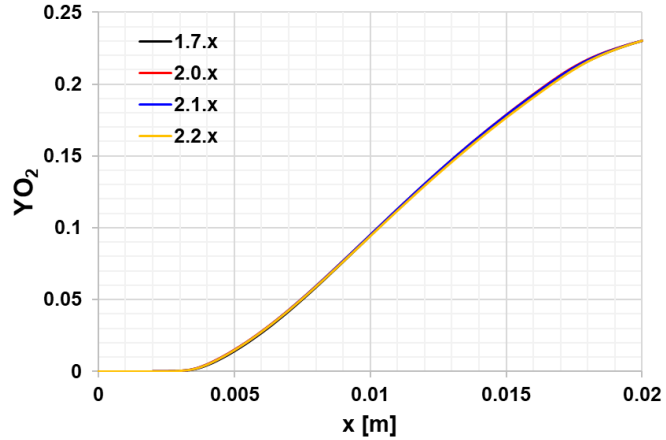
Intel icore5, 7.8Gb memory

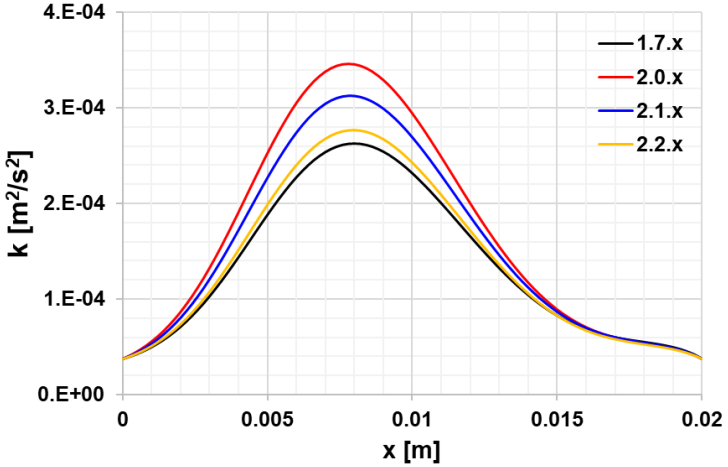
Ver.1.7.x～2.2.x

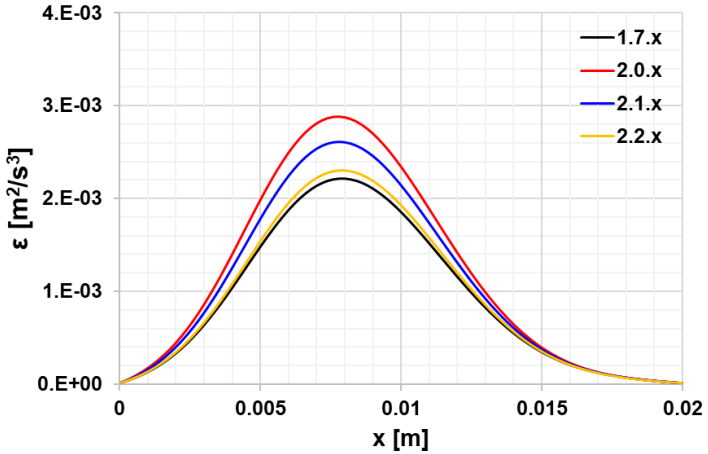

T [K]
x [m]
1.7.x
2.0.x
2.1.x
2.2.x


U [m/s]
x [m]
1.7.x
2.0.x
2.1.x
2.2.x

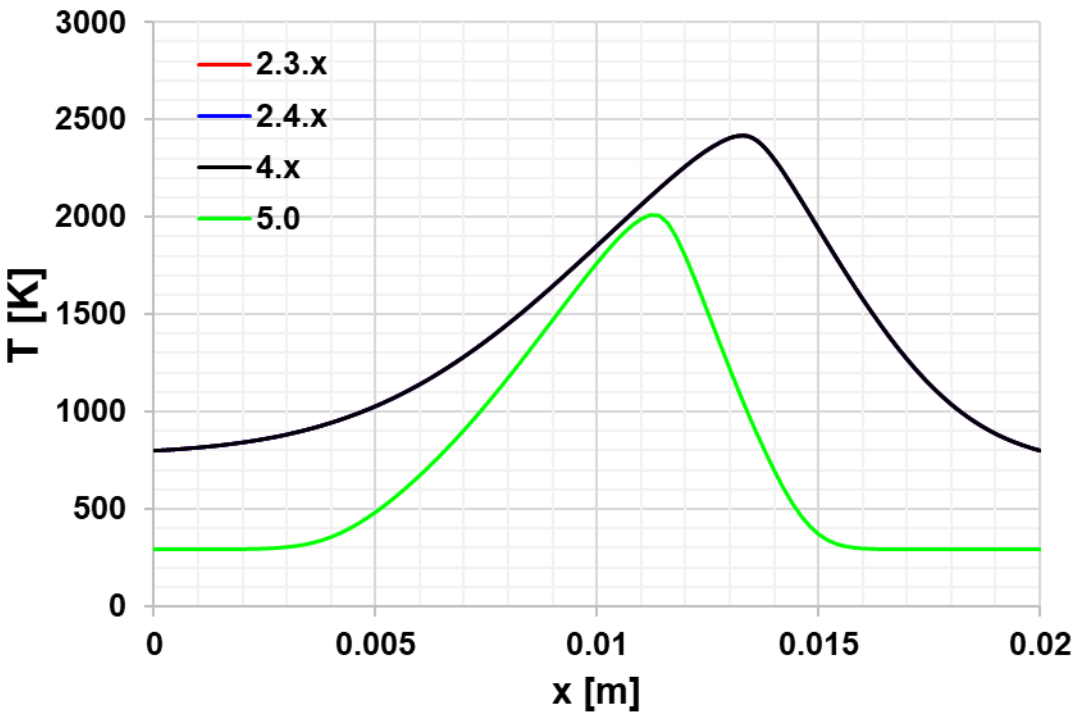

