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Particle Simulation with OpenFOAM®

Introduction, Fundamentals and Applications

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Outline

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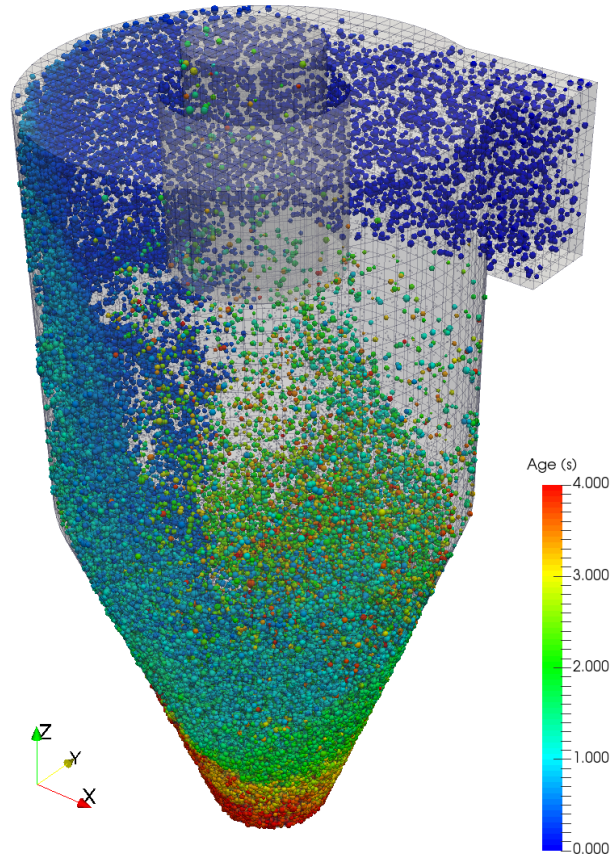
Why Particle Simulations with OpenFOAM?

- OpenFOAM is free and open source (customization and unlimited parallelization possible)
- OpenFOAM is constantly under development with a continuous growing community (academic research, R&D in companies)
- OpenFOAM includes solvers for any application of particle-laden flows (e.g. process engineering, mechanical engineering, civil engineering, physics,...)



Lagrangian-Particle-Tracking in OpenFOAM

- Solvers for any kind of particle-laden flow are already implemented[1]:
  - ***DPMFoam/MPPICFoam:*** Transient solver for the coupled transport of a single kinematic particle cloud including the effect of the volume fraction of particles on the continuous phase (Multi-Phase Particle In Cell modeling is used to represent collisions without resolving particle-particle interactions)
  - ***uncoupledKinematicParcelFoam:*** Transient solver for the passive transport of a single kinematic particle cloud
  - ***reactingParcelFilmFoam:*** Transient solver for compressible, turbulent flow with a reacting, multiphase particle cloud, and surface film modelling
  - ***sprayFoam***: Transient solver for compressible, turbulent flow with a spray particle cloud
  - ***...***
- No proper solver available? Customize one of the existing...

[1] based on OpenFOAM-4.x

Outline

Governing Equations of Lagrangian-Particle-Tracking

- Calculation of isothermal particle motions requires the solution of the following set of ordinary differential equations:

$$\frac{\mathrm{d}\mathbf{x}_p}{\mathrm{d}t} = \mathbf{u}_p, \qquad m_p \frac{\mathrm{d}\mathbf{u}_p}{\mathrm{d}t} = \sum \mathbf{F_i}, \qquad I_p \frac{\mathrm{d}\omega_p}{\mathrm{d}t} = \sum \mathbf{T} \tag{1}$$

- Newton's second law of motion presupposes the consideration of all relevant forces acting on the particle, e.g., drag, gravitational and buoyancy forces, pressure forces:

$$m_p \frac{\mathrm{d}\mathbf{u}_p}{\mathrm{d}t} = \sum \mathbf{F_i} = \mathbf{F_D} + \mathbf{F_G} + \mathbf{F_P} + \ldots \tag{2}$$

Drag Force

- Drag is the most important force (approx. 80 % of the total force) and is expressed in terms of the drag coefficient C_D:

$$\mathbf{F_D} = C_D \frac{\pi D_p^2}{8} \rho_f \left(\mathbf{u}_f - \mathbf{u}_p\right) \left|\mathbf{u}_f - \mathbf{u}_p\right| \tag{3}$$

Drag correlations (spherical particle)

- Schiller-Naumann (1935):

$$C_D = \begin{cases} \frac{24}{\mathrm{Re}_p}\left(1 + 0.15\mathrm{Re}_p^{0.687}\right) & \text{if } \mathrm{Re}_p \leq 1000 \\ 0.44 & \text{if } \mathrm{Re}_p > 1000 \end{cases} \tag{4}$$

- **Putnam (1961):**

$$C_D = \begin{cases} \frac{24}{\mathrm{Re}_p}\left(1 + \frac{1}{6}\mathrm{Re}_p^{2/3}\right) & \text{if } \mathrm{Re}_p \leq 1000 \\ 0.424 & \text{if } \mathrm{Re}_p > 1000 \end{cases} \tag{5}$$

