# *Tutorial: UDFs for a User-Defined Scalar*

## Introduction

ANSYS FLUENT solves the the transport equation for a user-defined scalar (UDS) in the same way as it solves the transport equation for a scalar in the core equations, such as a species mass fraction. The UDS capability can be used to implement a wide range of physical models in magnetohydrodynamics, electromagnetics, and more.

In this tutorial you will learn to solve a general scalar diffusion equation (1) with the possible types of boundary condition (BC) at the boundary (or a part of the boundary) of the domain.

$$c\frac{\partial \phi}{\partial t} - \nabla .\ (\Gamma \nabla \phi) = S_\phi,\ in\ \Omega,\ t > 0 \tag{1}$$

The possible types of boundary conditions are as follows:

- Dirichlet BC: $\phi = D_0$
- Neumann BC: $-\Gamma(\partial\phi/\partial n) = q_0$
- Mixed BC: $-\Gamma(\partial\phi/\partial n) = h_c(\phi - \phi_\infty)$

Here, $D_0$, $q_0$, $h_c$, and $\phi_\infty$ are constant values.

## Prerequisites

This tutorial is written with the assumption that you have completed Tutorial 1 from ANSYS FLUENT 12.0 Tutorial Guide, and that you are familiar with the ANSYS FLUENT navigation pane and menu structure. Some steps in the setup and solution procedure will not be shown explicitly.

For more details about UDFs, see ANSYS FLUENT 12.0 UDF Manual.

## Problem Description

As shown in the problem illustration, the problem is a 2D rectangle, with constant flux, constant value, and mixed boundary conditions along the boundary edges.

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For the problem,

| | | |
|---|---|---|
| $\Gamma$ | = | 0.162 W/(m K) |
| $C_p$ | = | Specific heat of the material [1650 J/(kg K)] |
| $\phi_\infty$ | = | $550^o$C |
| $h_C$ | = | 20 W/($m^2$K) |

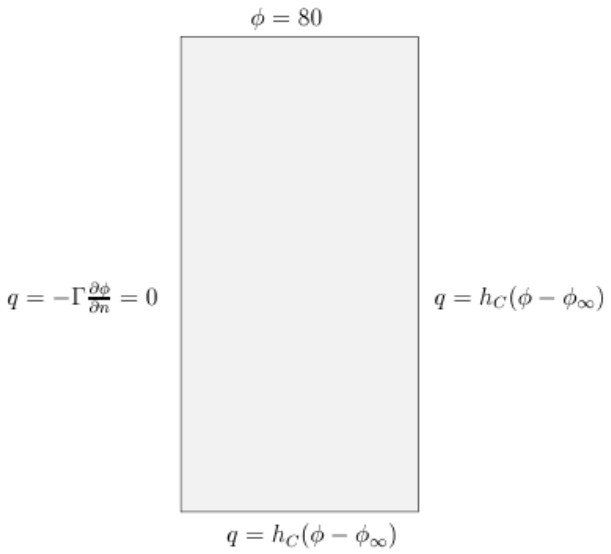


Figure 1: Schematic

## Setup and Solution: Steady-State Solver

## Preparation

1. Copy the files (`laplace.msh`, `mixedbc.c`, and `transientMixedBC.c`) to your working folder.

2. Use FLUENT Launcher to start the 2D version of ANSYS FLUENT.

   *For more information about* FLUENT Launcher *see Section* 1.1.2, Starting ANSYS FLUENT Using FLUENT Launcher *in* ANSYS FLUENT *12.0 User's Guide.*

3. Enable Double-Precision in the Options list.

4. Click the UDF Compiler tab and ensure that the Setup Compilation Environment for UDF is enabled.

   *The path to the* `.bat` *file which is required to compile the UDF will be displayed as soon as you enable* Setup Compilation Environment for UDF.

   *If the* UDF Compiler *tab does not appear in the* FLUENT Launcher *dialog box by default, click the* Show More >> *button to view the additional settings.*


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*The* Display Options *are enabled by default. Therefore, after you read in the mesh, it will be displayed in the embedded graphics window.*

### Step 1: Mesh

1. Read the mesh file (`laplace.msh`).

   File ⟶ Read ⟶ Mesh...

   *As the mesh file is read,* ANSYS FLUENT *will report the progress in the console.*

### Step 2: General Settings

1. Retain the default solver settings.

   General

2. Check the mesh.

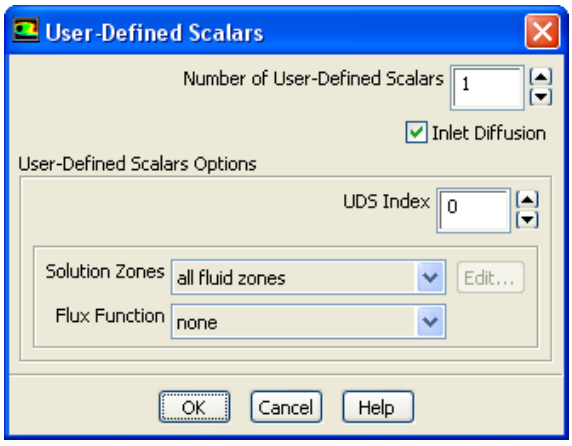
   General ⟶ Check

   ANSYS FLUENT *will perform various checks on the mesh and will report the progress in the console. Make sure the minimum volume reported is a positive number.*

### Step 3: User-Defined Functions

1. Set the UDS value.

   Define ⟶ User-Defined ⟶ Scalars...




