

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?

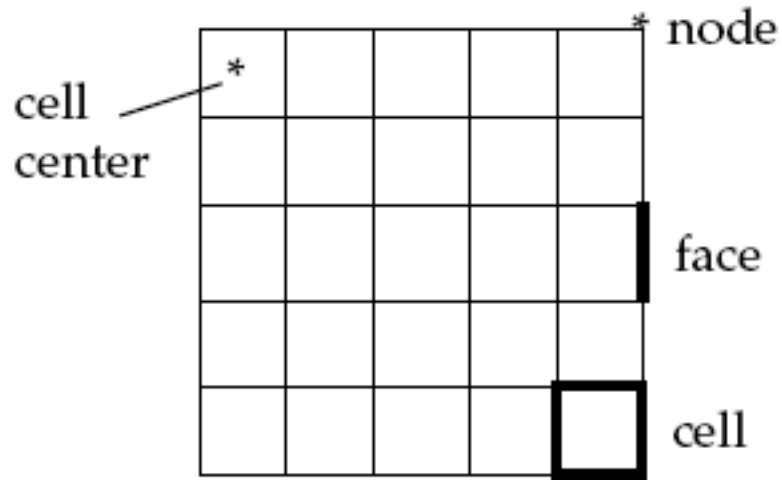
- The codes are general-purpose but cannot anticipate all needs
- New (physical) models can be developed in a user-friendly environment
- Large number of problems (test-cases) can be addressed with the same implementation

What is a the User Defined Function (UDF)?

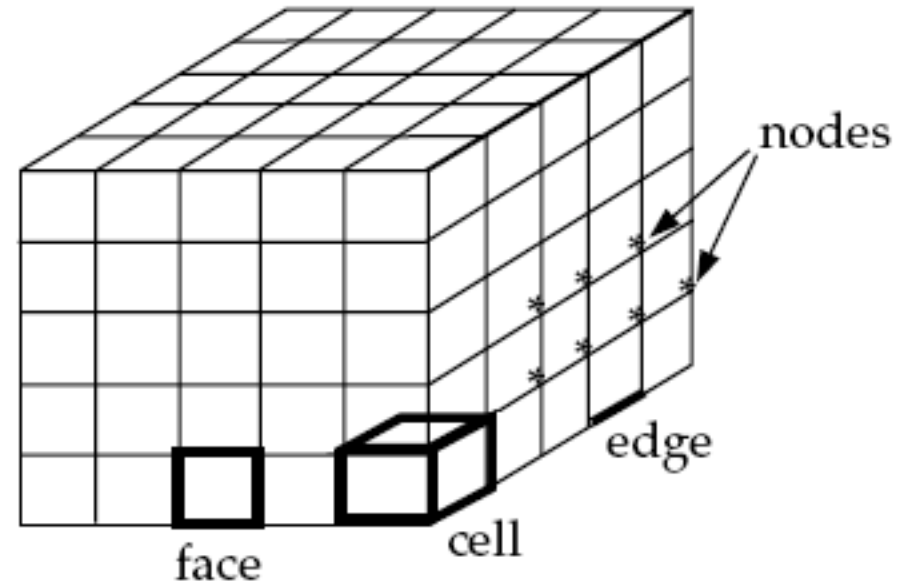
- **C (Fluent)** or **FORTRAN (StarCD, CFX)** routines programmed by the user linked to the solver to perform certain operations:
 - initialization
 - special boundary condition (i.e. space or time dependent)
 - material properties
 - source terms
 - reaction rates
 - postprocessing and reporting
 -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



Geometrical Entities - Reminder



2D



3D

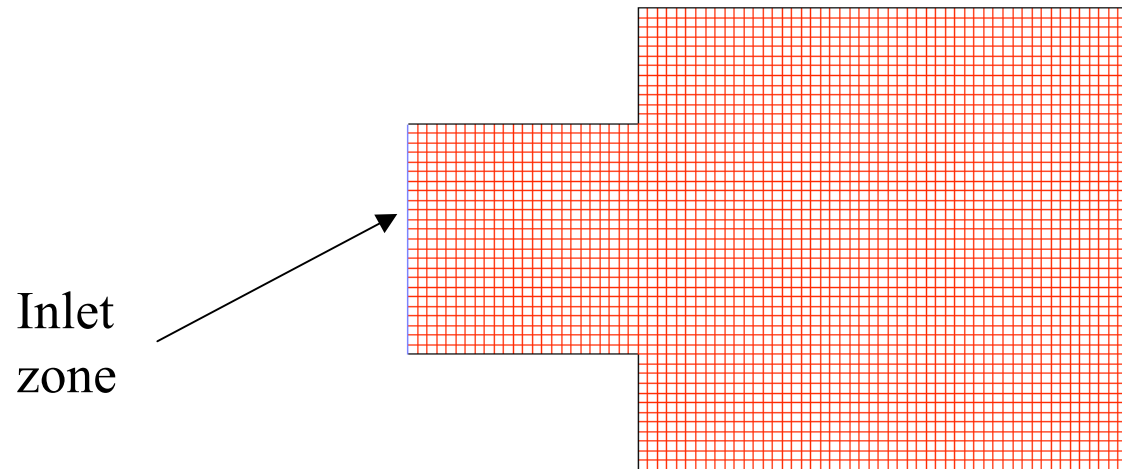
Collection of entities are called “zones”



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: $u = \frac{1}{2\rho\nu} \left(-\frac{dp}{dx} \right) y (h - y)$

function `inlet_parab`

Definitions

Loop over all the inlet cell faces

Evaluate the face centroid coordinates

The function return the velocity

```
winterm
#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 */
    begin_f_loop(f,thread)
    {
        F_CENTROID(x,f,thread); /* get the face centroid coordinates */
        y = x[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)

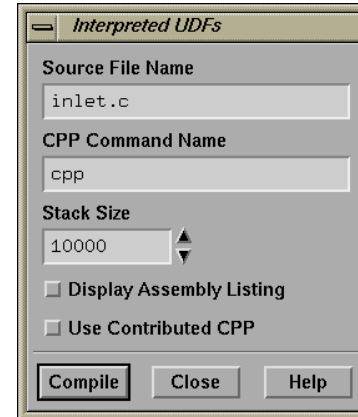
    /* finished */
}
```



A Simple UDF Example

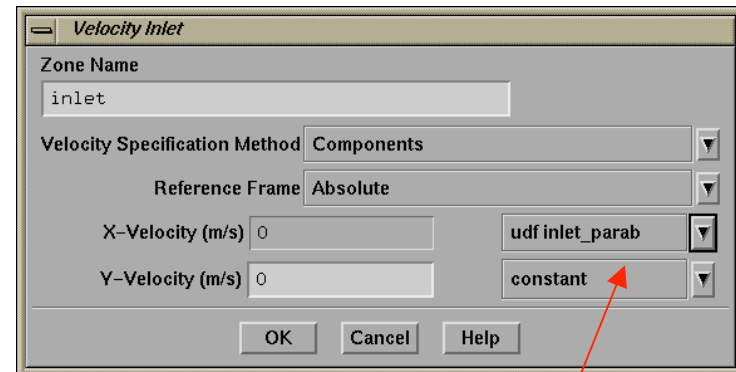
Compile/interpret the UDF:

Define → User Defined



Attach the profile to the inlet zone

Define → Boundary Condition



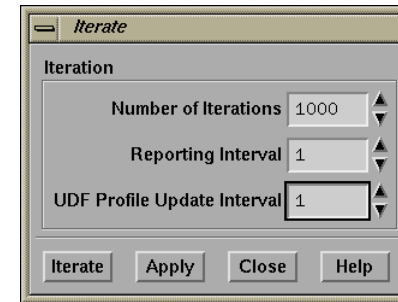
Equivalent to attach the profile from a separate simulation



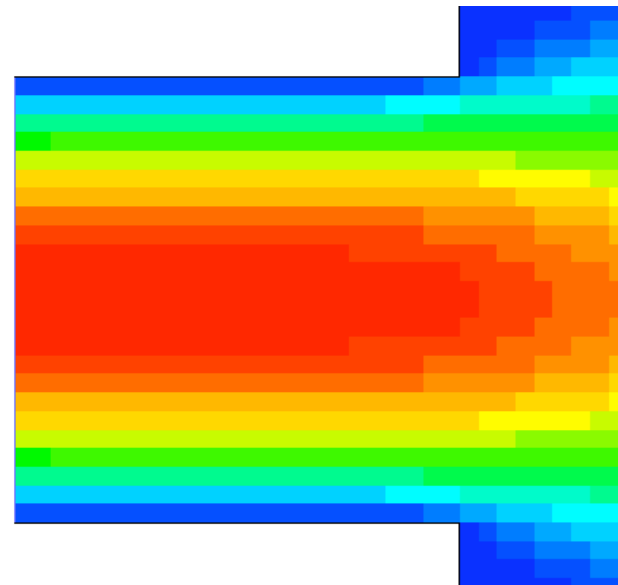
A Simple UDF Example

Solve the equations

Solve → Iterate



Final Result



C Programming

Typical C function:

```
/* 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 = mycompute(y, i, b);
```

