User Programming & Automation

• What are User Defined Functions
• Introduction to C
• Set-Up C User Routines in Fluent
• Programming in other CFD Commercial Codes
• Automation

Acknowledgement: this handout is partially based on Fluent training material
Introduction to UDF Programming

Why programming in commercial codes?

• The codes are general-purpose but cannot anticipate all needs
• New (physical) models can be developed in a user-friendly environment
• Large number of problems (test-cases) can be addressed with the same implementation

What is the User Defined Function (UDF)?

• C (Fluent) or FORTRAN (StarCD, CFX) routines programmed by the user linked to the solver to perform certain operations:
  • initialization
  • special boundary condition (i.e. space or time dependent)
  • material properties
  • source terms
  • reaction rates
  • postprocessing and reporting
  • debugging
  • ....
Geometrical Entities - Reminder

Collection of entities are called “zones”
A Simple UDF Example

Specify a Parabolic Velocity Profile at the Inlet

Goal: The UDF (inlet_parab) set the values of the x-velocity component at the cell faces of the inlet boundary zone

1) Determine the cell-faces belonging to the inlet zone
2) Loop on all those faces
3) Determine the coordinate of the face centroid
4) Specify the x-velocity component
A Simple UDF Example

Parabolic Velocity Profile: \[ u = \frac{1}{2\nu} \left( \frac{dp}{dx} \right) y (h - y) \]

function \texttt{inlet\_parab}

Definitions

Loop over all the inlet cell faces

Evaluate the face centroid coordinates

The function return the velocity

```c
#include "udf.h"

DEFINE_PROFILE(inlet_parab, thread, equation)
{
  float x[3], y;  /* face centroid coordinates */
  face_t f;       /* face identifier */
  float u;        /* x-velocity component */
  float rho = 1.0; /* density */
  float mu = 0.1; /* viscosity */
  float dp = 0.3; /* pressure gradient */
  float h = 2.0; /* height of the channel */

  /* Loop on all faces belonging to the current thread */
  for(f_loop(f, thread))
  {
    F CENTROID(x, f, thread); /* get the face centroid coordinates */
    y = F[1];                  /* get the y coordinate */
    u = dp*0.5/rho/mu*y*(y-h); /* exact solution to channel flow */

    F PROFILE(f, thread, equation) = u; /* output the velocity */
  }
  end_f_loop(f, thread)

  /* finished */
}
A Simple UDF Example

Compile/interpret the UDF:

Define → User Defined

Attach the profile to the inlet zone

Define → Boundary Condition

Equivalent to attach the profile from a separate simulation
A Simple UDF Example

Solve the equations

Solve → Iterate

Final Result
C Programming

Typical C function:

```c
/* A simple C function */
#include "udf.h"
#define PI 3.14159
float a = 1.2345;
int myfunction(int x)
{
    int y,z;
    y = 11;
    z = a*(x+y)*PI;
    printf("z = %d",z);
    return z;
}
```

- A comment line
- A preprocessor directive for including files
- A preprocessor directive for macro substitution
- A variable with "global" scope
- Function declaration (integer type)
- Left curly brace opens body of function
- Variable declarations
- Set y = 11
- Compute z
- Print output to screen
- Return integer value
- Right curly brace closes body of function
C vs. FORTRAN

/* A simple C function */
int myfunction(int x)
{
    int y,z;
    y = 11;
    z = x+y;
    printf("z = %d",z);
    return z;
}

C An equivalent FORTRAN function
INTEGER FUNCTION MYFUNCTION(X)
INTEGER X,Y,Z
Y = 11
Z = X+Y
WRITE (*,100) Z
MYFUNCTION = Z
100 FORMAT("Z = ",I5)
END
Basic Programming Rules

Statements MUST end with a semicolon → ;

Comments are placed anywhere in the program between → /* …… */

Statements are grouped by curly brackets → { …… }

Variables defined within the body functions are local
Variables defined outside the body functions are global and can be used by all the functions that follows

Variables MUST be ALWAYS defined explicitly

Integer/real/double functions have to return a integer/real/double value

C is case sensitive!
Basic Statements

Arithmetic expressions in C look like FORTRAN

\[ a = y + (i-b)/4; \]

Functions which return values can be used in assignment

\[ a = \text{mycompute}(y,i,b); \]

Functions which do not return values can be called directly

\[ \text{mystuff}(a,y,i,b); \]

Mathematical and various other default functions are available

\[ a = \text{pow}(b,2); \quad /* \text{pow}(x,y) \text{ returns } x \text{ raised to } y */ \]
Data Types and Arrays

Arrays of variables are defined using the notation