   (a) Set Number of User-Defined Scalars to 1.

   (b) Select none from Flux Function drop-down list.

   (c) Click OK to close User-Defined Scalars dialog box.

2. Compile the UDF (`mixedbc.c`).

   Define ⟶ User-Defined ⟶ Functions ⟶ Compiled...

(a) Click Add... and select the source file, mixedbc.c.

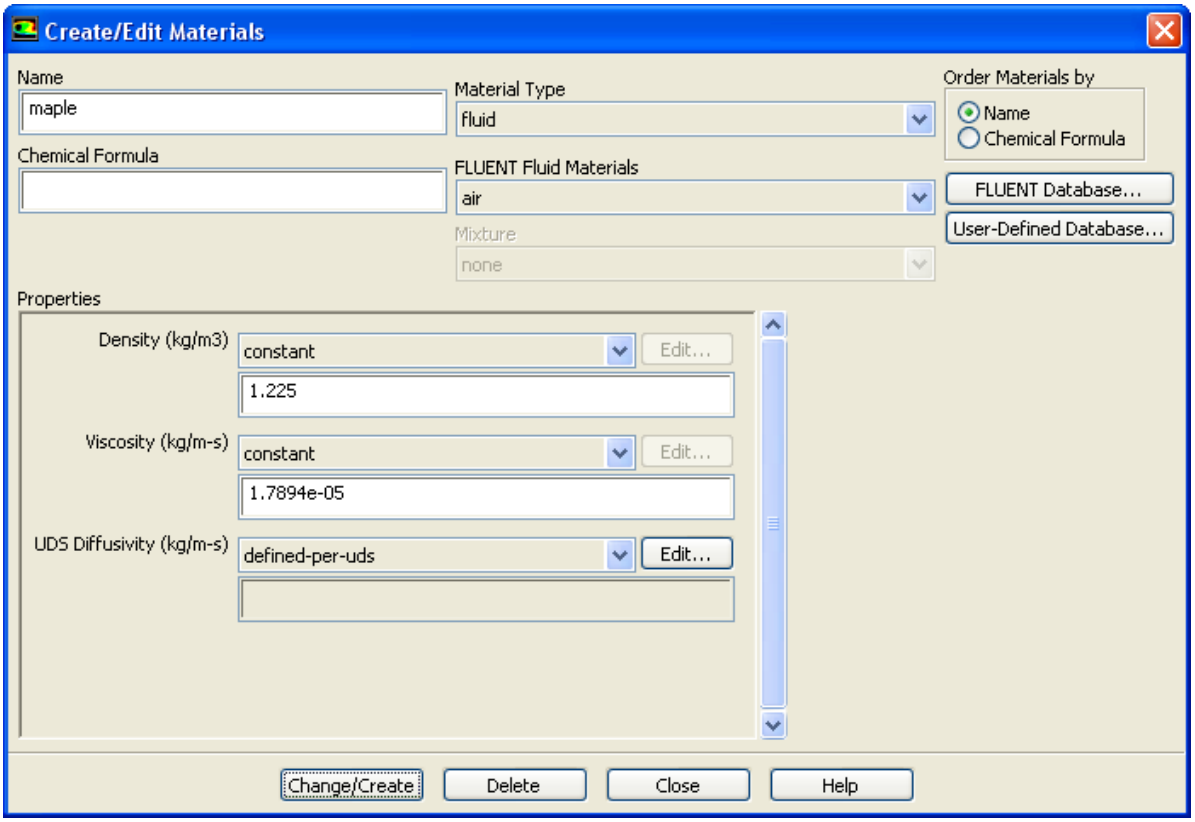
(b) Click Build to build the library.

*A* Warning *dialog box opens, asking you to ensure that the UDF source files are in the same folder that contains the case and data files. Click* OK.

(c) Click Load to load the newly created UDF library.

### Step 4: Materials

1. Create a new material (mapel).


(a) Retain the default values for Density and Viscosity.

(b) Click Edit... for UDS Diffusivity and enter `0.162` for the Coefficient.

(c) Enter `maple` for the Name.

(d) Click Change/Create.

*A* Question *dialog box appears, asking you whether to overwrite* air. *Click* Yes.

(e) Close the Create/Edit Materials dialog box.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### Step 5: Boundary Conditions

1. Set the boundary conditions for topwall.

   Boundary Conditions → topwall → Edit...

   (a) Click UDS tab.

   (b) Select Specified Value from the User Scalar 0 drop-down list in the User-Defined Scalar Boundary Condition group box.

   (c) Enter 80 for UDS Scalar 0 in the User-Defined Scalar Boundary Value group box.