Functions which do not return values can be called directly

```
mystuff(a, y, i, b);
```

Mathematical and various other default functions are available

```
a = pow(b, 2);    /* pow(x, y) returns x raised to y */
```



Data Types and Arrays

Arrays of variables are defined using the notation

```
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

```
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:

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

Set-up a pointer

```
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

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

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

Example

```
if (q != 1) {a = 0; b = 1;}
```

```
if (x < 0.)
    y = x/50.;
else
    y = x/25.;
```

C Equivalent FORTRAN code

```
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

end = 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

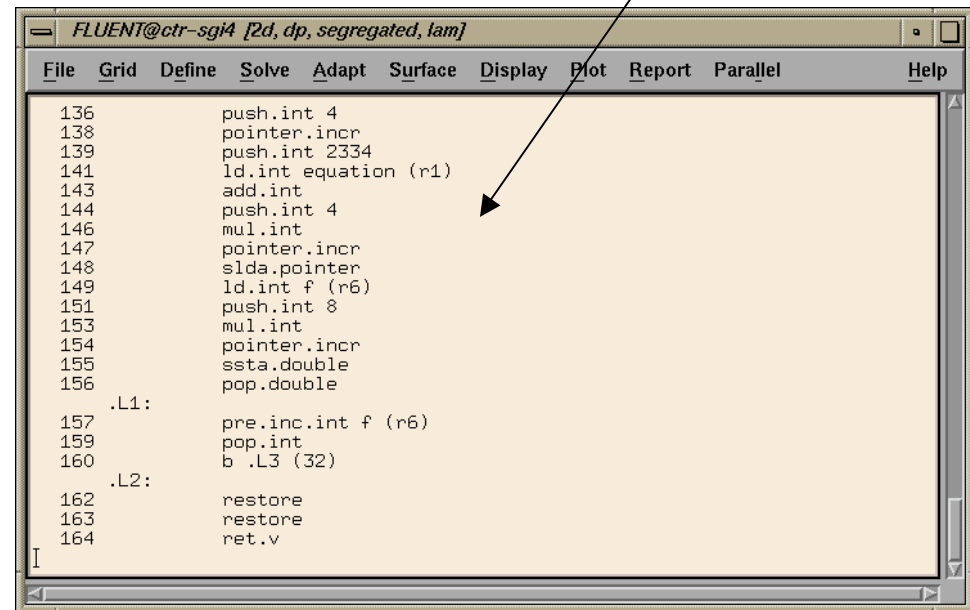
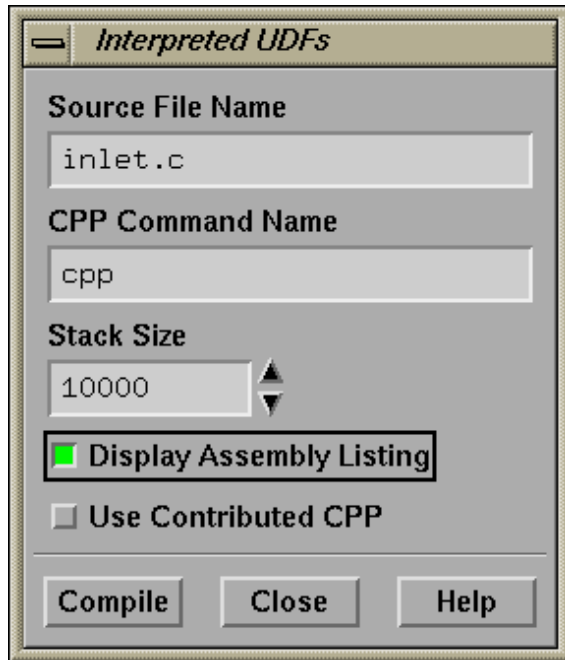
A library of UDF is compiled and linked to the main code
Overcomes all the disadvantages reported above



Interpret the UDFs

Define → User Defined → Interpreted

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

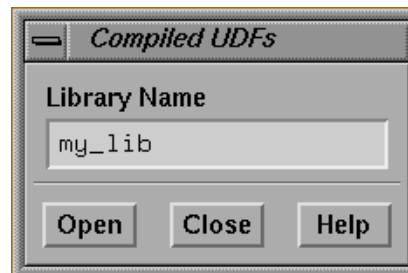


Default stack size might be too small for large arrays!



