



Incompressible flow simulation using regularized hydrodynamics equations in OpenFOAM v1912

Instructors: Tatiana V. Stenina, Aleksadr V. Ivanov

Authors: T.V. Stenina, A.V. Ivanov, M.V. Kraposhin, I.N. Sibgatullin

Training level: Intermediate

Session type: Lecture with examples **Software stack:** OpenFOAM v1912

https://github.com/unicfdlab





Plan of training course

- 1 Training course materials
- 2 Introduction to regularized/QHD equations History Application Key points of training course
- 3 Theoretical part
 Governing equations
 Boundary conditions
 Parameter τ
- 4 Practical part How to install QHD solver Stages of solution Basic case Results
- **5** Summary





Before we start

If you are listener of the course, you should:

- have basic knowledge of OpenFOAM
- know basic commands for Linux terminal
- have preinstalled OpenFOAM v1912 on your laptop OR ability to boot from USB
- have Internet connection





Training course materials

Course location: https://github.com/unicfdlab/TrainingTracks

• Folder QHDFoam-OFv1912

Folder Description

Cases Cases that will be used to demonstrate QHD solver's work during the track

This presentation and other materials that were used in this course

Full version of the solver is available at https://github.com/unicfdlab/QGDsolver





Part I Introduction

What is regularized hydrodynamics equations





History

1982 – QGD system derived from Boltzmann equation



Chetverushkin



Elizarova

1997 – QGD system formulated as conservation laws



Prof. Yu. V. Sheretov

From then to now regularized or sometime Quasi Gas Dynamic (QGD) and Quasi Hydro Dynamic (QHD) equations are extensively used for various flows simulations – incompressible, compressible, multicomponent, magnetohydrodynamic, porous flows, two-phase flows in Paris Fundamental Metablanting of Applied Metablanting of Ap

– in Russia, Europe and in Keldysh Institute of Applied Mathematics of the RAS <code>https://keldysh.ru/</code>





Pro's and Con's of QGD

Advantages of QGD algorithms

- they can work without flux limiters
- they converge monotonically to real solution
- they do not involve Rieman-solvers
- the procedure of approximation is universal for all types of flows
- they can be integrated with other OpenFOAM models
- by contrast to PISO/SIMPLE they don't involve non-orthogonal or pressure-velocity correctors
- all abovementined features make QGD algorithms a useful tool for studying transient flows phenomena

Drawbacks of QGD algorithms

- they are usually slower (3-4 times) than conventional PISO or Godunov-type methods
- additional conditions are imposed for stability criteria
- they require finer grids and smaller time steps in comparison with PISO algorithm for advection-dominated flows





QGD Target audience

According to stated advantages and drawbacks of QGD algorithms, they could be useful to:

- scientists, who want to solve complex set of equations, but still haven't elaborated PISO/SIMPLE or Godunov-type procedure
- researches or engineers who want to validate other methods and programs and numerical models, but they don't have analytic solution
- engineers, who want to simulate complex transient flows which could not be reproduced by PISO/SIMPLE algorithms





Key points of training course

The following points will be considered:

- a description of the basic principles of the solver (QHDFoam);
- setting the input parameters (initial and boundary conditions);
- running tutorials for OpenFOAM v1912.









 $Re = 10^{2}$

 $Re = 10^3$

 $Re = 10^4$

 $Re = 2 \times 10^4$

 $Re = 5 \times 10^4$





Part II Theoretical part

QHDFoam: how it works





Governing equations

Continuity equation:

$$\nabla \cdot \left(\vec{U} - \vec{W} \right) = 0, \quad \vec{W} = \tau \left((\vec{U} \cdot \nabla) \vec{U} + \frac{1}{\rho_0} \nabla \tilde{p} - \beta \vec{g} \tilde{T}) \right)$$

Momentum equation:

$$\frac{\partial \vec{U}}{\partial t} + \nabla \cdot \left(\left(\vec{U} - \vec{W} \right) \otimes \vec{U} \right) + \frac{1}{\rho_0} \nabla \tilde{p} = \frac{1}{\rho_0} \nabla \cdot \hat{\Pi} + \beta \vec{g} \tilde{T}$$

• Scalar (temperature) transport equation:

$$\frac{\partial T}{\partial t} + \nabla \cdot \left(\left(\vec{U} - \vec{W} \right) T \right) - \nabla \cdot \left(\tau \vec{U} \left(\vec{U} \cdot \nabla \right) T \right) - \nabla \cdot \left(\frac{\mu}{\rho_0 P r} \nabla T \right) = 0$$