   (d) Click OK.

2. Set the boundary conditions for leftwall.

   Boundary Conditions → leftwall → Edit...

   (a) Click UDS tab.

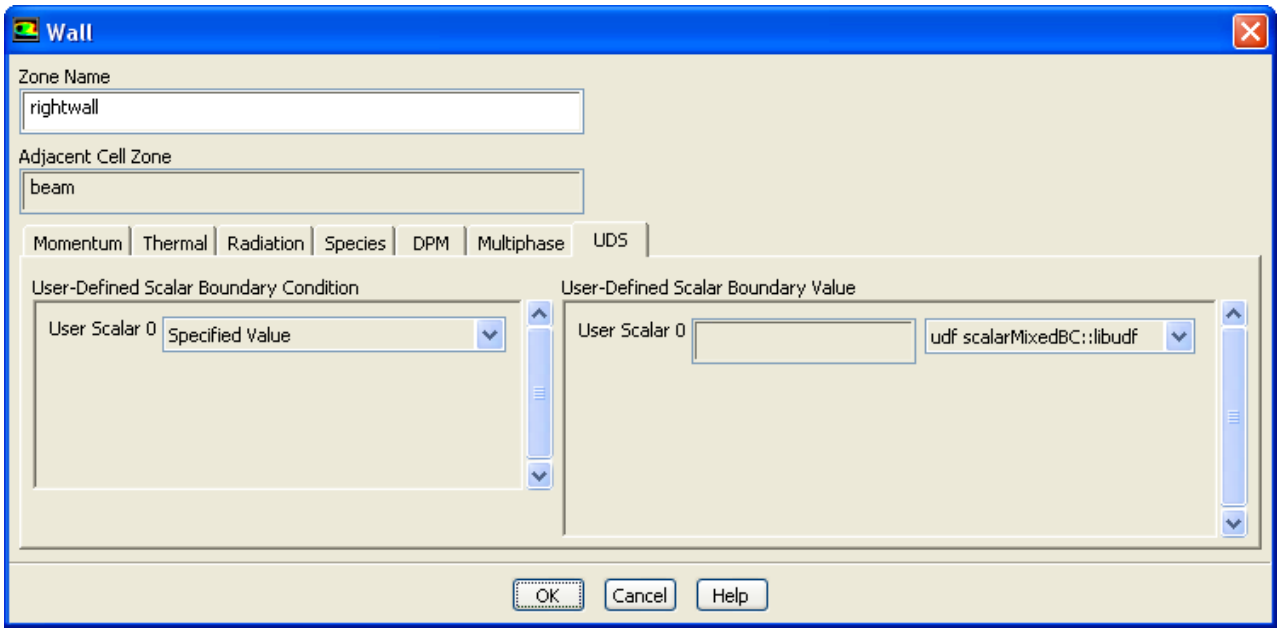
   (b) Ensure that Specified Flux is selected from the User Scalar 0 drop-down list.

   (c) Retain 0 for UDS Scalar 0.

   (d) Click OK.

3. Set the boundary conditions for rightwall.

   Boundary Conditions → rightwall → Edit...




   (a) Click UDS tab and select Specified Value from the User Scalar 0 drop-down list in the User-Defined Scalar Boundary Condition group box.

   (b) Select udf scalarMixedBC::libudf from the User Scalar 0 drop-down list in the User-Defined Scalar Boundary Value group box.

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(c) Click OK.

4. Set the similar boundary conditions for bottomwall. Repeat step 3 (previous step).

   *The following equation gives mixed boundary condition for* rightwall *and* bottomwall.

$$-\left(\Gamma\frac{\partial\phi}{\partial n}\right)_w = h_C(\phi - \phi_\infty) \tag{2}$$

   where,

| | | |
|---|---|---|
| $\Gamma$ | = | UDS diffusivity [0.162] |
| $h_C$ | = | 20 |
| $\phi_\infty$ | = | 550 |

**Step 6: Solution for Steady-State Solver**

1. Deselect the Flow equation.

   Solution Controls ⟶ Equations...

2. Disable Check Convergence for uds-0.

   Monitors ⟶ Residuals ⟶ Edit...

3. Define a point monitor.

   Surface ⟶ Point...

   (a) Enter `0.025` for x0 (m) and `0.05` for y0 (m).

   (b) Enter `middlepoint` for the Name.

   (c) Click Create and close Point Surface dialog box.

4. Enable the plotting of the point monitor.

   Monitors (Surface Monitors) ⟶ Create...

   (a) Enable Plot and Write.

   (b) Retain the selection of Iteration from the X Axis and Every drop-down lists.

   (c) Select Sum from the Report Type drop-down list.

   (d) Select User Defined Scalars... and Scalar-0 from the Field Variable drop-down lists.

   (e) Select middlepoint from the Surfaces list.

   (f) Click OK to close the Surface Monitor dialog box.

