

OpenFOAM 솔버 수렴특성

(Convergence characteristics of OpenFOAM solvers)

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한국해양대학교

- **Introduction**
 - Research background
 - OpenFOAM solver algorithm:
 - Solver modification
- **Convergence characteristics**
 - Numerical test of the solvers
- **summary**
 - Let's discuss what we do

Moderator circulation flow

- Buoyant and momentum forces acting on the fluid flow
 - Moderator flow around horizontal bundles inside an calandria tank of CANDU-6 reactors
 - Flow injection through inlet nozzles and volumetric heat source

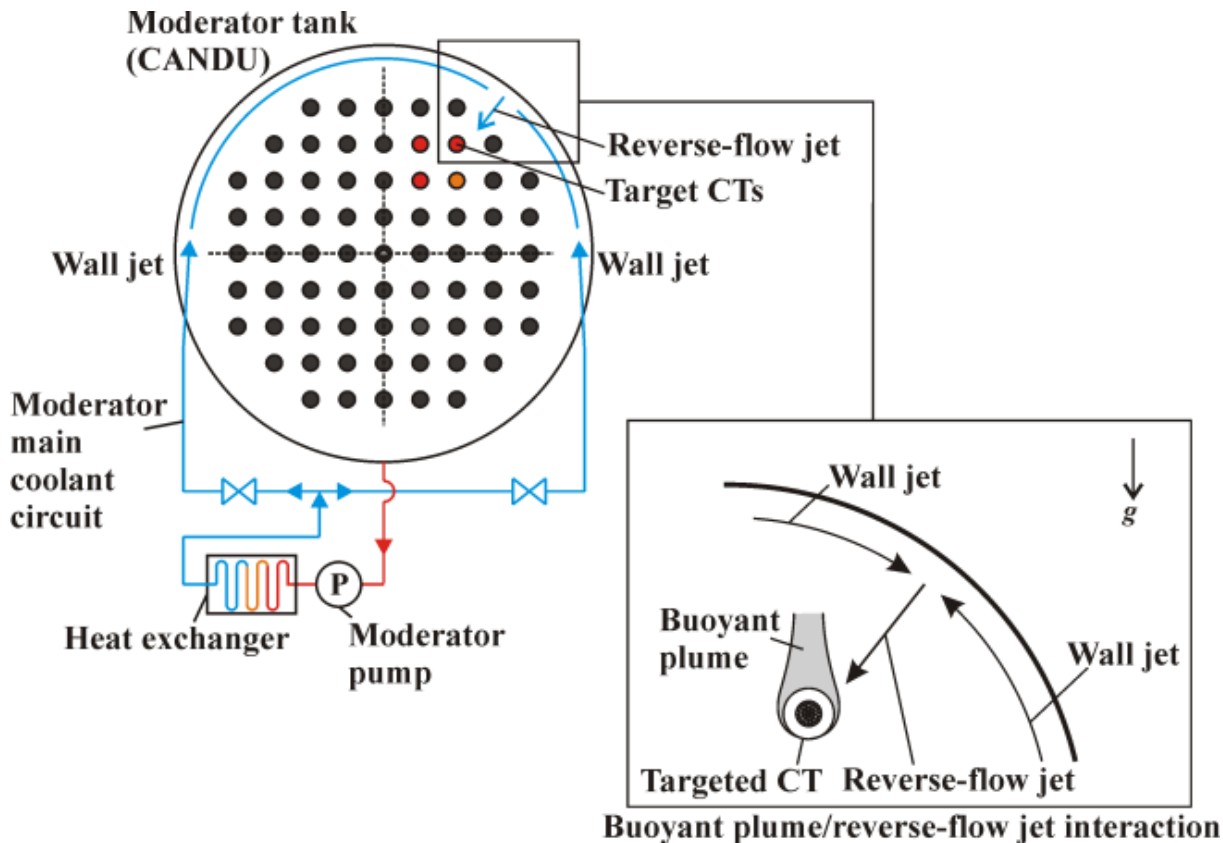
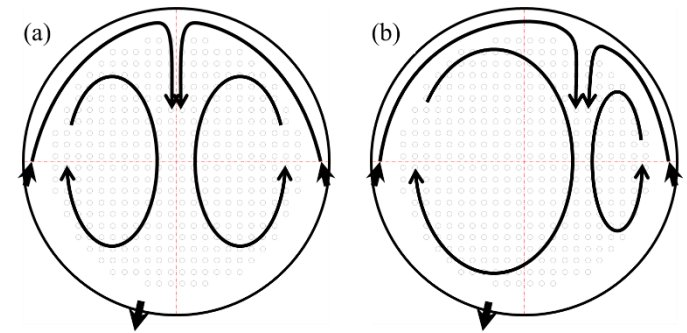


Fig. 1 Moderator circulation flow of CANDU-6



(a) Momentum-dominated flow (b) mixed flow

Fig. 2 Flow patterns of the moderator circulation

Moderator circulation flow

- Grid generation from geometry

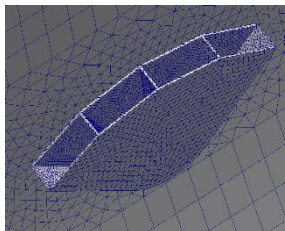
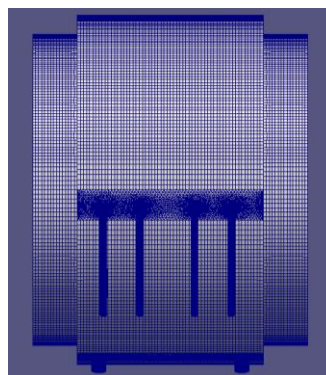
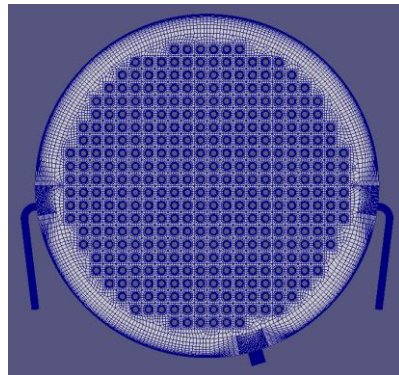
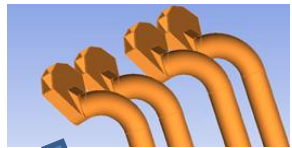
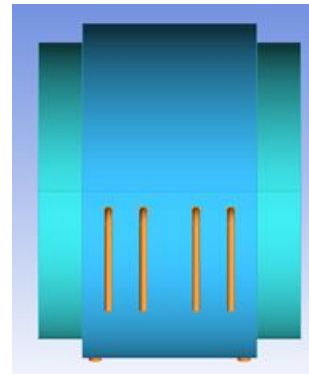
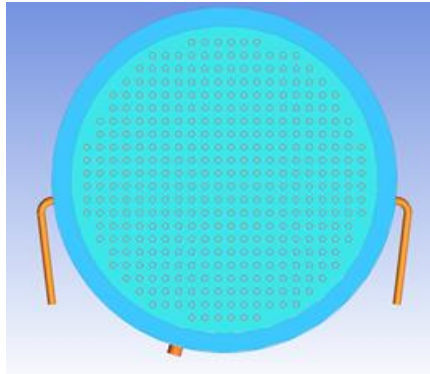
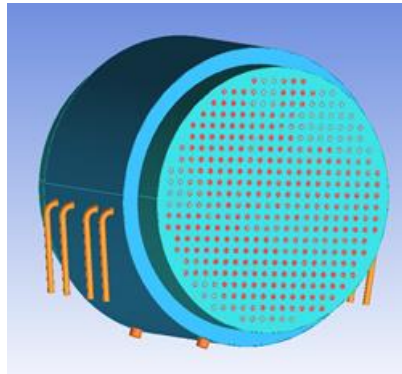


Table 1. Water properties

Parameter	Value
T (Inlet temperature)	47.3 °C
ρ	1085 kg/m ³
β	5×10^{-4} K ⁻¹
μ	5.5×10^{-4} kg/m-s
c_p	4,207 J/kg-K
k	0.659 W/m-K

Total # of elements: 6,740,446

- Hexahedron: 5,112,270
- Pyramid: 13,112
- Triangular: 1,615,064



Moderator circulation flow

- Total Thermal Power = 100 MW
 - Radial and axial power distribution

$$Q_s(r, z) = Q_s f_r(r) f_z(z)$$

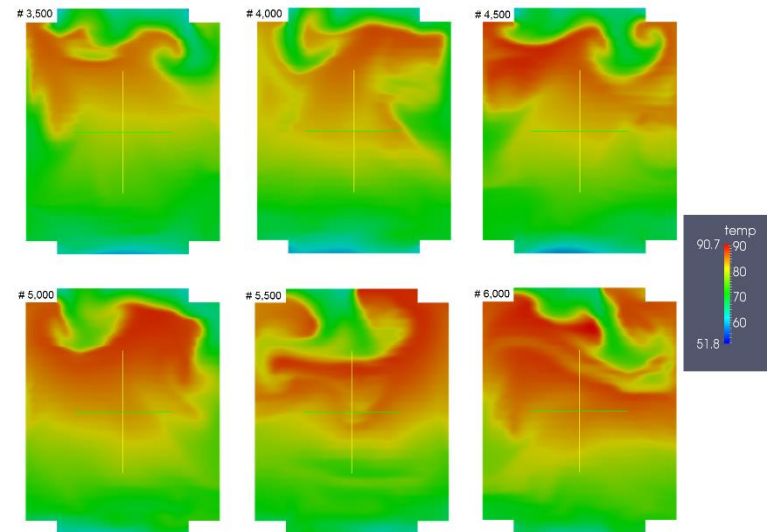
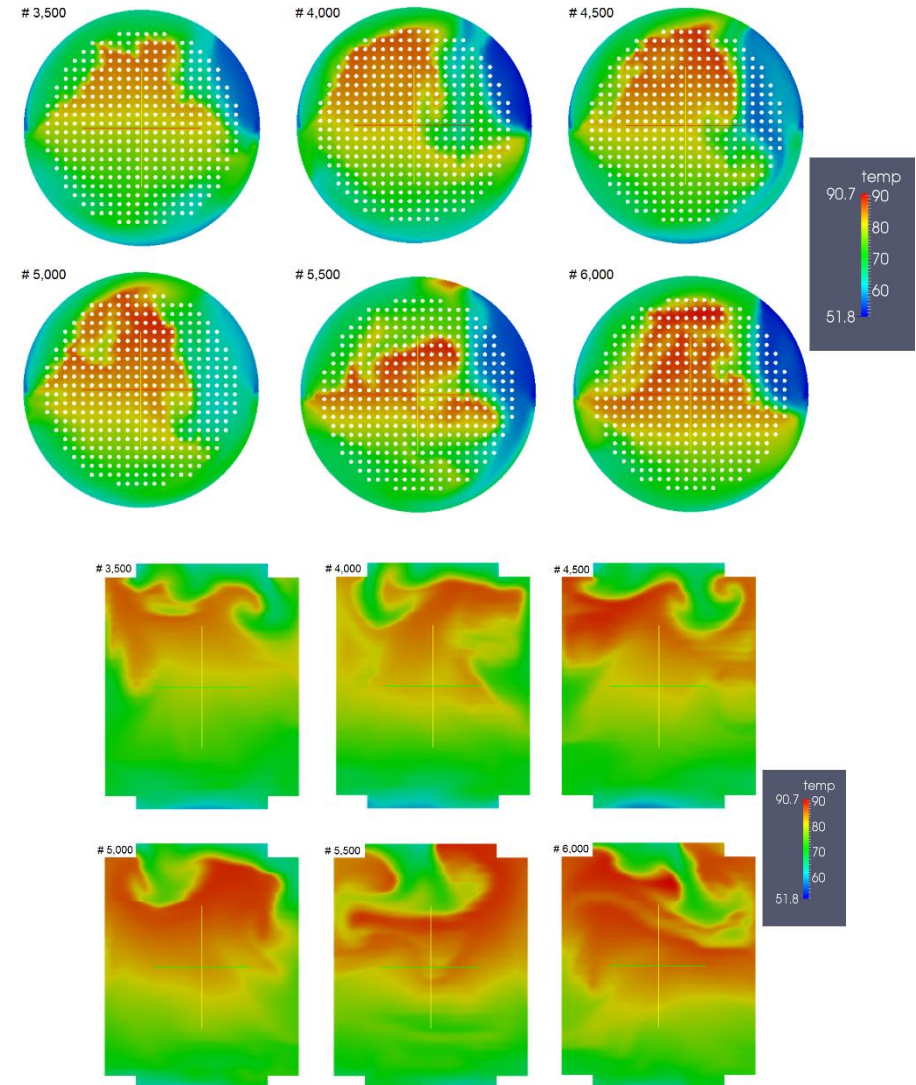
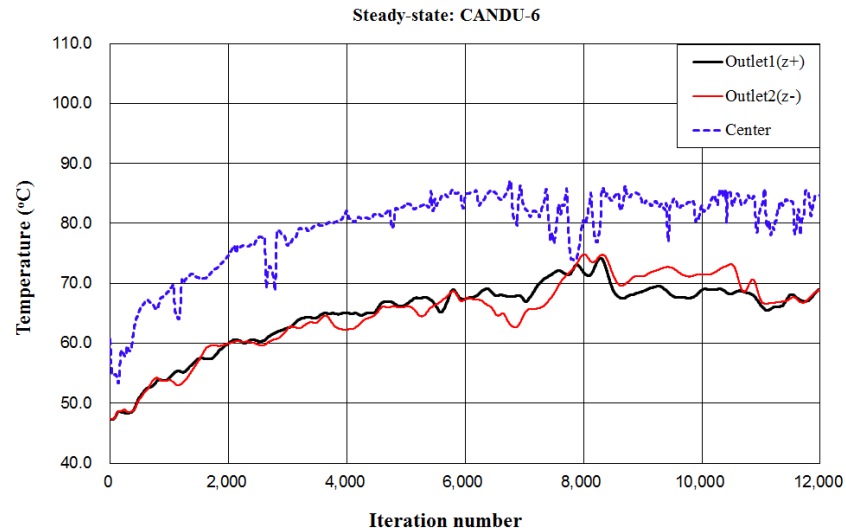
$$f_r(r) = 0.94588 - 0.01989r + 0.0995r^2 - 0.03888r^3 - 0.00256r^4 \quad (0.0 \leq r \leq 3.38 \text{ m})$$

$$f_z(z) = 1.0 - 0.1111z^2 \quad (-3.0 \leq z \leq 3.0 \text{ m})$$

- Boundary/initial conditions
 - Mass flow rate at each inlet = 127.4 kg/s (Total Massflow = 1,019 kg/s)
 - No-slip at the wall
 - Outlet pressure: fixed, & zero-gradient otherwise.
 - Inlet temperature = 47.3 degC
 - Adiabatic at the wall
 - Initially stationary & isothermal.

Moderator circulation flow

- Reference calculation with default options



OpenFOAM solver algorithm

- **Basics solution algorithm of the OpenFOAM solvers**

- ✓ Incompressible momentum equation

$$\frac{\partial}{\partial t}(\mathbf{U}) + \nabla \cdot (\mathbf{U}\vec{U}) + \nabla \cdot \mathbf{T} = -\nabla p + \mathbf{S}$$

- ✓ Discretized momentum equation

$$A_U \mathbf{U} = \mathbf{H}(\mathbf{U}) - \nabla p \quad \leftarrow \quad \mathbf{H}(\mathbf{U}) = -\sum_n A_n \mathbf{U}_n + \mathbf{S}_u$$

- ✓ predictor step

$$\mathbf{U}^* = \frac{\mathbf{H}(\mathbf{U}^*)}{A_U} - \frac{\nabla p}{A_U} \quad \phi^* = \mathbf{U}_f^* \cdot \vec{S}_f = \left(\frac{\mathbf{H}^*}{A_U} \right)_f \cdot \vec{S}_f - \left(\frac{1}{A_U} \nabla p \right)_f \cdot \vec{S}_f$$

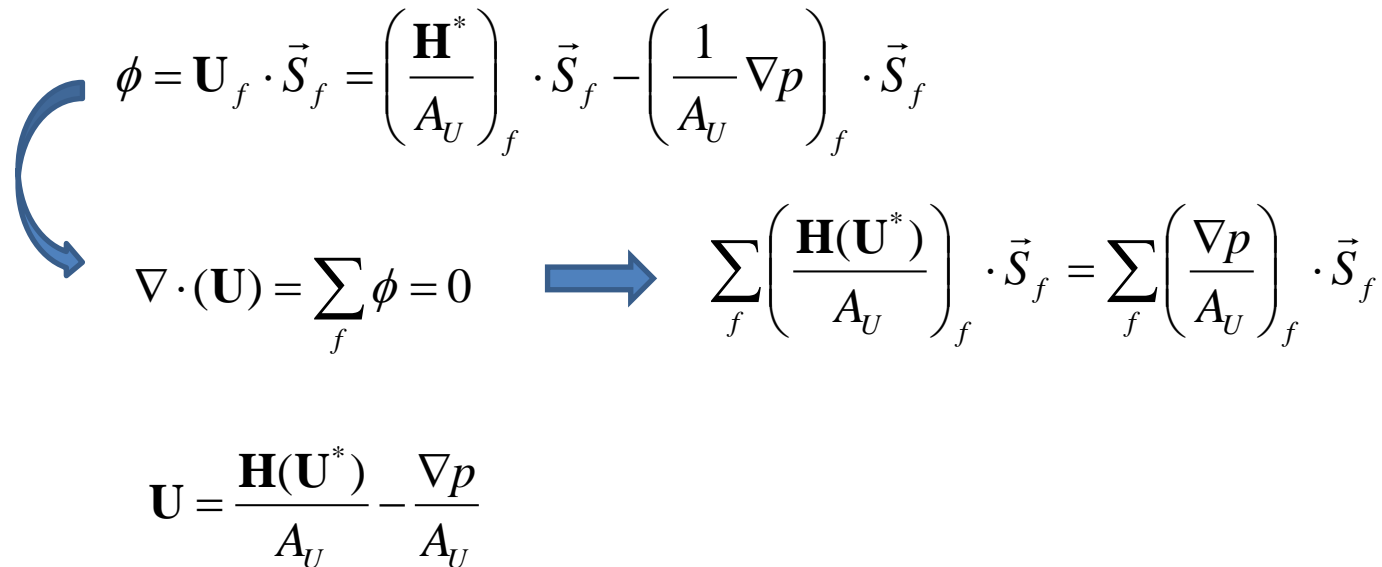
- ✓ Continuity equation

$$\nabla \cdot (\mathbf{U}) = 0$$

OpenFOAM solver algorithm (2)