YCH4
1.7.x
2.0.x
2.1.x
2.2.x

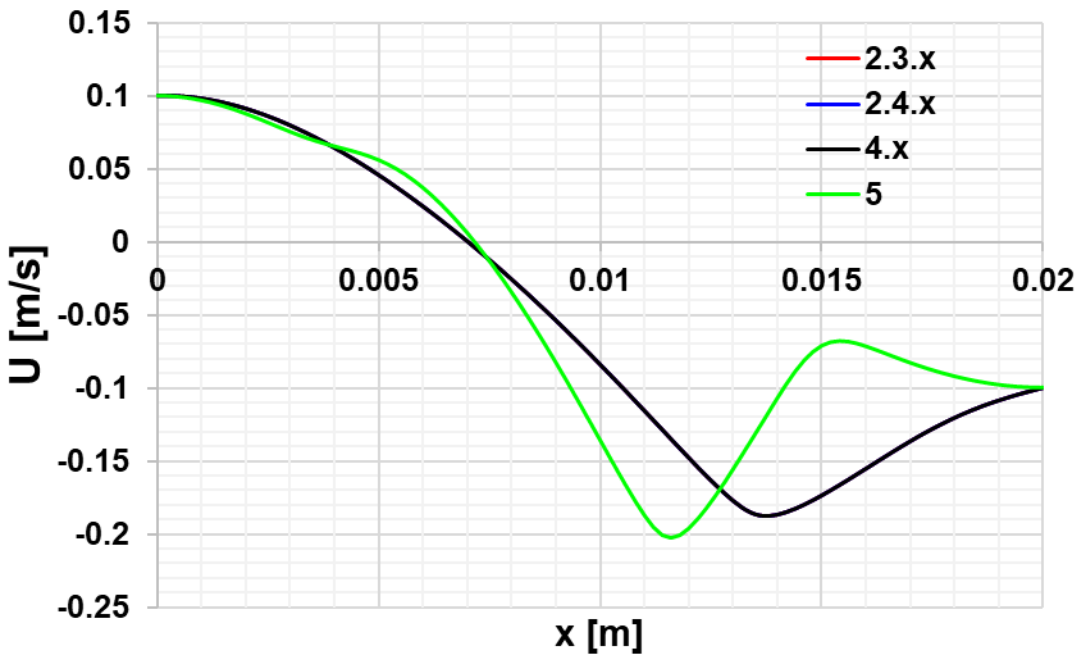

YO2
x [m]
1.7.x
2.0.x
2.1.x
2.2.x


k [m2/s2]
x [m]
1.7.x
2.0.x
2.1.x
2.2.x


ε [m2/s3]
x [m]
1.7.x
2.0.x
2.1.x
2.2.x

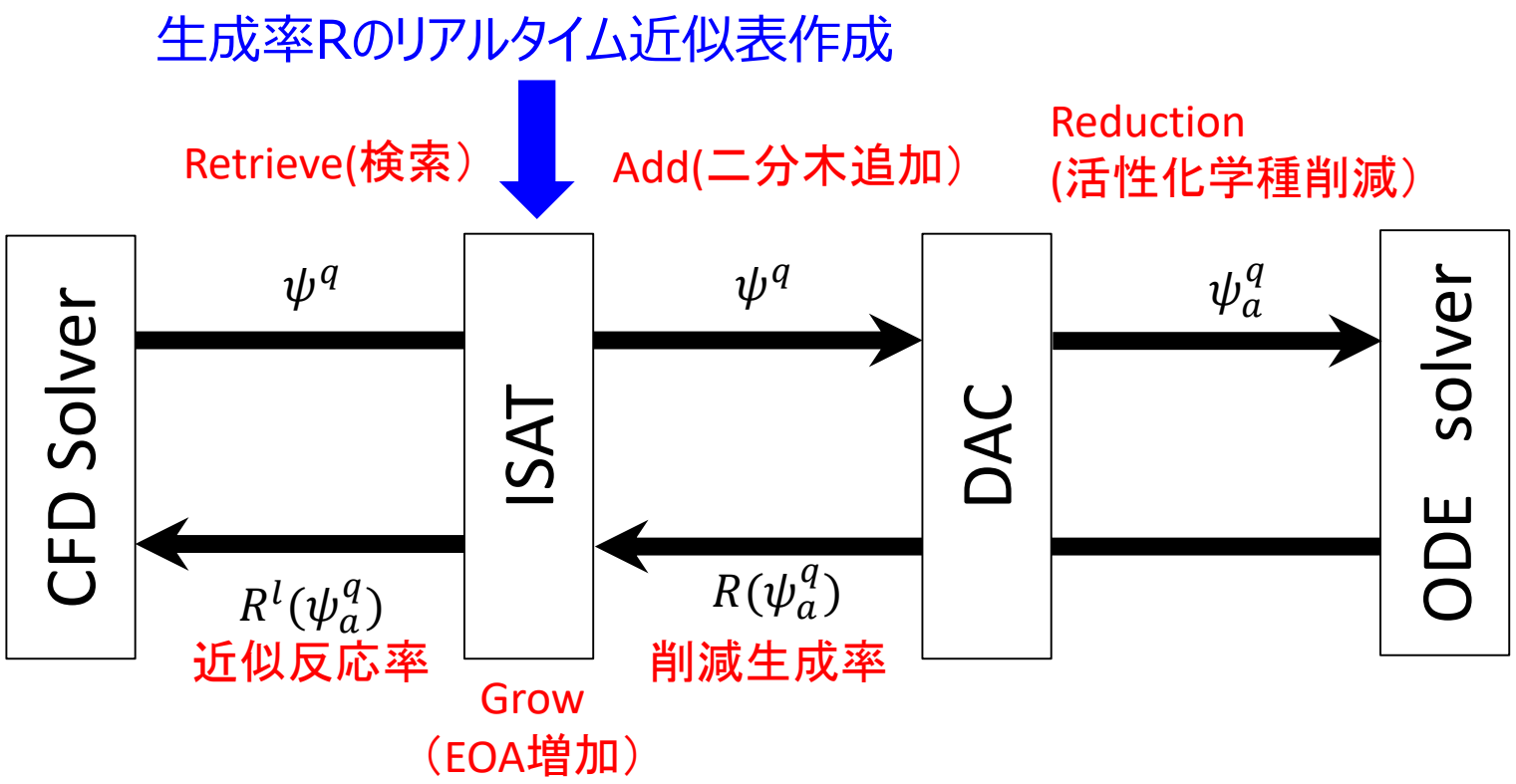
ver.2.3.x～5.0





5.0からT=800⇒300Kに境界条件を変更