• Incompressible EoS and regularized stress tensor:

$$\rho = \rho_0 \left(1 + \beta \tilde{T} \right), \ \hat{\Pi} = \rho \vec{U} \otimes \vec{W} + \hat{\Pi}_{NS}, \ \hat{\Pi}_{NS} = \mu \left[(\nabla \otimes \vec{U}) + (\nabla \otimes \vec{U})^T \right]$$

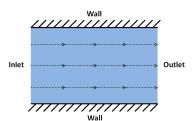




Boundary conditions

Types of boundary conditions:

- wall
- inlet
- outlet



The mathematical description of these BCs within the framework of regularized equations is set out on next slides.





Wall

Velocity of a fluid at a wall equals (0, 0, 0)

Mass flux through a wall equals 0

$$\vec{U} = (0, 0, 0)$$

$$\begin{split} \vec{n} \cdot (\vec{U} - \vec{W}) &= 0 \Rightarrow \\ \vec{n} \cdot \vec{U} - \tau (\vec{U} \cdot \nabla \vec{U} - \frac{1}{\rho_0} \nabla p) \cdot \vec{n} &= 0 \Rightarrow \\ \frac{\partial p}{\partial n} &= \rho_0 \vec{n} \cdot (-\vec{U} \cdot \nabla \vec{U}) \end{split}$$





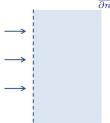


Inlet

Velocity of a fluid at the inlet is fixed

$$\vec{U} = \vec{U}_{in}$$

$$\begin{split} \vec{n} \cdot (\vec{U}_{in} - \vec{W}) &= \vec{n} \cdot \vec{U}_{in} \Rightarrow \\ \tau(\vec{U} \cdot \nabla \vec{U} - \frac{1}{\rho_0} \nabla p) \cdot \vec{n} &= 0 \Rightarrow \\ \frac{\partial p}{\partial n} &= -\rho_0 \vec{n} \cdot \vec{U} \cdot \nabla \vec{U} \end{split}$$



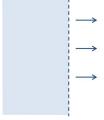




Outlet

Velocity gradient equals 0 Set the total pressure to maintain the mass flow

$$\begin{array}{l} \frac{\partial \vec{U}}{\partial \vec{n}} = \mathbf{0} \\ p = p_0 - \frac{\rho U^2}{2}, \ U^2 = \vec{U} \cdot \vec{U} \end{array}$$







Keywords in QHDFoam

There are prepared keywords for these boundary conditions in OpenFOAM.

For example, we want to set a specific pressure gradient for the wall:

```
wall
{
    type qhdFlux;
    value $internalField;
}
```

Or we want to set a fixed velocity for the inlet:

```
inlet
{
   type fixedValue;
   value uniform (1 0 0);
}
```





Keywords in OpenFOAM

slip This boundary condition provides a slip constraint:

 $\vec{n}\vec{U}_n = 0$, $\frac{\partial U_\tau}{\partial n}\tau = 0$

noSlip This boundary condition fixes the velocity to zero at

walls, similar to fixed Value = 0

fixedValue This boundary condition provides a fixed value

constraint, and is the base class for a number of other

boundary conditions

zeroGradient This boundary condition applies a zero-gradient in

normal direction condition

qhdFlux This boundary condition is a specific condition for ∇p :

 $\vec{n} \cdot \vec{U} - \tau (\vec{U} \cdot \nabla \vec{U} - \frac{1}{\rho_0} \nabla p) \cdot \vec{n} = 0$

totalPressure This boundary condition provides a total pressure

condition





Empty

This boundary condition provides an 'empty' condition for reduced dimensions cases, i.e. 1- and 2-D geometries. Apply this condition to patches whose normal is aligned to geometric directions which are not involved in simulation.