- Basics solution algorithm of the OpenFOAM solvers

- ✓ Corrector step


$$\phi = \mathbf{U}_f \cdot \vec{S}_f = \left(\frac{\mathbf{H}^*}{A_U} \right)_f \cdot \vec{S}_f - \left(\frac{1}{A_U} \nabla p \right)_f \cdot \vec{S}_f$$
$$\nabla \cdot (\mathbf{U}) = \sum_f \phi = 0 \quad \Rightarrow \quad \sum_f \left(\frac{\mathbf{H}(\mathbf{U}^*)}{A_U} \right)_f \cdot \vec{S}_f = \sum_f \left(\frac{\nabla p}{A_U} \right)_f \cdot \vec{S}_f$$
$$\mathbf{U} = \frac{\mathbf{H}(\mathbf{U}^*)}{A_U} - \frac{\nabla p}{A_U}$$

buoyantBoussinesqSimplefoam

- **Body force**

- ✓ Momentum equation with body force
 - Boussinesq assumption for incompressible flow

momentum eq.
$$\frac{\partial}{\partial t}(\rho \mathbf{U}) + \nabla \cdot (\rho \mathbf{U} \vec{U}) + \nabla \cdot \rho \mathbf{T} = -\nabla p + \rho \mathbf{g} + \rho \mathbf{S}$$


density
$$\rho = \rho_0 - \rho_0 \beta (T - T_0) \quad \longrightarrow \quad \frac{\rho}{\rho_0} = 1 - \beta (T - T_0) = 1 + \rho' = \rho_k$$

apply boussinesq assumption
$$\frac{\partial}{\partial t}(\rho_0 \mathbf{U}) + \nabla \cdot (\rho_0 \mathbf{U} \vec{U}) + \nabla \cdot \rho_0 \mathbf{T} = -\nabla p + \rho \mathbf{g} + \rho_0 \mathbf{S}$$

divide by ρ_0
$$\frac{\partial}{\partial t}(\mathbf{U}) + \nabla \cdot (\mathbf{U} \vec{U}) + \nabla \cdot \mathbf{T} = -\nabla p' + \rho_k \mathbf{g} + \mathbf{S}$$

● Body force

- ✓ Momentum equation with body force
 - Boussinesq assumption for incompressible flow

momentum eq. $\frac{\partial}{\partial t}(\mathbf{U}) + \nabla \cdot (\mathbf{U}\vec{U}) + \nabla \cdot \mathbf{T} = -\nabla p + \rho_k \mathbf{g} + \mathbf{S}$  $p' \Rightarrow p$

pressure and body force $-\nabla p + \rho_k \mathbf{g} = -\nabla(p - \rho_k gh) - gh \nabla \rho_k = -\nabla p_{rgh} - gh \nabla \rho_k$

modified momentum eq. $\frac{\partial}{\partial t}(\mathbf{U}) + \nabla \cdot (\mathbf{U}\vec{U}) + \nabla \cdot \mathbf{T} = -\nabla p_{rgh} - gh \nabla \rho_k + \mathbf{S}$

discretised momentum eq. $A_U \mathbf{U} = \mathbf{H}(\mathbf{U}) - \nabla p_{rgh} - gh \nabla \rho_k$

Body force induced problem

- Body force is strongly coupled with pressure gradient
 - ✓ Especially in low-momentum flow such as a natural convection, pressure gradient from the body force is bigger
 - ✓ In some cases, flow near wall is contaminated because of its low momentum
 - solution problem
 - checker-boarding pressure field
 - decoupling of pressure and velocity field
 - remedy
 - body force added on cell faces for the non-staggered mesh method
 - body force weighted pressure interpolation
 - wall pressure extrapolation using body force

$$p_b = p_0 + \nabla p_0 \cdot d\vec{s}_0 \quad \nabla p_0 = \rho \mathbf{g}$$

- cell-face pressure interpolation (*Numerical Heat transfer B 68, 2015*)

$$p_f = \frac{1}{2}(p_l + p_r) \quad p_l = p_i + \rho_i \mathbf{g} \cdot d\vec{r}_i \quad p_r = p_j + \rho_j \mathbf{g} \cdot d\vec{r}_j$$

p_{rgh} in buoyantBoussinesqSimpleFoam

● Pressure

- ✓ Pressure changed by
 - hydrodynamic, hydrostatic, thermodynamic et al.
- ✓ Pressure equation in buoyantBoussinesqSimpleFoam
 - hydrodynamic pressure

$$p_{rgh} = p - \rho_k gh$$

- ✓ on wall, $\mathbf{U} \approx 0$, then momentum equation becomes
 - In general solver

$$-\nabla p + \rho_k \mathbf{g} = 0 \quad \Rightarrow \quad \nabla p \cdot \vec{S}_f = \frac{dp}{dn} S_f = \rho_k \mathbf{g} \cdot \vec{S}_f \quad \Rightarrow \quad \frac{dp}{dn} = \rho_k \mathbf{g} \cdot \hat{n}$$

- In OpenFOAM

$$-\nabla p_{rgh} - gh \nabla \rho_k = 0 \quad \Rightarrow \quad \nabla p_{rgh} \cdot \vec{S}_f = -gh \nabla \rho_k \cdot \vec{S}_f \quad \Rightarrow \quad \frac{dp_{rgh}}{dn} = -gh \frac{d\rho_k}{dn}$$

- implemented in the solver and fixedFluxPressureFvPatch



Convergence problem

- **Solution oscillating**

- ✓ Physical oscillation → must be captured
- ✓ numerical oscillation → must be removed
- ✓ But sometimes it is difficult to distinguish the physical and numerical oscillation

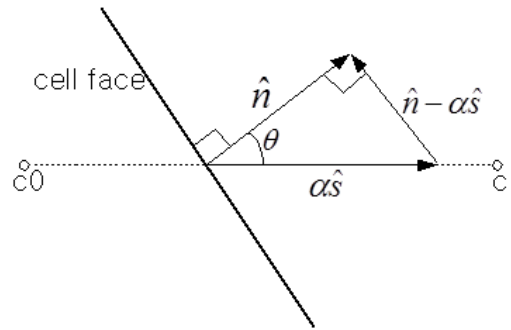
- **Why not converged or oscillating?**

- ✓ numerical schemes problem
- ✓ mesh non-orthogonality problem
- ✓ p-U/p-T-U coupling problem
- ✓ initialization problem
- ✓ physical model problem such as a turbulence model

Non-orthogonality correction in OpenFOAM

- **Need for non-orthogonality correction**

- ✓ Cross diffusion of the pressure Laplacian term is increased



- **It is different from standard SIMPLE algorithm**

- ✓ In standard SIMPLE algorithm pressure correction eq. is solved
- ✓ Before solving p' eq. it is not known

- **OpenFOAM solves pressure equation**

- ✓ Cross diffusion of the pressure Laplacian term can be calculated before solving the pressure equation

Modification of OpenFOAM solvers

● Pressure relaxation

- ✓ Before or after momentum correction? (NextFoam 길재흥, 2015 OKUCC)
- ✓ Many SIMPLE-based CFD codes do the p-relaxation after the velocity correction.

flux update
U update
pressure relax

- ✓ OpenFOAM does the p-relaxation before the velocity update .

flux update → $\phi = \phi H_{byA} - p_{rghEqn}.flux();$
p relax → $p_{rgh}.relax();$
U update → $U = H_{byA} + rAU*fvc::reconstruct((\phi_{ig} - p_{rghEqn}.flux())/rAUf)$

- ✓ Modified solver

$\phi = \phi H_{byA} - p_{rghEqn}.flux();$
 $U = H_{byA} + rAU*fvc::reconstruct((\phi_{ig} - p_{rghEqn}.flux())/rAUf)$
 $p_{rgh}.relax();$



Improvement of pressure implicitness

- Discretized momentum equation

$$A_U \mathbf{U}^* = \mathbf{H}(\mathbf{U}^*) - \nabla p^m$$

- ✓ \mathbf{U}^* is predicted value
- ✓ but, p^m is previous value. \Rightarrow semi-implicit

- Additional pressure equation

$$A_U \mathbf{U}^m = \mathbf{H}(\mathbf{U}^m) - \nabla p^*$$

- ✓ Before solving the momentum eq., construct pressure equation

$$\phi = \mathbf{U}_f^m \cdot \vec{S}_f = \left(\frac{\mathbf{H}(\mathbf{U}^m)}{A_U} \right)_f \cdot \vec{S}_f - \left(\frac{1}{A_U} \nabla p^* \right)_f \cdot \vec{S}_f \Rightarrow \sum_f \left(\frac{\mathbf{H}(\mathbf{U}^m)}{A_U} \right)_f \cdot \vec{S}_f = \sum_f \left(\frac{\nabla p^*}{A_U} \right)_f \cdot \vec{S}_f$$

- ✓ Now, we get a guessed pressure

$$A_U \mathbf{U}^* = \mathbf{H}(\mathbf{U}^*) - \nabla p^*$$

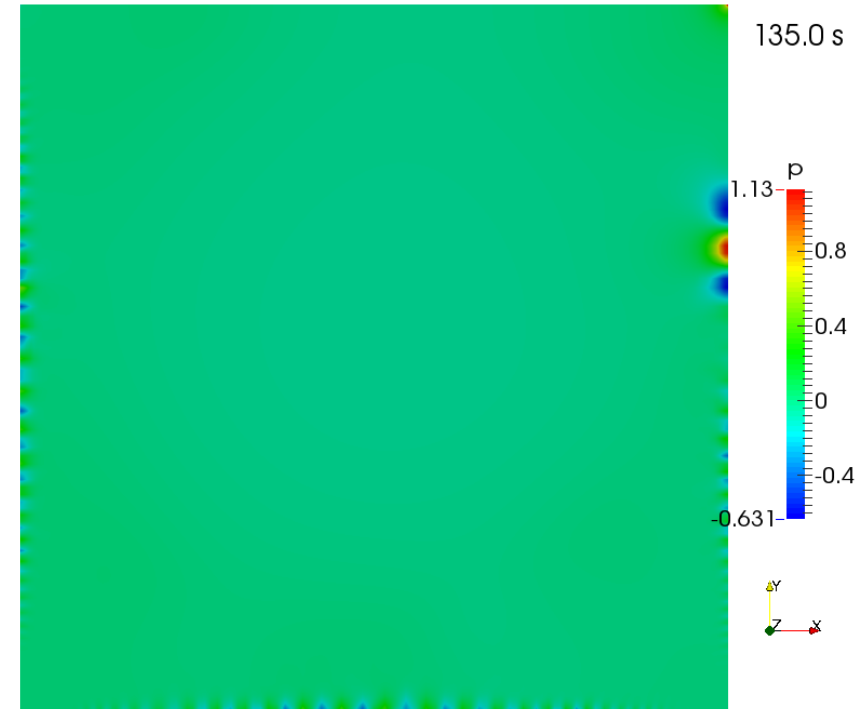
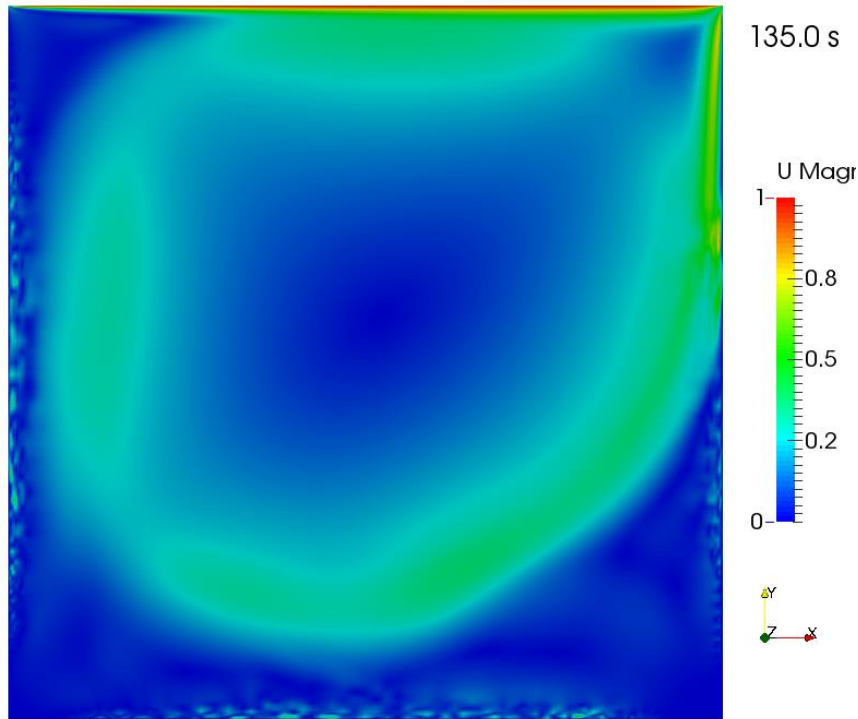
- **OpenFOAM version for numerical test**
 - ✓ OpenFOAM 2.4
 - ✓ OpenFOAM 3.0
 - ✓ OpenFOAM dev
- **OpenFOAM solvers for numerical test**
 - ✓ simpleFoam
 - ✓ buoyantBoussinesqSimpleFoam
 - ✓ buoyantBoussinesqPimpleFoam
 - ✓ buoyantSimpleFoam
 - ✓ buoyantPimpleFoam



- **OpenFOAM version**
 - ✓ OpenFOAM dev
- **Solver modification**
 - ✓ additional pressure prediction before solving momentum eq.
- **Test case**
 - ✓ lid-driven cavity flow problem
 - $Re = 10,000$

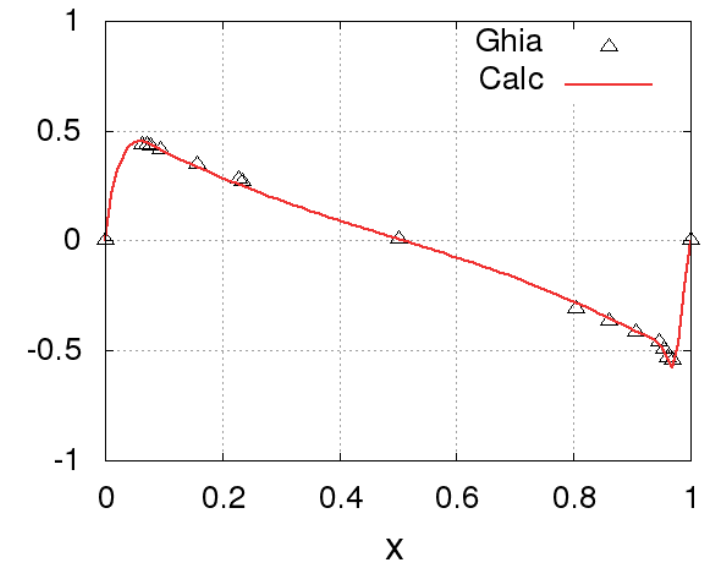
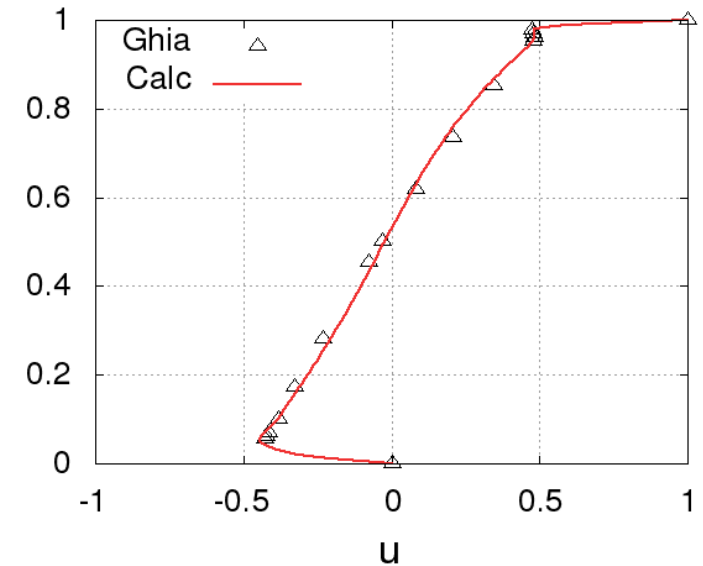
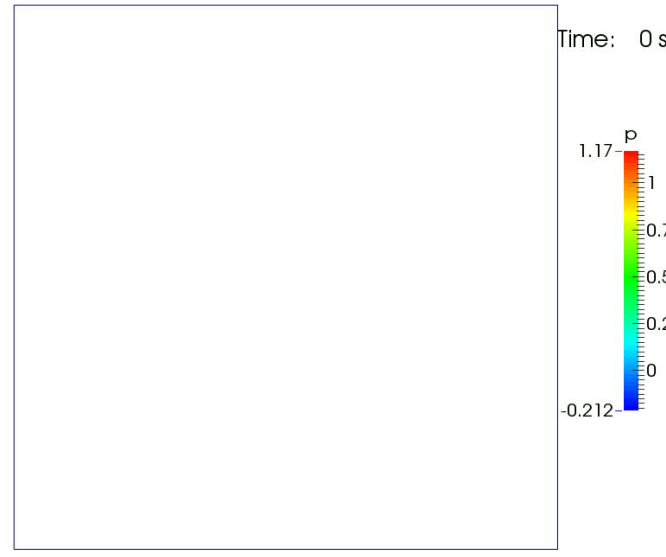
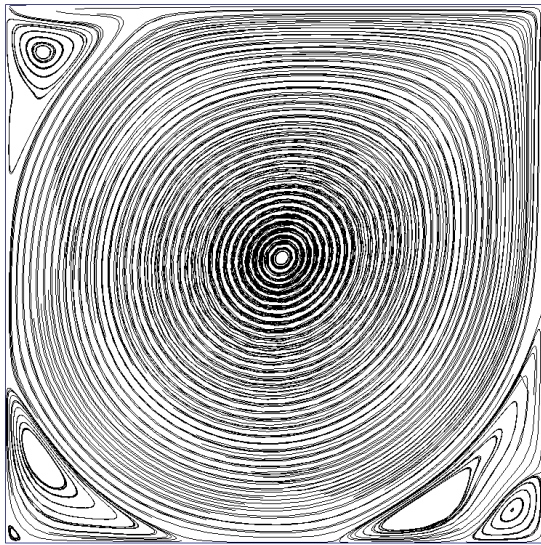
Lid-driven cavity flow

- Solver: pimpleFoam
- max Co number 50
 - ✓ run in PISO mode
- checker-board in pressure and velocity fields



Lid-driven cavity flow (2)

- Solver: modified pimplefoam
- max Co number 50
 - ✓ run in PISO mode
- checker-board in pressure and velocity >