5. Initialize the solution.

   Solution Initialization

6. Run the calculation for 50 iterations (see Figures 2 and 3).

   *As the value of $\phi$ remains constant after 40 iterations (Figure 2), you can consider that the solution as converged.*

7. Save the case and data files (`laplace.cas/dat.gz`).



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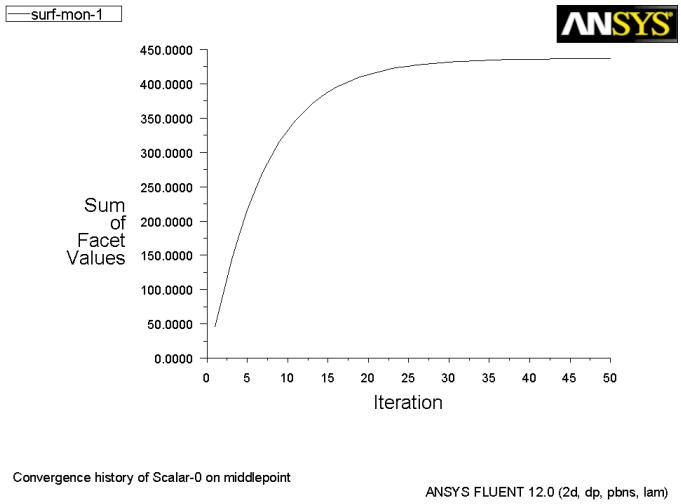


Figure 2: Monitor Plot

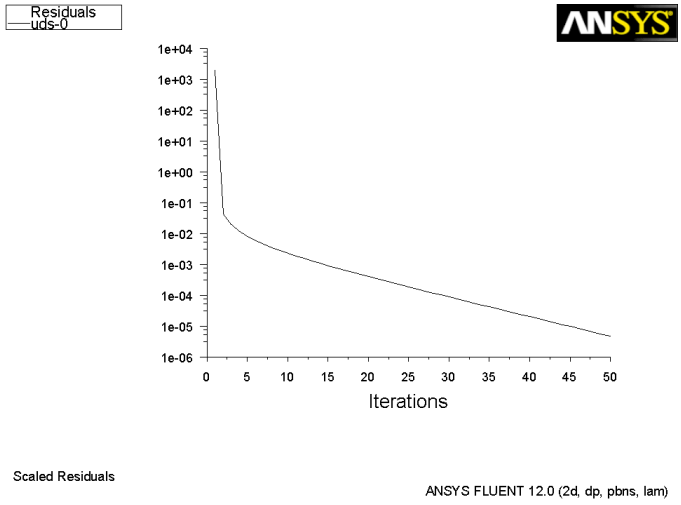


Figure 3: Residual Plot

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**Step 7: Postprocessing**

Display the contours of $\phi$.

1. Select User Defined Scalars... and Scalar-0 from the Contours of drop-down lists.
2. Click Display (see Figure 4).

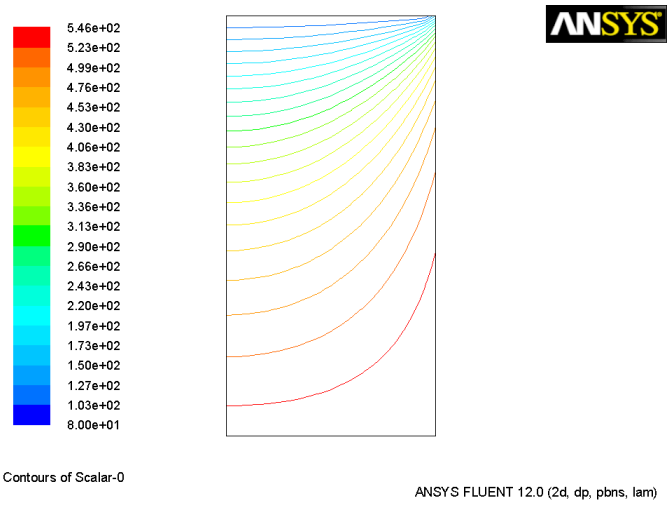


Figure 4: Contours of $\phi$

Since the problem is partially set up in the steady case, here only the unique steps for the setup of the unsteady solver are mentioned.

## Setup and Solution: Unsteady UDS Solver

The unsteady diffusion problem represented by equation 9 over the same rectangular domain is solved by a first-order implicit formulation. The boundary condition is also unchanged. The initial condition is $\phi = 80$ through the domain.

**Step 1: General Settings**

1. Read the case file `laplace.cas.gz`.
2. Enable the transient solver.
   General ⟶ Transient

**Step 2: User-Defined Functions**

1. Compile the UDF (`transientMixedBC.c`).
   Define ⟶ User-Defined ⟶ Functions ⟶ Compiled...


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(a) Click Add... and select the source file, transientMixedBC.c.

(b) Enter `libudf1` for the Library Name.