Compile the UDFs

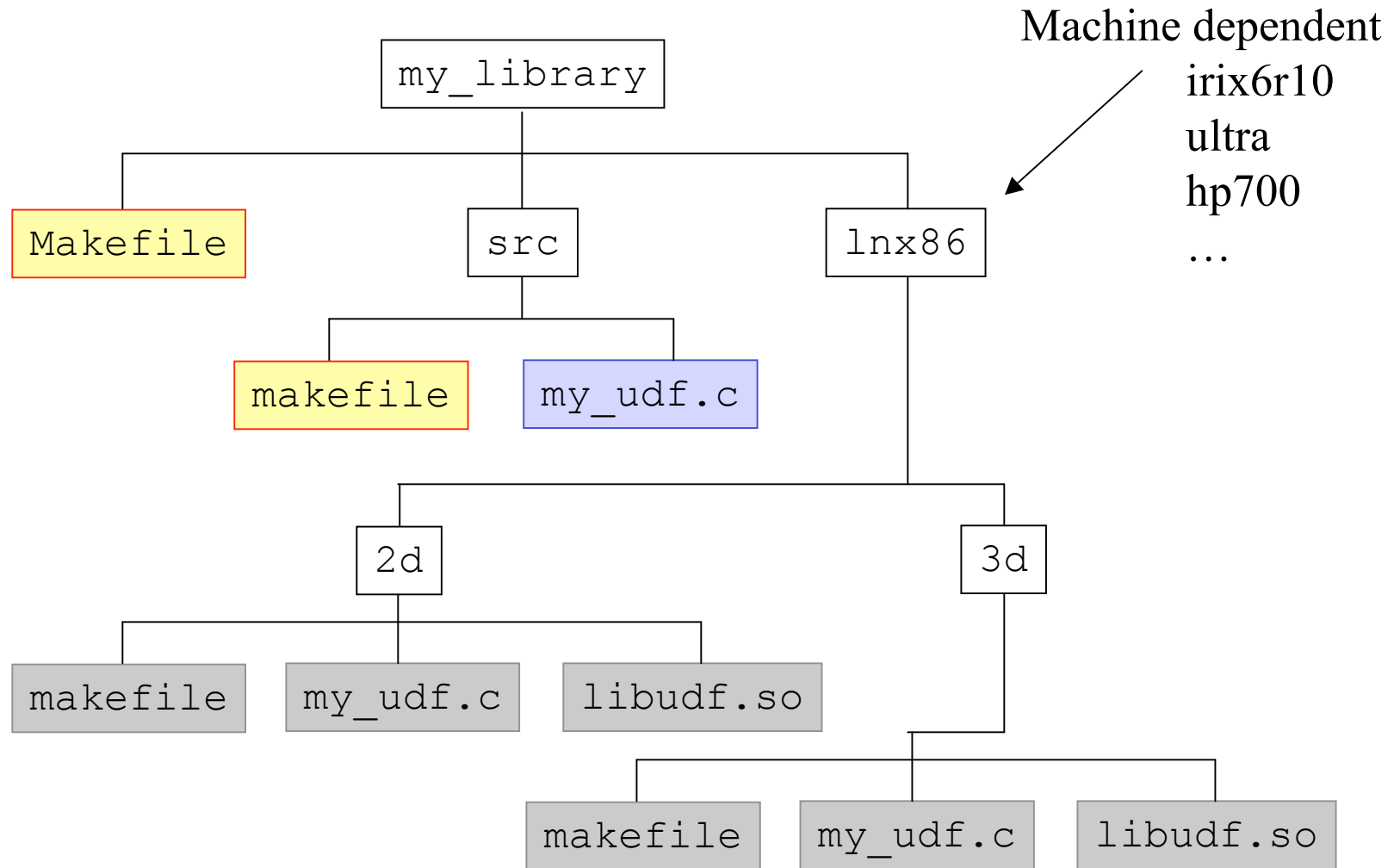
Define → User Defined → Compiled



The library **MUST** be precompiled in a directory tree



Directory tree for compiled UDFs



Makefiles for UDFs

In the directory

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

There are two files

```
akefile2.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.

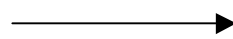
In the second one two macros **MUST** be modified

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



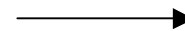
UDFs in FLUENT

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



Available MACROS

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



Programming
Tools

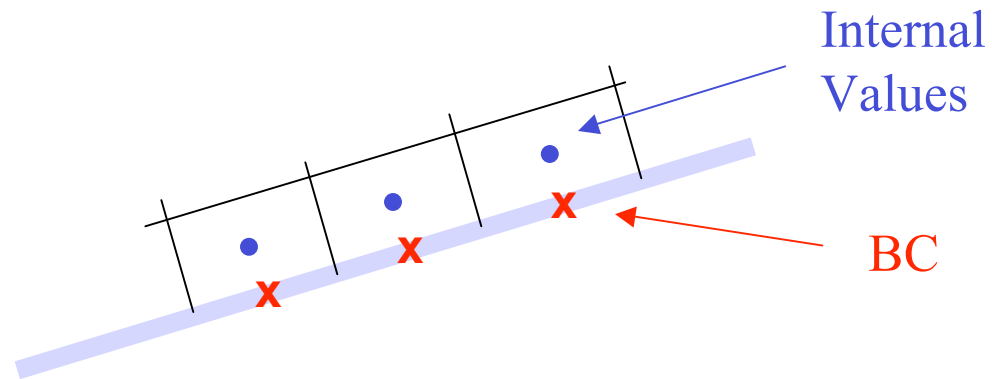


Boundary Conditions

The inlet profile specification is based on the macro `DEFINE_PROFILE`

`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

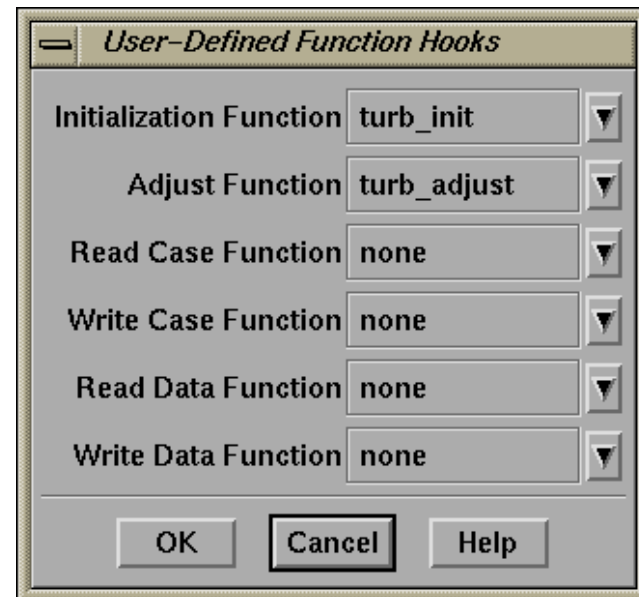
The initial condition specification can be performed using the macro `DEFINE_INIT`

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

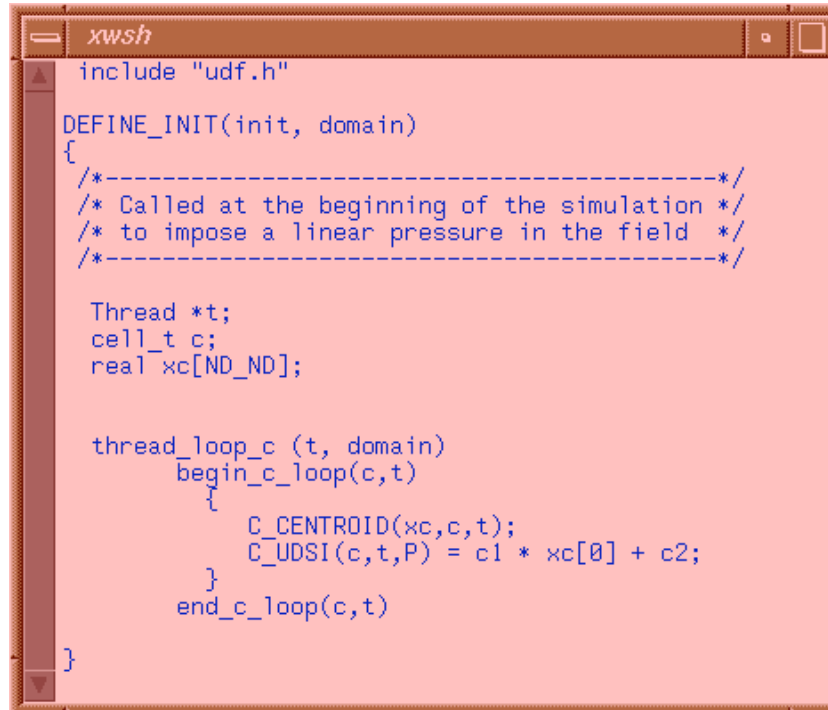
Define → User Defined → Function Hooks



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:



```
xwsh
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[ND_ND];