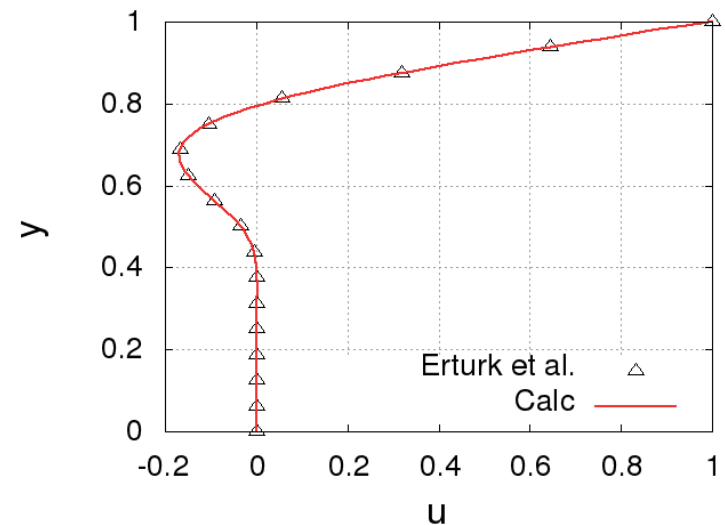
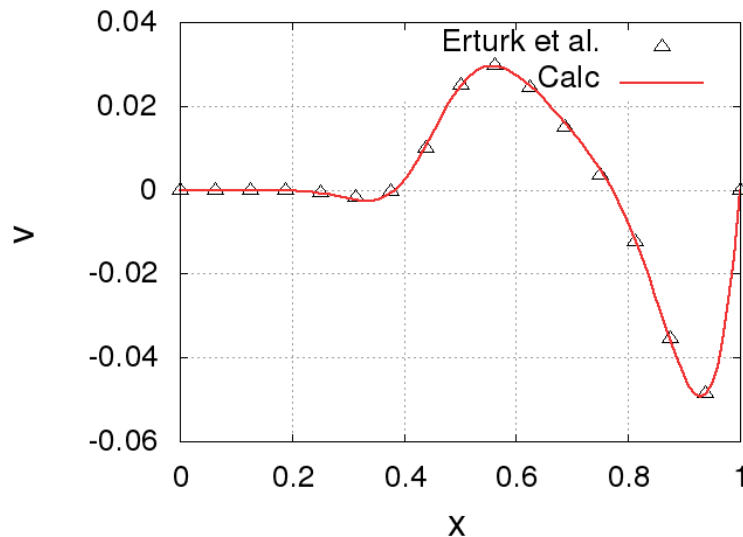
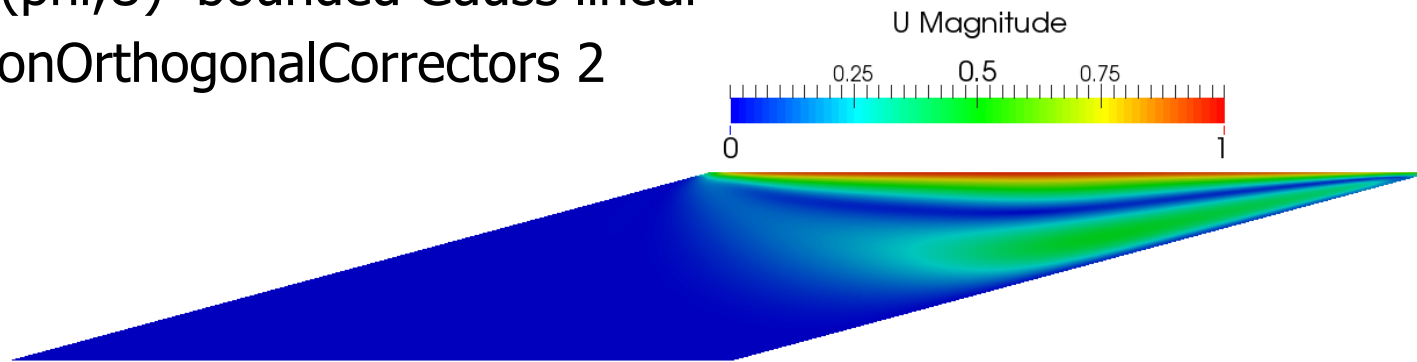




- **OpenFOAM version**
 - ✓ OpenFOAM dev
- **Solver modification**
 - ✓ additional pressure prediction before solving momentum eq.
- **Test case**
 - ✓ Skewed lid-driven cavity flow
 - cavity skew angle: 15°
 - $Re = 1 \times 10^3$



- Solver: standard simpleFoam
- Numerical schemes
 - ✓ $\text{div}(\phi, U)$ bounded Gauss linear
 - ✓ nNonOrthogonalCorrectors 2





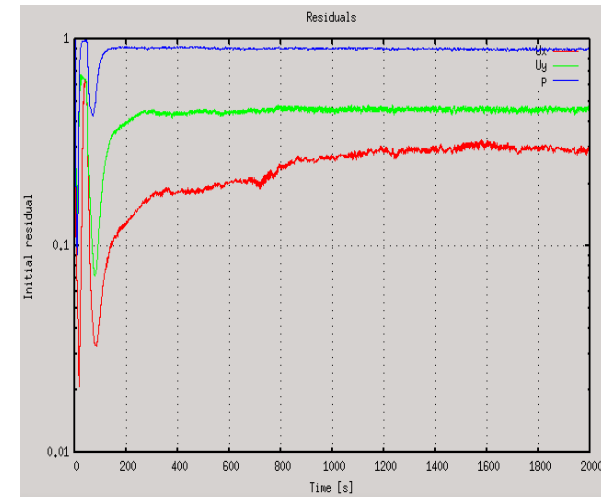
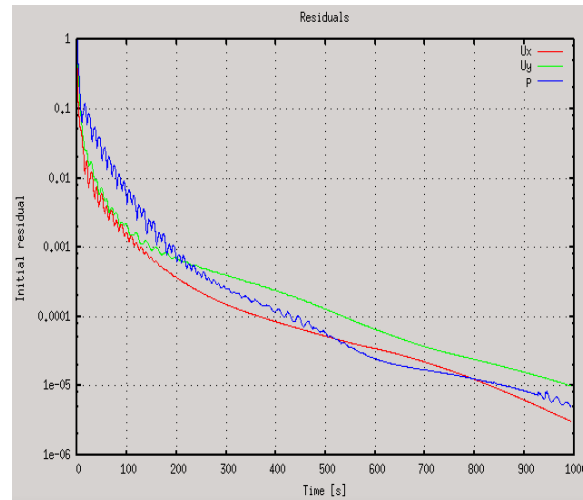
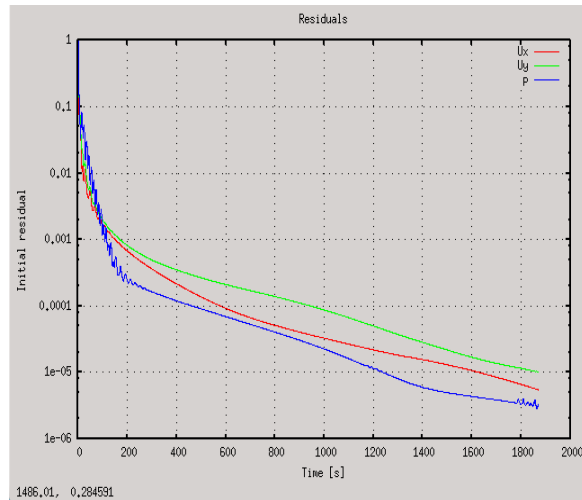
simpleFoam

$$\omega_p = 0.5, \quad \omega_U = 0.5$$

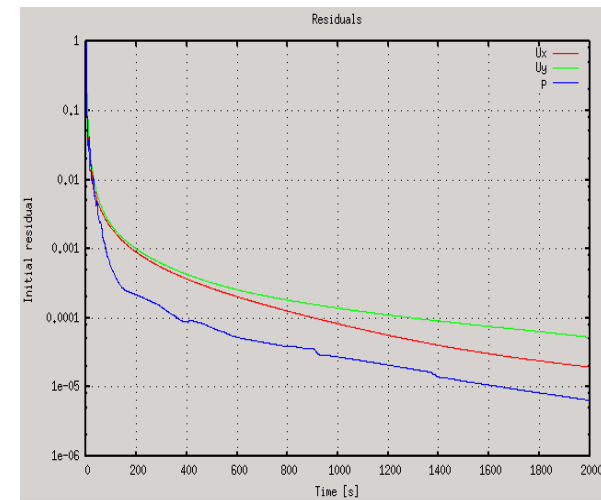
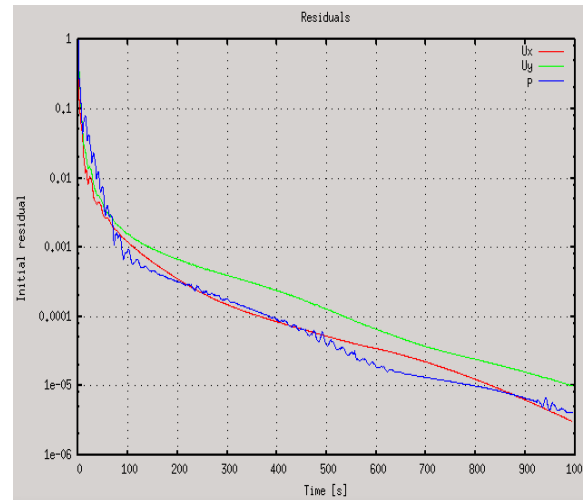
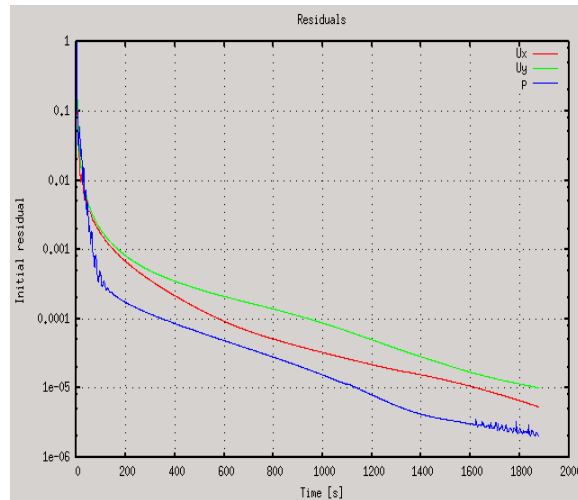
$$\omega_p = 0.3, \quad \omega_U = 0.7$$

$$\omega_p = 0.7, \quad \omega_U = 0.3$$

standard



modified





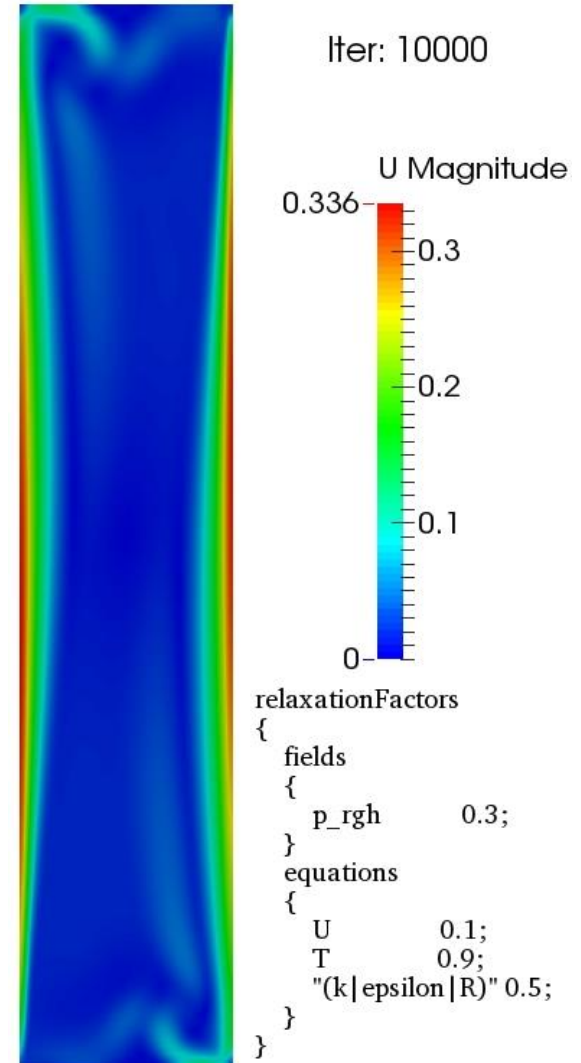
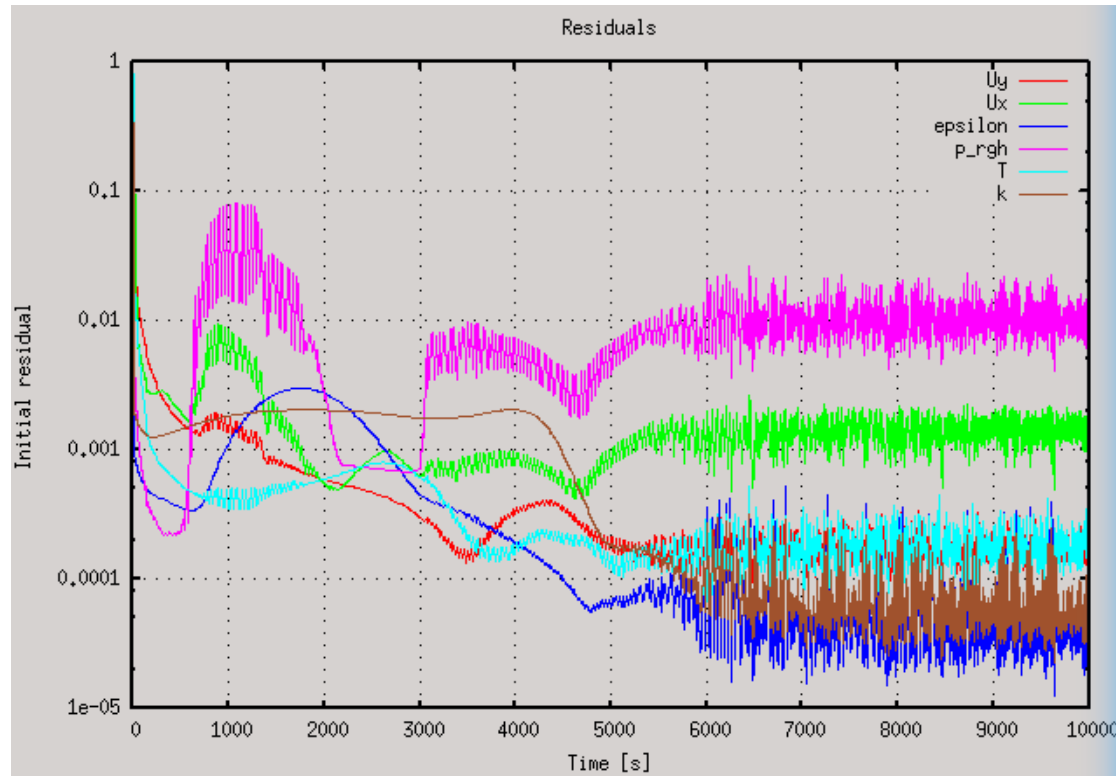
buoyantBoussinesqSimpleFoam

- **OpenFOAM version**
 - ✓ OpenFOAM 2.4
- **Solver modification**
 - ✓ pressure relaxation after velocity update
- **Test case**
 - ✓ King's natural convection problem
 - $Ra = 4.3 \times 10^{10}$
 - $Pr = 0.71$

Convergence characteristics (2)

buoyantBoussinesqSimpleFoam

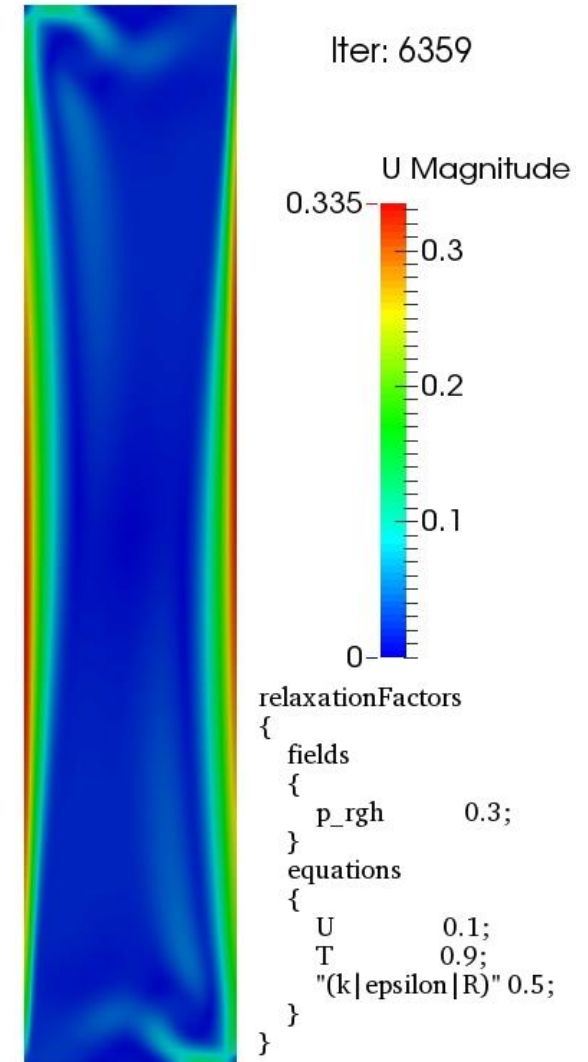
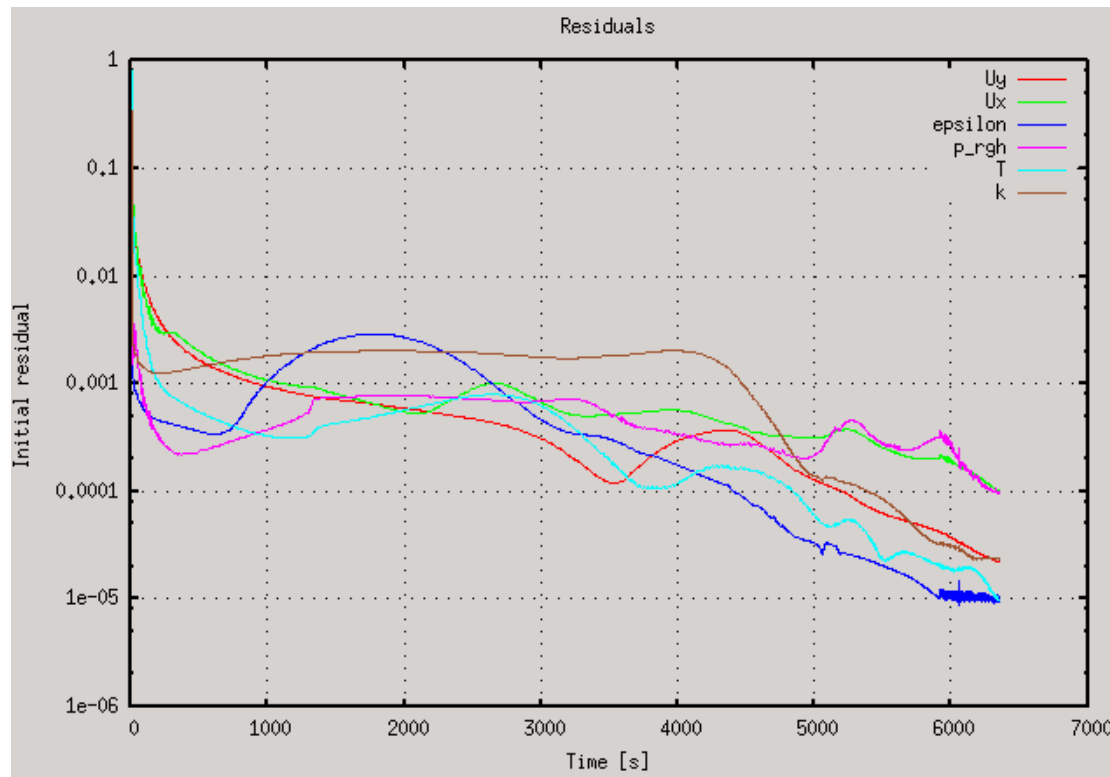
$$\omega_p = 0.3, \quad \omega_U = 0.1$$