Regularization parameter au

Value of τ ($[\tau]=s$) coefficient is selected to be equal or less than some characteristic hydrodynamic time using characteristic velocity magnitude U, kinematic viscosity ν , grid step Δx or other parameters:

- For simple cases, τ could be estimated from dimensionless numbers (like Re, Gr or others): $\tau \approx \tau_0 Re^{-1}$, $\tau \approx \tau_0 Gr^{-1}$;
- Through the max CFL $Co^{max}=|\vec{U}|^{max}\Delta t/\Delta x$ number: $au pprox \frac{Co^{max}\Delta x}{|\vec{U}|^{max}}C_{ au}$, where $C_{ au}$ is a constant less than 1

Three stability criteria are used:

- **1** $\Delta t < C_{\tau}^{-1}\tau$, where $C_{\tau} \leq \frac{1}{2}$. In some cases C_{τ} could be set to 0.75
- 2 $Co = U \frac{\Delta t}{\Delta x} < Co^{max}.$ The Co^{max} is usually about 0.1-0.2 in most cases
- 3 $\tau |\vec{U}| \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$





Regularization parameter au

Let us determine the value of the regularization coefficient τ using the Reynolds number:

$$\tau = \tau_0 Re^{-1}, \quad Re = \frac{Ul}{\nu}.$$

If $au_0 = rac{l}{U}$ then

$$au = \frac{\nu}{U^2},$$

where U is a value of characteristic speed, l is a characteristic size. The time integration step should not exceed au, and is often chosen as:

$$\triangle t = \frac{\tau}{2}.$$





Part III Practical part

How to set up cases





How to install QGDSolver

This is for OpenFOAM+ v1912, for other OpenFOAM version, different branches should be used.

 Download QGDSolver directly from https: //github.com/unicfdlab/QGDsolver/tree/digitef-dev-1912 you can try short link: https://clck.ru/QgNJy or using git clone:

```
git clone https://github.com/unicfdlab/QGDsolver.git git checkout digitef-dev-1912
```

Install QGDSolver:

```
./Allwmake
```





QHDFoam case ... other fields constant/ polyMesh/ thermophysicalProperties turbulencelProperties gravitationalProperties system/ controlDict fvSchemes fvSolution

... other settings

QHDFoam case structure

It is similar to ${\it rhoPimpleFoam}$ case structure

Initial and boundary conditions

Initial conditions are set in the folder "0". Three fields are mandatory to start a simulation: pressure "p", velocity "U" and temperature "T"

Fluid properties

Thermophysical fluid properties (density, heat capacity coefficients, viscosity and heat conductivity coefficients) are set in "thermophysicalPropertis" dictionary. By default the turbulence modelling is turned off in the

"turbulenceProperties" dictionary. Value and direction of gravity bulk field is set in "gravitationalProperties"

Numerical schemes

Numerical schemes settings are stored in "fvSchmes" and "fvSolution", time advancement control is in "controlDict"





Stages of solution

See folder QHDFoam-OFv1912

• prepare new case folder:

cp cases/cavity cases/cavityRe1000 -r

- mesh generation
- boundary conditions setup
- physical properties setup
- au selection
- advancement time settings
- numerical schemes settings



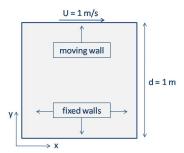


Basic case

Case set up

See folder QHDFoam-OFv1912. The case is in the folder cases/

- 2D case (cavity): square with side d = 1 m
- one moving top wall: $\vec{U} = (1~0~0)~\text{m/s}$
- fluid: rho = 1000, mu = 1
- stable flow: Re = 1000







See file system/blockMeshDict Set scale:

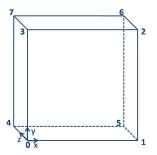
```
convertToMeters 1;
```

Set vertices:

```
vertices
(

(0 0 0)  // 0
(1 0 0)  // 1
(1 1 0)  // 2
(0 1 0)  // 3
(0 0 0.1)  // 4
(1 0 0.1)  // 5
(1 1 0.1)  // 6
(0 1 0.1)  // 7
```

Mesh generation







Mesh generation

Create one box:

```
blocks
(
hex (0 1 2 3 4 5 6 7) (50 50 1) simpleGrading (1 1 1)
);
```

Describe boundaries:

```
boundary
(
movingWall
{
type wall;
faces
(
(3 7 6 2)
);
}
```





Mesh generation

```
fixedWalls
        type wall;
       faces ( (0 4 7 3) (2 6 5 1) (1 5 4 0) );
   frontAndBack
        type empty;
        faces ( (0 3 2 1) (4 5 6 7) );
);
```

Command: blockMesh





Boundary conditions

See folder 0/

Name	U, m/s	p, Pa	T, K
movingWall	fixedValue	qhdFlux	zeroGradient
	(1 0 0)		
fixedWalls	noSlip	qhdFlux	zeroGradient
frontAndBack	empty	empty	empty





Physical properties

```
See folder constant/
See file thermophysicalProperties
Set density:
```

```
equationOfState
{
    rho 1000;
}
```