    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)
}
}
```



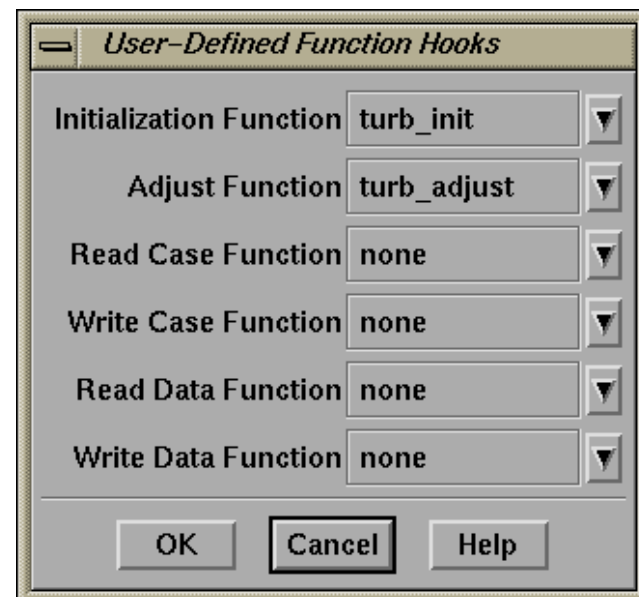
Adjust Function

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!)

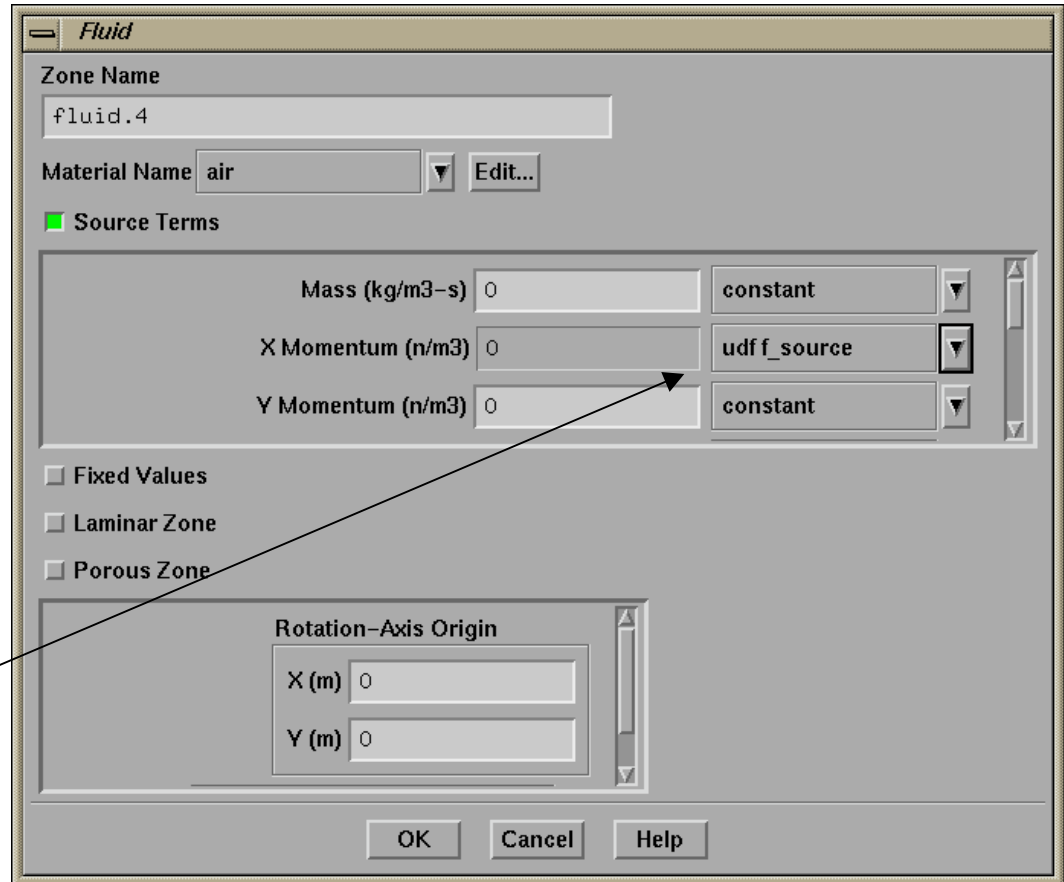


Source Terms

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 ϕ is the dependent variable

A is treated explicitly and B ϕ 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

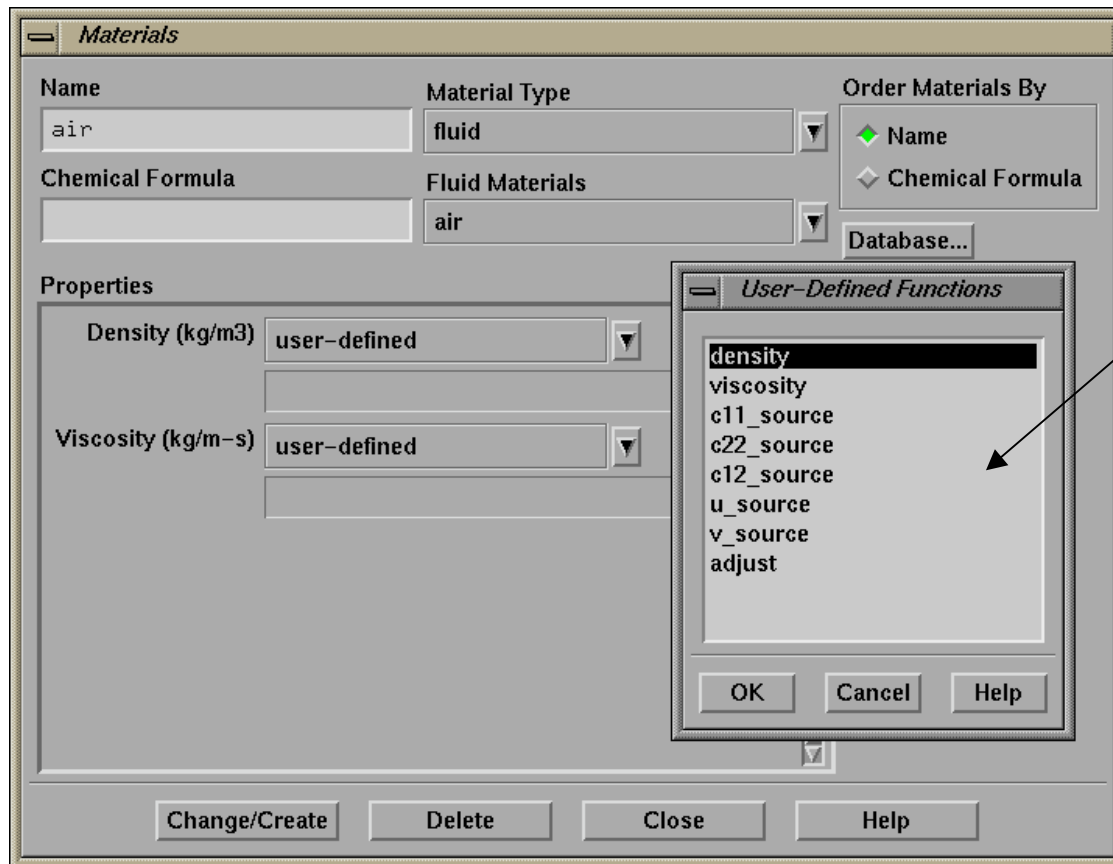
....

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 : EXECUTE_ON_DEMAND

It is executed when activated by the user

Can be used for:

Debugging

Postprocessing

....

Define → User Defined → Execute on Demand



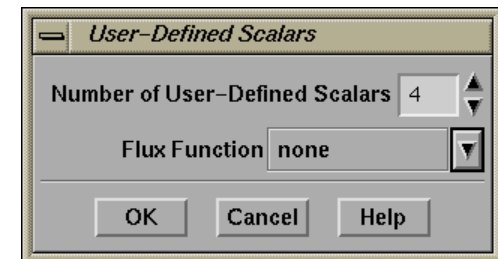
User Defined Scalar

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

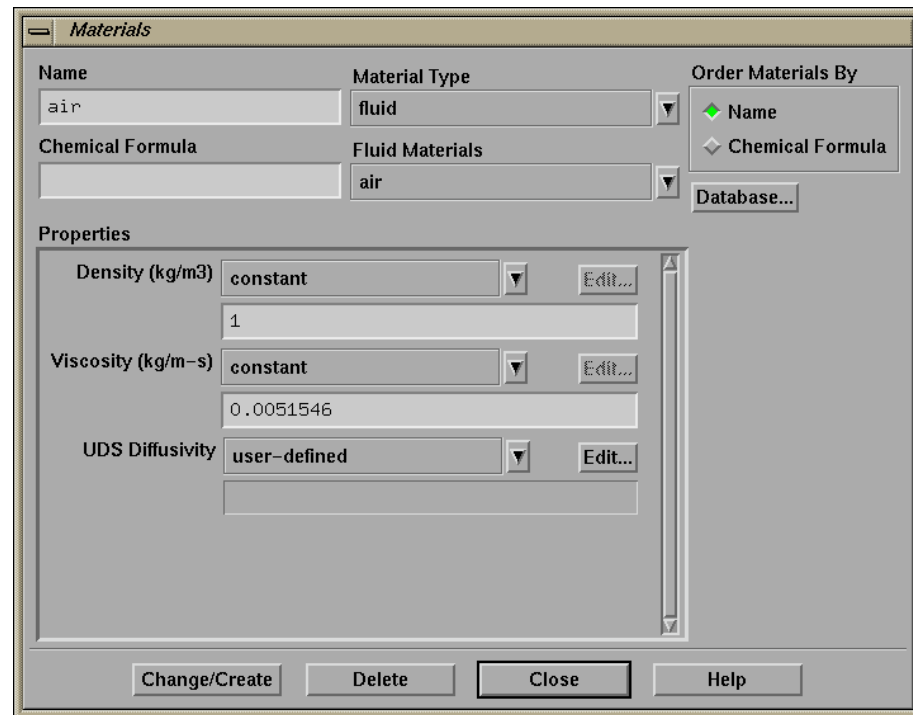
$$\frac{\partial \phi}{\partial t} + U_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D_\phi \frac{\partial U_i}{\partial x_j} \right) + S_\phi$$



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!

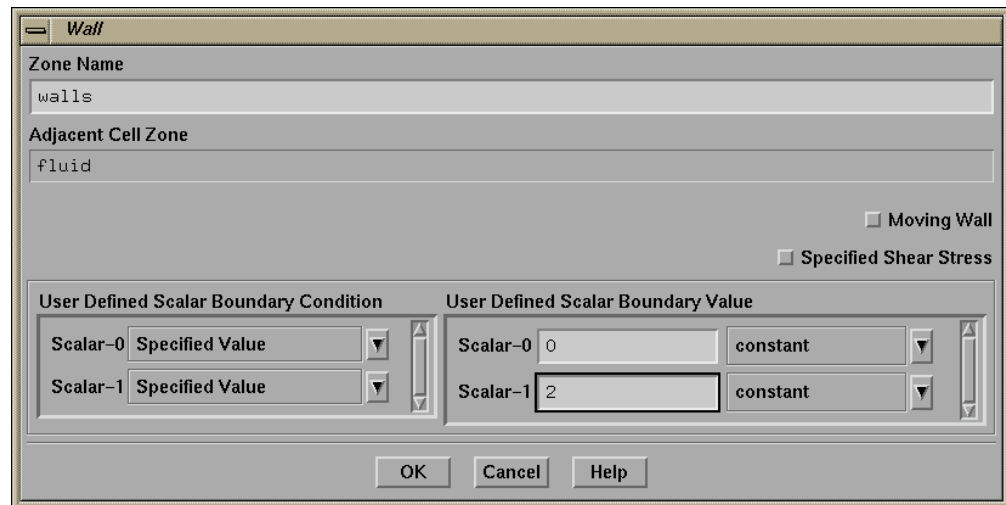


User Defined Scalar

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

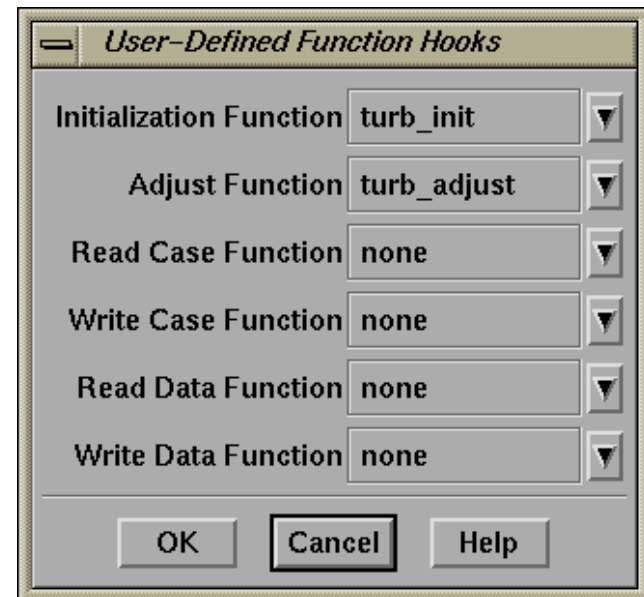


I/O in UDF

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 is introduced

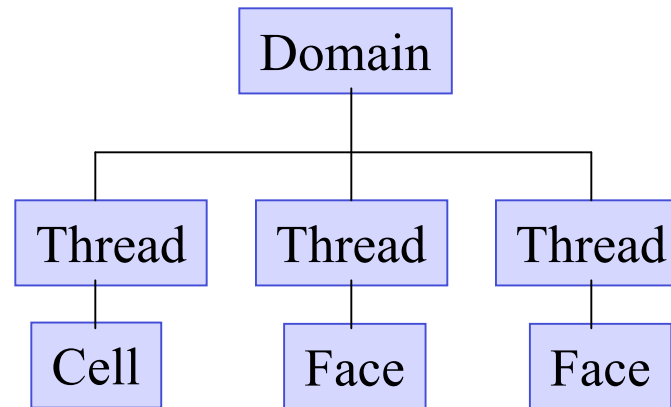


Data Structure

It is based on a hierarchy of structures

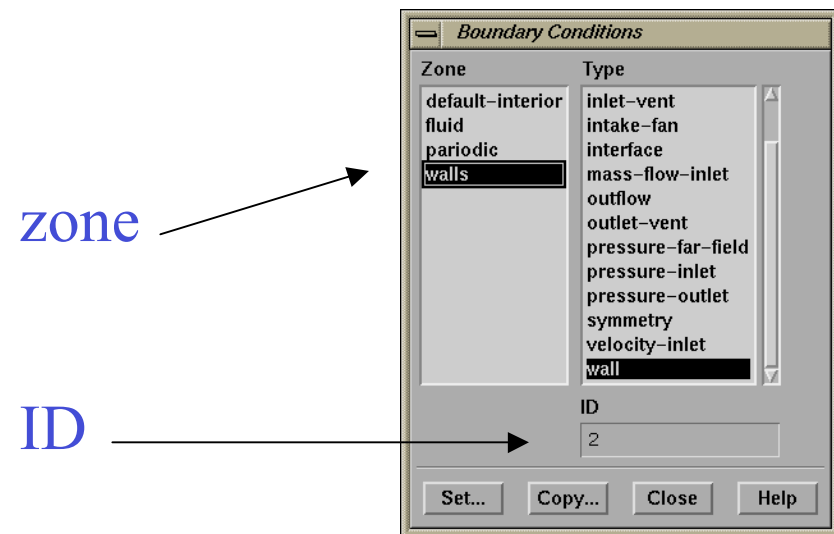
Threads (zones) are collection of cells or faces

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:

```
Thread *tf = Lookup_Thread(domain, ID);
```

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

```
ID = THREAD_ID(thread);
```



Loop Macros

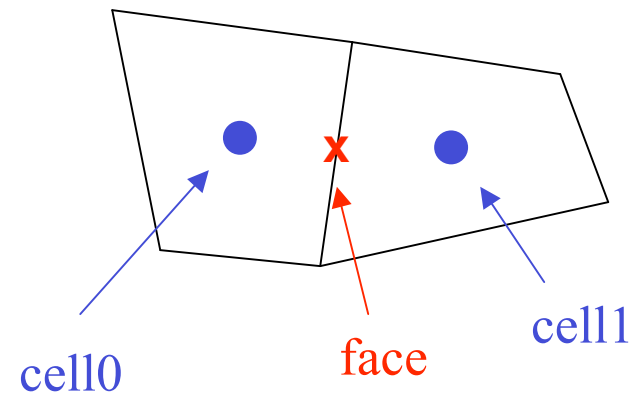
- ◆ `thread_loop_c(t, d);`
- ◆ `thread_loop_f(t, d);`
- ◆ `begin_c_loop(c, t);`
`end_c_loop(c, t);`
- ◆ `begin_f_loop`
`end_f_loop`
- ◆ `f_edge_loop(f, t, n);`
- ◆ `f_node_loop(f, t, n);`
- ◆ `c_node_loop(c, t, n);`
- ◆ `c_face_loop(c, t, n);`
- ◆ Loop over cell threads
- ◆ Loop over face threads
- ◆ 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:

```
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:

```
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:

```
if(!Data_Valid_P())  
    return;
```

◆ `boolean
FLUID_THREAD_P(t0)`

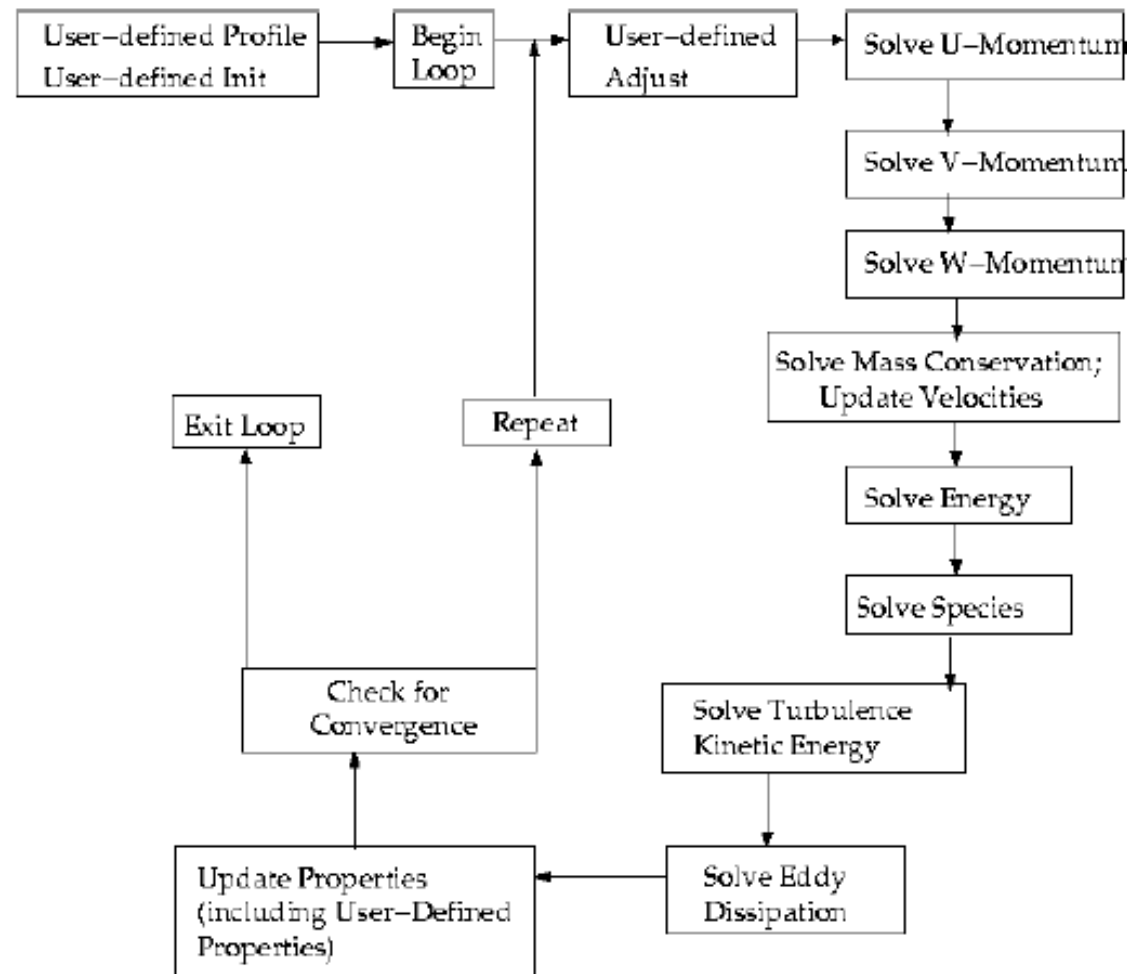
◆ Checks to see if thread `t0` fluid thread

◆ `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

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:

$U(I, J, K) \rightarrow U(IJK)$ where $IJK = (K-1) * NI * NJ + (J-1) * NI$

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

USRBC

USRSRC

USRDI F

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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



FLUENT Example of Scheme file for Adaptation