Convergence characteristics

modified buoyantBoussinesqSimpleFoam

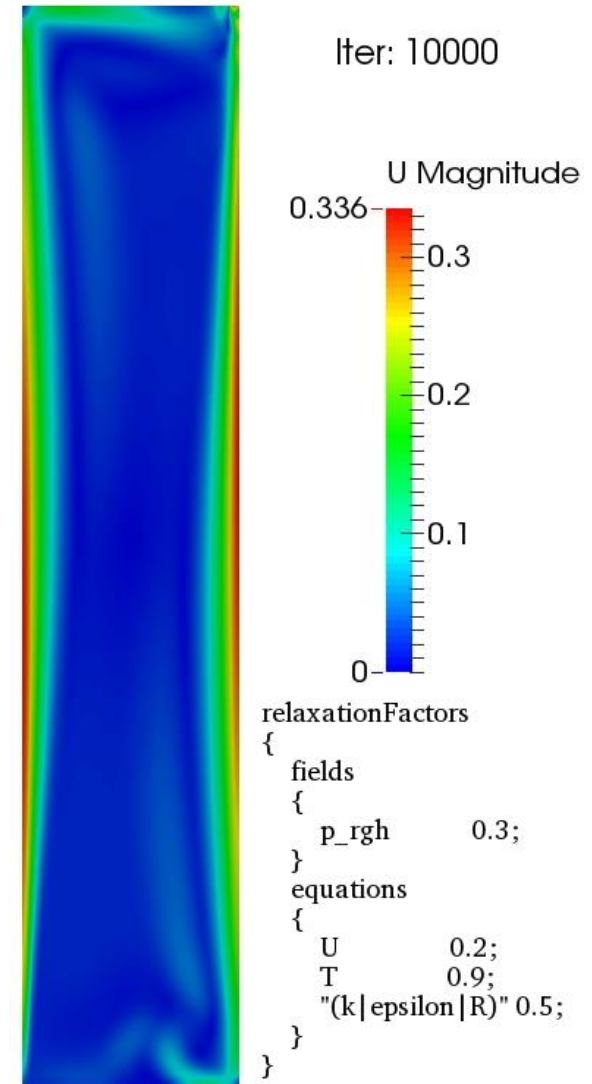
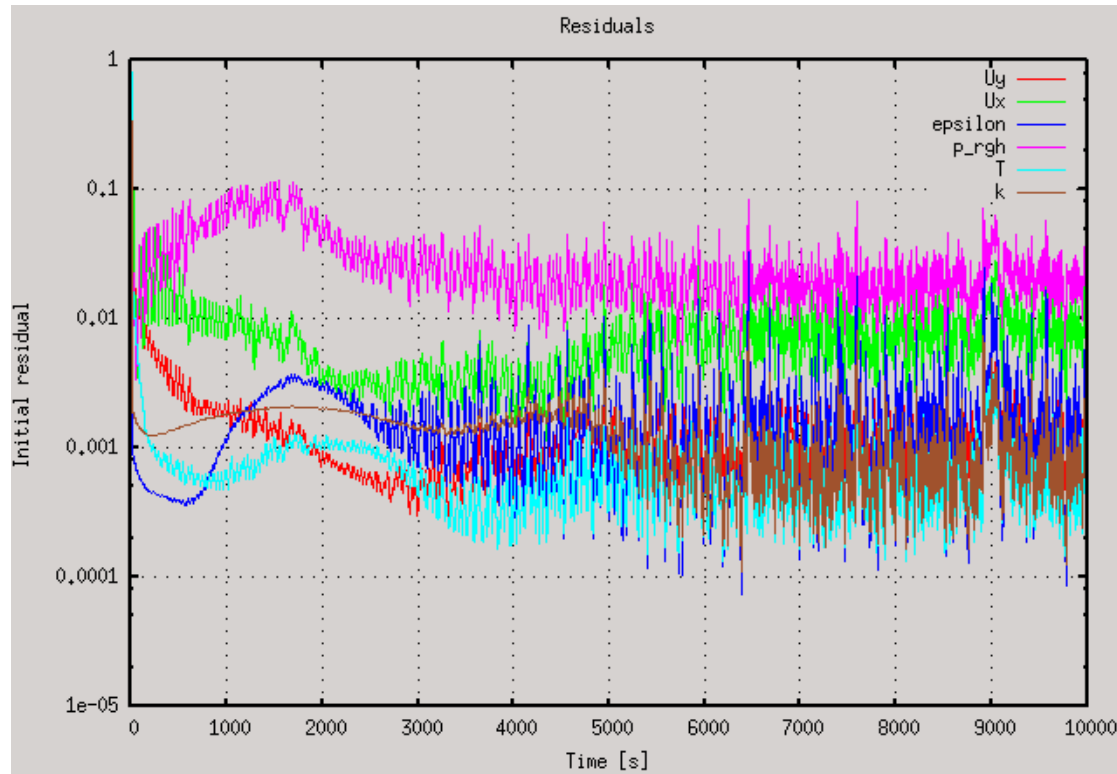
$$\omega_p = 0.3, \quad \omega_U = 0.1$$



Convergence characteristics (4)

buoyantBoussinesqSimpleFoam

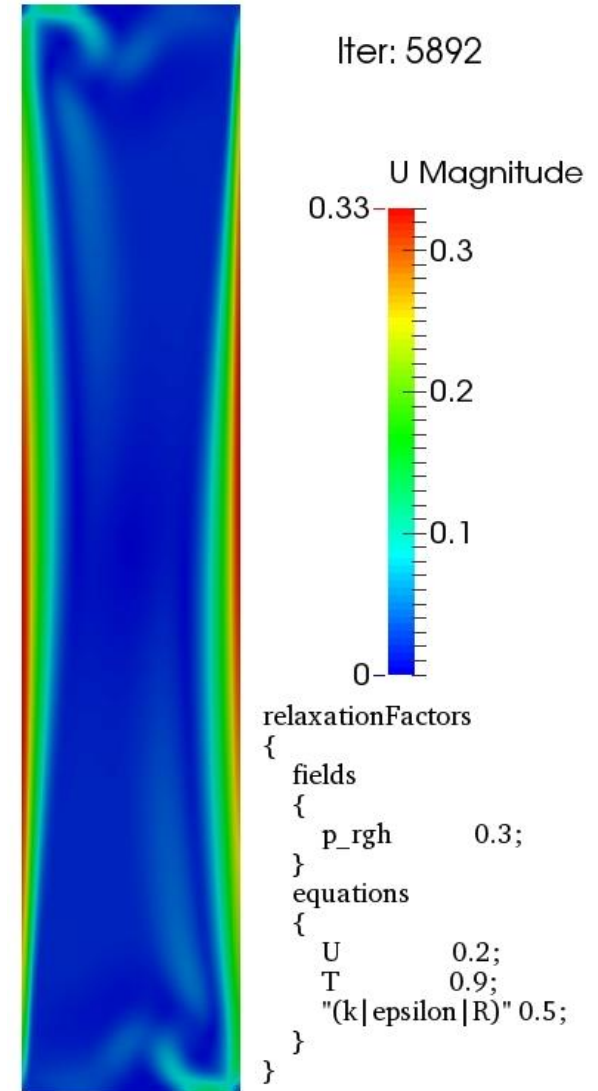
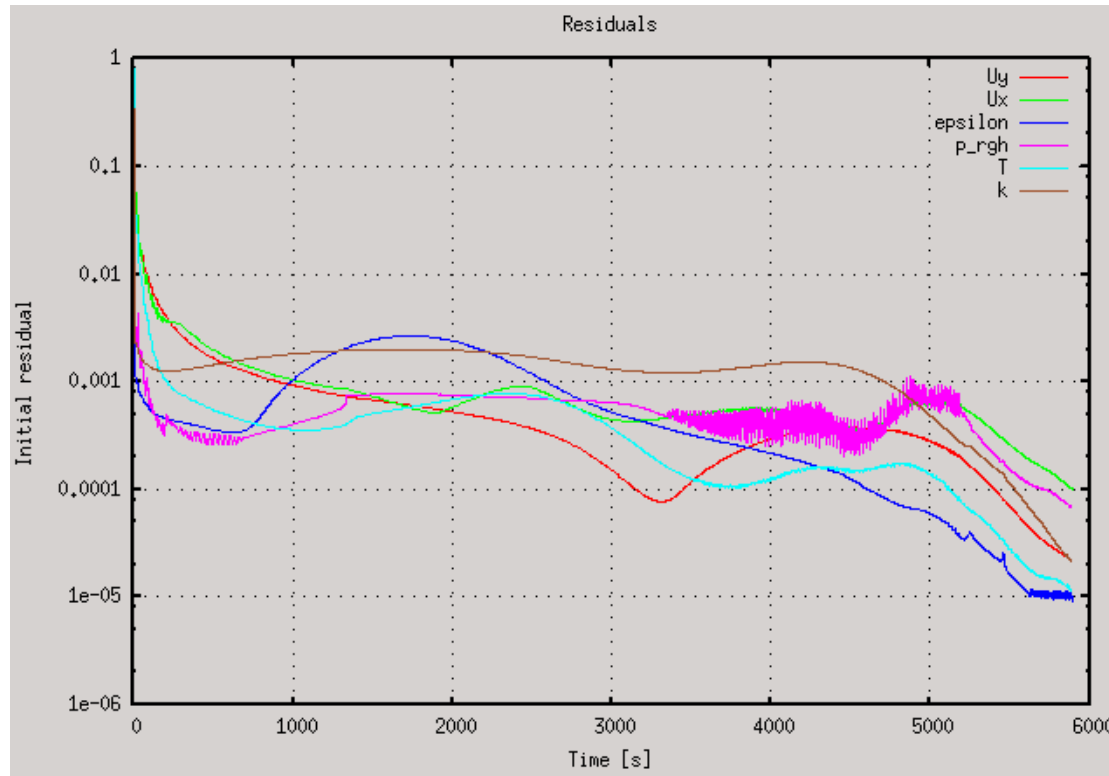
$$\omega_p = 0.3, \quad \omega_U = 0.2$$



Convergence characteristics (3)

modified buoyantBoussinesqSimpleFoam

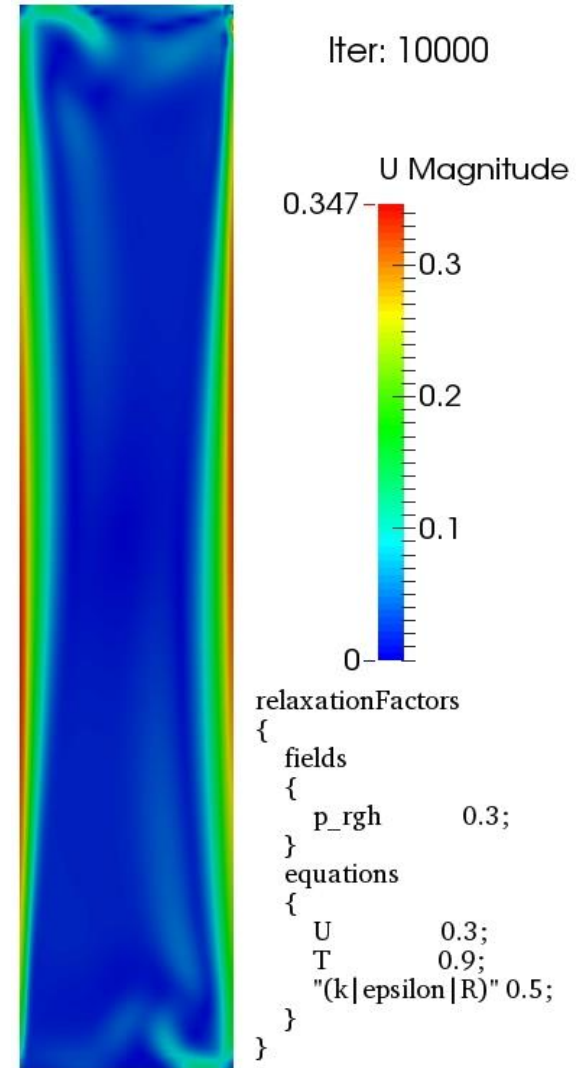
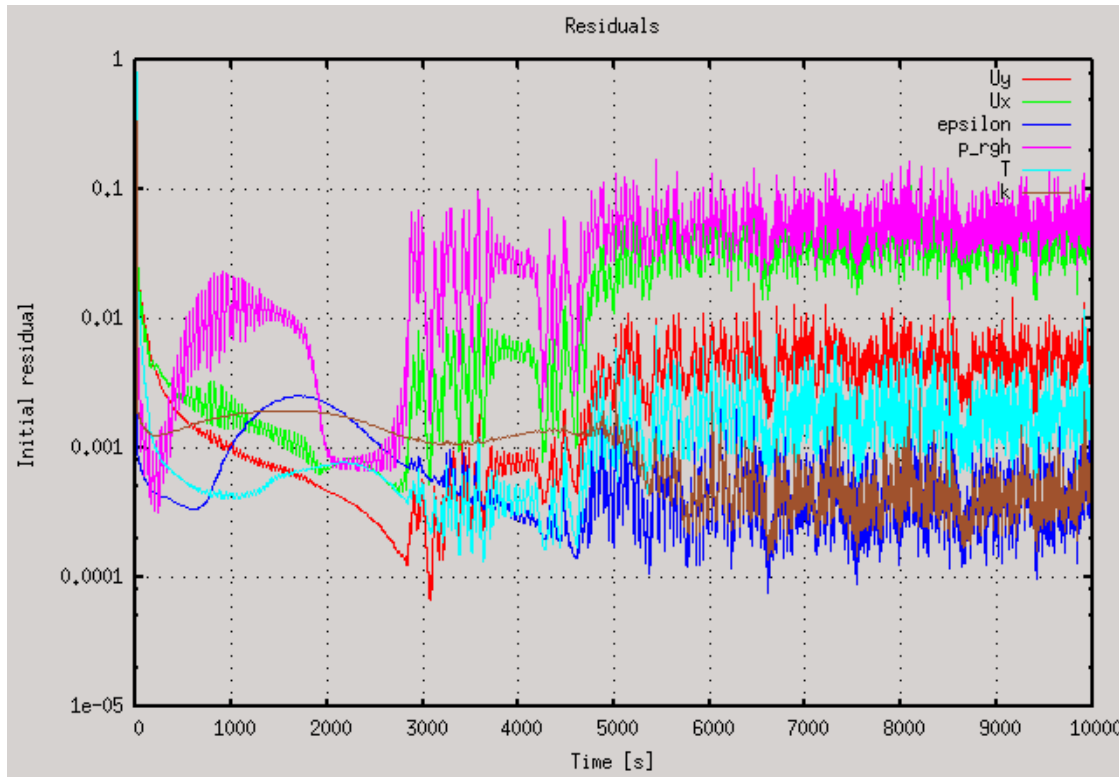
$$\omega_p = 0.3, \quad \omega_U = 0.2$$