Drag Force

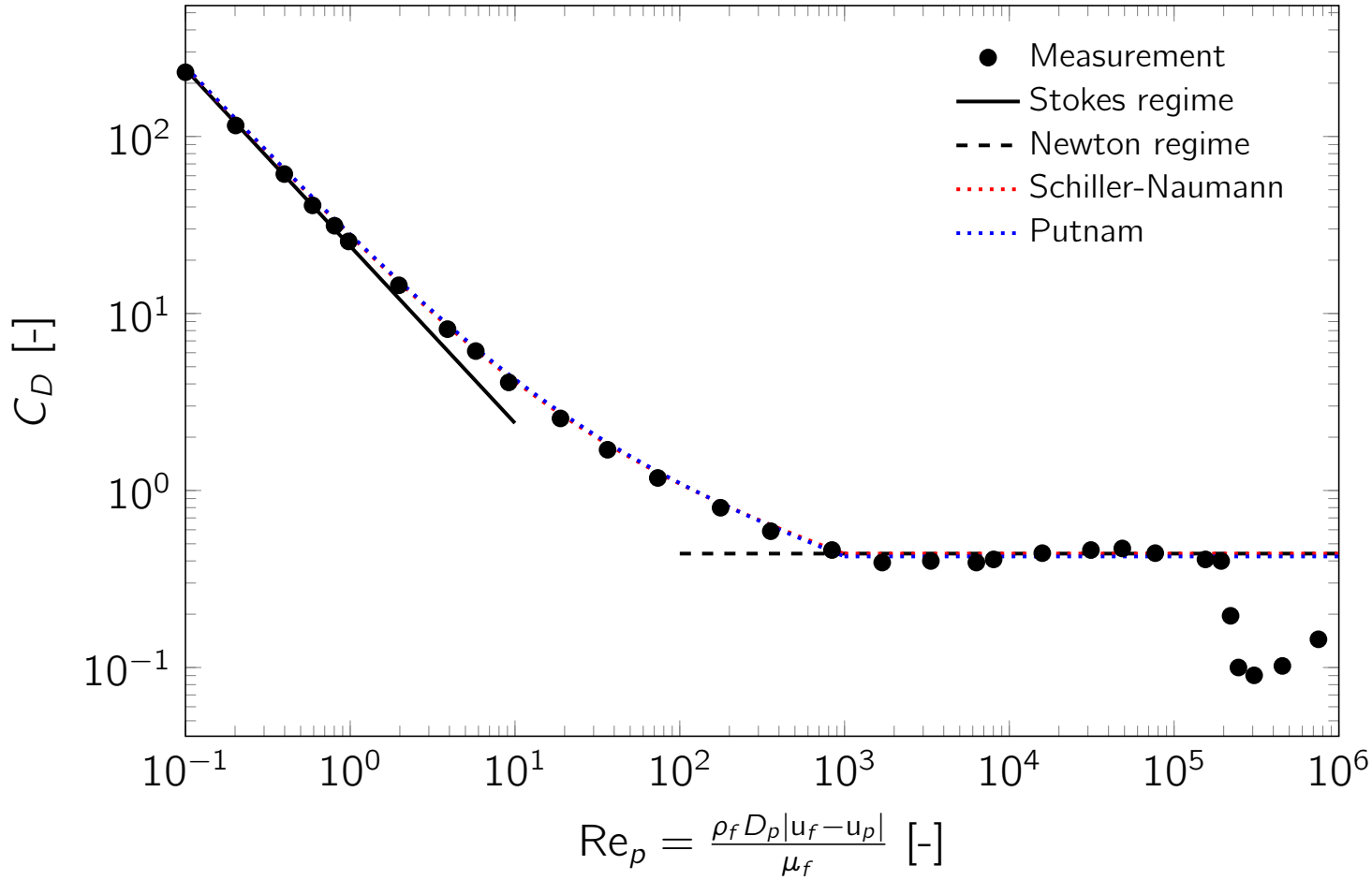


Figure: Drag coefficient as a function of particle Reynolds number, comparison of experimental data with correlations of Schiller-Naumann (1935) and Putnam (1961)

Gravity/Buoyancy and Pressure Gradient Force

- Gravitational and Buoyancy force is computed as one total force:

$$\mathbf{F_G} = m_p \mathbf{g} \left(1 - \frac{\rho_f}{\rho_p}\right) \tag{6}$$

- The force due to a local pressure gradient can be expressed for a spherical particle simply as:

$$\mathbf{F_P} = -\frac{\pi D_p^3}{6} \nabla p \tag{7}$$

- Expressing the local pressure gradient ∇p in terms of the momentum equation leads to the final pressure gradient force:

$$\mathbf{F_p} = \rho_f \frac{\pi D_p^3}{6} \left(\frac{\mathrm{D}\mathbf{u}_f}{\mathrm{D}t} - \nabla \cdot \nu \left(\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T\right)\right) \tag{8}$$

Other Forces

- **Added mass force:** particle acceleration or deceleration in a fluid requires also an accelerating or decelerating of a certain amount of the fluid surrounding the particle (important for liquid-particle flows)
- **Slip-shear lift force:** particles moving in a shear layer experience a transverse lift force due to the nonuniform relative velocity over the particle and the resulting nonuniform pressure distribution
- **Slip-rotation lift force:** particles, which are freely rotating in a flow, may also experience a lift force due to their rotation (Magnus force)
- **Thermophoretic force:** a thermal force moves fine particles in the direction of negative temperature gradients (important for gas-particle flows)
- ...

Particle Response Time

- Particle response time is used to characterize the capability of particles to follow sudden velocity changes in the flow
- Starting from the equation of motion considering only drag force (divided by particle mass and in terms of the particle Reynolds number):

$$\frac{\mathrm{d}u_p}{\mathrm{d}t} = \frac{18\mu_f}{\rho_p D_p^2}\frac{C_D\,\mathrm{Re}_p}{24}(u_f - u_p) \;\rightarrow\; \frac{\mathrm{d}u_p}{\mathrm{d}t} = \frac{1}{\tau_p}(u_f - u_p) \tag{9}$$

Particle response time & Stokes number

$$\tau_p = \frac{\rho_p D_p^2}{18\mu_f f_D}, \quad \mathrm{St} = \tau_p/\tau_f \tag{10}$$

$\rightarrow$ The Stokes number St is the ratio of the particle response time and a characteristic time scale of the flow

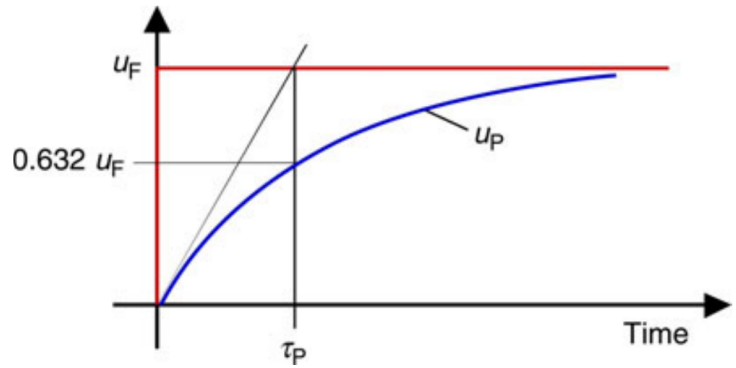
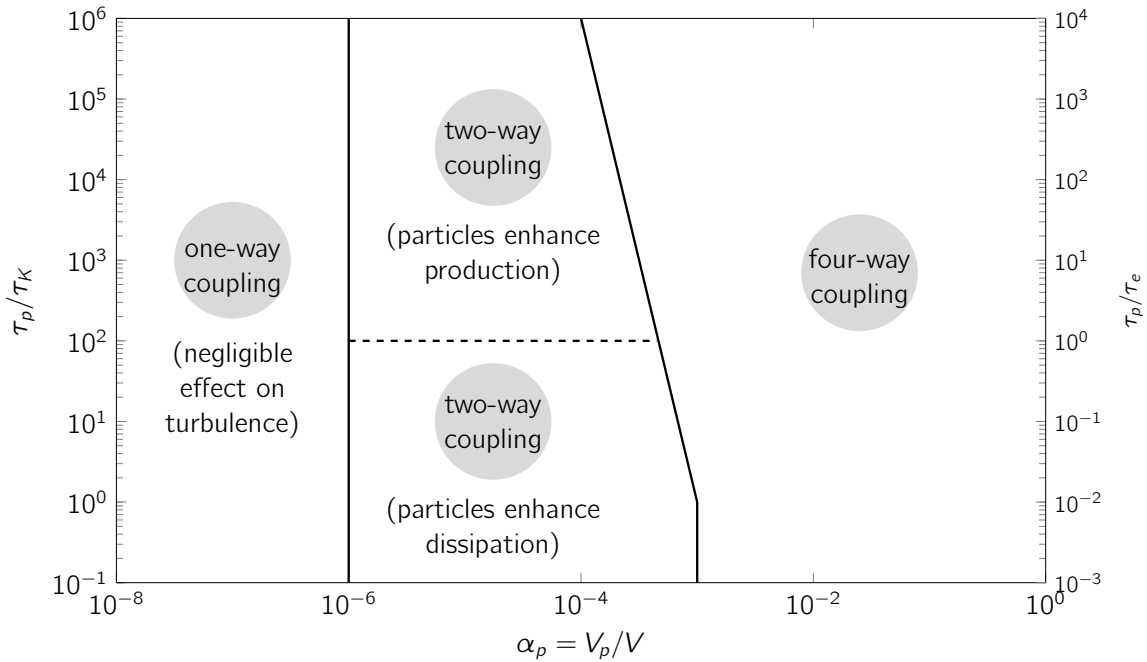


