

German OpenFOAM User meeting 2017 (GOFUN 2017)

Particle Simulation with OpenFOAM[®]

Introduction, Fundamentals and Applications

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Outline

Introduction

- Motivation
- Lagrangian-Particle-Tracking in OpenFOAM

Fundamentals of Lagrangian-Particle-Tracking

- Governing Equations
- Particle Forces
- Particle Response Time
- Phase-Coupling Mechanisms
- Particle-Particle Interaction

Application

- How to build your own Eulerian-Lagrangian Solver in OpenFOAM
- How to use your own Eulerian-Lagrangian Solver in OpenFOAM
- Post-Processing with OpenFOAM/Paraview

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Fundamentals of Lagrangian-Particle-Tracking

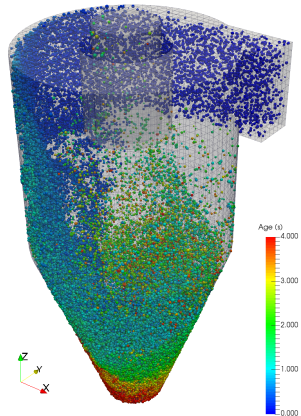
- Governing Equations
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Why Particle Simulations with OpenFOAM?

- 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 implemented¹:
 - ***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...

¹based on OpenFOAM-4.x

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Governing Equations of Lagrangian-Particle-Tracking

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

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p, \quad m_p \frac{d\mathbf{u}_p}{dt} = \sum \mathbf{F}_i, \quad I_p \frac{d\omega_p}{dt} = \sum \mathbf{T} \quad (1)$$

- 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:

$$m_p \frac{d\mathbf{u}_p}{dt} = \sum \mathbf{F}_i = \mathbf{F}_D + \mathbf{F}_G + \mathbf{F}_P + \dots \quad (2)$$

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 :

$$\mathbf{F}_D = C_D \frac{\pi D_p^2}{8} \rho_f (\mathbf{u}_f - \mathbf{u}_p) |\mathbf{u}_f - \mathbf{u}_p| \quad (3)$$

Drag correlations (spherical particle)

- Schiller-Naumann (1935):

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

- Putnam (1961):

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

Drag Force

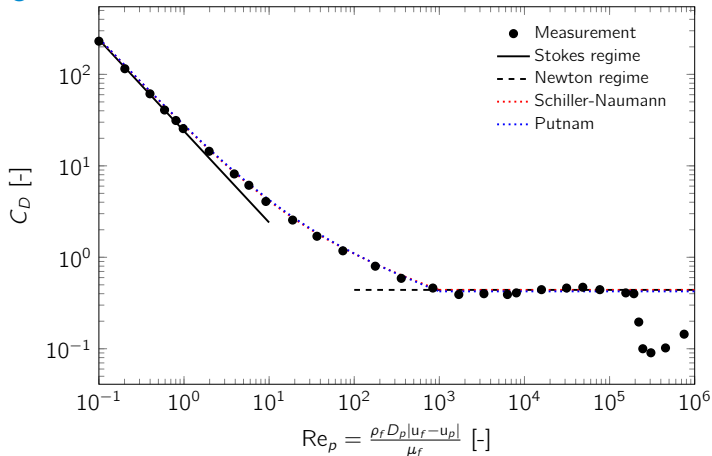


Figure: Drag coefficient as a function of particle Reynolds number, comparison of experimental data with correlations of Schiller-Naumann (1935) and Putnam (1961)

Gravity/Buoyancy and Pressure Gradient Force

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

$$\mathbf{F}_G = m_p \mathbf{g} \left(1 - \frac{\rho_f}{\rho_p} \right) \quad (6)$$

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

$$\mathbf{F}_P = -\frac{\pi D_p^3}{6} \nabla p \quad (7)$$

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

$$\mathbf{F}_P = \rho_f \frac{\pi D_p^3}{6} \left(\frac{D\mathbf{u}_f}{Dt} - \nabla \cdot \nu \left(\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T \right) \right) \quad (8)$$