TDAC
(Tubulation Dynamic Adaptive Chemistry)



ISAT（In situ adaptive talulation）

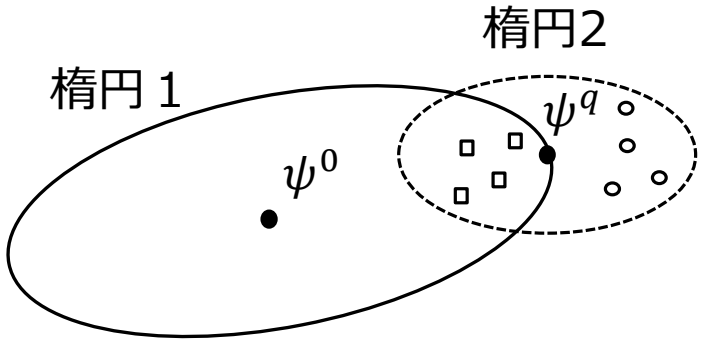
$\psi = \{Y_i, T, p\}$

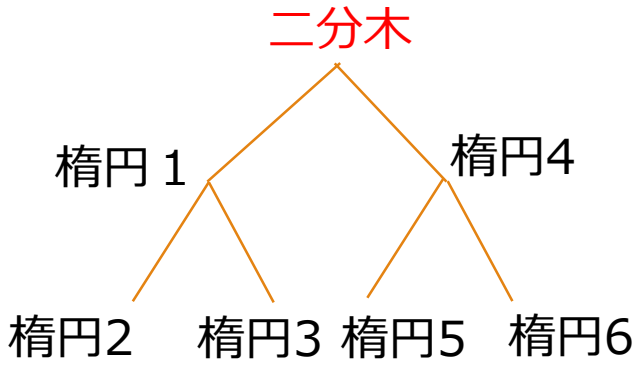
$R(\psi^q) \approx R^l(\psi^q) = R(\psi^0) + \dfrac{\partial R_i(\psi^0)}{\partial \psi_i}(\psi^q - \psi^0)$