Figure: Graphical illustration of the particle response time (Sommerfeld, 2011)

Phase-Coupling Mechanisms

- Phase-coupling mechanisms strongly influences the behavior of the continous and dispersed phase:
  - **One-way coupling:** fluid $\rightarrow$ particles
  - **Two-way coupling:** fluid $\leftrightarrows$ particles
  - **Four-way coupling:** fluid $\leftrightarrows$ particles + particle collisions
- Classification of phase-coupling mechanisms according to Elghobashi (1994):



Particle-Particle Interaction

- OpenFOAM uses the soft-sphere-model (DSEM)
- Particle-particle collisions are considered using a spring, friction slider and dash-pot
- **Normal force** is expressed according to the *Hertzian contact theory*:

$$F_{n,ij} = \left(-k_n \delta_n^{3/2} - \eta_{n,j} \mathbf{G} \cdot \mathbf{n}\right) \mathbf{n} \qquad (11)$$

- **Tangential force** is expressed by:

$$F_{t,ij} = -k_n \delta_t - \eta_{t,j} \mathbf{G}_{ct} \quad \text{or} \qquad (12)$$

$$F_{t,ij} = -\mu \left|\mathbf{F}_{n,ij}\right| \mathbf{t} \quad \text{if} \quad \left|F_{t,ii}\right|_j > \mu \left|\mathbf{F}_{n,ij}\right| \qquad (13)$$

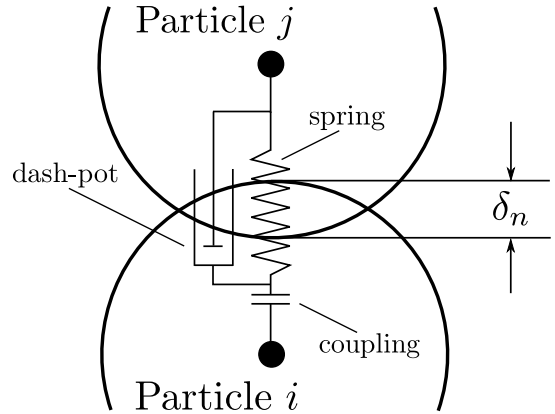


Figure: Normal force

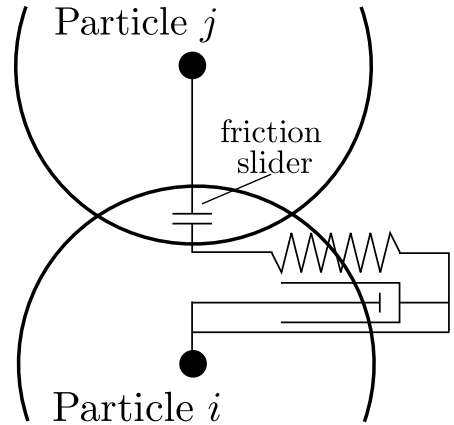


Figure: Tangential force

Outline

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

- **Problem:** no proper solver is available for your requirements? ☹
- **Solution:** customize an existing solver for your own purposes! ☺

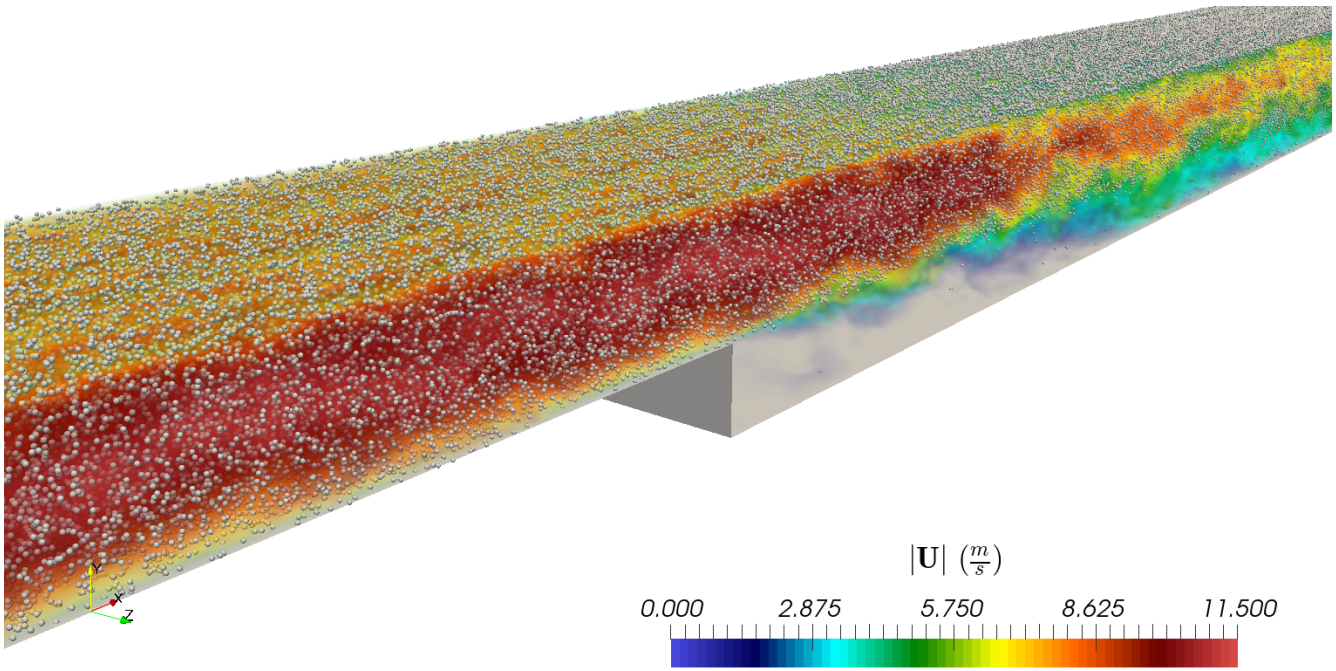


Figure: Particle-laden backward-facing step flow according to Fessler & Eaton (1999)