Set dynamic viscosity:

```
transport
{
    mu 1;
    Pr 0.73;
    beta 0.0; // buoyancy factor
}
```





au calculation

See file thermophysicalProperties

```
QGD
   implicitDiffusion true; // approximation of viscous terms
   QGDCoeffs constTau; // choice of calculation option for \tau
   constTauDict.
        Tau 1e-3; // \tau \sim \tau_0 = \frac{\nu}{U^2} = \frac{10^{-3}}{1^2} = 10^{-3}
   pRefCell 0;
   pRefValue 0;
```

In a closed incompressible system such as the cavity, pressure is relative: it is the pressure range that matters not the absolute values. In cases such as this, the solver sets a reference level by pRefValue in cell pRefCell. In this example both are set to 0.





implicitDiffusion

true

Implicit approximation of viscous terms: $\nabla \cdot (\frac{1}{\rho_0} \hat{\Pi})$ and $\nabla \cdot \left(\frac{\mu}{\rho_0 Pr} \nabla T\right)$

false

Explicit approximation of viscous terms: $\nabla \cdot (\frac{1}{\rho_0} \hat{\Pi})$ and $\nabla \cdot \left(\frac{\mu}{\rho_0 Pr} \nabla T\right)$





QGDCoeffs

We have different methods for τ calculation:

- H2bynuQHD
- HbyUQHD
- T0byGr
- constTau





H2bynuQHD

 $\tau = \frac{h^2}{\nu},$ where h is a grid step, ν is a kinematic viscosity.

```
QGD
{
    implicitDiffusion true;
    QGDCoeffs H2bynuQHD;
    pRefCell 0;
    pRefValue 0;
}
```





HbyUQHD

 $\tau = \frac{h}{U},$

where h is a grid step, U is a magnitude of characteristic velocity.

```
QGD
   implicitDiffusion true;
   QGDCoeffs HbyUQHD;
   HbyUQHDDict
       UQHD 1; // value of characteristic speed
   pRefCell 0;
   pRefValue 0;
```





T0byGr

$$\tau = \frac{\tau_0}{Gr},$$

where τ_0 is a characteristic time, Gr is a Grashof number.

$$Gr = \frac{g\beta(T_s - T_0)L^3}{\nu^2}$$

where g is acceleration of gravity, β is the coefficient of thermal expansion, T_s is the surface temperature, T_0 is a bulk temperature, L is the characteristic length, ν is a kinematic viscosity.

```
QGD { implicitDiffusion true; QGDCoeffs T0byGr; T0byGrDict { Gr 100; T0 1e-2; //T0 = \tau_0 } pRefCell 0; pRefValue 0; }
```





constTau

 $\tau = constant$

```
QGD
  implicitDiffusion true;
  QGDCoeffs constTau;
  constTauDict
       Tau 1e-3;
  pRefCell 0;
  pRefValue 0;
```





Physical properties

See file *gravitationalProperties* Set acceleration of gravity:

g g [0 1 -2 0 0 0 0] (0 -10 0); //
$$g=g_y=-10$$

See file *turbulenceProperties* Set flow type:

simulationType laminar; // uses no turbulence models





Advancement time settings

See file system/controlDict to create time settings:

• time step interval

```
deltaT 0.5e-3;
```

write interval

```
writeInterval 1;
```

• CFL number and parameter C_{τ}^{-1} (any value less than 1)

```
writeControl adjustableRunTime;
adjustableTimeStep true;
maxCo 0.5;
cTau 0.3;
```





Advancement time settings

• Start time of calculations

```
startTime 0;
```

• End time of calculations

```
endTime 20;
```





Numerical schemes settings. Running

See file system/fvSchemes and system/fvSolution.

The user specifies the choice of finite volume schemes in the *fvSchemes* dictionary. In file *fvSchemes* you can see that we use only central difference scheme.

The specification of the linear equation solvers and tolerances and other algorithm controls is made in the *fvSolution* dictionary.

You can start application by QHDFoam command.

Sequence of all commands is placed in the script file: ./Allrun. Clean results: ./Allclean.