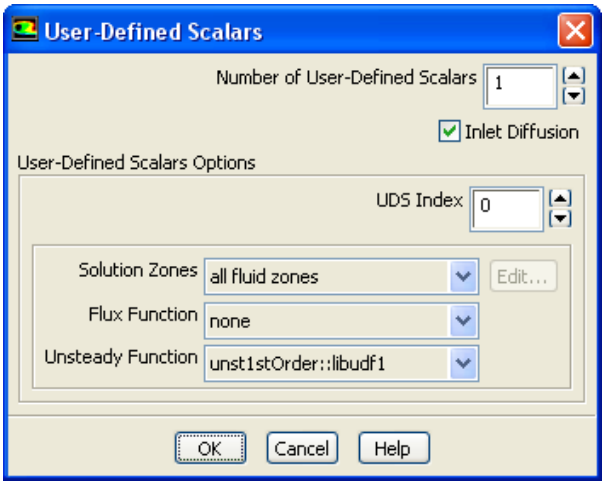
(c) Click Build to build the library.

*A* Warning *dialog box opens, asking you to ensure that the UDF source files are in the same folder that contains the case and data files. Click* OK.

(d) Click Load to load the newly created UDF library.

2. Select first-order unsteady UDF.

Define ⟶ User-Defined ⟶ Scalars...




(a) Retain Number of User-Defined Scalars to 1.

(b) Retain the selection of none from Flux Function drop-down list.

(c) Select unst1storder::libudf1 from Unsteady Function drop-down list.

(d) Click OK to close User-Defined Scalars dialog box.

### Step 3: Solution for Unsteady Solver

1. Initialize the solution by setting User Scalar 0 to 80.

Solution Initialization

2. Autosave the data files every 10 steps.

Calculation Activities

(a) Enter 10 for Autosave Every (Time Steps).

(b) Click Edit... to open Autosave dialog box.

i. Retain the default settings.

ii. Click OK to close the Autosave dialog box.

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3. Set the time-stepping parameters.

   Run Calculation

   (a) Enter `0.1` s for Time Step Size.

   (b) Enter 200 for Number of Time Steps.

   (c) Enter 40 for Max Iterations/Time Step.

   (d) Click Calculate.

### Step 3: Postprocessing

1. Display the contours of $\phi$ at t = 1 s.

   *For displaying the contours t = 1 s, you need to read the data file (*`laplace-1-00010.dat`*).*

   (a) Select User Defined Scalars... and Scalar-0 from the Contours of drop-down lists.

   (b) Click Display (see Figure 5).

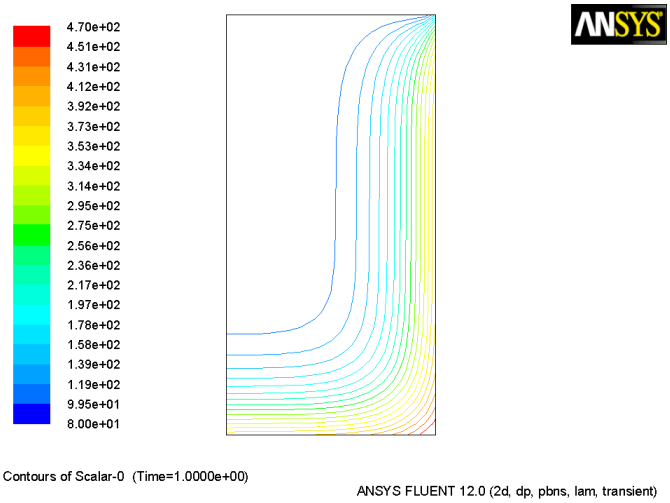


Figure 5: Contours of $\phi$ at t = 1 s

2. Similarly, display contours of $\phi$ at t = 2 s, t = 3 s, and t = 4 s reading appropriate data files (Figures 6–8).

   *The diffusion of $\phi$ into the domain due to high $\phi_\infty$ in the ambient is clearly visible via the mixed (convective) boundary condition.*


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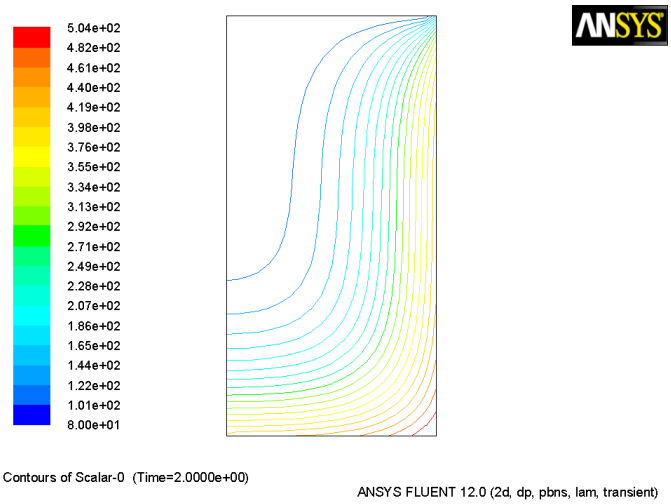