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

1. Open a terminal and source OpenFOAM-4.x (if not already done)

2. Create a working directory for our Eulerian-Lagrangian solver and move into it:

```
mkdir solver/

cd solver/
```

3. Copy the original **pimpleFoam** solver (Large time-step transient solver for incompressible, turbulent flow, using the PIMPLE (merged PISO-SIMPLE) algorithm) from OpenFOAM-4.x and rename it:

```
cp -r $FOAM_SOLVERS/incompressible/pimpleFoam/ .

mv pimpleFoam pimpleLPTFoam/

cd pimpleLPTFoam/
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

4. After moving into the pimpleLPTFoam directory, change the name of the pimpleFoam.C file, remove the pimpleDyMFoam and SRFPimpleFoam sub-solver directories:

```
mv pimpleFoam.C pimpleLPTFoam.C

rm -r pimpleDyMFoam/ SRFPimpleFoam/

mkdir lagrangian
```

5. Copy the lagrangian library **intermediate** (includes submodels for particle forces, particle collisions, injection and dispersion models,...) from OpenFOAM-4.x:

```
cp -r $FOAM_SRC/lagrangian/intermediate/ lagrangian/
```

6. Open the createFields.H file with a text editor for some customizations:

```
vi createFields.H
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

7. Add the following code lines after `#include "createMRF.H"` to create and read the fluid density from the transportProperties and calculate the inverse fluid density:

createFields.H

```
Info« "Reading transportProperties\n" « endl;
IOdictionary transportProperties
(
      IOobject
      (
           "transportProperties",
           runTime.constant(),
           mesh,
           IOobject::MUST_READ_IF_MODIFIED,
           IOobject::NO_WRITE
      )
);
dimensionedScalar rhoInfValue
(
      transportProperties.lookup("rhoInf")
);
dimensionedScalar invrhoInf("invrhoInf",(1.0/rhoInfValue));
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

8. Create a volScalarField for the fluid density and the dynamic fluid viscosity:

createFields.H

```
volScalarField rhoInf
(
      IOobject
      (
           "rho",
           runTime.timeName(),
           mesh,
           IOobject::NO_READ,
           IOobject::AUTO_WRITE
      ),
      mesh,
      rhoInfValue
);
```

createFields.H

```
volScalarField mu
(
      IOobject
      (
           "mu",
           runTime.timeName(),
           mesh,
           IOobject::NO_READ,
           IOobject::AUTO_WRITE
      ),
     laminarTransport.nu()
     *rhoInfValue
);
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

9. Initialize the basicKinematicCollidingCloud (includes particle-particle interactions):

createFields.H

```
const word kinematicCloudName
(
    args.optionLookupOrDefault<word>("cloudName", "kinematicCloud")
);
Info« "Constructing kinematicCloud " « kinematicCloudName « endl;
basicKinematicCollidingCloud kinematicCloud
(
    kinematicCloudName,
    rhoInf,
    U,
    mu,
    g
);
```

10. Open the pimpleLPTFoam.C file for some customizations:

```
vi pimpleLPTFoam.C
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

11. Add the basicKinematicCollidingCloud.H and readGravitationalAcceleration.H to the existing header files:

pimpleLPTFoam.C

```
...
#include "turbulentTransportModel.H"
#include "pimpleControl.H"
#include "fvOptions.H"
#include "basicKinematicCollidingCloud.H"

// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

int main(int argc, char *argv[])
{
    #include "setRootCase.H"
    #include "createTime.H"
    #include "createMesh.H"
    #include "readGravitationalAcceleration.H"
    #include "createControl.H"
    #include "createTimeControls.H"
    #include "createFields.H"

...
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

12. Add the kinematicCloud.evolve() function after the PIMPLE corrector loop:

pimpleLPTFoam.C

```
// -- Pressure-velocity PIMPLE corrector loop
while (pimple.loop())
{
    #include "UEqn.H"

    // -- Pressure corrector loop
    while (pimple.correct())
    {
        #include "pEqn.H"
    }
    if (pimple.turbCorr())
    {
        laminarTransport.correct();
        turbulence->correct();
    }
}

Info« "\nEvolving " « kinematicCloud.name() « endl;
kinematicCloud.evolve();

runTime.write();
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

13. Open the UEqn.H file for some customizations:

```
vi UEqn.H
```

14. Expand the momentum equation for two-way coupling:

UEqn.H

```
tmp<fvVectorMatrix> tUEqn
(
      fvm::ddt(U) + fvm::div(phi, U)
      + MRF.DDt(U)
      + turbulence->divDevReff(U)
      ==
      fvOptions(U)
      + invrhoInf*kinematicCloud.SU(U)
);
fvVectorMatrix& UEqn = tUEqn.ref();

UEqn.relax();
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

15. The implementation is (almost) done, but we need some customizations within the Make directory of the intermediate library in order to compile everything correctly:

```
vi intermediate/Make/options
```

16. We want our own customized intermediate library (maybe to implement a own particle force model or similar), so replace the last code line of the files file by:

files

```
LIB = $(FOAM_USER_LIBBIN)/libPimpleLPTLagrangianIntermediate
```

17. Tell the solver where he can find our intermediate library (and some additional too):

```
vi Make/options
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

options

```
EXE_INC =
      -Ilagrangian/intermediate/lnInclude \
      -I$(LIB_SRC)/TurbulenceModels/turbulenceModels/lnInclude \
      -I$(LIB_SRC)/TurbulenceModels/incompressible/lnInclude \
      -I$(LIB_SRC)/transportModels \
      -I$(LIB_SRC)/transportModels/incompressible/singlePhaseTransportModel \
      -I$(LIB_SRC)/finiteVolume/lnInclude \
      -I$(LIB_SRC)/meshTools/lnInclude \
      -I$(LIB_SRC)/sampling/lnInclude \
      -I$(LIB_SRC)/lagrangian/basic/lnInclude \
      -I$(LIB_SRC)/regionModels/surfaceFilmModels/lnInclude \
      -I$(LIB_SRC)/regionModels/regionModel/lnInclude

EXE_LIBS = \
      -L$(FOAM_USER_LIBBIN) \
      -lPimpleLPTLagrangianIntermediate \
      -llagrangian\
      -lturbulenceModels \
      -lincompressibleTurbulenceModels \
      -lincompressibleTransportModels \
      -lfiniteVolume \

...
```

How to build your own Eulerian-Lagrangian Solver in OpenFOAM

18. Tell the compiler the name of our new Eulerian-Lagrangian solver:

