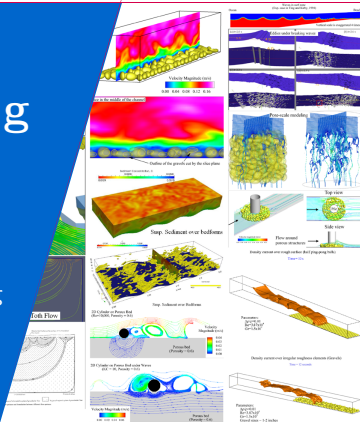


# Chapter 5: Programming and customization

Xiaofeng Liu, Ph.D., P.E.  
 Assistant Professor  
 Department of Civil and Environmental Engineering  
 Pennsylvania State University  
 xliu@engr.psu.edu



# What will be covered in this chapter?

2/31

This chapter is for intermediate and advanced level users:

- ▶ Develop a new solver
- ▶ Develop a new boundary condition
- ▶ Develop a new utility tool
- ▶ Debugging

Overview

Develop a new solver

Develop a new B.C.

Develop a new utility tool

Debugging

# The structure of OpenFOAM

4/31

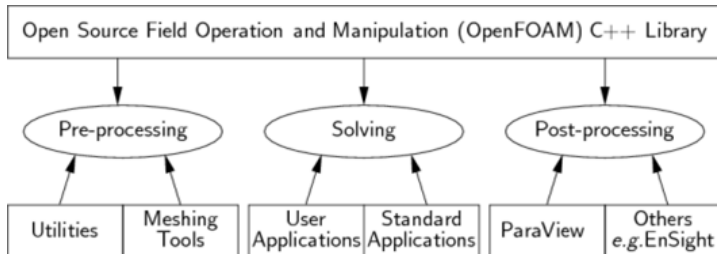


Figure: Structure of the OpenFOAM® platform

Before you do anything, search or ask!

- ▶ Do not re-invent the wheel!
- ▶ The OpenFOAM® user community is getting so big and the applications are very broad
- ▶ There might be someone has done similar work
- ▶ Try search the web by using key words (including OpenFOAM® of course)
- ▶ Or ask the community (the CFD-online forum, OF extend project, etc.)

## Code organization and compilation:

- ▶ Best place to start is the OpenFOAM<sup>®</sup> code itself
- ▶ Usually we find the closest code and make a copy (with a different name of course).
  - For example, to write a new solver, just copy a similar existing solver
  - Change the name of the files and resulting executable
  - Modify code and compile
  - Use the new solver
- ▶ OpenFOAM<sup>®</sup> uses `wmake` to organize the compilation process
- ▶ Detailed instructions:

<http://www.openfoam.org/docs/user/compiling-applications.php>

Usage of wmake:

- ▶ `files`: specify what C++ source files to compile, the result name, and where to put it.
- ▶ The targeted result can be executables (solver and utility tools)

`newApp.C`

`EXE = $(FOAM_USER_APPBIN)/newApp`

or library

`newLib.C`

`LIB = $(FOAM_USER_LIBBIN)/libnewLib`

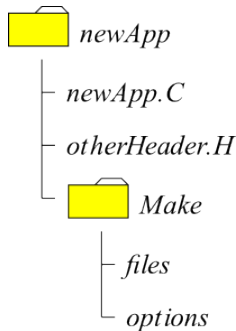


Figure: wmake

## Usage of wmake:

- ▶ options: specify the paths to the header files to be included and the libraries to be linked.

```
EXE_INC = \  
    -I<directoryPath1> \  
    -I<directoryPath2> \  
    \  
    -I<directoryPathN>
```

```
EXE_LIBS = \  
    -L<libraryPath1> \  
    -L<libraryPath2> \  
    \  
    -L<libraryPathN> \  
    -l<library1> \  
    -l<library2> \  
    \  
    -l<libraryN>
```

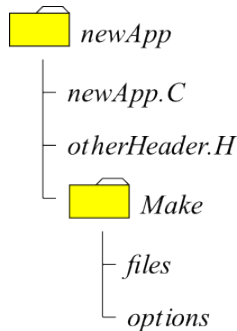


Figure: wmake



Usage of `wmake`:

- ▶ To compile: just type `wmake`
- ▶ In OpenFOAM<sup>®</sup>, `wmake` uses a lot of environmental variables, such as `WM_PROJECT`, `FOAM_USER_LIBBIN`, etc
- ▶ `wmake` generates a lot of intermediate files.
- ▶ It is a good idea to cleanup using the `wclean` command before compilation

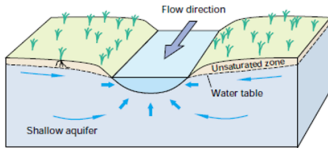
- ▶ OpenFOAM® comes with a lot of pre-defined solvers
- ▶ However, they might not meet your needs.
- ▶ Examples:
  - Your problem is totally new and has not been implemented in OpenFOAM®
  - Your problem is not totally new but you need to modify existing solver.
  - You need to add more physics to the problem, say add scalar transport to the `pisoFoam` solver.