$\left|R(\psi^q) - R^l(\psi^q)\right| \leq \varepsilon_{ISAT}$ Torelance：大きいと計算高速となるが精度が悪化

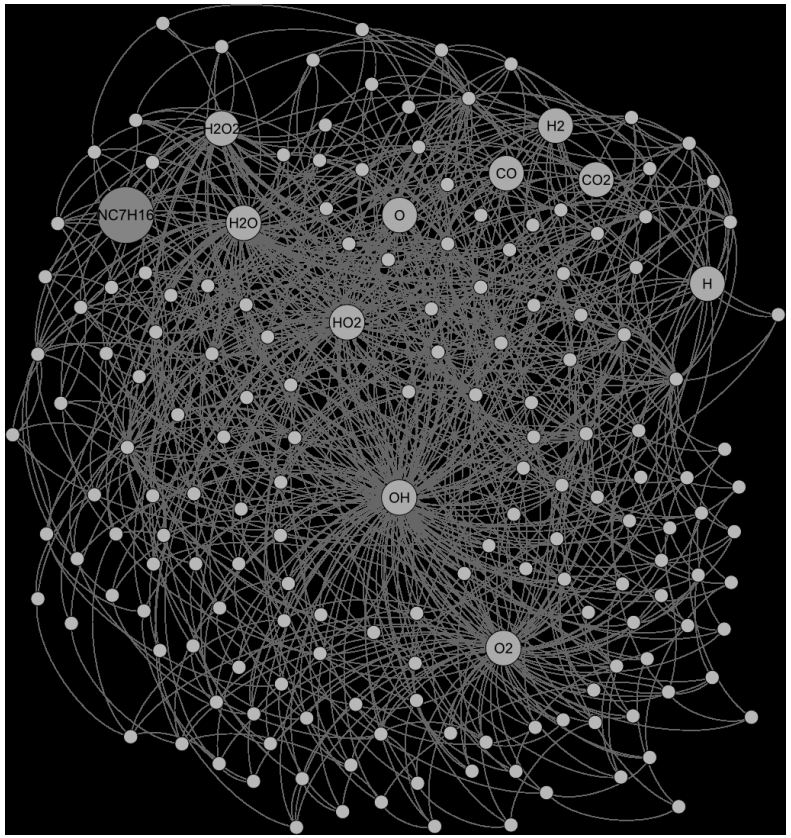
$(Ellipsoid\ Of\ Accuracy)\ EOA \triangleq \delta\psi^{\mathrm{T}}\widetilde{A^T}B^T B\tilde{A}\delta\psi \leq \varepsilon_{ISAT}^2$