```c
int a[10]; /*define an array of ten integers */
```

Note the brackets are square [] not round ()!!

Note that the arrays ALWAYS start from 0

Standard C types are: Integer, Real, Double, Char

C allows to define additional types

```c
typedef struct list{int id, float x[3], int id_next};
```
Pointers

A pointer is a variable which contain the address of another variable

Pointers are defined as:

```c
int *a_p;    /* pointer to an integer variable */
int a;       /* an integer variable */
```

Set-up a pointer

```c
a = 1;
a_p = &a;   /* &a return the address of variable a */

*a_p returns the content of the address pointed by a_p```
Operators

Arithmetic Operators

=  assignment
+  addition
-  subtraction
*  multiplication
/  division
%  modulo
++ increment
-- decrement

Logical Operators

<  less than
<= less than or equal to
>  greater than
>= greater than or equal to
== equal to
!= not equal to
Conditional Statements

**if and if-else**

```plaintext
if (logical-expression)
    {statements}
else
    {statements}
```

**Example**

```plaintext
if (q != 1) {a = 0; b = 1;}
if (x < 0.)
    y = x/50.;
else
    y = x/25.;
```

**C Equivalent FORTRAN code**

```plaintext
IF (X.LT.0.) THEN
    Y = X/50.
ELSE
    Y = X/25.
ENDIF
```
Loop Procedure

for loops

for (begin ; end ; increment)

{statements}

where:

begin = expression which is executed at beginning of loop

d = logical expression which tests for loop termination

increment = expression which is executed at the end of each loop iteration (usually incrementing a counter)

Example

/* Print integers 1-10 and their squares */

int i, j, n = 10;
for (i = 1 ; i <= n ; i++)

{  j = i*i;
    printf("%d %d\n",i,j);
}

C Equivalent FORTRAN code

INTEGER I,J

N = 10

DO I = 1,10

J = I*I

WRITE (*,*), I,J

ENDDO
C Preprocessor

It handles Macro substitutions

#define A B
#define my_f(x,y) x+y*3-5

The preprocessor replaces A with B

It also handles file inclusion

#include “udf.h”
#include “math.h”

The files to be included MUST reside in the current directory
Programming in C

Of course much more than just this…. 

Additional information are: 

http://www.cs.cf.ac.uk/Dave/C/CE.html

Plenty of books:

“The C Programming Language”, Kernighan & Ritchie, 1988
UDF in Commercial CFD Codes

Commercial CFD codes allow the development of User Defined Functions for various applications. Anyway, the core of the software is closed.

UDF must be compiled and linked to the main code

Most codes provide macros and additional tools to facilitate the use of UDFs

In Fluent there are two options:

Interpreted
The code is executed on a “line-by-line” basis at run time
+ does not need a separate compiler (completely automatic)
- slows down the execution and uses more memory
- somewhat limited in scope

Compiled
A library of UDF is compiled and linked to the main code
Overcomes all the disadvantages reported above
Interpret the UDFs

Define → User Defined → Interpreted

Display of code translation in assembly (and eventual compiling errors)

Default stack size might be too small for large arrays!
Compile the UDFs

Define → User Defined → Compiled

The library MUST be precompiled in a directory tree
Directory tree for compiled UDFs

- my_library
  - Makefile
  - src
    - makefile
    - my_udf.c
  - lnx86
    - 2d
      - makefile
      - my_udf.c
      - libudf.so
    - 3d
      - makefile
      - my_udf.c
      - libudf.so

Machine dependent
- irix6r10
- ultra
- hp700
- ...
Makefiles for UDFs

In the directory

```
/usr/local/Fluent.Inc/fluent6/src
```

There are two files

- `makefile2.udf` to be copied in the directory `my_library`.
- `makefile.udf` to be copied in the directory `my_library/src`

The first one does not require modifications.
In the second one two macros MUST be modified

```
SOURCE = my_udf.c
FLUENT_INC = /usr/local/Fluent.Inc
```
UDFs in FLUENT

Boundary Conditions
Initial Conditions
Adjust Function
Source Terms
Material Properties
Execute on Demand
User Defined Scalars
User Defined Memory

Pointers to threads
Geometry Macros
Cell and Face Variables
Arithmetic and Trigonometric Functions

Available MACROS

Programming Tools
Boundary Conditions

The inlet profile specification is based on the macro `DEFINEPROFILE`.