# Develop a new solver

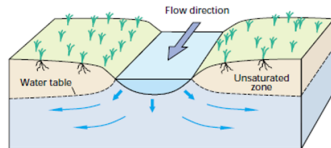
11/31

New solver examples in porous media and groundwater flows:

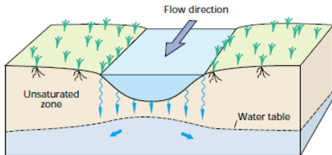
- ▶ Saturated (Darcy law, diffusion equation, linear, easy)
- ▶ Unsaturated (Richardson equation, non-linear, not easy)



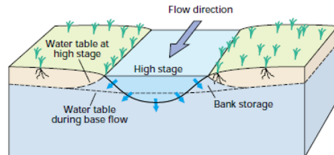
Gaining stream



Losing stream



Disconnected stream



Bank storage

Figure: Surface water-groundwater interactions

Saturated groundwater flow:

- ▶ Darcy law, diffusion equation, linear, easy
- ▶ This governing equation is a simple heat equation. The solution of which is very easily implemented in OpenFOAM® using tensor notations.
- ▶ The new solver: `groundWaterFoam`

$$S_s \frac{\partial h}{\partial t} = K \nabla^2 h + Q$$

where  $h$  is the pressure head,  $S_s$  is the specific storage coefficient,  $K$  is hydraulic conductivity,  $Q$  is source/sink.

# Develop a new solver

13/31

The new solver: groundWaterFoam:

```
while (simple.loop())
{
    Info<< "Time = " << runTime.timeName() << nl << endl;

    for (int nonOrth=0; nonOrth<=simple.nNonOrthCorr(); nonOrth++)
    {
        solve
        (
            fvm::ddt(h)
            - fvm::laplacian(K/Ss, h)
            ==
            Q_o_Ss
        );
    }

    #    include "write.H"

    Info<< "ExecutionTime = " << runTime.elapsedCpuTime() << " s"
        << "    ClockTime = " << runTime.elapsedClockTime() << " s"
        << nl << endl;
}
```

# Develop a new solver

14/31

The new solver: groundWaterFoam

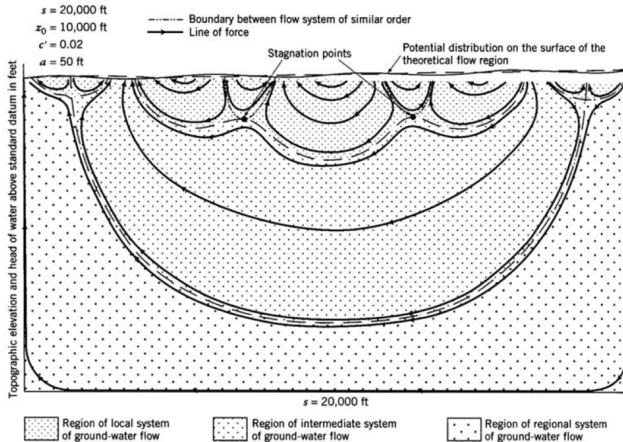


Figure: Scheme of Toth flow (Toth, 1963)

The top boundary condition for  $h$  used groovyBC.

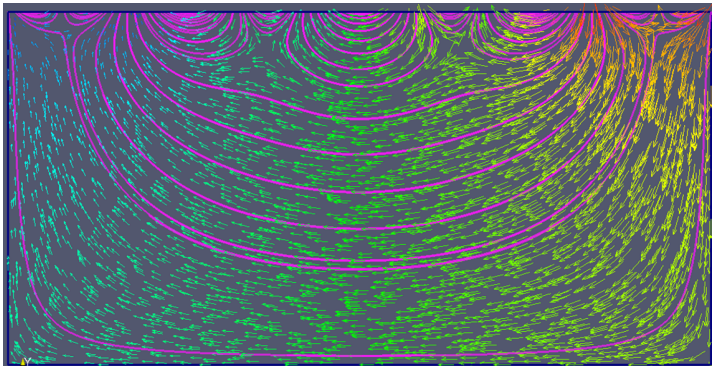


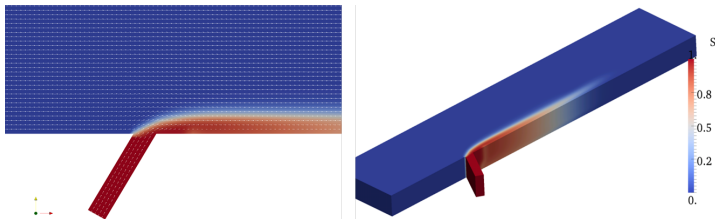
Figure: Simulation result of Toth flow (Toth, 1963)

# Develop a new solver

16/31

In the tutorial, you will learn how to adapt the `pisoFoam` solver for adding a scalar transport equation:

$$\frac{\partial S}{\partial t} + \nabla \cdot (\mathbf{u}S) = \nabla \cdot (D\nabla S) \quad (1)$$





# Develop a new B.C.

17/31

- ▶ OpenFOAM® also comes with a lot of pre-defined boundary conditions
- ▶ However, they might not meet your needs.
- ▶ Examples:
  - You need to specify velocity distribution at the inlet.
  - You need to specify a boundary condition change with time
  - Other boundary conditions needs to be hard-coded
- ▶ Again, before you do, search and ask!