B: $optional\ scaling\ matrix$ （特定の変数の$torelance$を改善）
$\widetilde{A}$: $modified\ A\ matrix$ （極端に大きい楕円主軸を防止ため特異値を制限）





DAC（Dynamic Aaptive Chemistry）



反応パスで重要度が低いものを削減し、骨格反応機構（reduced mechanism,skeletal mechanism)を探索

<パス削減手法> DACなど５つの手法が使える
DAC:Dynamic Aaptive Chemistry
DRG:Directed Relation Graph
DRGEP:DRG with Error Propagation
EFA : Element Flux Analysis
PFA : Path Flux Analysis
デフォルトではDAC

＜DACアルゴリズム＞
①各化学種の生成率と消費率の他の化学種の寄与率を計算
②初期設定化学種 {fuel,CO,HO_2}について全ての化学種に対する反応パスの強度を計算
③ユーザーが定めたtorelance以下の化学種を削減

chemistryProperties （1）

```
chemistryType
{
    chemistrySolver   ode;
    chemistryThermo   psi;
    TDAC              on;
}
chemistry       on;
initialChemicalTimeStep 1e-7;
odeCoeffs
{
    solver          seulex;
    absTol          1e-12;
    relTol          1e-1;
}
```

chemistryProperties（2）

```
reduction
{
    // Activate reduction
    active  on;
    // Switch logging of the reduction statistics and performance
    log         on;
    // Tolerance depends on the reduction method, see details for each method
    tolerance   1e-4;
    // Available methods: DRG, DAC, DRGEP, PFA, EFA
    method DAC;
    // Search initiating set (SIS) of species, needed for most methods
    initialSet
    {
        CO;
        CH4;
        HO2;
    }
```

chemistryProperties（3）

```
tabulation
 {
    // Activate tabulation
    active      on;
    // Switch logging of the tabulation statistics and performance
    log         on;
    printProportion    off;
    printNumRetrieve   off;
    // Tolerance used for retrieve and grow
    tolerance   1e-3;
    // ISAT is the only method currently available
    method    ISAT;
```

chemistryProperties（4）

```
// Scale factors used in the definition of the ellipsoid of accuracy
scaleFactor
{
    otherSpecies 1;
    Temperature  25000;
    Pressure     1e15;
    deltaT       1;
}
// Maximum number of leafs stored in the binary tree
maxNLeafs  2000;
// Maximum life time of the leafs (in time steps) used in unsteady
// simulations to force renewal of the stored chemPoints and keep the tree small
chPMaxLifeTime 100;
// Maximum number of growth allowed on a chemPoint to avoid distorted chemPoints
maxGrowth  10;
```