`DEFINE_PROFILE` can be used for wall boundary conditions as well to impose temperature, velocity, shear stress, etc.

It is possible to specify a constant value, a position-dependent or time-dependent values and to link the values on the boundary to the values in the internal cells.

Note that the BCs are applied to the faces of the cells (face centroids).
Initial Conditions

The initial condition specification can be performed using the macro `DEFINE_INIT`

Space-dependent conditions might be imposed

The routine is executed once at the beginning of the solution process

It is attached in the UDFs hooks

Define → User Defined → Function Hooks
Initial Conditions

Note that the difference between the DEFINE_PROFILE and DEFINE_INIT is that the former performs a loop on the face-centroids belonging to a certain zone whereas the latter loops on the cell-centroids.

Example:

```c
#include 'udf.h'

DEFINE_INIT(init, domain)
{
    /* Called at the beginning of the simulation */
    /* to impose a linear pressure in the field */
    
    Thread *t;
    cell_t c;
    real xc[NOD_NO];

    thread_loop_c (t, domain)
        begin_c_loop (c, t)
        {
            C_CENTROID(xc, c, t);
            C_UDSI(c, t, P) = c1 * xc[0] + c2;
        }
    end_c_loop (c, t)
}
```
Adjust Function

Similar to the DEFINE_INIT but it is executed every iteration: `DEFINE_ADJUST`

Can be used for postprocessing, clipping, etc.

It is attached in the UDFs hooks

Define → User Defined → Function Hooks
Source Terms

To add a source term in the equations: DEFINE_SOURCE

Can be used for:
  Continuity
  Momentum (component by component)
  Turbulent quantities
  Energy

It is different from the previous macros because it works on a cell-by-cell basis (no need to perform loops!)
Source Terms

Define → Boundary Conditions → Fluid

Activate source terms

Attach the UDF
Source Terms

In FLUENT the source terms are written in the form

\[ S(\phi) = A + B \phi \]

where \( \phi \) is the dependent variable

A is treated explicitly and B \( \phi \) is treated implicitly

In the DEFINE_SOURCE both terms A and B have to be specified
Material Properties

To define the properties of the materials: **DEFINE_PROPERTIES**

Can be used for:
- Viscosity
- Density
- Thermal Conductivity
  
- ....

As for the source terms works on a cell-by-cell basis
Material Properties

Define → Material Property

All the available UDFs are shown in the menu.
Execute on Demand

To perform operations instantaneously: \texttt{EXECUTE\_ON\_DEMAND}

It is executed when activated by the user

Can be used for:
- Debugging
- Postprocessing
- ...

Define \rightarrow User Defined \rightarrow Execute on Demand
User Defined Scalar

In addition to the Continuity and Momentum Equations (and Energy) generic transport equations can be solved (up to 50!)

To include scalars in the calculations

1) Define the number of scalars

   Define → User Defined → User Defined Scalars

2) Define the diffusion and source terms in the generic equation

\[ \frac{\partial \phi}{\partial t} + U_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_\phi \frac{\partial U_i}{\partial x_j} \right) + S_\phi \]
User Defined Scalar

When UDS are defined in the material property panel the diffusivity of the scalars MUST be defined.

Define → Material Property

Note that the default diffusivity for the scalars is constant and equal to 1!
User Defined Scalar

Boundary conditions for the scalars can be defined as

- Constant Value
- Constant Gradient
- User Defined

Define → Boundary Conditions → Wall
User Defined Scalar

The Source terms for the scalars are set using the DEFINE_SOURCE macro Introduced before

The scalar equations can be further customized

1) Convective terms can be modified using the macro
   DEFINE_UDS_FLUX

2) Unsteady term can be modified using the macro
   DEFINE_UDS_UNSTEADY
User Defined Memory

The User Defined Scalars are used to solve additional equations eventually coupled to the mean flow equations.

Sometimes it is useful to define temporary field variables to store and retrieve values not directly available.

UDM are defined: Define → User Defined → User Defined Memory

More efficient storage compared to User Defined Scalars.
I/O in UDF

User Defined Scalars and User Defined Memory are AUTOMATICALLY Stored in the Fluent Data files

Additional I/O (from and to the Fluent Case and Data files) can be Accomplished using the macro DEFINE_RW_FILE

Define → User Defined → Function Hooks
Detailed Programming

The macros introduced before are interpreted/compiled and attached to the various Fluent panels.

The detailed programming is based on additional macros that allow to loop on cells to retrieve field variables, etc.