# Develop a new B.C.

18/31

- ▶ There are at least two ways to do it
  - Add the implement of new BC directly into your solver
  - Write a new library implementing the new BC and dynamically load it at run time
- ▶ Pros and cons of both methods

Option 1: Implement the new BC into your solver:

- ▶ The generic BCs in OpenFOAM are located in  
`$FOAM_SRC/finiteVolume/fields/fvPatchFields/`
- ▶ Find the one closest to your needs
- ▶ Copy its files to the solver's code directory
- ▶ Change the files according to your needs
- ▶ Modify `Make/files` and `Make/options` and instruct the compiler to compile these new BC files
- ▶ Recompile the solver

# Develop a new B.C.

20/31

Option 1: Implement the new BC into your solver:

- ▶ Demonstration: Modify the `oscillatingFixedValue` BC

## Option 2: Write a new library for the BC

- ▶ The generic BCs in OpenFOAM are located in  
`$FOAM_SRC/finiteVolume/fields/fvPatchFields/`
- ▶ Find the one closest to your needs
- ▶ Copy its files to the solver's code directory
- ▶ Change the files according to your needs
- ▶ Modify `Make/files` and `Make/options` and instruct the compiler to compile these new BC files
- ▶ Compile these new BC files to a library

# Develop a new B.C.

22/31

Option 2: Write a new library for the BC

- ▶ Demonstration: Create a new library for the new `oscillatingFixedValue` BC

A closer look at the boundary condition code

- ▶ It has several .H and .C files
- ▶ First, it defines a unique name by  
`Typename(myOscillatingFixedValueq)`  
in the `myOscillatingFixedValueFvPatchField.H` head file
- ▶ This head file also defines the class  

```
template<class Type>
class myOscillatingFixedValueFvPatchField
:   public fixedValueFvPatchField<Type>
```
- ▶ It is templated, i.e., good for Type scalar, vector, and tensor fields.

A closer look at the boundary condition code

- ▶ It has three private data

```
Field<Type> refValue_  
scalar amplitude_  
scalar frequency_;
```

- ▶ Each boundary condition class has an `updateCoeffs` member function, which is called every time step to update the boundary condition

```
void myOscillatingFixedValueFvPatchField<Type>::updateCoeffs()
```

- ▶ You need to change here according to your needs



# Develop a new utility tool

25/31

- ▶ OpenFOAM<sup>®</sup> comes with a lot of pre-defined tools (in applications/utilities)
- ▶ However, they might not meet your needs.
- ▶ Examples:
  - You need to convert OF result to certain format for visualization
  - You need to calculate flow rate across some surface
  - You need to calculate the total kinetic energy in the simulation domain
  - ...

# Develop a new utility tool

26/31

Implement a new utility tool:

- ▶ The generic tools in OpenFOAM® are located in `$FOAM_APP/utilities/`
- ▶ Find the one closest to your needs
- ▶ Copy its files to a new directory
- ▶ Change the files according to your needs
- ▶ Modify `Make/files` and instruct the compiler to compile these new files
- ▶ Recompile the tool

# Develop a new utility tool

27/31

- ▶ Demonstration: new utility tool `oneFieldToTecplot`

- ▶ What if something is not right with your code?
- ▶ You need to do debugging.
- ▶ Ways to do it:
  - Print information to the screen/file
    - Use `Info << something << A_variable << endl;`
    - `Info` is a pre-defined object of class `messageStream` which handles messages
    - Most of classes in OpenFOAM® implement the `<<` operator.
    - So `Info << U << endl;` will dump everything about velocity  $U$  field to the screen.

## ► Ways to do it:

- Use DebugSwitches

- Defined in file \$WM\_PROJECT\_DIR/etc/controlDict
- It has the following information

```
DebugSwitches
{
    Analytical    0;
    ...
    fvVectorMatrix 0;
    ...
}
```

- Switch 0 turns off the debug information; 1, 2, 3, etc. turns on different levels of debug information
- You don't need to run the debug version of OpenFOAM® to use DebugSwitches
- Each simulation case can have its own definition of DebugSwitches in system/controlDictfile

- ▶ Ways to do it:
  - Use gdb (Gnu Debugger)
    - It is the professional way to do debugging
    - It is doable
    - But I have not done it so far.
    - You need to recompile a debug version of OpenFOAM® by  
export WM\_COMPILE\_OPTION=Debug  
in file \$WM\_PROJECT\_DIR/etc/bashrc
    - Then you need to load the executable into gdb to do things like stepping, break, print variables, etc.

Questions?