Convergence characteristics (5)

modified buoyantBoussinesqSimpleFoam

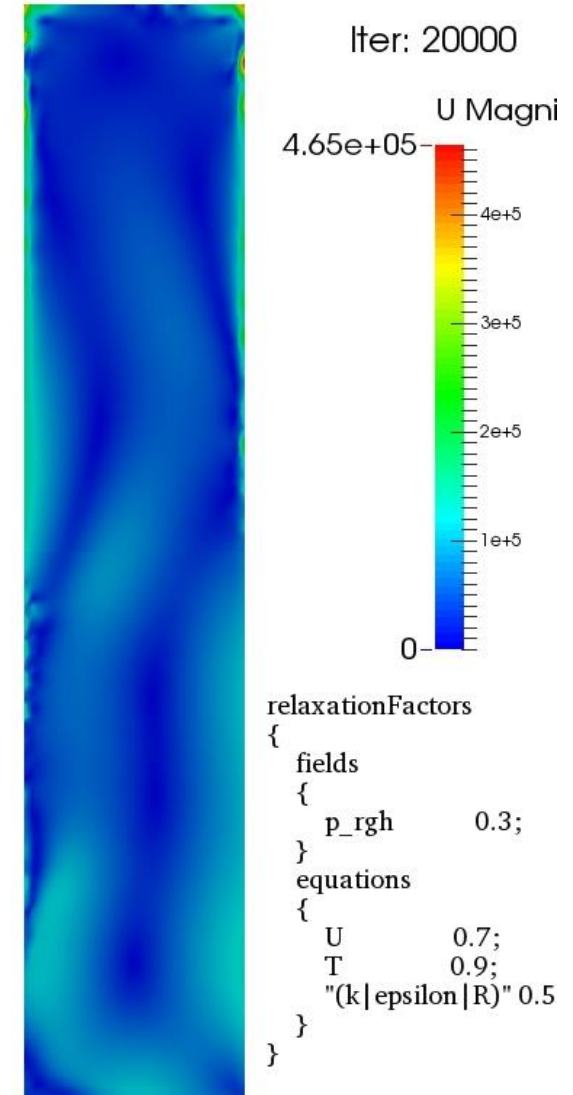
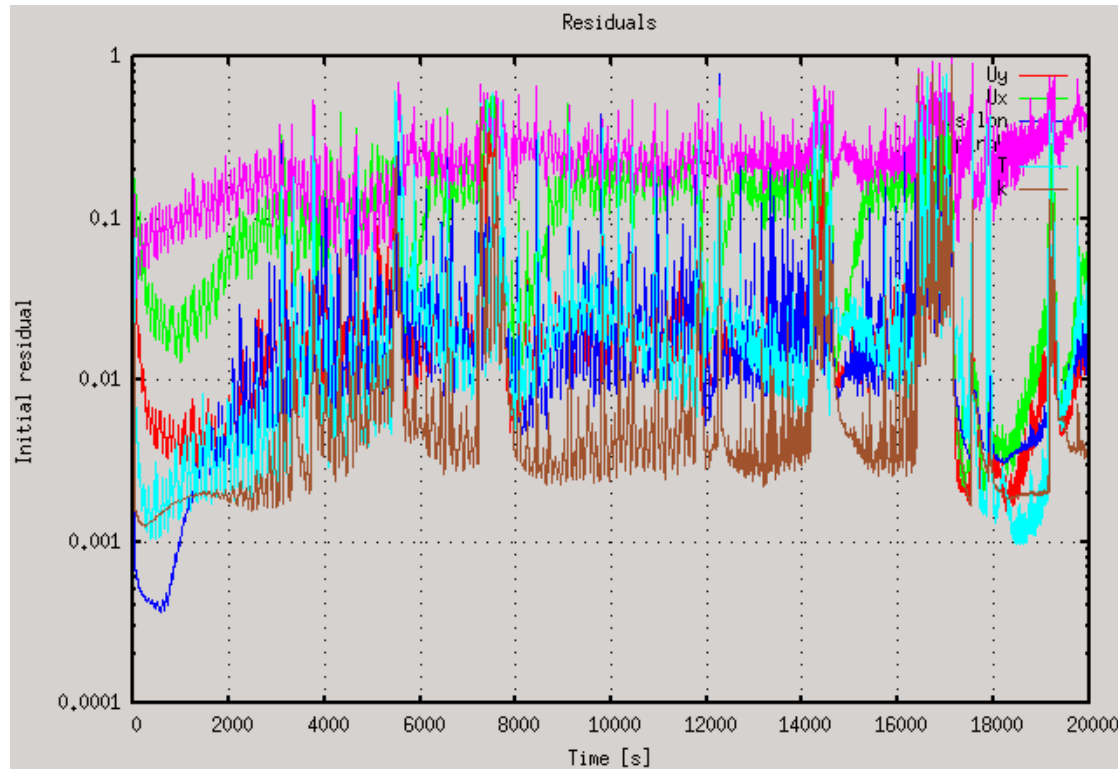
$$\omega_p = 0.3, \quad \omega_U = 0.3$$



Convergence characteristics (6)

modified buoyantBoussinesqSimpleFoam

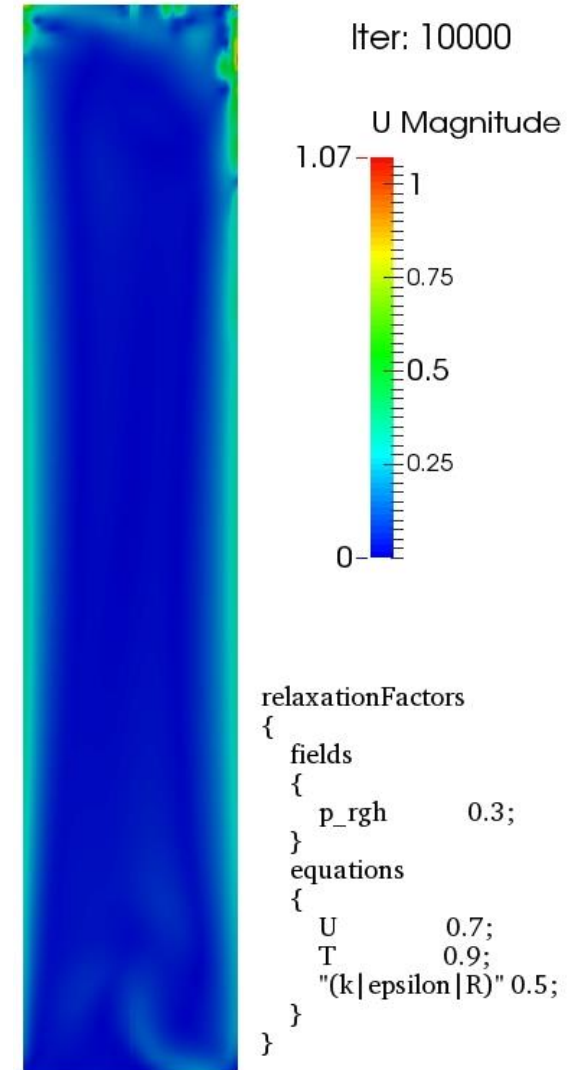
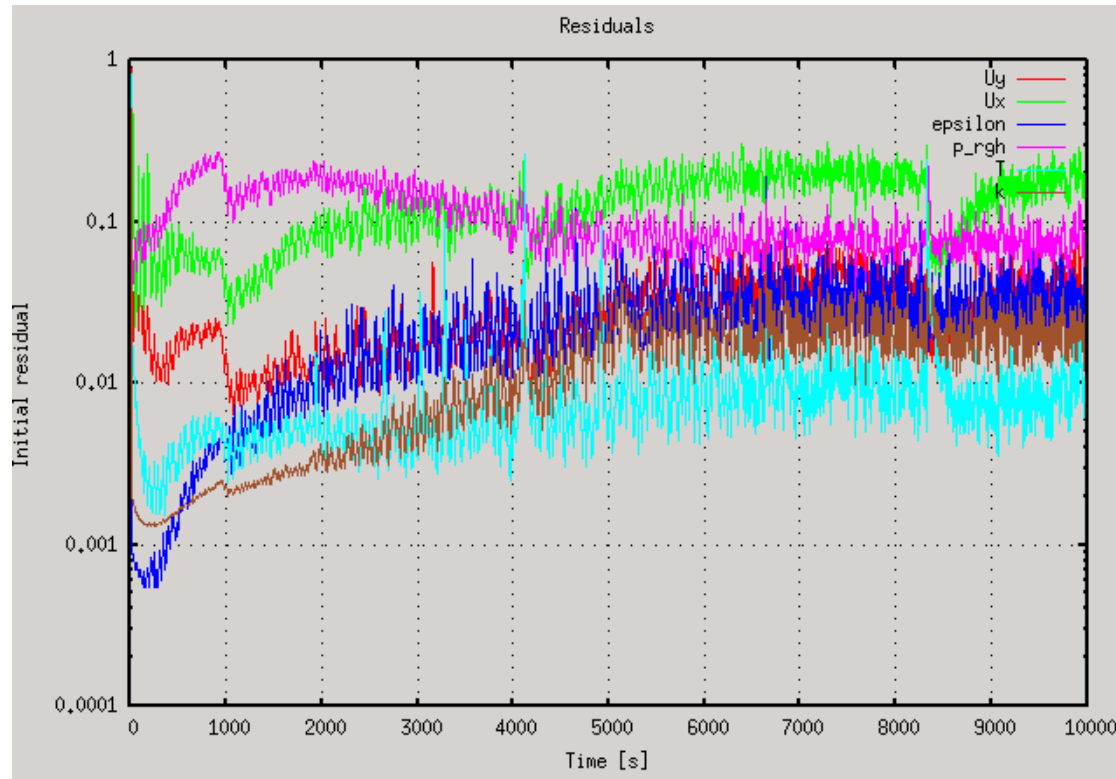
$$\omega_p = 0.3, \quad \omega_U = 0.7$$



Convergence characteristics (7)

buoyantBoussinesqSimpleFoam

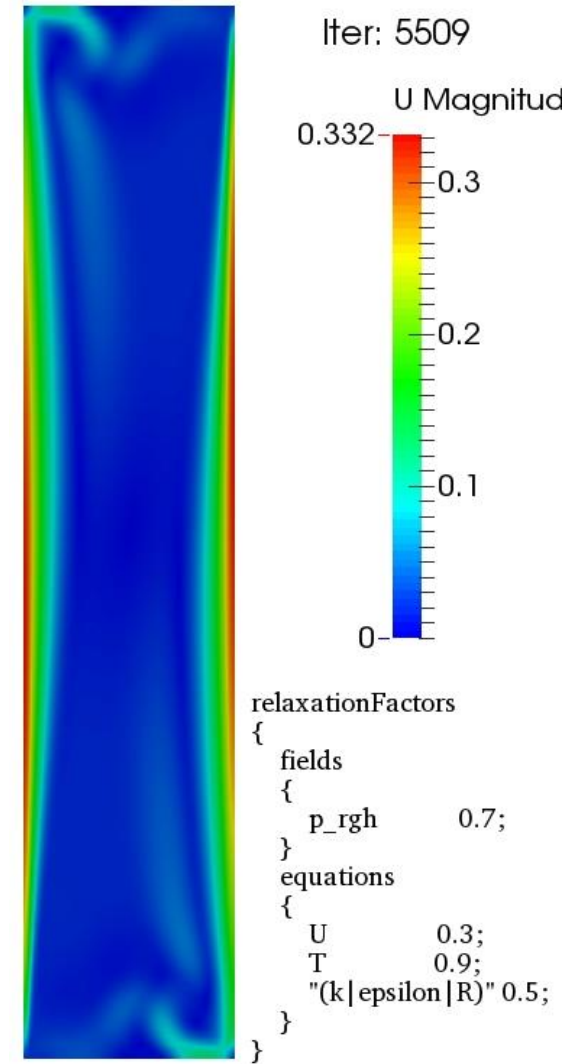
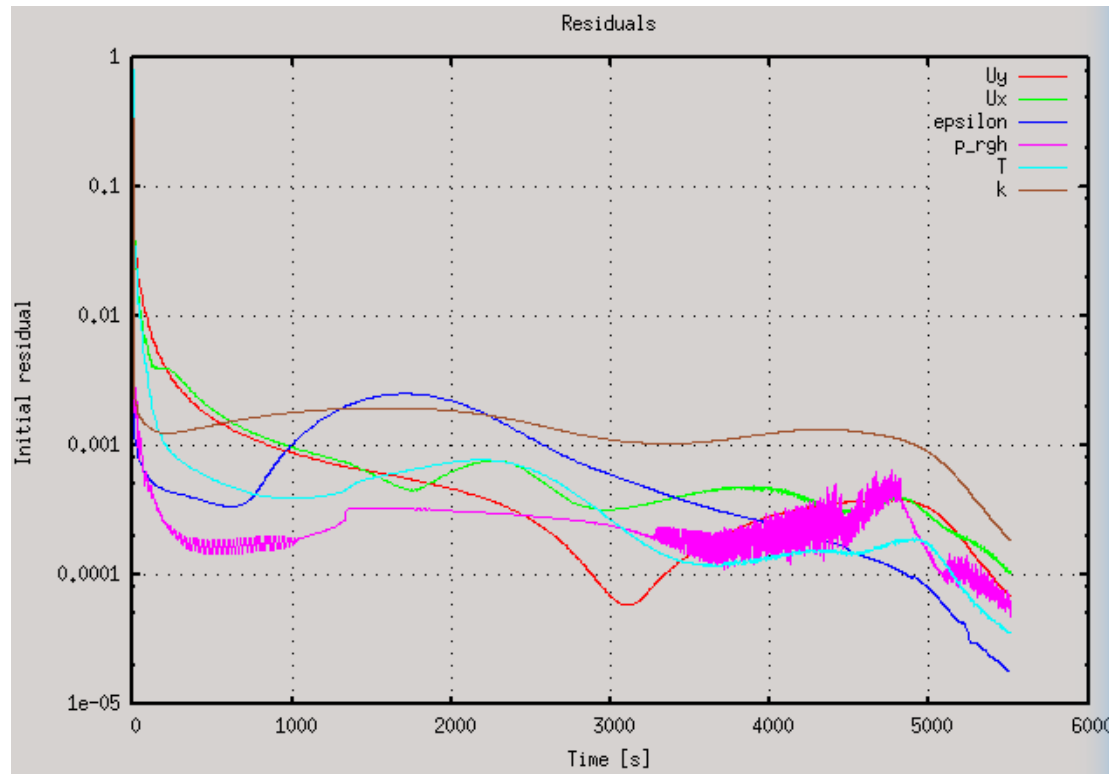
$$\omega_p = 0.3, \quad \omega_U = 0.7$$



Convergence characteristics (9)

modified buoyantBoussinesqSimpleFoam

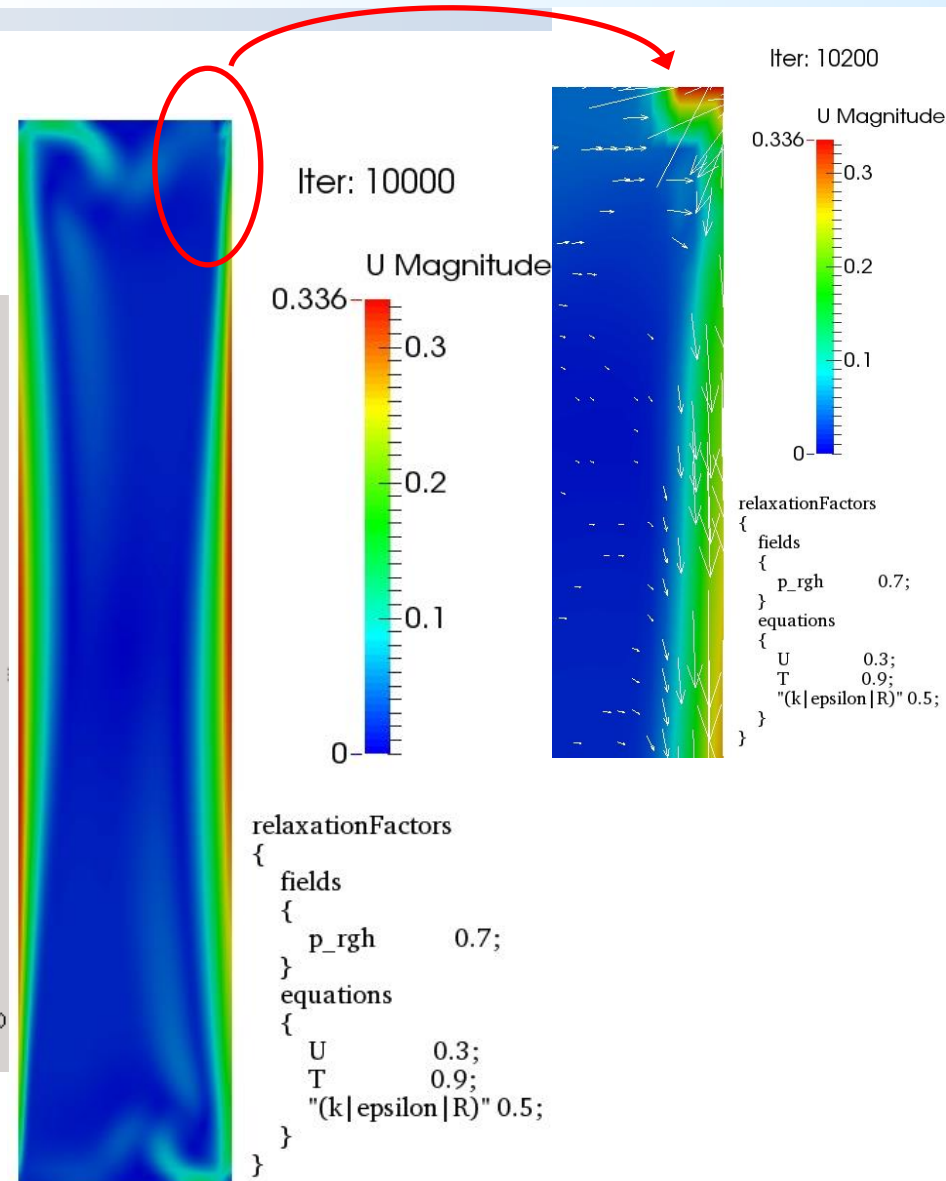
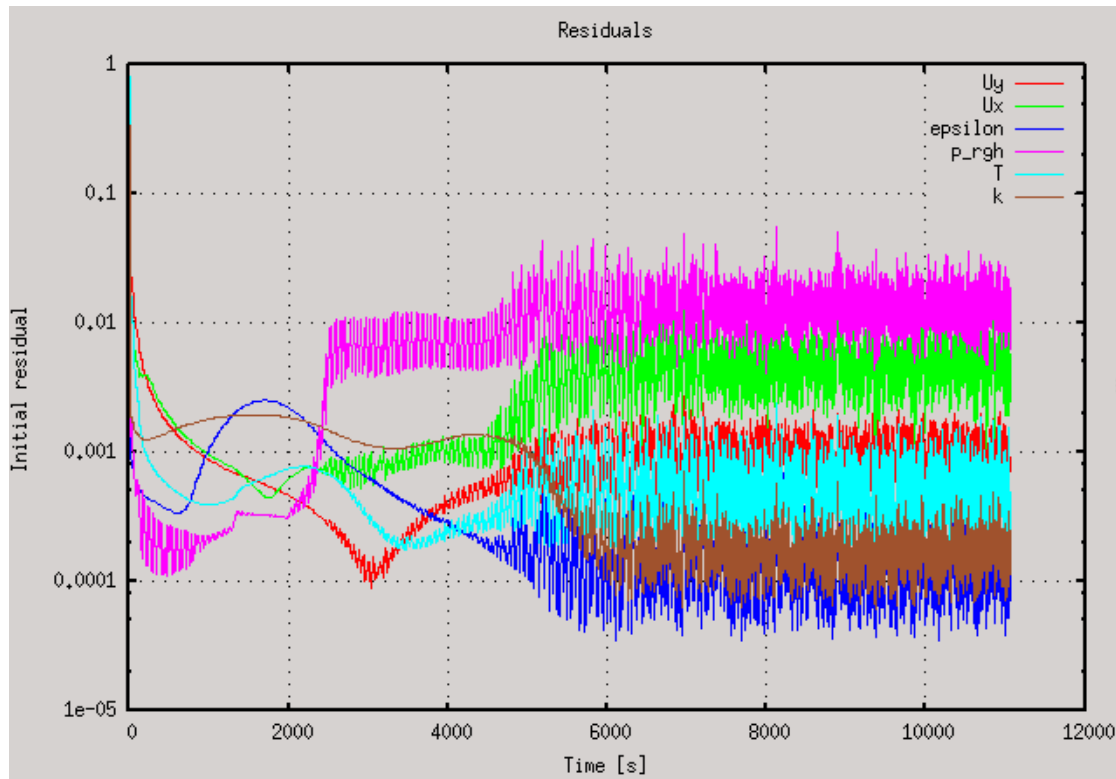
$$\omega_p = 0.7, \quad \omega_U = 0.3$$