```
;;;
(custom-field-function/define ,....) ...      ! Define Adaptation Function
;;;
;;; set few parameters
;;;
(define maxcells 200000) ...                ! Set Control 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
```



Example of Automatic Adaptation

Driven Cavity Problem

Start Initial Conditions - Uniform Grid

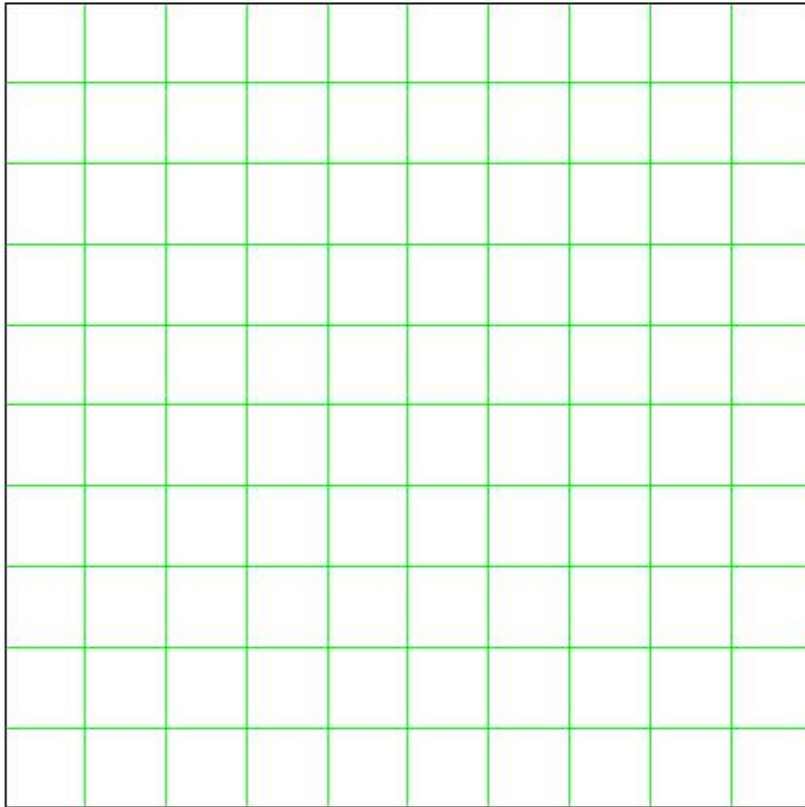
Perform 5 Steps of Adaptation Using Hanging Nodes

Adaptation Function is:

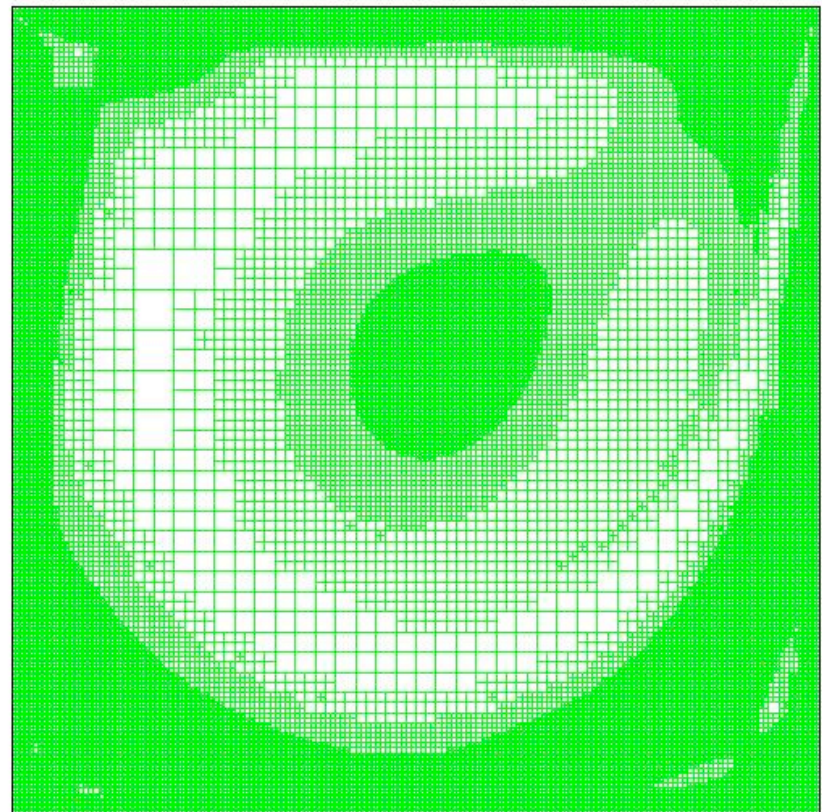
Scaled Velocity Difference =
 $(\text{Velocity Gradient} * \text{Volume}^{1/3}) / \text{Velocity}$



Example of Automatic Adaptation