Re = 1000

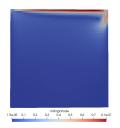
After the entering the QHDFoam command, you will see on the screen:

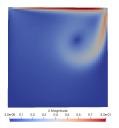
```
HPC CLUSTER bi220 (na 872d80377e3b)
File Edit View Terminal Tabs Help
ime = 1.6205
GAMGPCG: Solving for p, Initial residual = 0.000160216, Final residual = 0.36112e-11, No Iterations 9
GAMGPCG: Solving for Ux, Initial residual = 9.03893e-05, Final residual = 2.03472e-19, No Iterations 1
GAMGPCG: Solving for Uy, Initial residual = 0.000138275, Final residual = 2.11342e-19, No Iterations 1
AMGPCG: Solving for T, Initial residual = 0.00102896, Final residual = 1.20196e-15, No Iterations 1
max/min of T: 300/300
ExecutionTime = 212.64 s ClockTime = 214 s
Time = 1.621
GAMGPCG: Solving for p, Initial residual = 0.000160193, Final residual = 8.33544e-11, No Iterations 9
AMGPCG: Solving for Ux, Initial residual = 9.83804e-05, Final residual = 1.95165e-19, No Iterations 1
SAMGPCG: Solving for Uy, Initial residual = 0.000138239, Final residual = 1.93586e-19, No Iterations 1
AMGPCG: Solving for T, Initial residual = 0.0010174, Final residual = 1.18932e-15, No Iterations 1
max/min of T: 300/300
xecutionTime = 212.7 s ClockTime = 214 s
GAMGPCG: Solving for p, Initial residual = 0.000160169, Final residual = 8.30978e-11, No Iterations 9
AMARPICO. Solving for UK. Initial residual = 9.83714e-85. Enual residual = 2.08372e-19. No Iterations 1
AMARPICO. Solving for UK. Initial residual = 0.80018204. Final residual = 2.10833e-19. No Iterations 1
AMARPICO. Solving for IT. Initial residual = 0.00101204. Final residual = 1.10042e-15. No Iterations 1
Max/Inio of IT. 300/300
ExecutionTime = 212.75 s ClockTime = 214 s
ime = 1.622
AMGPCG: Solving for p, Initial residual = 0.000160144, Final residual = 8.28416e-11, No Iterations 9
GAMGPCG: Solving for Ux. Initial residual = 9.83624e-05, Final residual = 1.9487e-19, No Iterations 1
GAMGPCG: Solving for Uy, Initial residual = 0.00013817, Final residual = 1.79713e-19, No Iterations 1
AMGPCG: Solving for T, Initial residual = 0.00100914, Final residual = 1.17235e-15, No Iterations 1
max/min of T: 300/300
ExecutionTime = 212.81 s ClockTime = 214 s
Time = 1.6225
GAMGPCG: Solving for p, Initial residual = 0.000160119, Final residual = 8.25859e-11, No Iterations 9
GAMGPCG: Solving for Ux, Initial residual = 9.83532e-05, Final residual = 2.03838e-19, No Iterations 1
AMGPCG: Solving for Uy, Initial residual = 0.800138135, Final residual = 2.36318e-19, No Iterations 1
AMGPCG: Solving for T, Initial residual = 0.00100385, Final residual = 1.16152e-15, No Iterations 1
max/min of T: 300/300
xecutionTime = 212.87 s ClockTime = 214 s
AMGPCG: Solving for p. Initial residual = 0.080160094, Final residual = 8.23308e-11, No Iterations 9
```





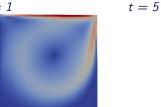
Re = 1000

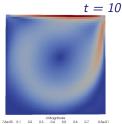






t = 1





$$t = 15$$









$$Re = 100$$

- mesh: 100 × 100;
- $\mu = 10$;

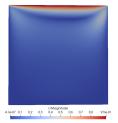
•
$$\tau \sim \tau_0 = \frac{\nu}{U^2} = \frac{10^{-2}}{1^2} = 10^{-2}$$
;

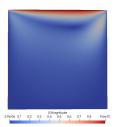
- $\Delta t = \frac{\tau}{2} = 0.5 \cdot 10^{-2}$;
- startTime = 0;
- endTime = 5;
- writeInterval = 0.5;





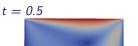
Re = 100

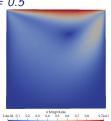


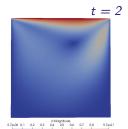


t = 1

















Summary

- We look how QHDFoam for OpenFOAM v1912 works;
- We learned how to set boundary conditions for QHDFoam;
- We studied how to solve cases step-by-step on the basic example.

Let's talk about training track. Some questions?





Contacts

Telegram: https://t.me/qgd_qhd

GitHub: https://github.com/unicfdlab/libAcoustics/issues