Convergence characteristics (9)

buoyantBoussinesqSimpleFoam

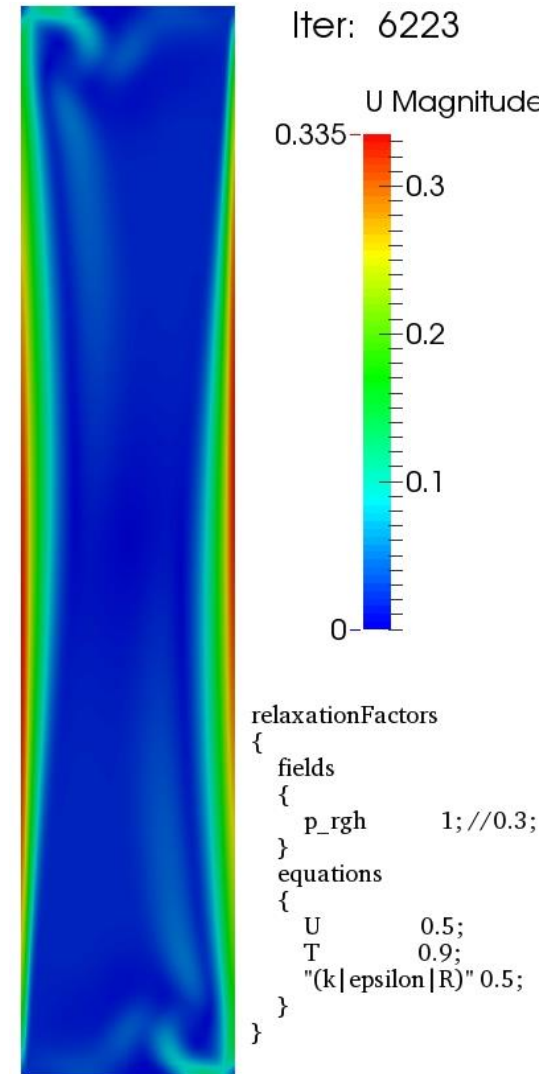
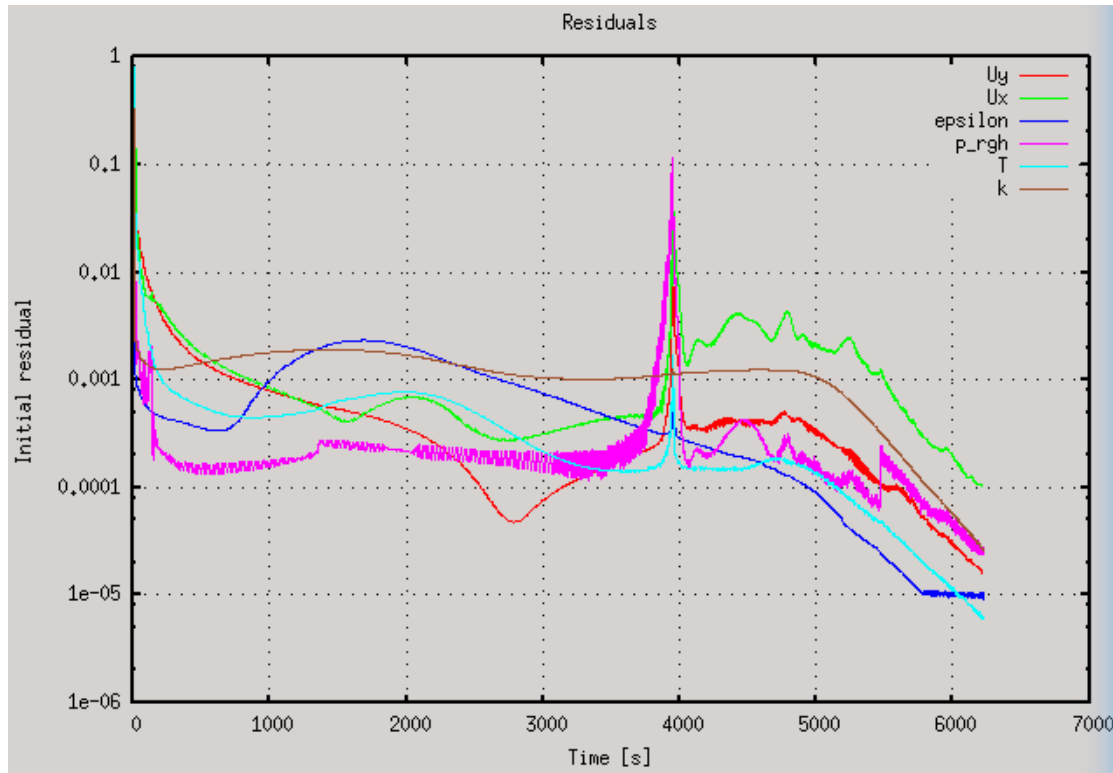
$$\omega_p = 0.7, \quad \omega_U = 0.3$$



Convergence characteristics (8)

modified buoyantBoussinesqSimpleFoam

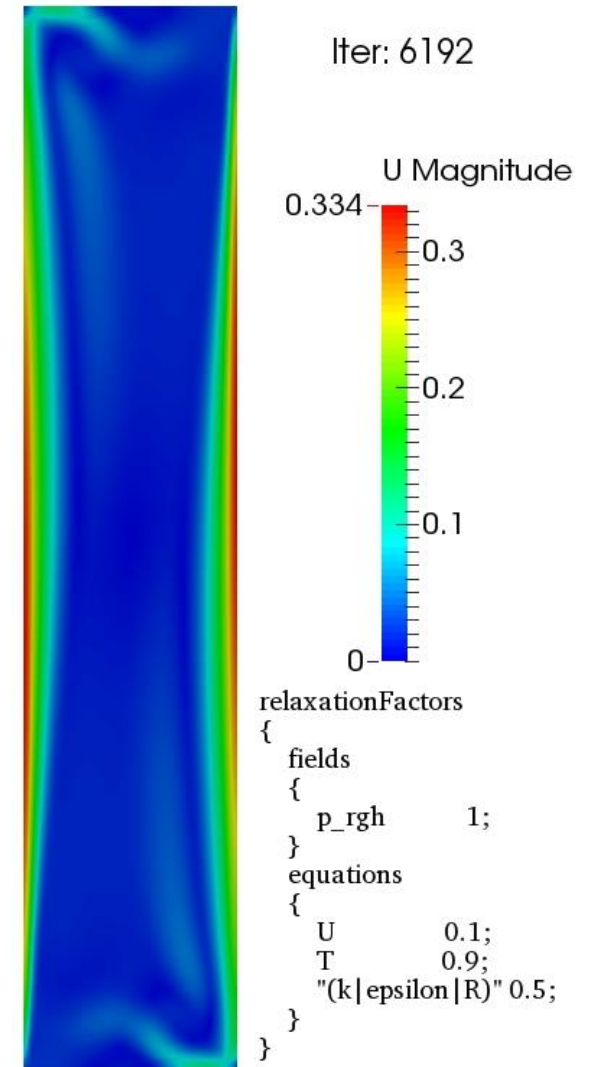
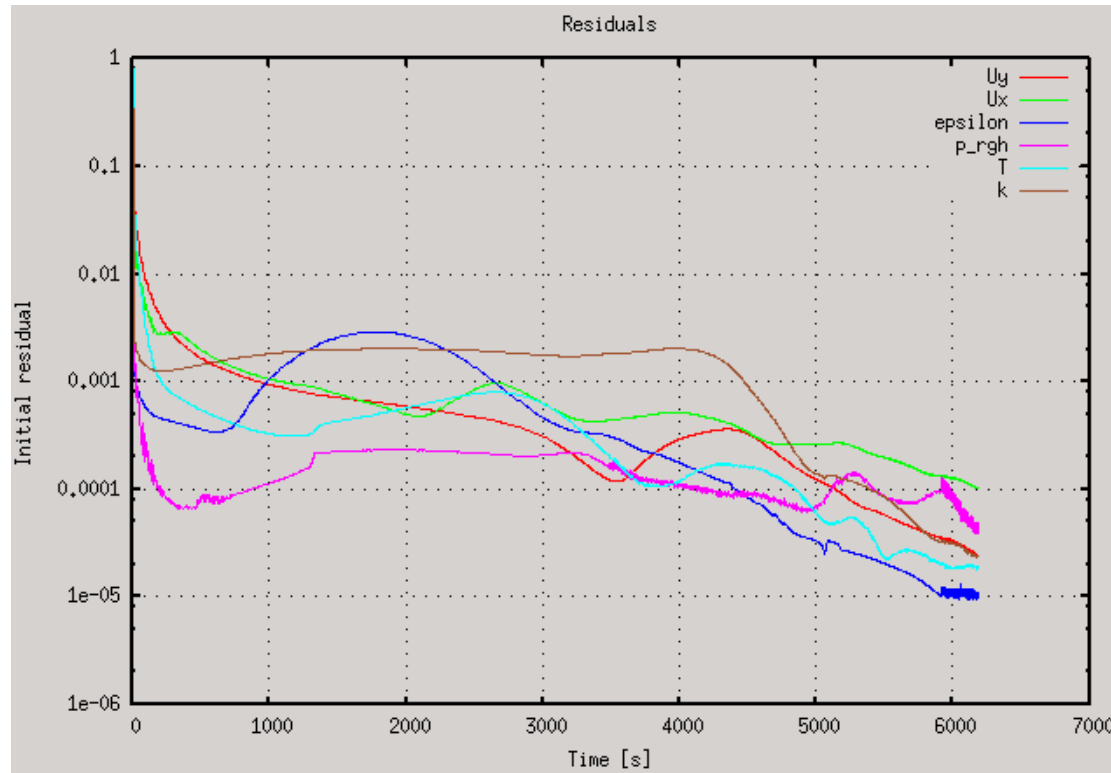
$$\omega_p = 1, \quad \omega_U = 0.5$$



Convergence characteristics (9)

modified buoyantBoussinesqSimpleFoam

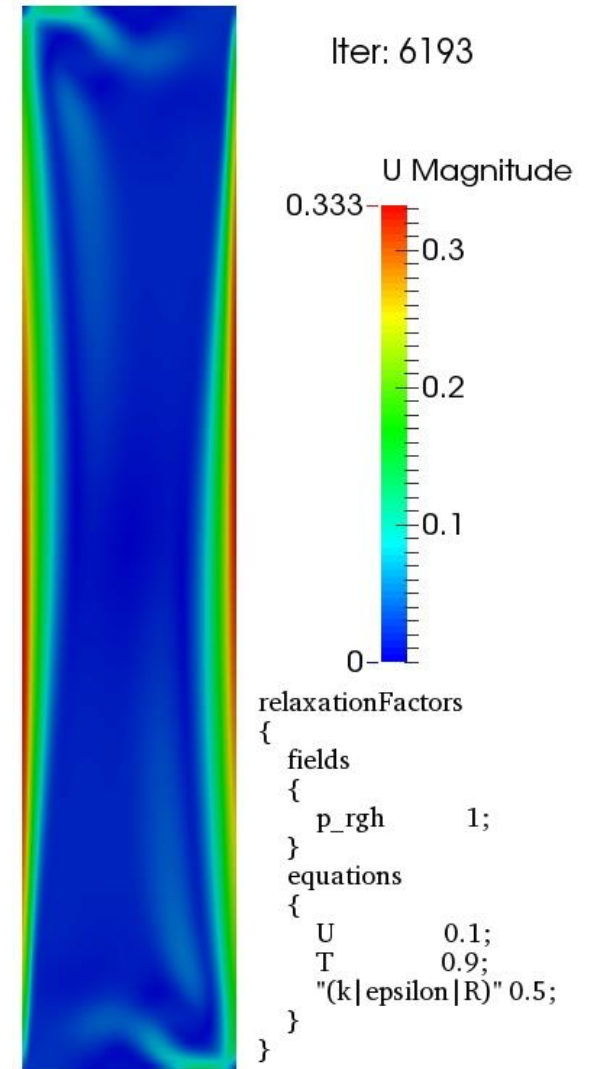
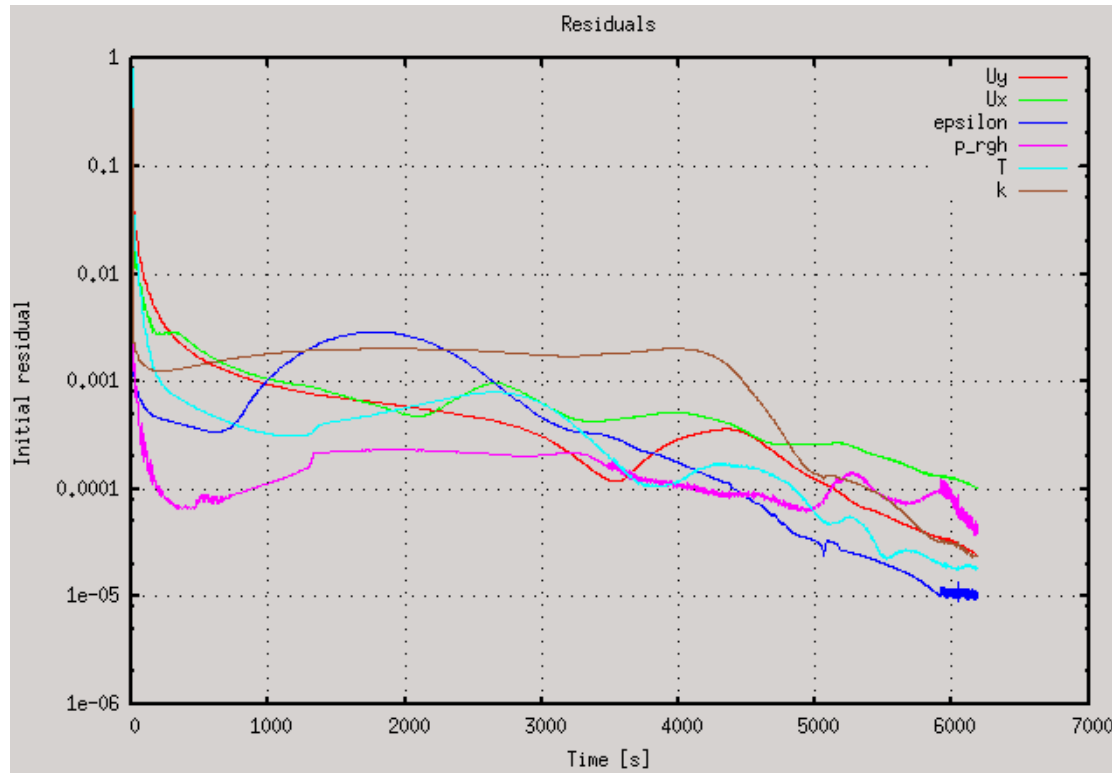
$$\omega_p = 1, \quad \omega_U = 0.1$$



Convergence characteristics (10)

buoyantBoussinesqSimpleFoam

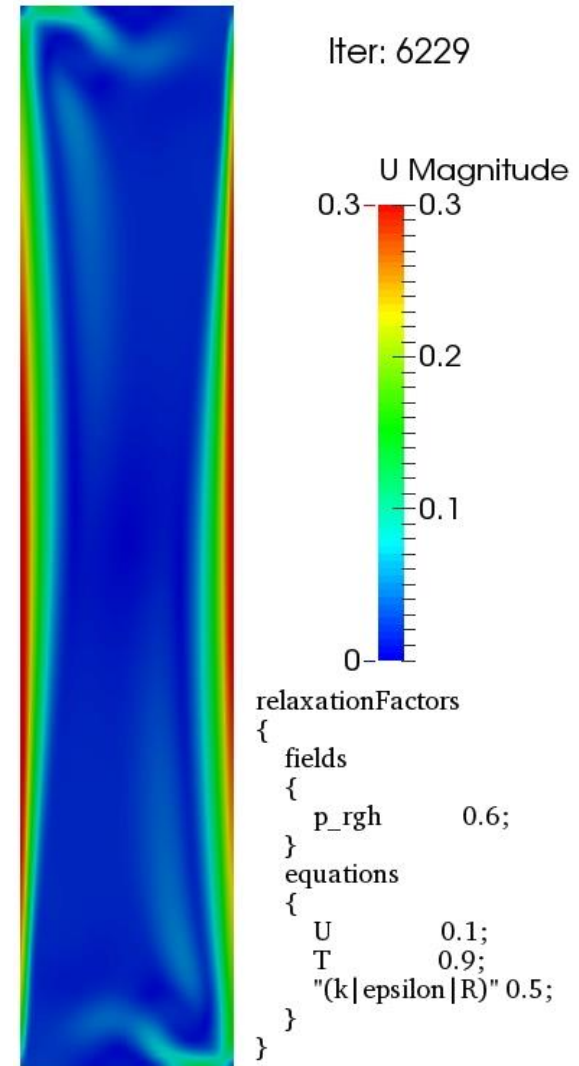
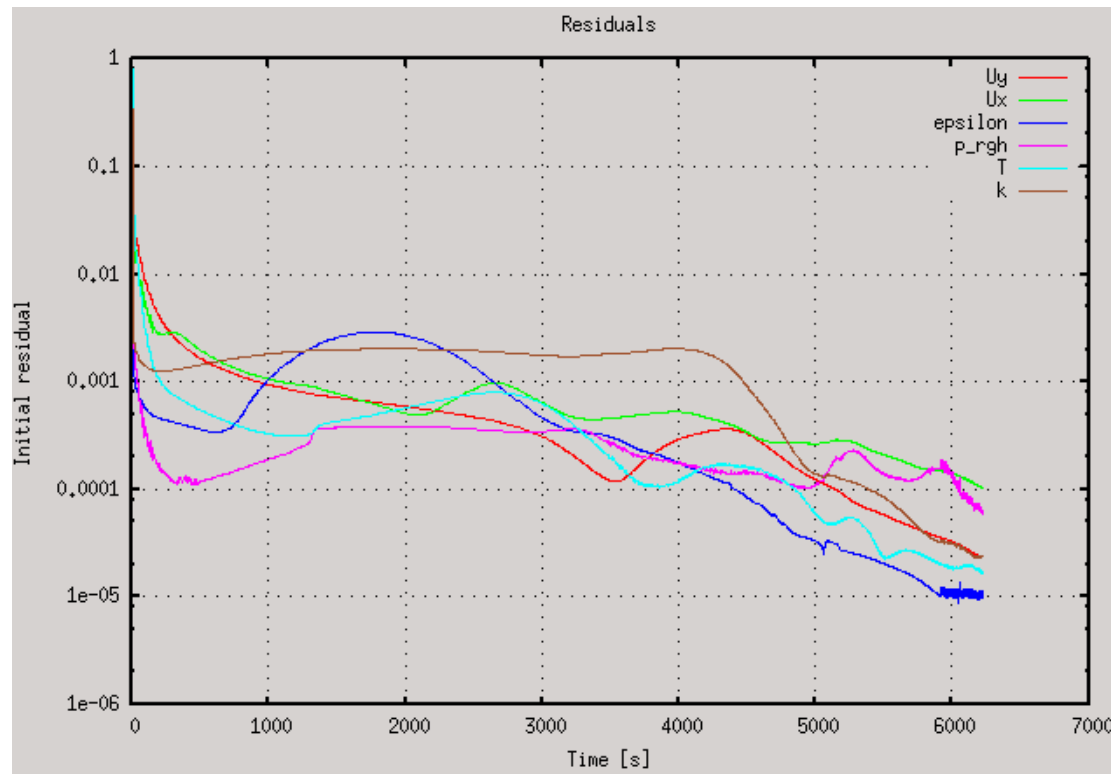
$$\omega_p = 1, \quad \omega_U = 0.1$$