chemistryProperties（5）

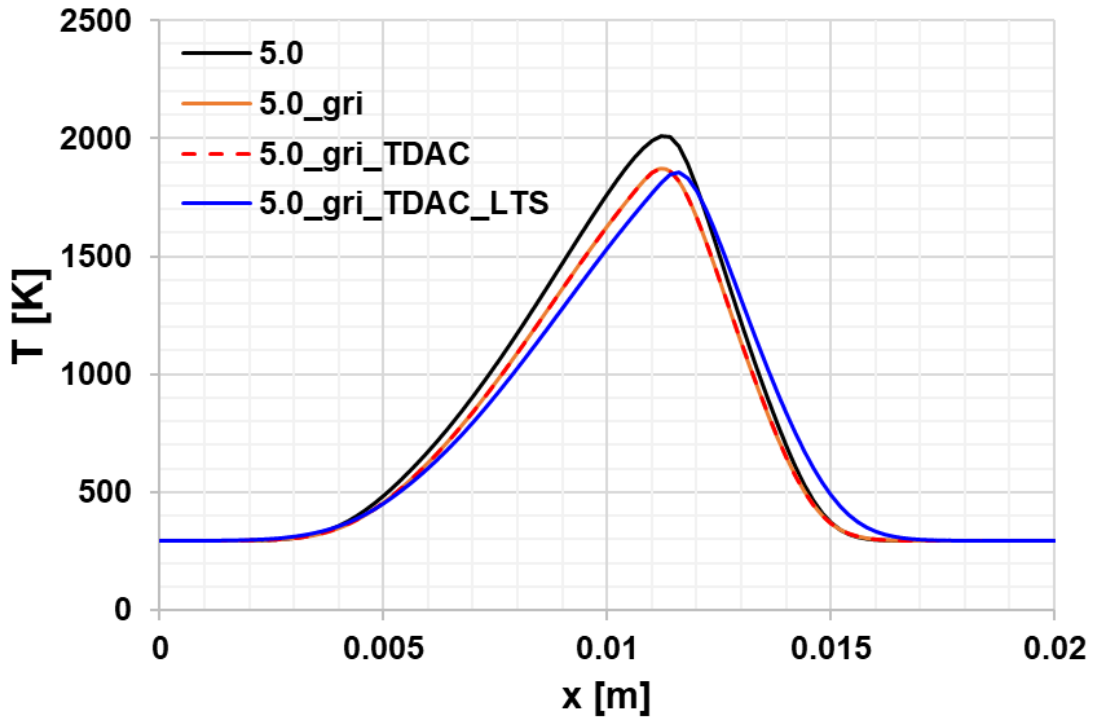
```
// Number of time steps between analysis of the tree to remove old  chemPoints or try to balance it
checkEntireTreeInterval  5;
// Parameters used to decide whether to balance or not if the tree's depth
// is larger than maxDepthFactor*log2(nLeafs) then balance the tree
maxDepthFactor   2;
// Try to balance the tree only if the size of the tree is greater
minBalanceThreshold 30;
// Activate the use of a MRU (most recently used) list
MRURetrieve false;
// Maximum size of the MRU list
maxMRUSize 0;
// Allow to grow points
growPoints  true;
// When mechanism reduction is used, new dimensions might be added
// maxNumNewDim set the maximum number of new dimensions added during a  growth
maxNumNewDim 10;
}
```