Figure 6: Contours of $\phi$ at t = 2 s

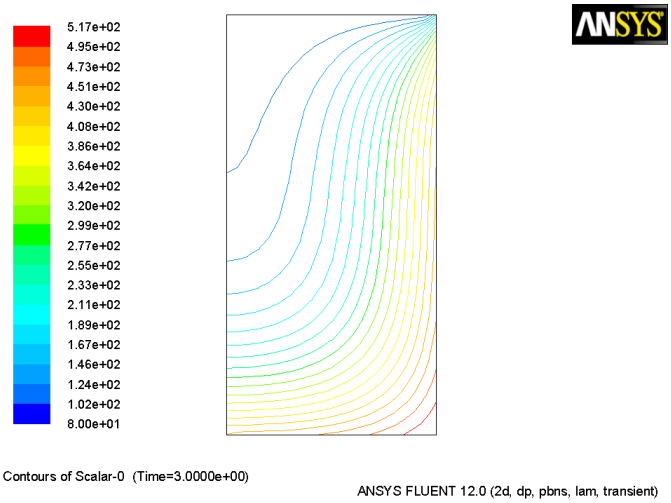


Figure 7: Contours of $\phi$ at t = 3 s

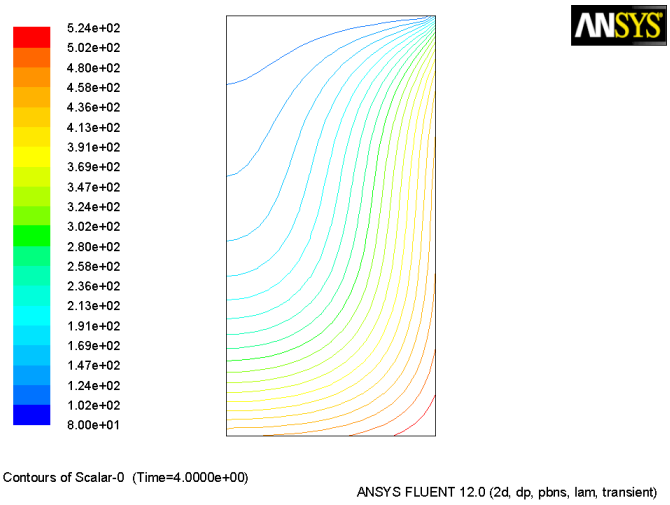


Figure 8: Contours of $\phi$ at t = 4 s


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## Appendix A: Steady-State Solver

Consider a steady-state scalar equation with constant $\Gamma$ and zero source term ($S_\phi = 0$) as follows:

$$-\nabla \cdot (\Gamma \nabla \phi) = 0 \tag{3}$$

This is the Laplace's equation. Solving the Laplaces's equation using the ANSYS FLUENT UDS solver does not necessarily require user-defined functions (UDFs). You can activate the UDS from the graphical user interface. ANSYS FLUENT UDS provides only Dirichlet and Neumann conditions for the boundaries. Hence, you need to use the UDF to apply the mixed boundary condition for the UDS equation.

**Formulation of the Mixed Boundary Condition**

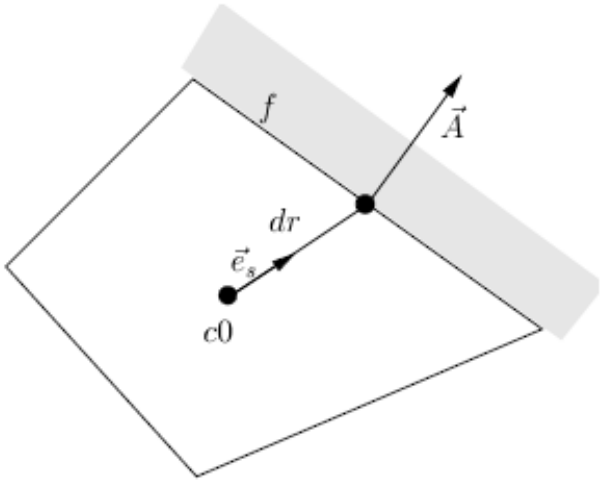


Figure 9: Mixed Boundary Condition

For a generic cell $c0$ adjacent to the boundary, the diffusive flux across the boundary face $f$ of the cell is expressed as follows:

$$-\int_f \Gamma \left(\frac{\partial \phi}{\partial n}\right) dS = \int_f h_C(\phi - \phi_\infty) dS \tag{4}$$

Using the mid-point rule of surface integral, the diffusive flux can be approximated as:

$$-\Gamma_f \left(\frac{\partial \phi}{\partial n}\right)_f A_f = h_C(\phi_f - \phi_\infty) A_f \tag{5}$$

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In ANSYS FLUENT, the diffusive flux is approximated in two parts:

1. The primary gradient is evaluated implicitly along the line connecting the cell centroid $c0$ to the centroid face $f$.
2. It is corrected by a *secondary* gradient (or cross diffusion) term evaluated explicitly by the gradient obtained from the previous iteration ($\overline{\nabla\phi}$).

$$\Gamma_f \left(\frac{\partial\phi}{\partial n}\right)_f A_f \approx \underbrace{\Gamma_f \frac{(\phi_f - \phi_{c0})}{dr}\left(\frac{\vec{A}\ .\ \vec{A}}{\vec{A}\ .\ \vec{e_s}}\right)}_{primary} + \underbrace{\Gamma_f \left(\overline{\nabla\phi}\ .\ \vec{A}\ -\ \overline{\nabla\phi}\ .\ \vec{e_s}\ \frac{\vec{A}\ .\ \vec{A}}{\vec{A}\ .\ \vec{e_s}}\right)}_{secondary} \tag{6}$$

ANSYS FLUENT provides you with two macros:

- `BOUNDARY_FACE_GEOMETRY(f, t, A, ds, es, A_by_es, dr0)`: a macro which defines the necessary geometrical variables of the cell.
- `BOUNDARY_SECONDARY_GRADIENT_SOURCE(source,SV_UDSI_G(i),dG,es,A_by_es,k)`: a macro which calculates the secondary gradient term in equation 6.