- Loop Macros
- Geometry Macros
- Field Variable Macros
- Control Macros
- Arithmetic and Trigonometric Macros

Before looking at the Macros, the Fluent Data structure in introduced.
Data Structure

It is based on a hierarchy of structures

Threads (zones) are collection of cells or faces
Domain is a collections of threads
Threads

Every zone is associated to a single ID (available in the boundary conditions menu)

Given the ID of a thread the pointer can be retrieved as:

\[
\text{Thread } *tf = \text{Lookup\_Thread(domain, ID)};
\]

Given the thread pointer the ID of the zone can be retrieved as:

\[
\text{ID } = \text{THREAD\_ID(thread)};
\]
Loop Macros

- `thread_loop_c(t, d);`
- `thread_loop_f(t, d);`
- `begin_c_loop(c, t);`
  `end_c_loop(c, t);`
- `begin_f_loop`
  `end_f_loop`
- `f_edge_loop(f, t, n);`
- `f_node_loop(f, t, n);`
- `c_node_loop(c, t, n);`
- `c_face_loop(c, t, n);`
- Loop over cell threads
- Loop over face threads
- Loop over cells in a cell thread
- Loop over faces in a face thread
Cell-face connectivity

When looping on faces the surrounding cells can be accessed using the macros:

```c
cell0_thread = F_C0_THREAD(face, thread)
cell1_thread = F_C1_THREAD(face, thread)
cell0_id = F_C0(face, thread)
cell1_id = F_C1(face, thread)
```

When looping on cells adjacent faces and cells can be accessed using the macros:

```c
for (nf=0; nf<C_NFACES(cell, thread); nf++)
{
    face_id = C_FACE(cell, thread, nf);
    face_thread = C_FACE_THREAD(cell, thread, nf);
}
```

Number of faces of each cell is unknown
Geometry Macros

- C_CENTROID(x, c, t);
- F_CENTROID(x, f, t);
- F_AREA(A, f, t);
- C_VOLUME(c, t);
- C_VOLUME_2D(c, t);
- C_NNODES(c, t);
- C_NFACES(c, t);
- F_NNODES(f, t);
- x, y, z-coordinates of cell centroids
- These definitions are in metric.h and mem.h files.
- No of nodes in a cell
- No. of faces in a cell
- No. of nodes in a face

Many more available; refer to the FLUENT UDF Manual
Field Variables Macros

- $C_R(c,t)$
- $C_P(c,t)$
- $C_U(c,t)$
- $C_V(c,t)$
- $C_W(c,t)$
- $C_T(c,t)$
- $C_H(c,t)$
- $C_K(c,t)$
- $C_D(c,t)$
- $C_YI(c,t,i)$
- $C_UDSI(c,t,i)$
- (mem.h) density
- Pressure
- Velocity components
- Temperature
- Enthalpy
- Turbulent kinetic energy
- Turbulent energy dissipation
- Species mass fraction
- User defined scalar
Field Variables Macros

- \( c_{DUDX}(c,t) \)
- \( c_{DUDY}(c,t) \)
- \( c_{DUDZ}(c,t) \)
- \( c_{DVDX}(c,t) \)
- \( c_{DVDY}(c,t) \)
- \( c_{DVDZ}(c,t) \)
- \( c_{DWDX}(c,t) \)
- \( c_{DWDY}(c,t) \)
- \( c_{DWDZ}(c,t) \)
- \( c_{MU\_L}(c,t) \)
- \( c_{MU\_T}(c,t) \)
- \( c_{MU\_EFF}(c,t) \)
- \( c_{K\_L}(c,t) \)

- Velocity derivatives
- Viscosities
- Thermal conductivity

Many more available; refer to the FLUENT UDF Manual
Control Macros

- **boolean Data_Valid_P()**
  - Equals 1 if data is available, 0 if not.
  - Usage:
    ```c
    if(!Data_Valid_P())
        return;
    ```

- **boolean FLUID_THREAD_P(t0)**
  - Checks to see if thread t0 fluid thread

- **NULLP(T_STORAGE_R_NV(t0, SV_UDSI_G(p1)))**
  - Checks for storage allocation of user defined scalars
Code FlowChart - Segregated Solver
Additional Information

Many additional macros are available to implement different physical models
combustion models
particles-based models
....

It is formally possible to develop additional numerical methods
flux discretizations
variable reconstruction and clipping
....
UDF in other commercial CFD Codes

CFX (v4) is a structured code; the data structure is much simpler because the field variables are accessed directly. It uses 1D arrays where the quantities are stored in succession.