```
vi Make/files
```

files

```
pimpleLPTFoam.C

EXE = $(FOAM_USER_APPBIN)/pimpleLPTFoam
```

19. Finally, we can compile the intermediate library and the solver:

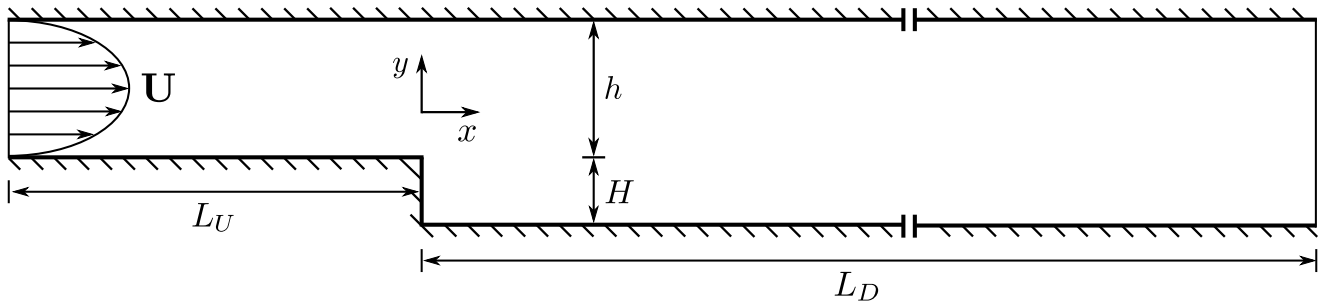
```
wmake all
```

You received no error messages from the compiler?
Congratulations, your new Eulerian-Lagrangian solver is ready...
but how to use it? ☺

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

Particle-laden backward-facing step flow (Fessler & Eaton, 1999)

- Geometry:
  - Step height: $H = 26.7\,\mathrm{mm}$
  - Channel height/width: $h = 40\,\mathrm{mm}$, $B = 457\,\mathrm{mm}$
  - Length inlet and expansion channel: $L_U = 5h$, $L_D = 35h$



- Flow and particle characteristics:
  - Centerline velocity and Reynolds number: $U_0 = 10.5\,\mathrm{m/s}$, $\mathrm{Re}_0 = U_0 H/\nu = 18.600$
  - Particle type: copper $\rightarrow D_p = 70\,\mu\mathrm{m}$, $\rho_p = 8800\,\mathrm{kg/m^3}$
  - Stokes number: $\mathrm{St} = \frac{\tau_p}{\tau_f} = \rho_p D_p^2 U_0/(90\mu H) = 6.9$

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

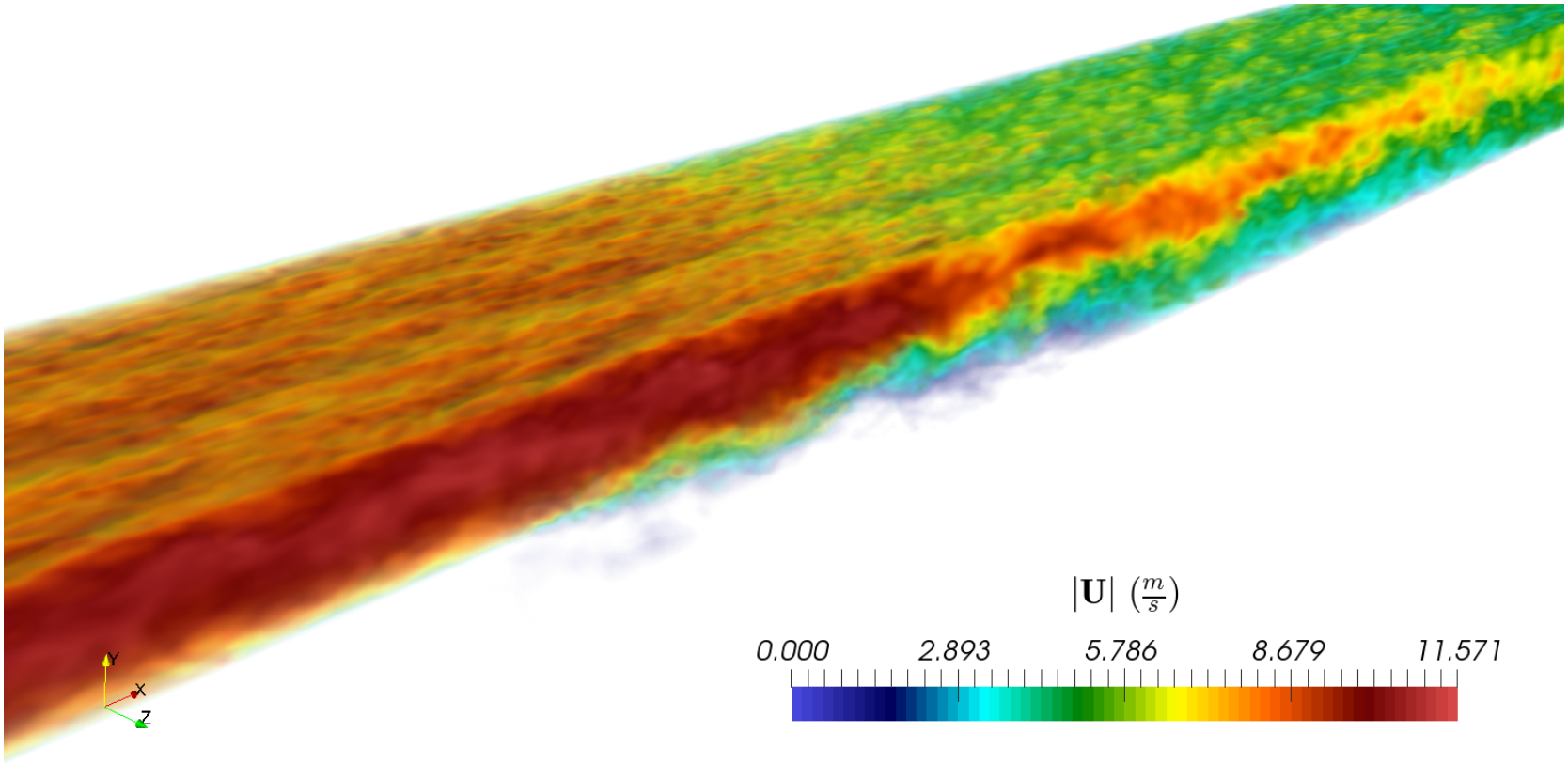


Figure: Snapshot of the instantaneous velocity field $|\mathbf{U}|$ obtained from Large Eddy Simulation (sub-grid scale turbulence model: Dynamic Smagorinsky (DSM)) for $\mathrm{Re}_0 = 18.600$

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

- Basic folder structure of any OpenFOAM case:

0: includes the initial boundary conditions

constant: includes the mesh (polyMesh folder), physical properties of the fluid (transportProperties), particle properties and settings (kinematicCloudProperties),...

system: includes the simulation settings (controlDict), settings for numerical schemes (fvSchemes) and solver for the algebraic equations systems (fvSolution), decomposition methods (decomposeParDict), ...

- Download the current tutorial case setup using the git clone command:

Git repository on Bitbucket