If you designate the secondary gradient term in equation 6 as $\beta_0$, and $(\vec{A}\ .\ \vec{A})/(\vec{A}\ .\ \vec{e_s})$ as $A_{be}$, equations 5 and 6 can be written as:

$$-h_C(\phi_f - \phi_\infty)A_f = \Gamma_f \frac{(\phi_f - \phi_{c0})}{dr} A_{be} + \beta_0 \tag{7}$$

$\phi_f$ can be expressed as follows:

$$\phi_f = \frac{\Gamma_f (A_{be}/dr)\phi_{c0} - \beta_0 + h_C A_f \phi_\infty}{h_C A_f + \Gamma_f (A_{be}/dr)} \tag{8}$$

The mixed boundary condition for the UDS is ready to be specified by boundary profile $\phi_f$ in equation 8 through the UDF macro `DEFINED_PROFILE()`.


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### UDF Code

The UDF code for steady state is as follows:

```
/*****************************************************************************/
/* Implementation of the mixed boundary condition for a UDS (or multiple):   */
/*            q = hC ( phi - PHI_inf)                                        */
/*****************************************************************************/

#include "udf.h"
#include "sg.h"     /* needed for the boundary and secondary gradient macros */

/*===========================================================================*/

#define CP 1650.0   /* heat capacity for maple in (J/kg K)  */
#define HTC 20.0    /* heat transfer coefficient for the problem */
#define TINF 550    /* ambient temperature of the problem */
/*===========================================================================*/

/* Names of the user-defined scalar to be used */
enum
{
  phi1,
  N_REQUIRED_UDS
};

DEFINE_PROFILE(scalarMixedBC, thread, nv)
{
   /*constants must be specified correctly for the mixed BC */
   real hC, PHI1_inf;

   /* ====================== */
   face_t f;

   real A[ND_ND], dG[ND_ND], dr0[ND_ND], es[ND_ND], dr, A_by_es;
   real Af;
   real beta0, gamma;
   real temp1, temp2;
   Thread *t0=thread->t0;

   hC=HTC;
   PHI1_inf=TINF;

   begin_f_loop(f, thread)
     {

      /* identify the cell thread adjecent to the face thread f */
       cell_t c0 = F_C0(f, thread);

       BOUNDARY_FACE_GEOMETRY(f, thread, A, dr, es, A_by_es, dr0);
       Af=NV_MAG(A);
       gamma=C_UDST_DIFF(c0, t0, phi1);

    if (NULLP(T_STORAGE_R_NV(t0, SV_UDST_G(phi1))))
      beta0=0;   /*if gradient is not allocated and stored yet,
                   bypass the following macro (it happens
   when case/data files are being read */
    else
      BOUNDARY_SECONDARY_GRADIENT_SOURCE(beta0, SV_UDSI_G(phi1), dG,
          es, A_by_es, gamma);
```

```
/* temporary variables used in the profile expression */
    temp1=gamma*A_by_es/dr;
    temp2=hC*Af;

    F_PROFILE(f, thread, nv)
      = (temp1*C_UDSI(c0, t0, phi1)- beta0 + temp2*PHI1_inf)/(temp2 + temp1);
  }
end_f_loop(f, thread)
  }
}
```


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## Appendix B: Unsteady Solver

The unsteady user-defined scalar equation is as follows:

$$c\frac{\partial \phi}{\partial t} - \nabla \cdot (\Gamma \nabla \phi) = 0, \; in \; \Omega, t > 0 \tag{9}$$

It has to be solved with the same boundary conditions and given initial condition. When the transient term is $\partial(\rho\phi)/\partial t$, ANSYS FLUENT can readily handle this unsteady UDS term when you enable the unsteady solver (either first or second-order). But if the transient term of the user's equation is not the same as the given form, you must supply the unsteady term through the `DEFINE_UDS_UNSTEADY()` macro.

For example, in equation 9, $c$ is a variable. For an unsteady heat conduction problem in dimensional form it represents $\rho c_p$ of the solid material.