CFX UDFs are written in FORTRAN

For example:

\[ U(I,J,K) \rightarrow U(IJK) \text{ where } IJK = (K-1) \times NI \times NJ + (J-1) \times NI \]

There are no macros, but examples of subroutines to perform the customization:

USRBC
USRSRC
USRDIFF
...
UDF in other commercial CFD Codes

Star-CD

StarCD is an unstructured code similar to Fluent in term of data organization
But similar to CFX for the organization of the UDF.

StarCD has threads (as Fluent) and the UDF work normally on a cell-by-cell basis

StarCD UDFs are written in FORTRAN

There are no macros, but examples of subroutines to perform the customization

BCDEFW
SORSCA
DIFFUS
...

Automation
CFD Solver Automation

• FLUENT can save a “journal” file
  To start saving: File → Write → Start Journal
  To stop saving: File → Write → Stop Journal

• Journal file are ASCII editable files

• Commands are somewhat “obscure” (keywords, etc.)

• They can be made general by introducing User Defined Parameters
FLUENT Journal Files

Fluent GUI is developed using a LISP dialect called SCHEME.

To interact with Fluent Journal files via parameters it is necessary to use SCHEME commands.

For example to fix the under-relaxation in the momentum equation the command is:

```
solve/set/under-relaxation/momentum 0.7
```

Otherwise we can define a variable:

```
(define my_url 0.7)
solve/set/under-relaxation/momentum my_url
```
FLUENT Journal Files

With SCHEME you can perform standard operations:

```
(define my_new_url (+ my_url 0.1))
```

To interact with Fluent Journal files via parameters it is necessary to use SCHEME commands.

Loops and conditional statements

```
(if (> 3 2) 'yes 'no)
```
FLUENT Batch Execution

Batch NO GUI:  fluent 2ddp -g -i <journalfile.jou>
Batch with GUI: fluent 2ddp -i <journalfile.jou>

Unfortunately journal files automatically saved by FLUENT contain commands that operate directly on the GUI:

(cx-do-gui cx-activate-item "MenuBar*WriteSubMenu*Stop Journal")

Therefore even for batch executions the GUI has to be activated to use journal files!

The other option is to generate the command files directly using the text-command And NOT the GUI!!!

Many examples on the Web site of journal files that can be run in batch
(define maxcells 200000) ! Set Control Parameters

;;;
;;; set few parameters
;;;
(define minref .1)

;;;
(do ((j 0) ! Adaptation Loop
     (i 0 (+ i 1)))
    ((= i 5) j)
    (format "\n Iteration ~a step - STARTED   " i)

;;;
(cx-gui-do cx-activate-item ...) ! Display Adaptation function

;;;
(cx-gui-do cx-activate-item "MenuBar*AdaptMenu*Iso-Value...") ! Adapt

;;;
(cx-gui-do cx-activate-item "MenuBar*SolveMenu*Iterate...") ! Iterate

;;;
(format "\n Iteration ~a step - FINISHED \n" i)
)

! End Adaptation Loop

Available as adapt.scm from the Website
Example of Automatic Adaptation

Driven Cavity Problem

Start Initial Conditions - Uniform Grid

Perform 5 Steps of Adaptation Using Hanging Nodes

Adaptation Function is:

\[
\text{Scaled Velocity Difference} = \frac{(\text{Velocity Gradient} \times \text{Volume}^{1/3})}{\text{Velocity}}
\]
Example of Automatic Adaptation

**Initial Grid**: 100 elements

**Final Grid**: 40,000 elements
Example of Automatic Adaptation

Initial Grid: 100 elements
Final Grid: 40,000 elements
Optimization

Objective: Automatically find the best solution according to a certain goal (cost function)

Approach: Requires several “similar” CFD simulations obtained by varying one or few parameters (geometry, flow conditions, etc.)

Scripts allow to perform this task very easily!
Optimization Procedure

PROCESS CONTROLLER

GAMBIT → FLUENT → COST FUNCTION EVALUATION → END

GAMBIT → FLUENT

GAMBIT → FLUENT
Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship

By T. Doyle
Optimization Procedure Example
Design and Trim Sails for a Modern Clipper Ship

Aerodynamic Force Definitions

One cost function is defined as Lift/Drag
Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship

Grid Generation
Optimization Procedure Example
Design and Trim Sails for a Modern Clipper Ship

Flow Solutions
Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship

Optimized Solution for Different Wind Directions