```
$ git clone https://slint@bitbucket.org/slint/gofun2017_particletut.git
```

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

1. We start with the mesh generation → move into the tutorial directory and build the 2D mesh using OpenFOAM's blockMesh utility and check the mesh quality:

```
cd gofun2017_particletutorial/tutorial/BFS/

blockMesh

checkMesh
```

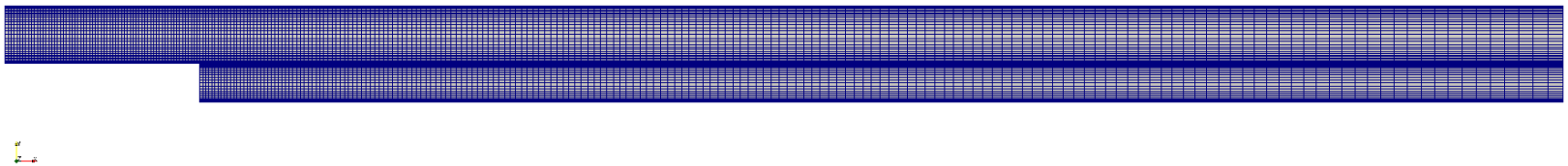


Figure: Two-dimensional block-structured mesh for the particle-laden backward-facing step flow

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

2. Let's see how to define initial boundary conditions (at the example of the velocity field):

U

```
dimensions [0 1 -1 0 0 0 0];

internalField uniform (0 0 0);

boundaryField
{
        inlet
        {
                type fixedValue;
                value uniform (9.39 0 0);
        }
        outlet
        {
                type zeroGradient;
        }
        walls
        {
                type noSlip;
        }
        sides
        {
                type empty;
        }

}
```

- OpenFOAM needs the dimension of the flow field in SI-units (see OpenFOAM user guide)
- You can set an initial flow field if present
- Each patch needs an initial boundary condition
- Boundary conditions in OpenFOAM:
  - Dirichlet (fixedValue)
  - Neumann (fixedGradient/zeroGradient)
  - Special types: cyclic, symmetry, empty (for 2D caes), ...

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

3. Let's see how to set up the particle cloud:

kinematicCloudProperties

```
solution
{
        active true;
        coupled true;
        transient yes;
        cellValueSourceCorrection off;
        maxCo 0.3;
        interpolationSchemes
        {
                rho cell;
                U cell;
                mu cell;
        }
        integrationSchemes
        {
                U Euler;
        }
sourceTerms
{
        schemes
        {
                U semiImplicit 1;
        }

}
```

- Activate/de-activate the particle cloud
- Enable/disable phase coupling
- Transient/steady-state solution (max. Courant number)
- Enable/disable correction of momentum transferred to the Eulerian phase
- Choose interpolation/integration schemes for the LPT and treatment of source terms

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

kinematicCloudProperties

```
constantProperties
{
        rho0 8800;
        youngsModulus 1.3e5;
        poissonsRatio 0.35;
}

subModels
{
        particleForces
        {
                sphereDrag;

                gravity;

                pressureGradient
                {
                        U U;
                }
        }
```

- Define the physical particle properties:
  - Density
  - Young's module (elastic modulus)
  - Poisson's ratio
- Define the relevant particle forces:
  - Drag force
  - Gravition/Buoyancy force
  - Pressure drag force

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

kinematicCloudProperties

```
injectionModels
{
        model1
        {
                type patchInjection;
                patchName inlet;
                duration 1;
                parcelsPerSecond 33261;
                massTotal 0;
                parcelBasisType fixed;
                flowRateProfile constant 1;
                nParticle 1;
                SOI 0.4;
                U0 (9.39 0 0);
                sizeDistribution
                {
                        type fixedValue;
                        fixedValueDistribution
                        {
                                value 0.00007;
                        }
                }
        }
}
```

- Setup of the particle injection:
  - Injection model + injection patch name
  - Total duration of particle injection
  - Injected parcels/particles per second
  - Number of particles per parcel
  - Start-of-injection time (SOI)
  - Initial parcel/particle velocity (U_0)
  - Size distribution model (normal size distribution, ...)

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

kinematicCloudProperties

```
dispersionModel none;

patchInteractionModel
standardWallInteraction;

standardWallInteractionCoeffs
{
        type rebound;
        e 0.97;
        mu 0.09;
}

surfaceFilmModel none;

stochasticCollisionModel none;

collisionModel pairCollision;
```

- Specify the sub-models for the particle simulation:
  - Turbulent dispersion models (Discrete Random Walk model and Gradient Dispersion model)
  - Patch interaction model + coefficients (rebound, stick or escape)
  - Surface film model for dripping and film interaction (absorb, bounce and splash)
  - Stochastic collision/pair collision model (spring, slider and dash-pot)
  - Further sub-models: heat transfer (only Ranz-Marshall correlation), phase change,...

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

kinematicCloudProperties

```
pairCollisionCoeffs
{
        maxInteractionDistance 0.00007;
        writeReferredParticleCloud no;
        pairModel pairSpringSliderDashpot;
        pairSpringSliderDashpotCoeffs
        {
                useEquivalentSize no;
                alpha 0.12;
                b 1.5;
                mu 0.52;
                cohesionEnergyDensity 0;
                collisionResolutionSteps 12;
        };
        wallModel wallSpringSliderDashpot;
        wallSpringSliderDashpotCoeffs
        {
                useEquivalentSize no;
                collisionResolutionSteps 12;
                youngsModulus 1e10;
                poissonsRatio 0.23;
                alpha 0.12;
                b 1.5;
                mu 0.43;
                cohesionEnergyDensity 0;
        };

}
```

- Adjust the particle-particle and particle-wall interaction model coefficients:
  - α: coefficient related to the coefficient of restitution e (see diagram)
  - b: Spring power $\rightarrow b = 1$ (linear) or $b = 3/2$ (Hertzian theory)
  - μ: friction coefficient

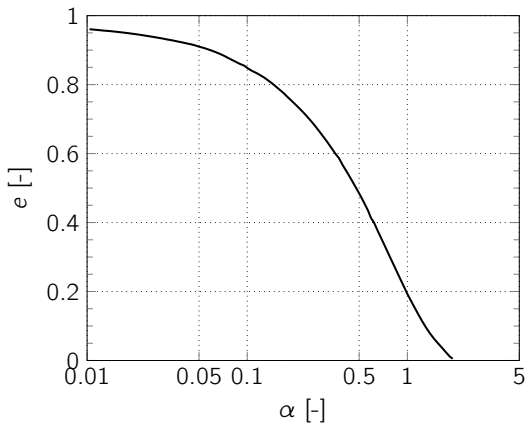


Figure: Relationship between α and the coefficient of restitution e (Tsuji et al., 1992)

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

kinematicCloudProperties