**First-Order Unsteady Formulation**

In finite-volume methods, the transient term is first approximated by first or second-order finite-difference expression, then integrated with respect to the cell volume. The ANSYS FLUENT solver expects this transient term to be moved to the right-hand side of the governing equation and included in the discretized equation as a source term.
The first-order finite-difference backward differencing approximation gives:

$$\frac{\partial \phi}{\partial t} \approx \frac{\phi^n - \phi^{n-1}}{\Delta t} \tag{10}$$

where,

| | | |
|---|---|---|
| $\phi^n$ | = | the value of $\phi$ at the current time level |
| $phi^{n-1}$ | = | the value at the previous time level |
| $\Delta t$ | = | the time-step size |

Hence,

$$-\int c\frac{\partial \phi}{\partial t} dV \approx \underbrace{\left(-c\frac{\Delta V}{\Delta t}\right)}_{A_{pu}} \phi^n + \underbrace{c\frac{\Delta V}{\Delta t}}_{S_u} \phi^{n-1} \tag{11}$$

where,

| | | |
|---|---|---|
| $\Delta V$ | = | the volume of each individual cell |
| $A_{pu}$ | = | the coefficient multiplying $\phi^n$ (the implicit part) |
| $S_u$ | = | the explicit part (because it is expressed by known values at the previous time-step) |

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You can rewrite the volume integral of the unsteady term as:

$$-\int c\frac{\partial\phi}{\partial t}dV = A_{pu}\ \phi^n + S_u \tag{12}$$

and it is ready to be coded in the unsteady macro `DEFINE_UDS_UNSTEADY()`.

**UDF Code**

The UDF code for unsteady solver is as follows:

```
/*****************************************************************************/
/*  Implementation of                                                        */
/*                                                                           */
/*    the unsteady term for the user-defined scalar (1st-order)              */
/*                                                                           */
/*****************************************************************************/


DEFINE_UDS_UNSTEADY(unst1stOrder, c, t, i, apu, su)
{
  /* if the unsteady term is different from the default term: d(rho*phi)
                                                             ----------
                                                                dt
     this macro is used to specify the appropriate unsteady term           */

  real volume, cp=CP, deltaTime=CURRENT_TIMESTEP;

  volume=C_VOLUME(c, t);

  /* the transient term is moved to the RHS of the equation and is split
    into two parts---check the FVM algorithm for detail. First-order
    backward differencing is implemented below:                            */

   *apu = -cp*volume/deltaTime;
   *su  = cp*volume*C_UDSI_M1(c, t, i)/deltaTile;

}
```

**Note:** *Before compiling the source code, add the program fragment to the code given in Appendix A. The complete UDF is in* `transientMixedBC.c`.


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## Further Improvements

### Second-Order Unsteady Formulation

It can be shown that the following finite-difference backward differencing approximation to $\partial\phi/\partial t$ is second-order accurate in time:

$$\frac{\partial \phi}{\partial t} \approx \frac{3\phi^n - 4\phi^{n-1} + \phi^{n-2}}{2\Delta t} \tag{13}$$

It involves the values of $\phi$ at three different time levels: $\phi^n$, $\phi^{n-1}$, and $\phi^{n-2}$.

You can use the first-order implicit UDF code in the appendix as a useful guide to come up with your own second-order implicit unsteady UDF code. A few hints for the exercise:

- In the *first step* of unsteady simulation ($n = 1$), $\phi^{n-2}$ is not available yet ($\phi^{n-1}$ is the initial condition). Therefore you can use the first-order formulation in this step in order to advance to the second time step ($n = 2$).
- $\phi^{n-2}$ is represented by `C_UDSI_M2(c,t,i)` for each cell.
- The transient term is moved to the right hand side of the equation as a source term. Hence, remember to get the signs right.
- Select second-order unsteady formulation before starting the iteration.

### Non-Constant Source Term

You can implement a non-constant source term in equation 1. The macro, `DEFINE_SOURCE` (`name`, `c`, `t`, `dS`, `eqn`) is called to represent $S_\phi$. The finite-volume solver of ANSYS FLUENT expects the source term to be *linearized* according to the following convention:

$$S_\phi = A + B\phi = \underbrace{\left(S^* - \left(\frac{\partial S_\phi}{\partial \phi}\right)^* \phi^*\right)}_{A} + \underbrace{\left(\frac{\partial S_\phi}{\partial \phi}\right)^*}_{B} \phi \tag{14}$$

where,

| | | |
|---|---|---|
| $*$ | = | Value at the previous iteration |
| $A$ | = | `source` |
| $B$ | = | `dS[eqn]` |

$A$ and $B$ can be coded explicitly by using currently known value of $\phi$. The general UDF for all variables is `DEFINE_SOURCE()`. To use it for a UDS ($\phi$), you need to hook it up in the boundary condition dialog box to the cell zone where $\phi$ is be solved.

There are various ways to linearize a source term, but the general requirement is that $B$ (the slope) should be non-positive to enhance convergence of the iterative solution process. The convergence is better with more negative slope.

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## Summary

In this tutorial, you modeled the UDS scalar diffusion equation by using UDFs in ANSYS FLUENT. Some details of the finite-volume method used by the solver were carefully discussed when implementing terms in the governing equation and BC. However, treatment of the advective term $\nabla \cdot \overrightarrow{F}\phi$ ($\overrightarrow{F}$ is the general flux vector), is not covered here.


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