Convergence characteristics (11)

modified buoyantBoussinesqSimpleFoam

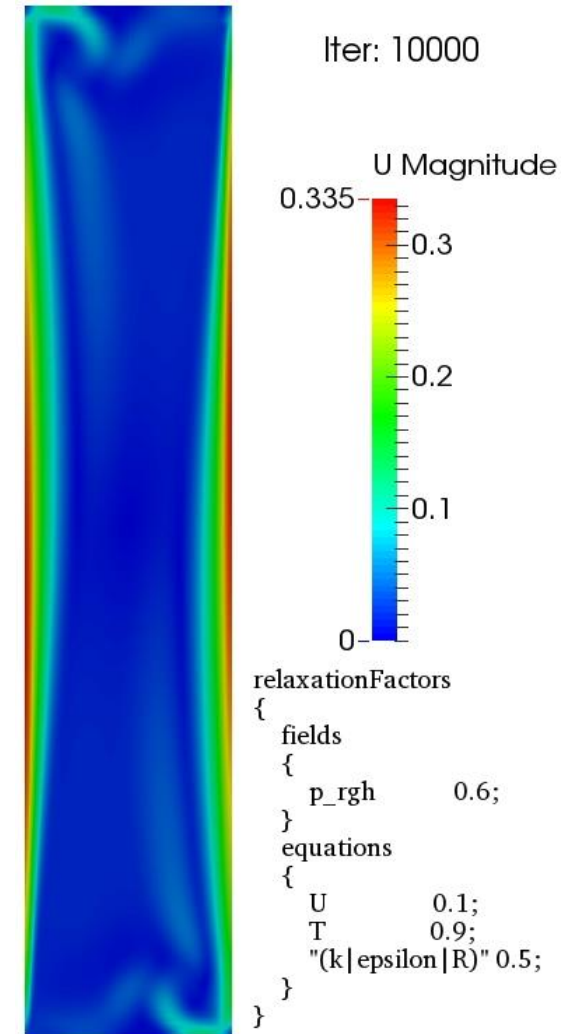
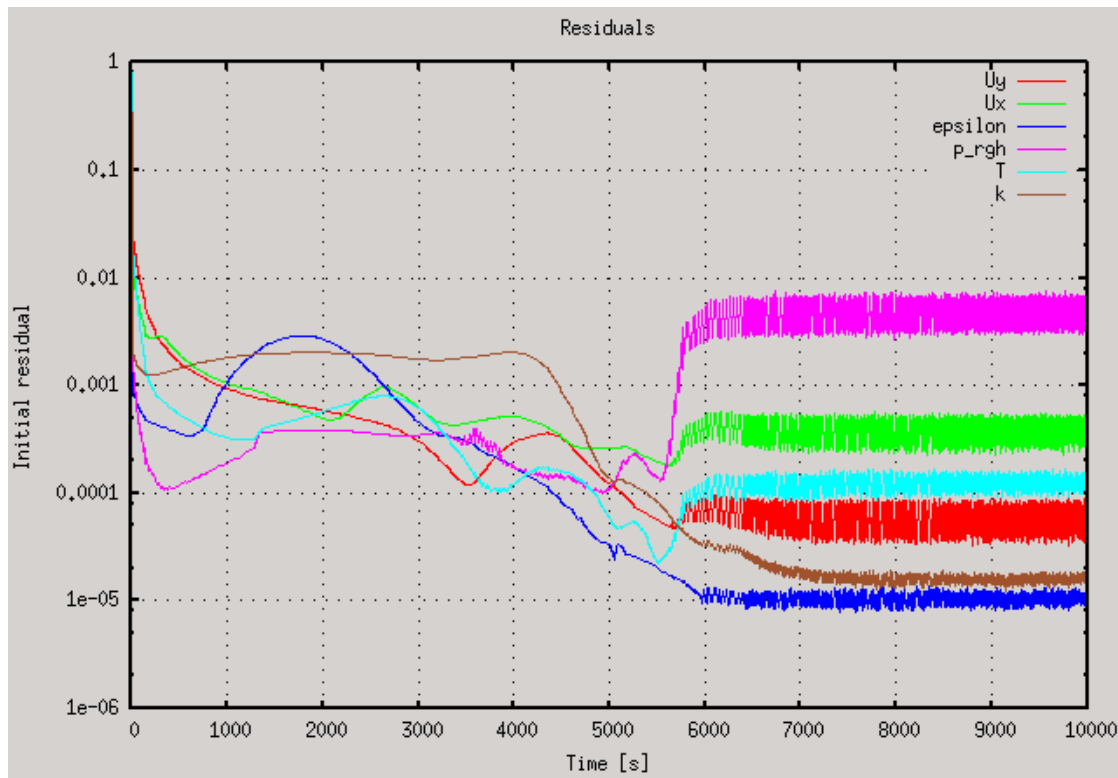
$$\omega_p = 0.6, \quad \omega_U = 0.1$$



Convergence characteristics (12)

buoyantBoussinesqSimpleFoam

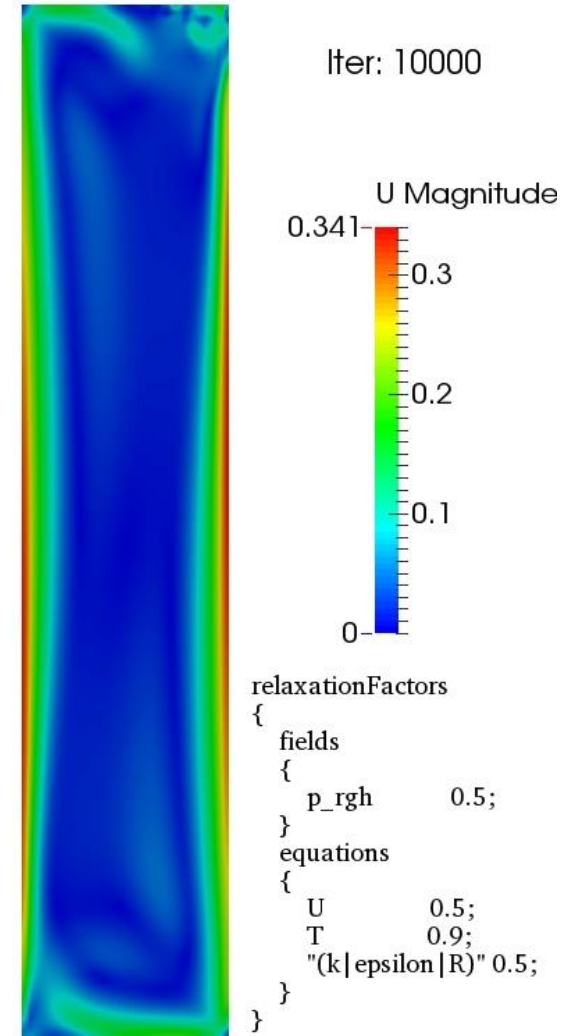
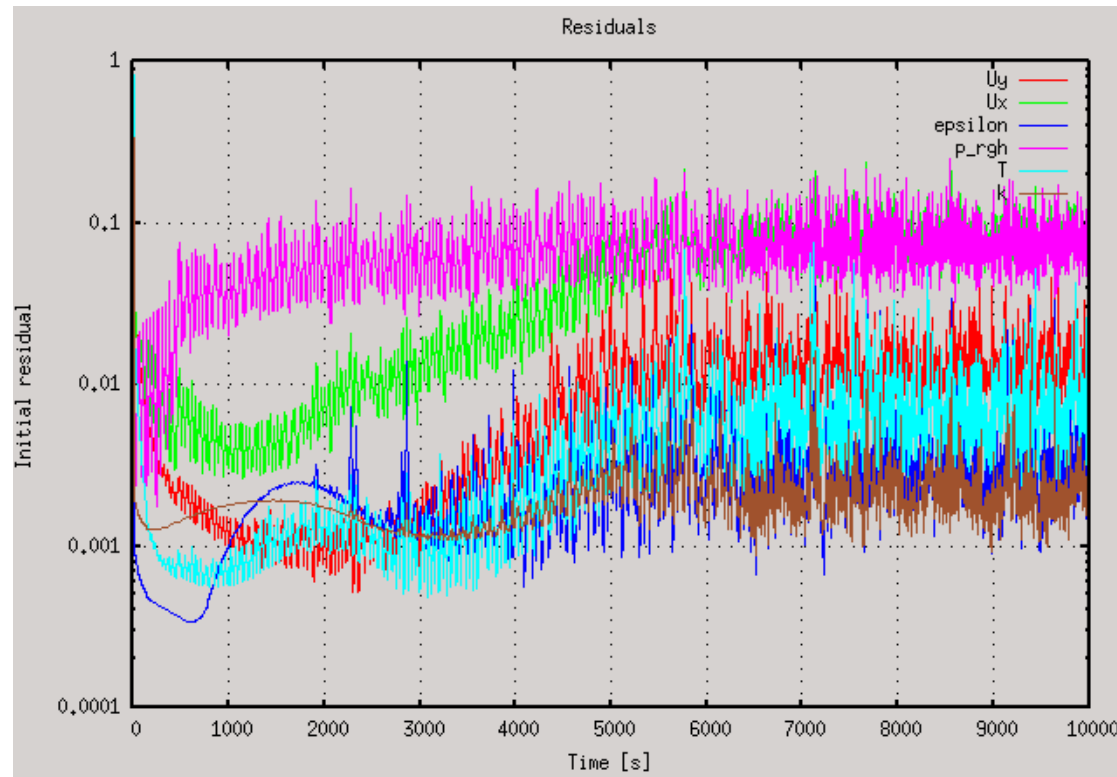
$$\omega_p = 0.6, \quad \omega_U = 0.1$$



Convergence characteristics (13)

modified buoyantBoussinesqSimpleFoam

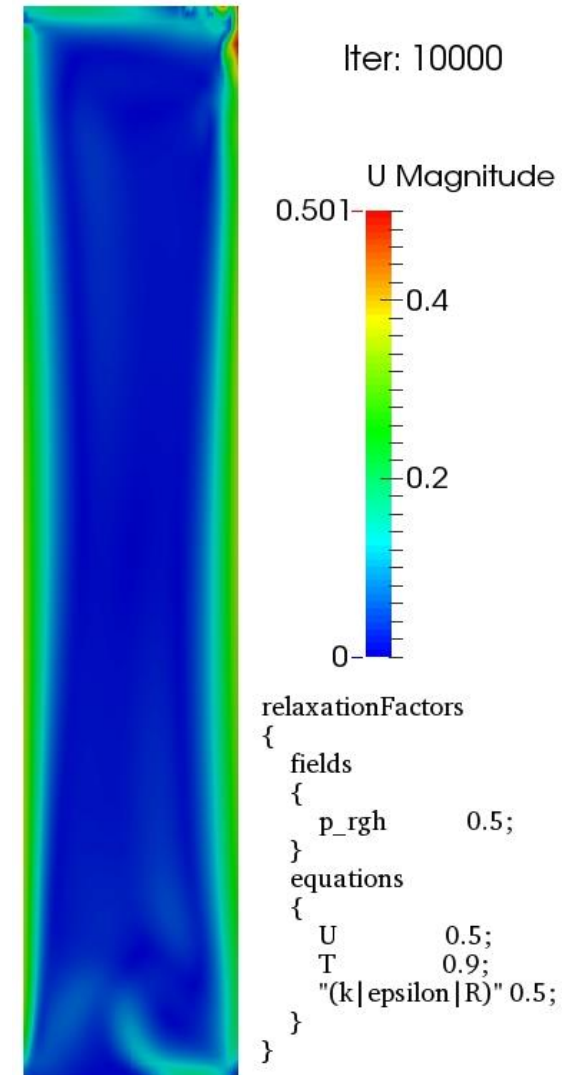
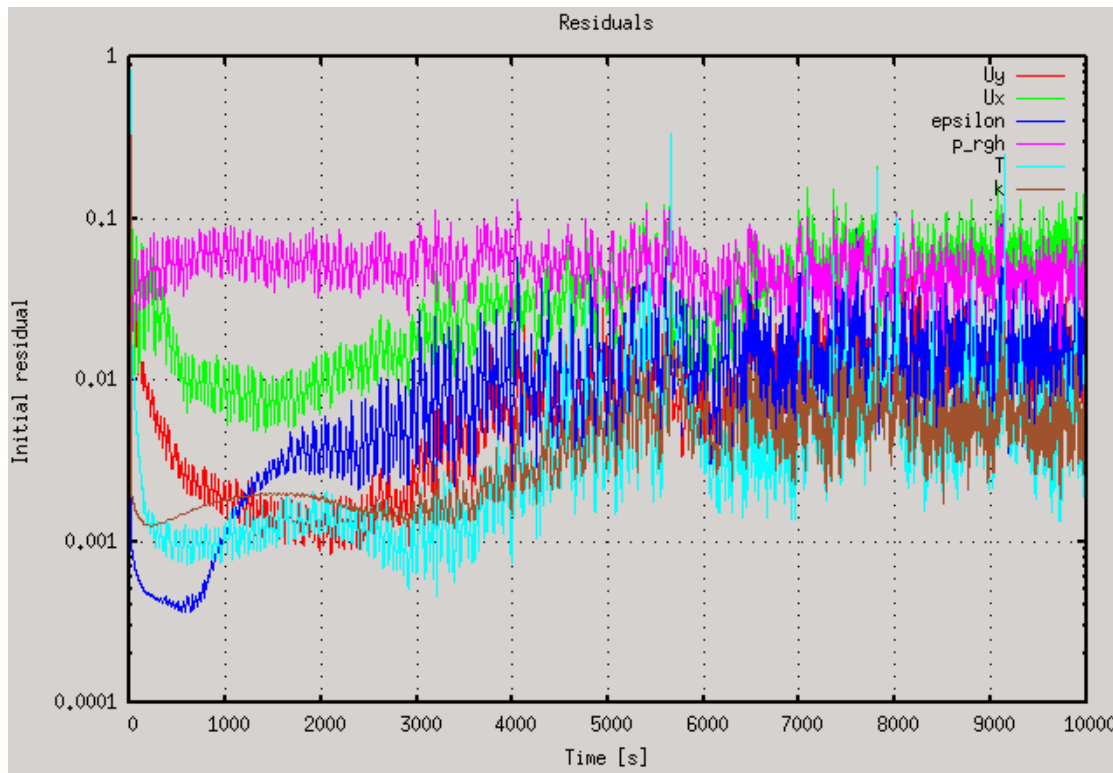
$$\omega_p = 0.5, \quad \omega_U = 0.5$$



Convergence characteristics (14)

buoyantBoussinesqSimpleFoam

$$\omega_p = 0.5, \quad \omega_U = 0.5$$



Summary of Convergence characteristics

modified buoyantBoussinesqSimpleFoam

ω_p	ω_u	Converged (iter.)
1	0.5	6223
0.3	0.7	diverged
0.7	0.3	5509
0.5	0.5	oscillating
0.3	0.3	oscillating
1	0.1	6192
0.6	0.1	6229
0.3	0.1	6359
0.3	0.2	5892

buoyantBoussinesqSimpleFoam

ω_p	ω_u	Converged (iter.)
1	0.5	6223
0.3	0.7	oscillating
0.7	0.3	oscillating
0.5	0.5	oscillating
0.3	0.3	oscillating
1	0.1	6193
0.6	0.1	oscillating
0.3	0.1	oscillating
0.3	0.2	oscillating



buoyantBoussinesqPimpleFoam

- **OpenFOAM version**
 - ✓ OpenFOAM 2.4
- **Solver modification**
 - ✓ pressure relaxation after velocity update
 - ✓ additional pressure prediction before solving momentum eq.
- **Test case**
 - ✓ King's natural convection problem
 - $Ra = 4.3 \times 10^{10}$
 - $Pr = 0.71$

Standard *buoyantBoussinesqPimpleFoam*

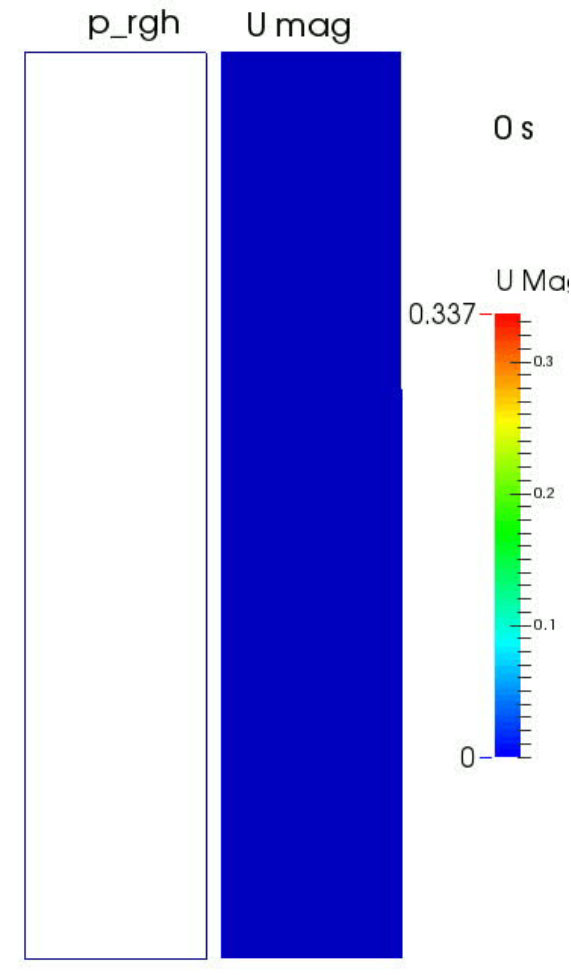
- Solver options

- ✓ PISO mode ($n_{\text{OuterCorrectors}} = 1$, $n_{\text{Correctors}} = 3$) → no relaxation