```
cloudFunctions
{
        voidFraction1
        {
                type voidFraction;
        }

}
```

- Use cloudFunctions to record particle tracks, calculate particle erosion, ...

4. The last step is to define the vector of the gravitational acceleration:

g

```
dimensions [0 1 -2 0 0 0 0];

value ( 0 -9.81 0 );
```

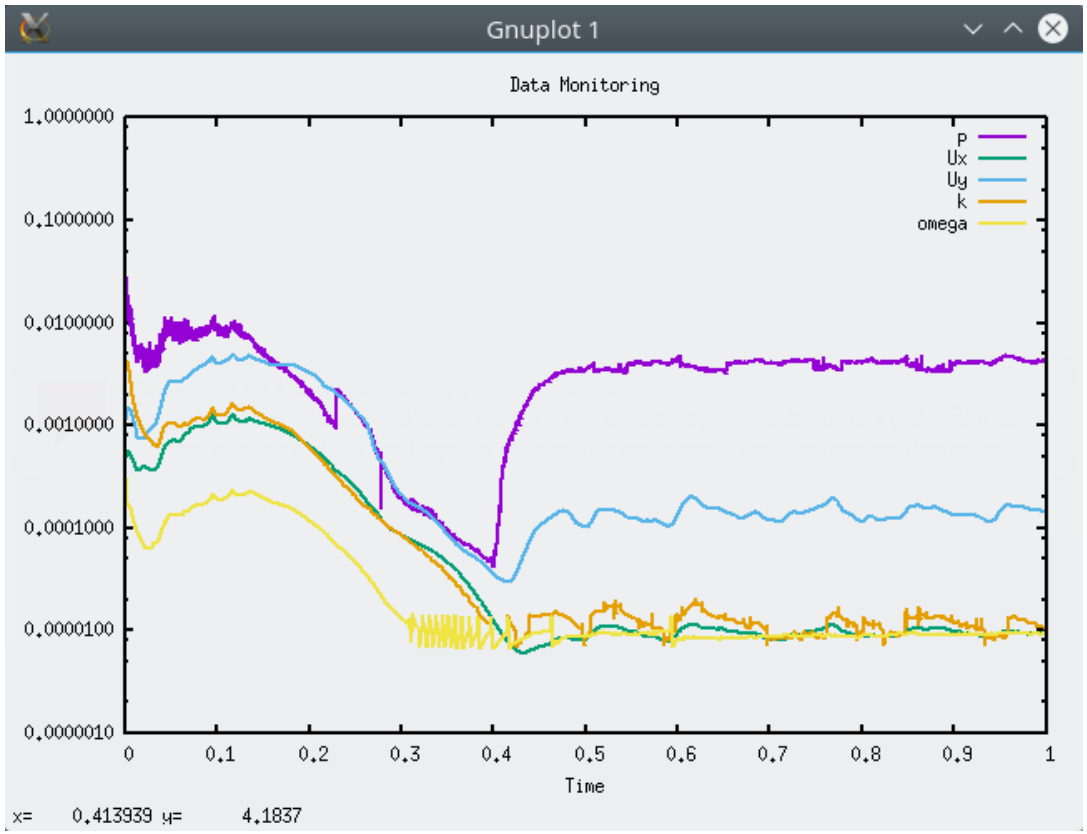
5. Finally, start our solver (and write a log file):

```
pimpleLPTFoam > run.log &
```

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

6. Use OpenFOAM's foamMonitor utility to check the convergence:

```
foamMonitor -l postProcessing/residuals/0/residuals.dat
```



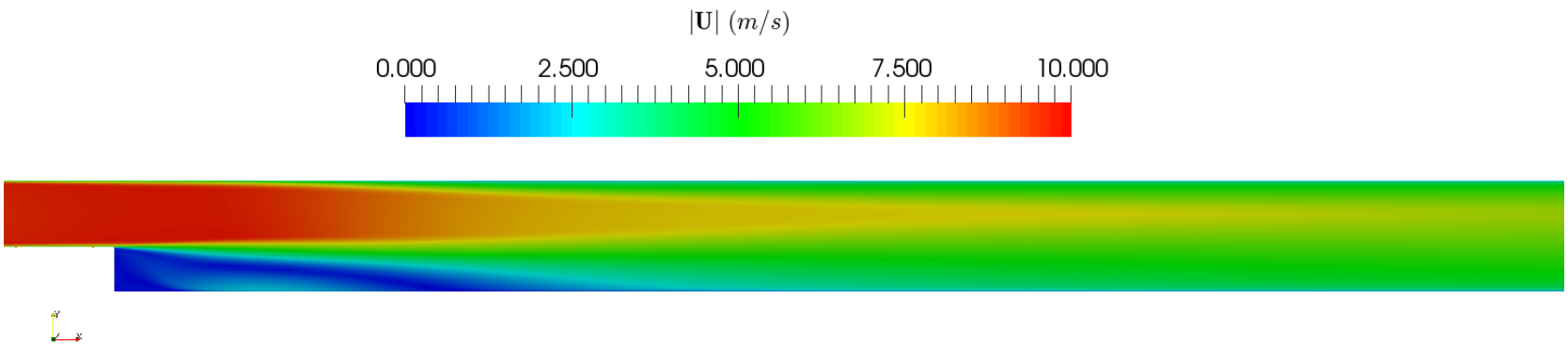
Post-Processing with OpenFOAM/Paraview

- OpenFOAM provides many utilities (e.g. sampling of data) and functionObjects (e.g. calculation of forces and turbulence fields) for the analysis of simulation results
- The standard program for the graphical post-processing of OpenFOAM cases is Paraview (see OpenFOAM user guide)

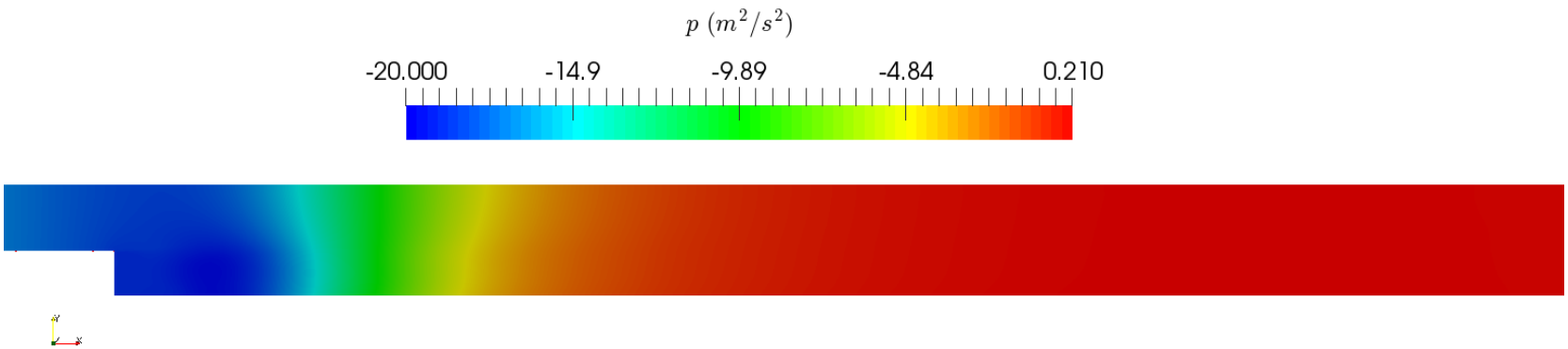
1. Start post-processing with Paraview by typing:

```
paraFoam
```

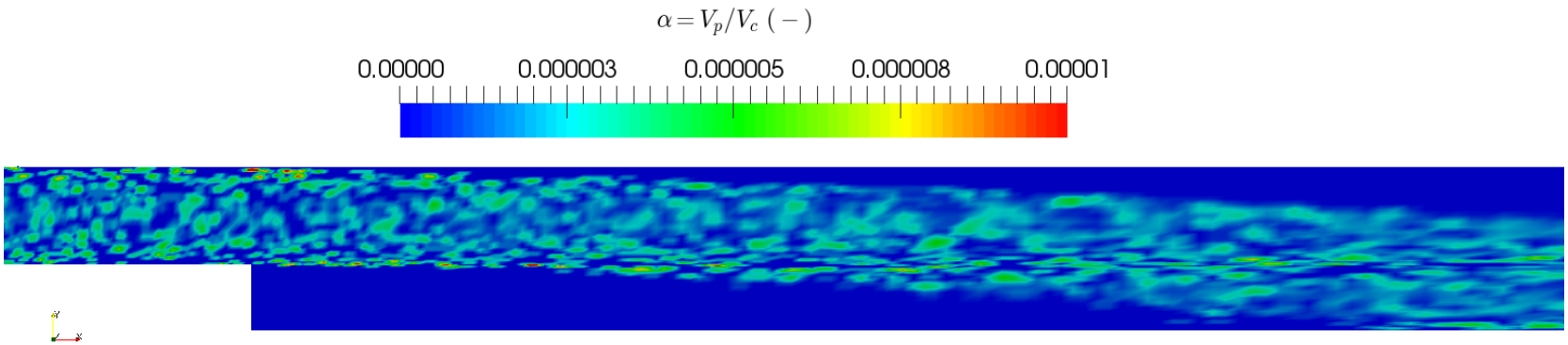
2. Load the last time step and check the velocity and pressure field:



Post-Processing with OpenFOAM/Paraview

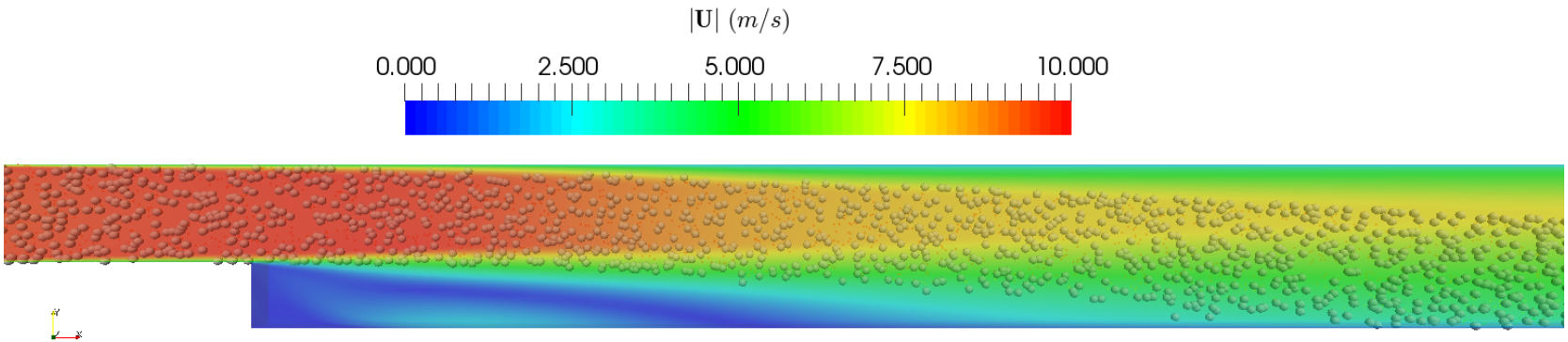


3. Let's check how much volume of each grid cell is occupied by particles (void fraction $\alpha = V_p/V_c$):

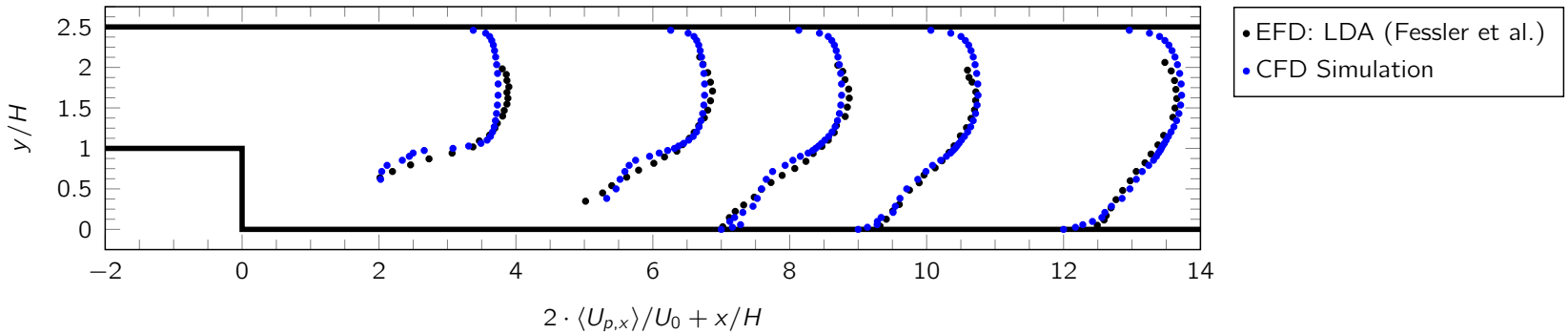


Post-Processing with OpenFOAM/Paraview

3. Apply the **Extract Block** filter on the kinematicCloud and scale the particles using the **Glyph** filter:



4. Sample the flow and particle velocity using OpenFOAM's sample utility (see OpenFOAM user guide) and plot the velocity profiles:



Further Information and References


OpenFOAM User/Programmers Guide (www.openfoam.org)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Thank you for your attention!

Any questions?

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