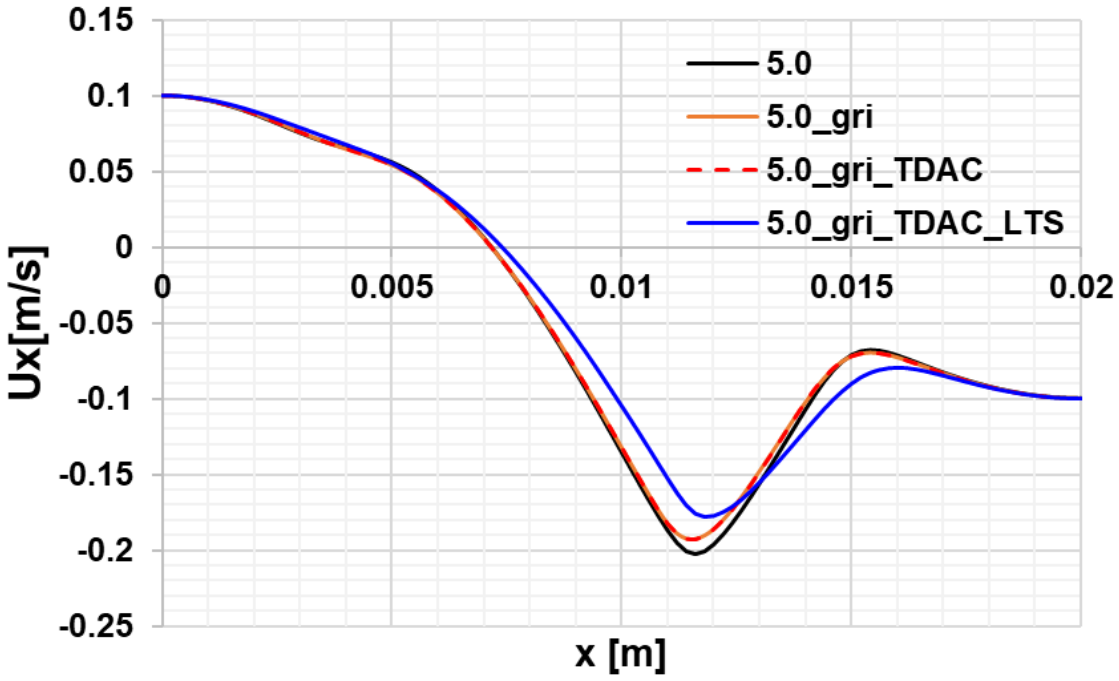
LTS

fvSchemeで以下の指定をする。

```
ddtSchemes
{
    default         localEuler;
}
```

ver.5.0



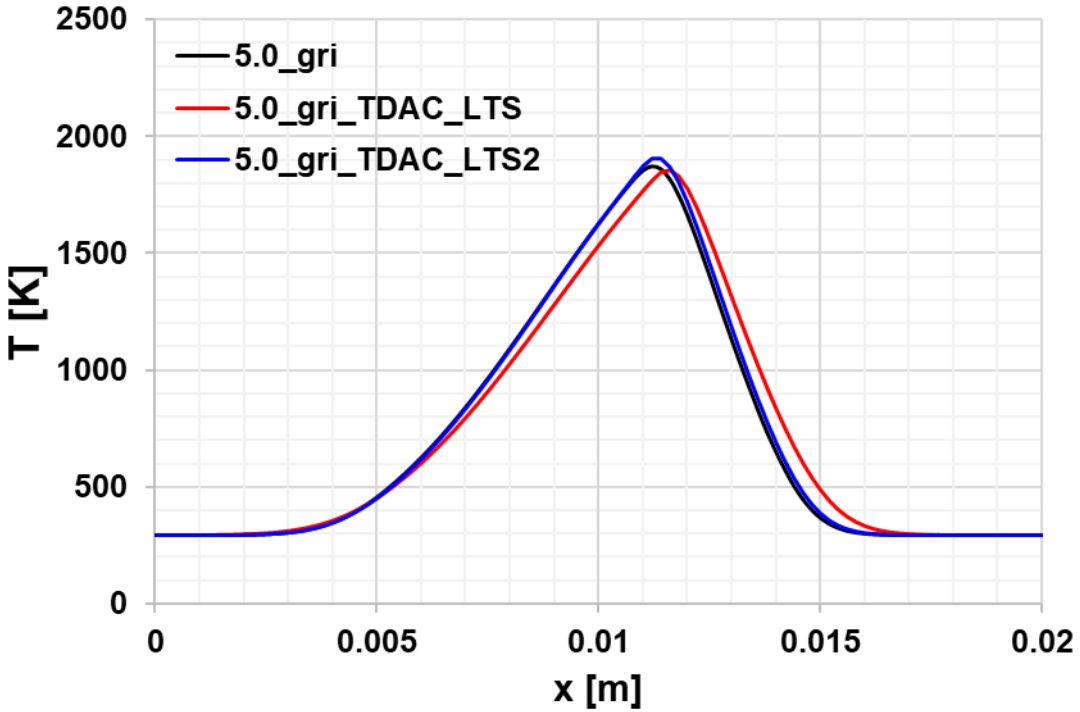


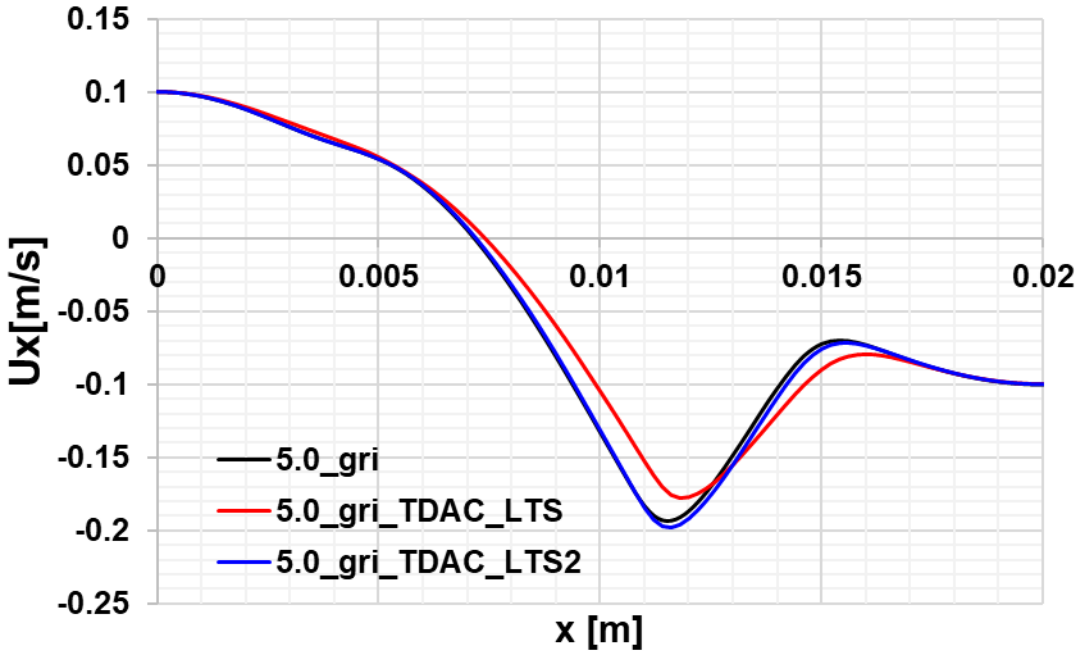
gri_TDAC_LTSとgriの差異が大きい。収束していない?!

計算時間

Tutorial	Core	End Time [s] or Itaration	Execution Time [s]
counterFlowFlame2D	1	0.5	57
counterFlowFlam2D_GRI	4	0.5	10,107
counterFlowFlame2D_GRI_TDAC	4	0.5	3,850
counterFlowFlame2DLTS_GRI_TDAC	4	1000	1,718

Ver5.0 LTS再計算





LTS:反復回数1000 ➡LTS2:反復回数2000
精度が改善

文献

(1)Bachelor Thesis : Implementation and Validation of a Solver for Direct Numerical Simulations of Turbulent Reacting Flows in OpenFOAM By cand. chem. ing. Henning Bonart October 2012

(2)Francesco Contino, Herve Jeanmart, Tommaso Lucchini, Gianluca D'Errico, Coupling of in situ adaptive tabulation and dynamic adaptive chemistry: An effective method for solving combustion in engine simulations, Proc. Combust. Inst. (2010)

(3)Francesco Contino, Tommaso Lucchini, Gianluca D'Errico, Catherine Duynslaegher, Veronique Dias & Herve Jeanmart, Simulations of advanced combustion modes using detailed chemistry combined with tabulation and mechanism reduction techniques, 2012-01-0145, 2012 SAE International.