- Time step control

- ✓ $\text{maxDeltaT} = 0.1$, $\text{maxCo} = 50$

- ✓ runtime calculated $\text{maxCo} = 1.85$



Standard *buoyantBoussinesqPimpleFoam*

- **Solver options**

- ✓ Pimple mode ($nOuterCorrectors = 2$, $nCorrectors = 3$)

- **Relaxation**

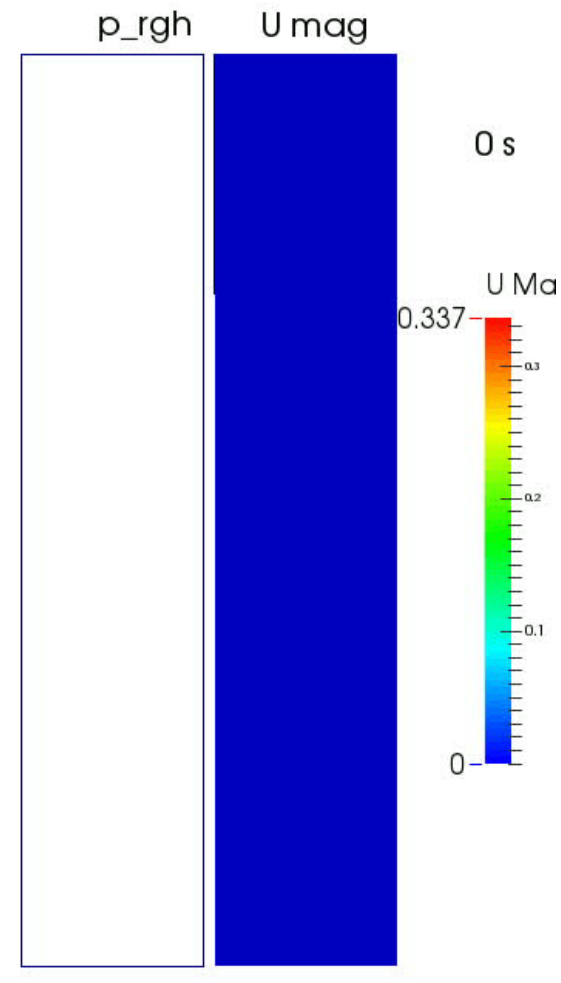
- ✓ $p_rgh = 0.5$, $p_rghFinal = 1$

- ✓ $U = 0.5$, $Ufinal = 1$

- **Time step control**

- ✓ $maxDeltaT = 0.1$

- **No effect of relaxation step change**



Modified *buoyantBoussinesqPimpleFoam*

- Solver options

- ✓ Pimple mode ($nOuterCorrectors = 2$, $nCorrectors = 3$)

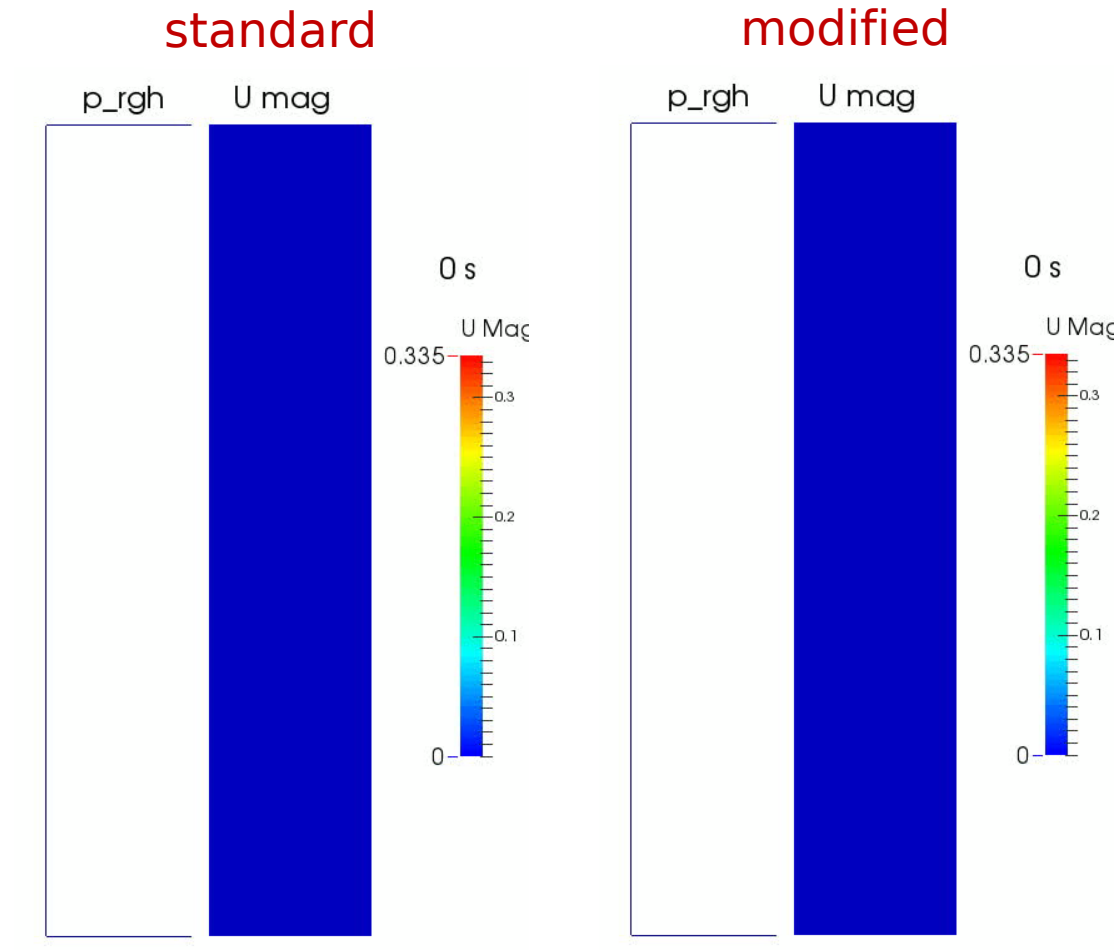
- Relaxation

- ✓ $p_rgh = 0.5$, $p_rghFinal = 1$

- ✓ $U = 0.5$, $U_{final} = 1$

- Time step control

- ✓ $maxCo = 10$





buoyantPimpleFoam

- **OpenFOAM version**
 - ✓ OpenFOAM dev
- **Solver modification**
 - ✓ pressure relaxation after velocity update
 - ✓ additional pressure prediction before solving momentum eq.
- **Test case**
 - ✓ tutorial/heatTransfer/buoyantPimplefoam/hotroom

Standard buoyantPimpleFoam

- **Solver options**

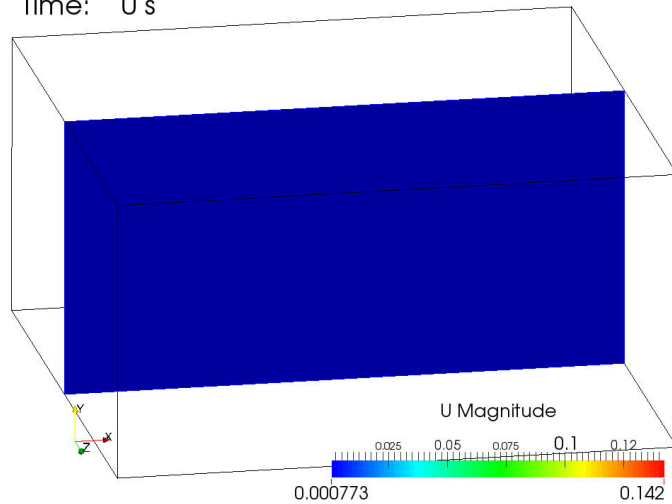
- ✓ PISO mode ($n_{\text{OuterCorrectors}} = 1$, $n_{\text{Correctors}} = 2$)

- **Convergence**

- only if $dt \leq 2$

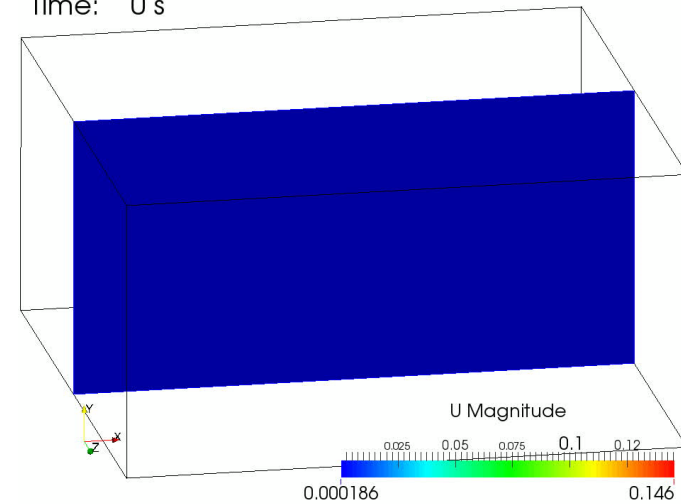
$dt = 1$, $\max Co = 0.3$

Time: 0 s



$dt = 2$, $\max Co = 0.6$

Time: 0 s



p-relax modified buoyantPimpleFoam

- Solver options

- ✓ PISO mode ($n_{\text{OuterCorrectors}} = 1$, $n_{\text{Correctors}} = 2$)

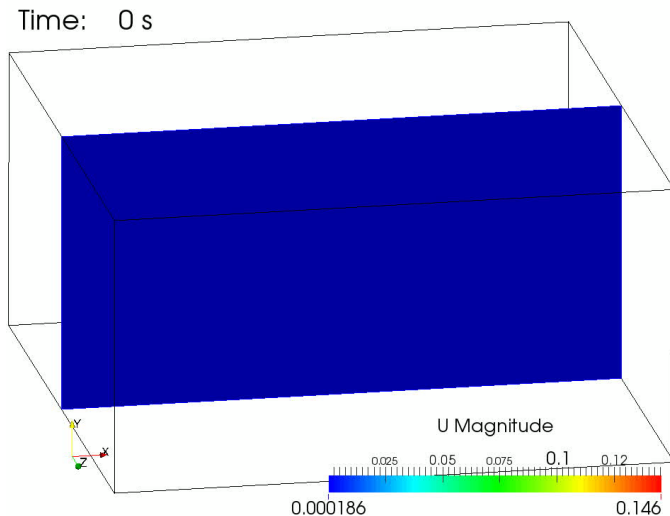
- Convergence

- ✓ only if $dt \leq 2$

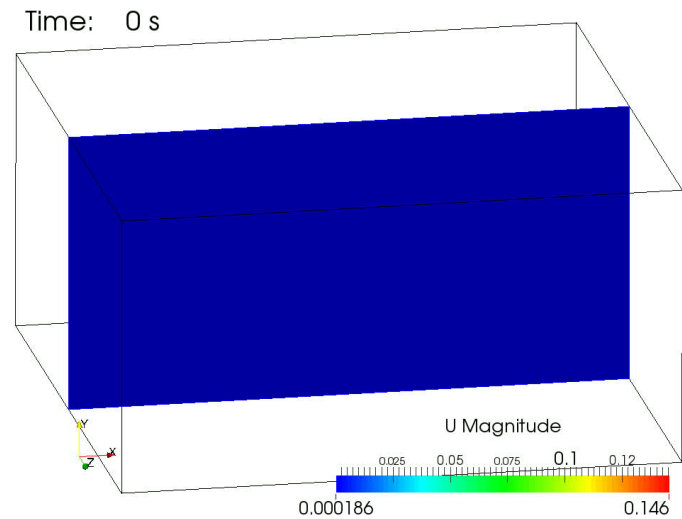
- In the PISO mode, no relaxation is used

- ✓ Convergence characteristics are same as standard solver

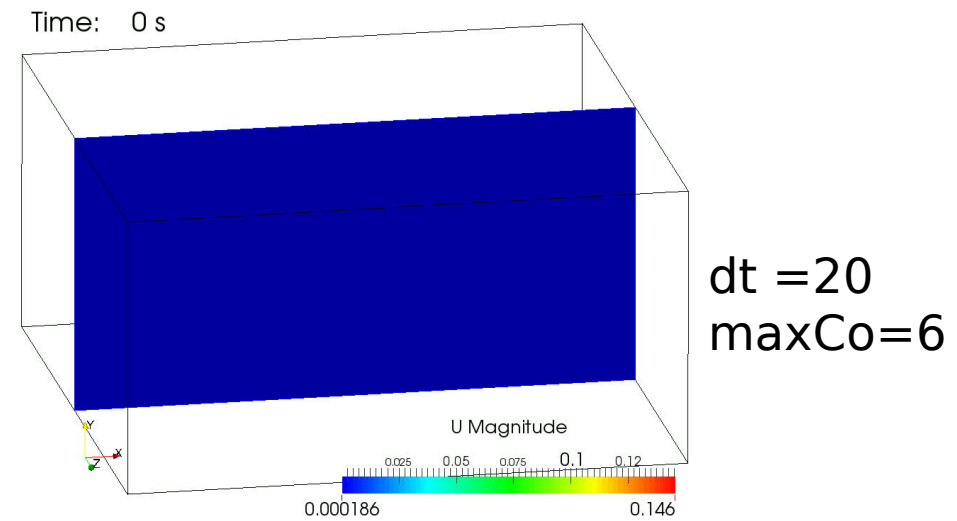
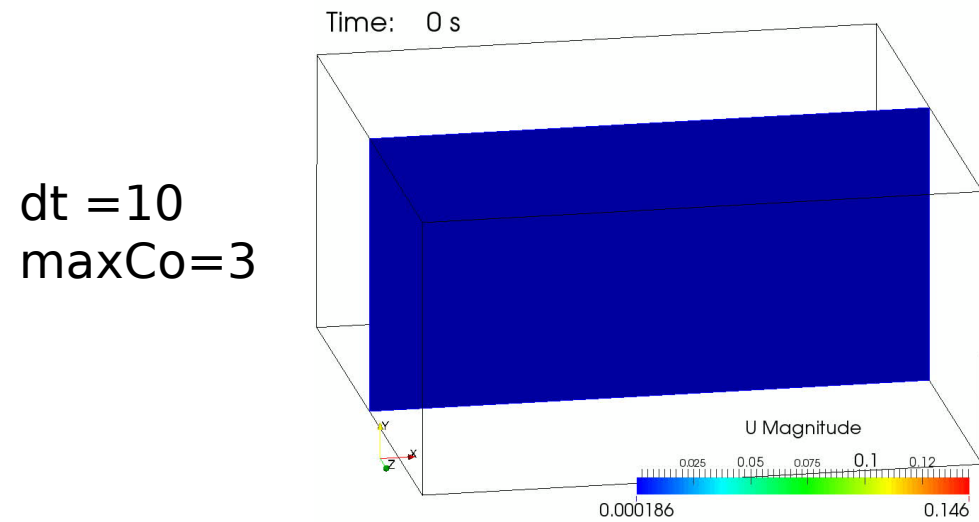
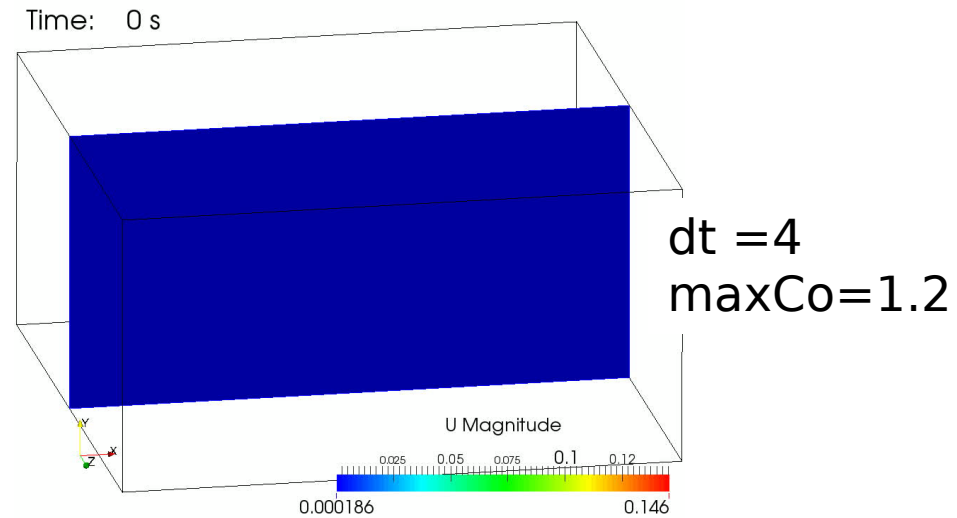
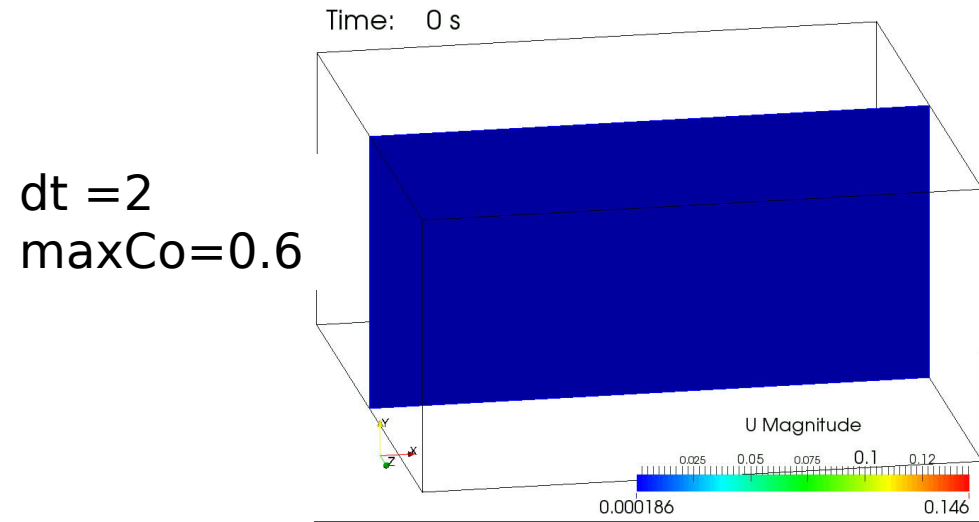
$dt = 1$, $\max Co = 0.3$



$dt = 2$, $\max Co = 0.6$



buoyantPimpleFoam with pressure prediction



- **Modification of the pressure relaxation step**

- ✓ It is effective for convergence enhancement of buoyantBoussinesq-SimpleFoam

- **Addition of pressure prediction step**

- ✓ Increase stability range of relaxation factors in Simple mode and max. Courant number in Piso mode.

- **It is still under evaluation**

- **A critical point to solution divergence**

- ✓ turbulence model is very critical to the solution convergence

Thank you for your attention