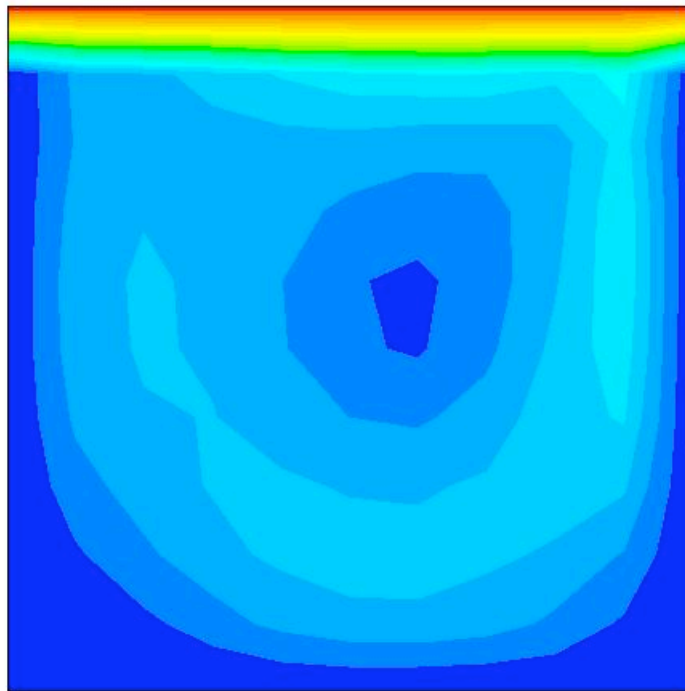
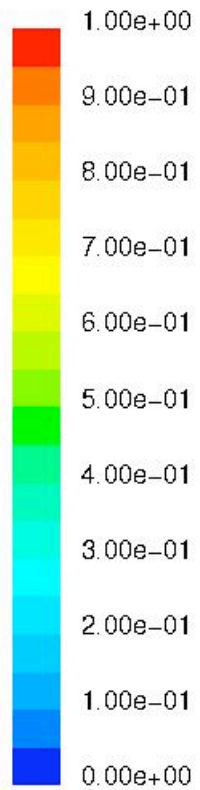
Initial Grid: 100 elements



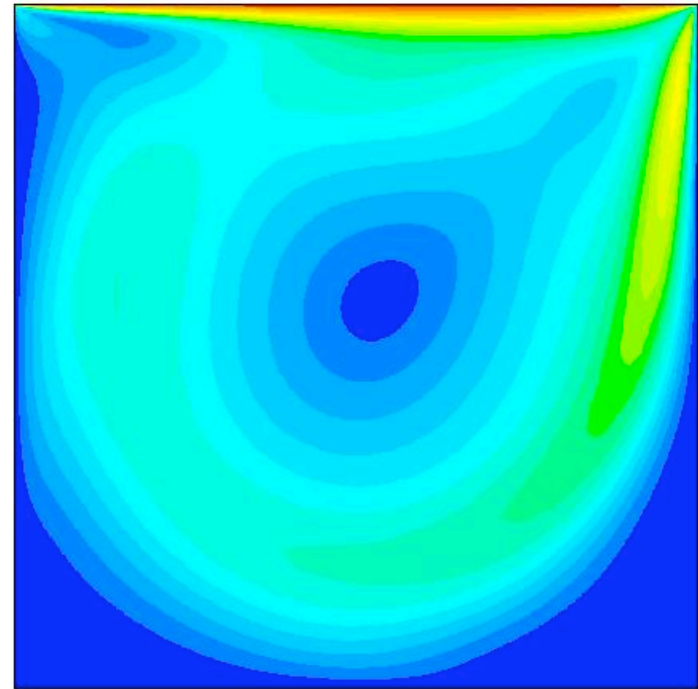
Final Grid: 40,000 elements



Example of Automatic Adaptation



Initial Grid: 100 elements



Final Grid: 40,000 elements



Optimization

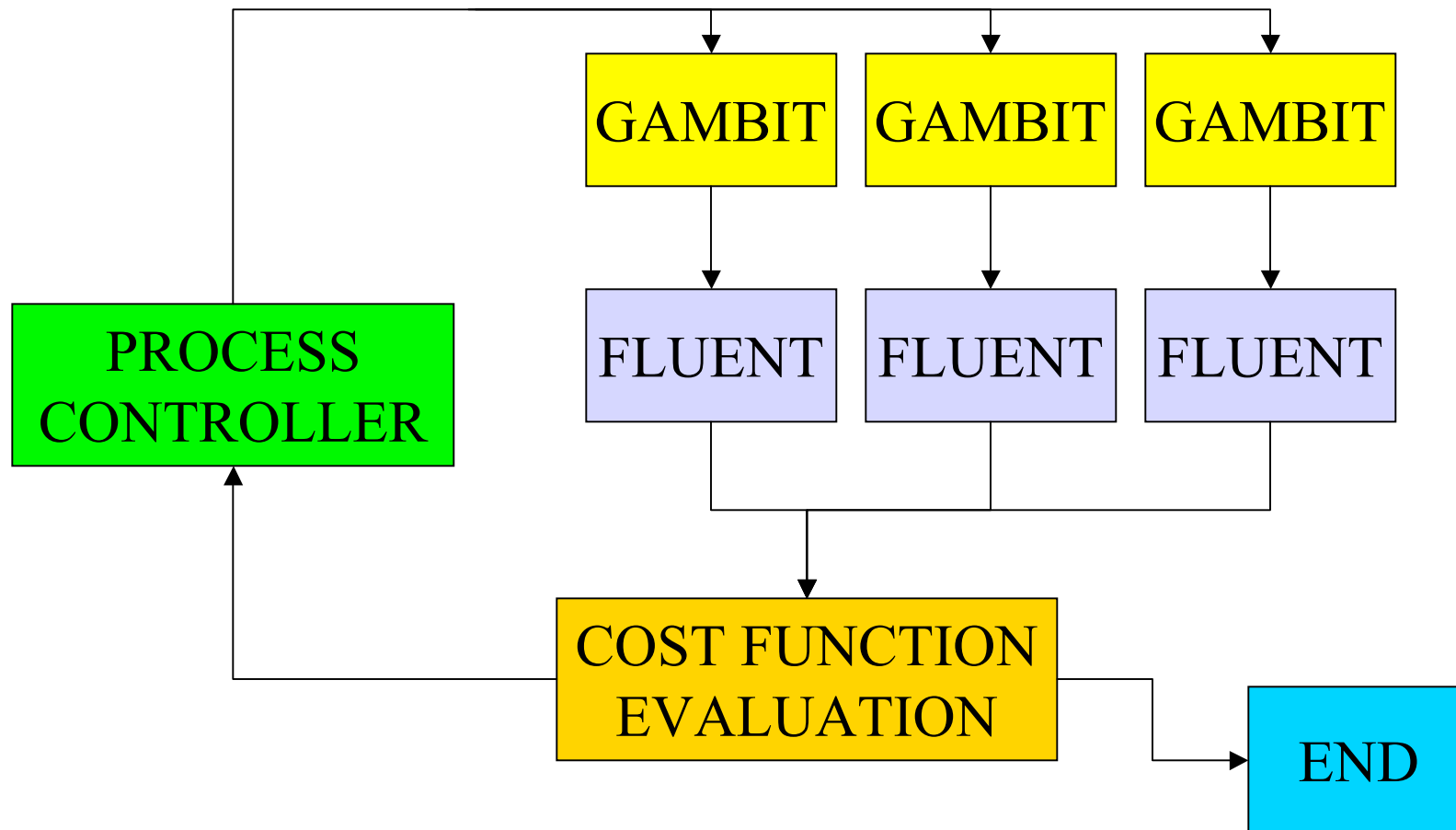
Objective: Automatically find the best solution according to a certain goal (cost function)

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!

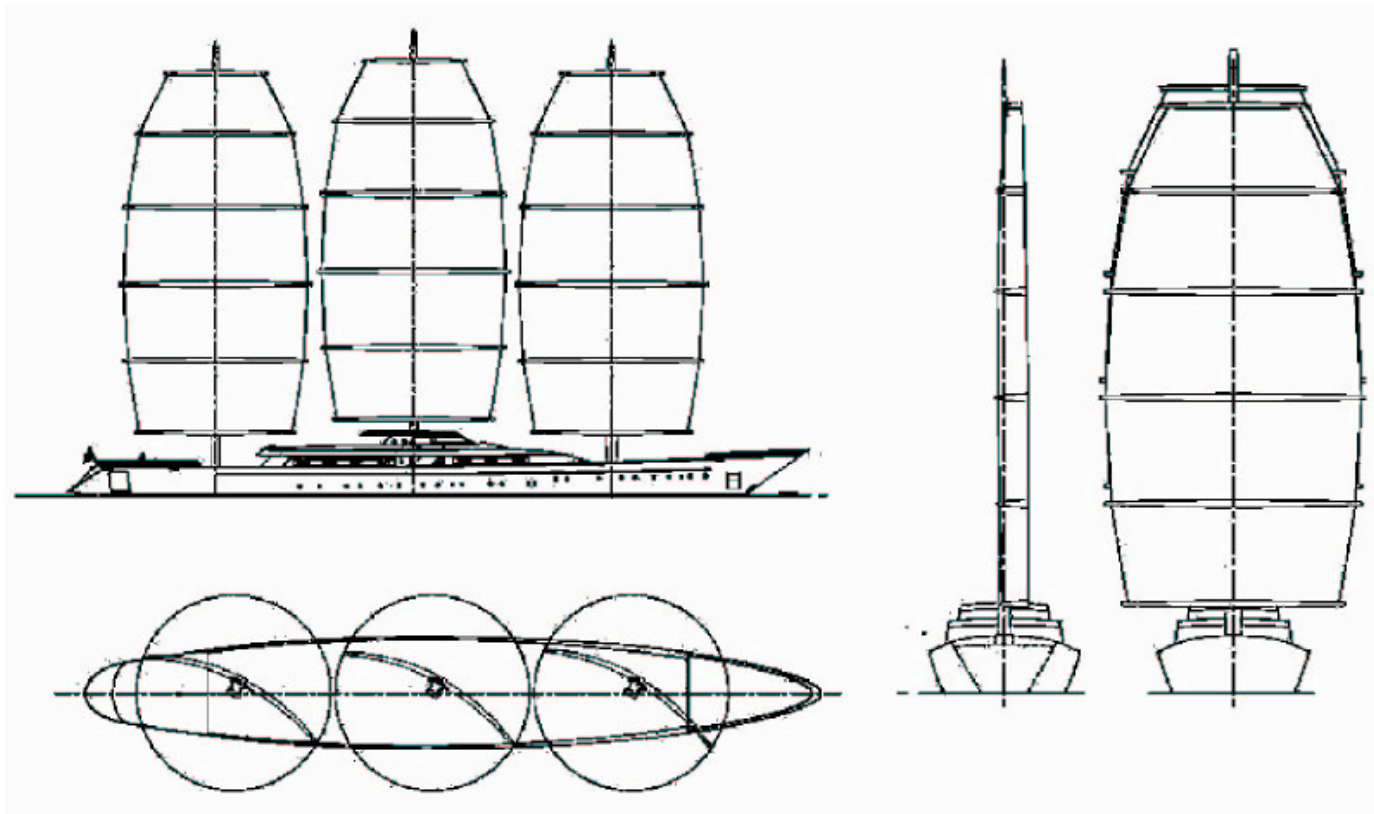


Optimization Procedure



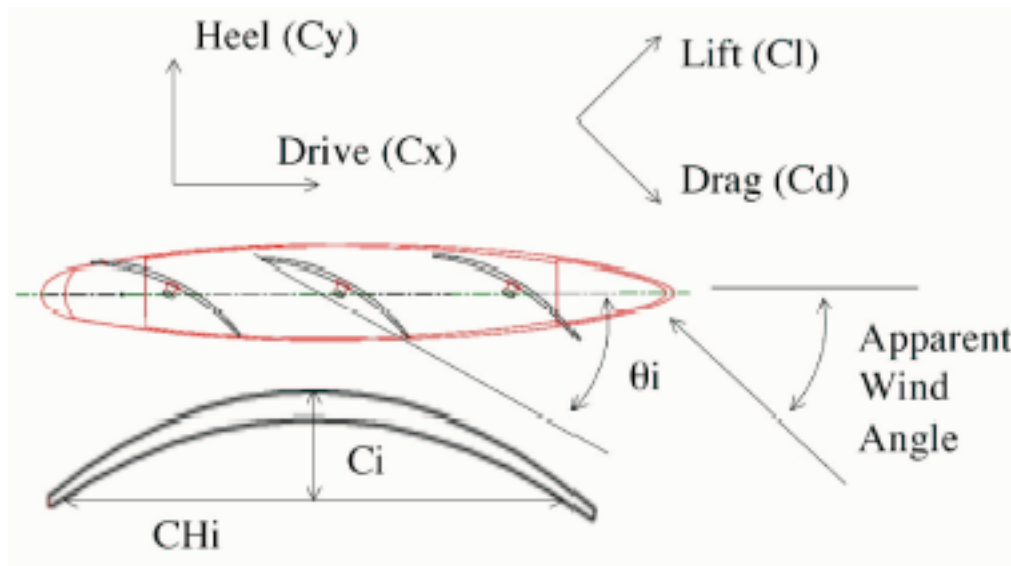
Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship



Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship



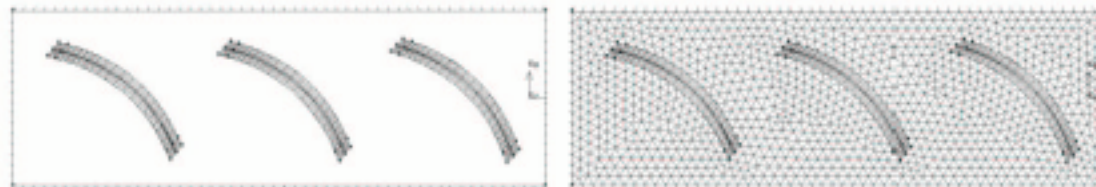
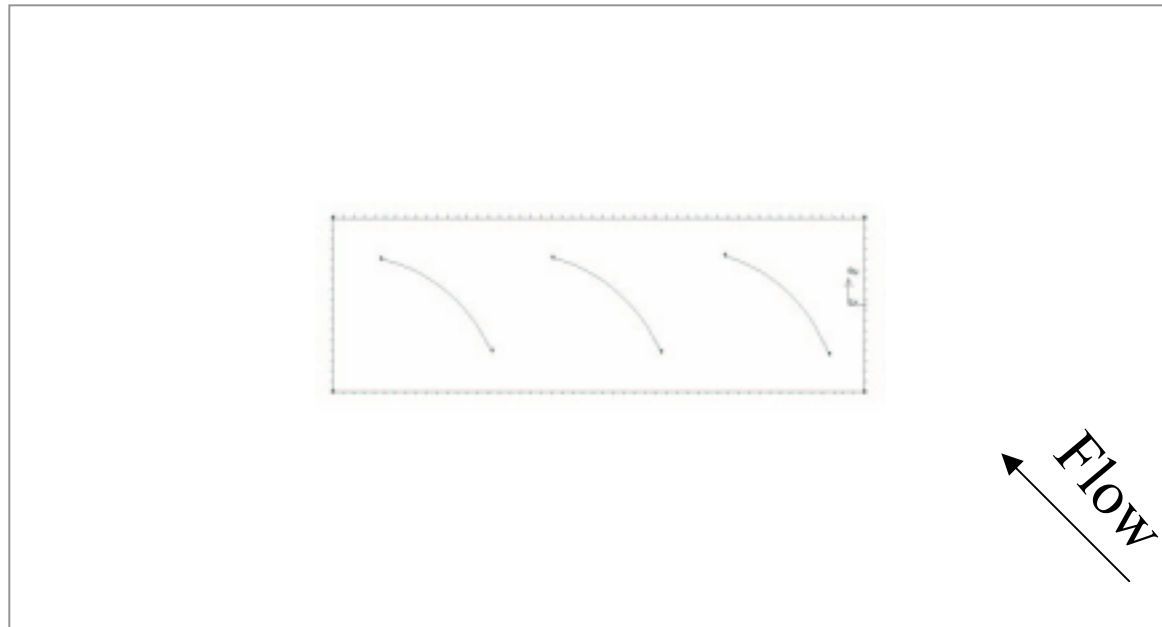
Aerodynamic Force Definitions

One cost function is defined as Lift/Drag



Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship

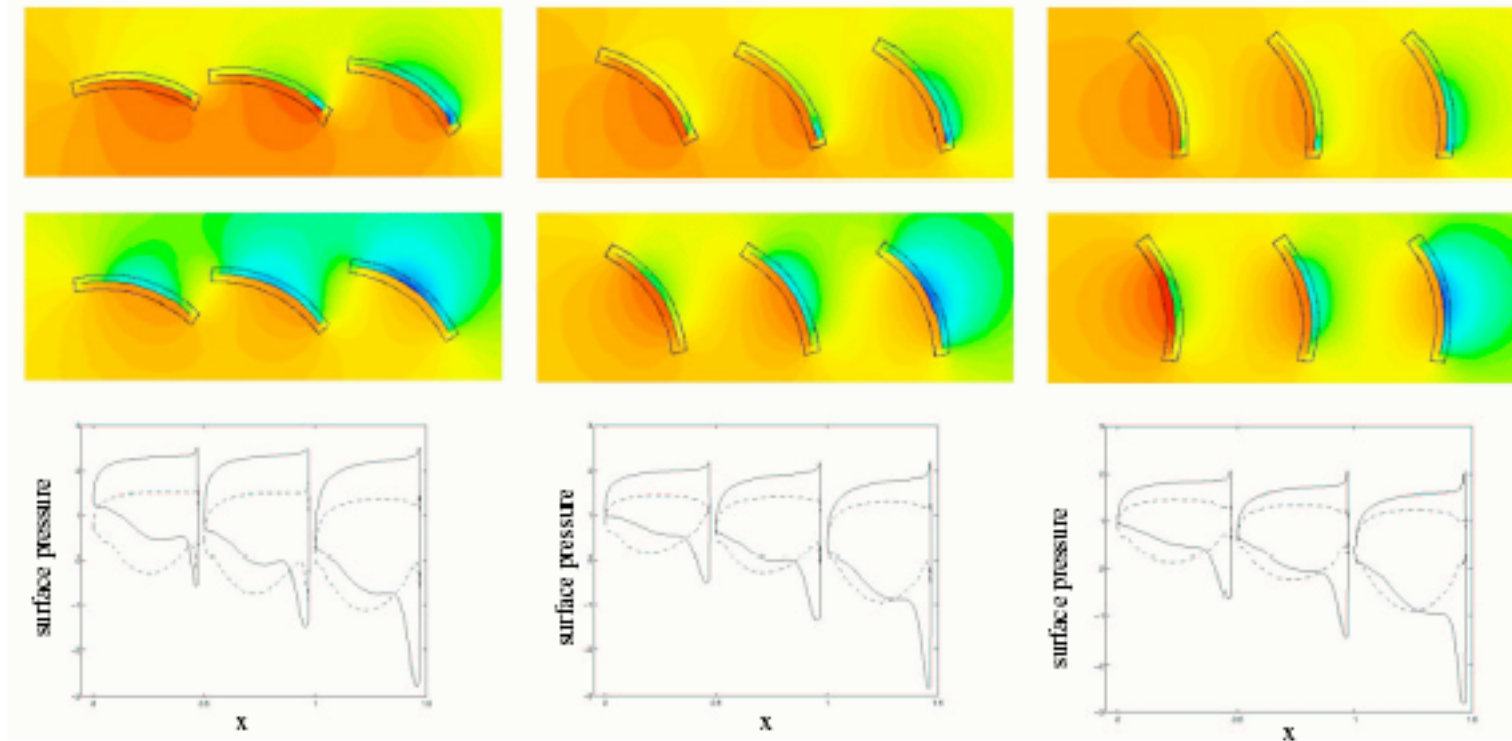


Grid Generation



Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship

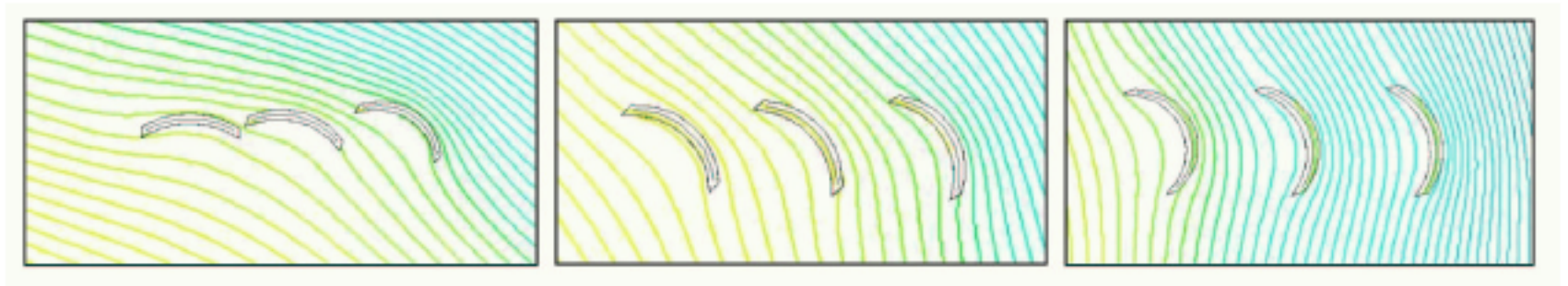


Flow Solutions



Optimization Procedure Example

Design and Trim Sails for a Modern Clipper Ship



Optimized Solution for Different Wind Directions