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):

$$\frac{du_p}{dt} = \frac{18\mu_f}{\rho_p D_p^2} \frac{C_D Re_p}{24} (u_f - u_p) \rightarrow \frac{du_p}{dt} = \frac{1}{\tau_p} (u_f - u_p) \quad (9)$$

Particle response time & Stokes number

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

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

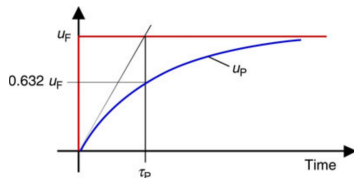
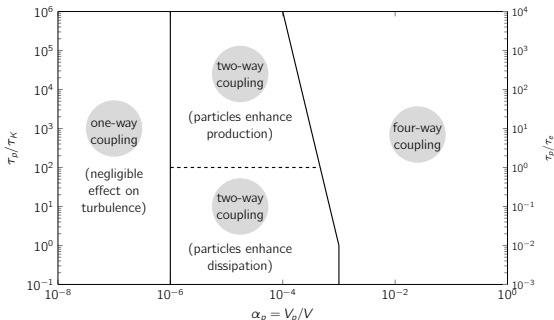


Figure: Graphical illustration of the particle response time (Sommerfeld, 2011)

Phase-Coupling Mechanisms

- Phase-coupling mechanisms strongly influences the behavior of the continuous and dispersed phase:
 - One-way coupling:** fluid \rightarrow particles
 - Two-way coupling:** fluid \leftrightarrow particles
 - Four-way coupling:** fluid \leftrightarrow 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*:

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

- **Tangential force** is expressed by:

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

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

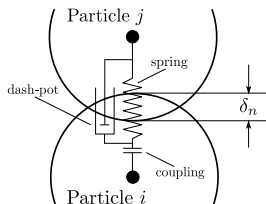


Figure: Normal force

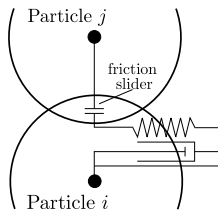


Figure: Tangential force

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How to build your own Eulerian-Lagrangian Solver in OpenFOAM

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

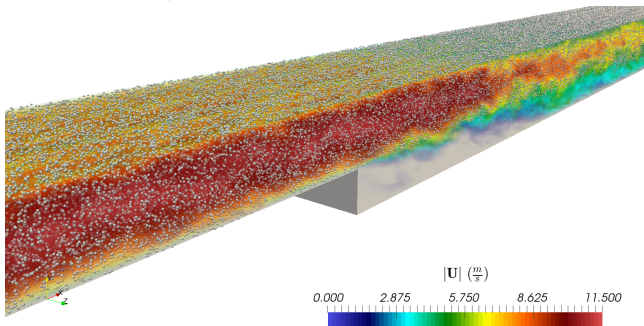


Figure: Particle-laden backward-facing step flow according to Fessler & Eaton (1999)

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 =

```
-llagrangian/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:

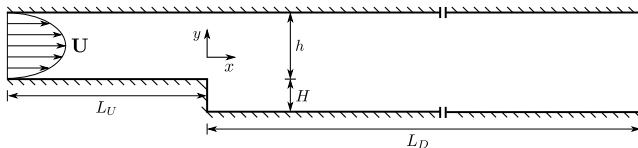
```
wmake all
```

**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: $H = 26.7$ mm
 - Channel height/width: $h = 40$ mm, $B = 457$ mm
 - Length inlet and expansion channel: $L_U = 5h$, $L_D = 35h$



- Flow and particle characteristics:
 - Centerline velocity and Reynolds number: $U_0 = 10.5$ m/s, $Re_0 = U_0 H / \nu = 18.600$
 - Particle type: copper $\rightarrow D_p = 70$ μ m, $\rho_p = 8800$ kg/m³
 - Stokes number: $St = \frac{\tau_p}{\tau_f} = \rho_p D_p^2 U_0 / (90 \mu H) = 6.9$

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

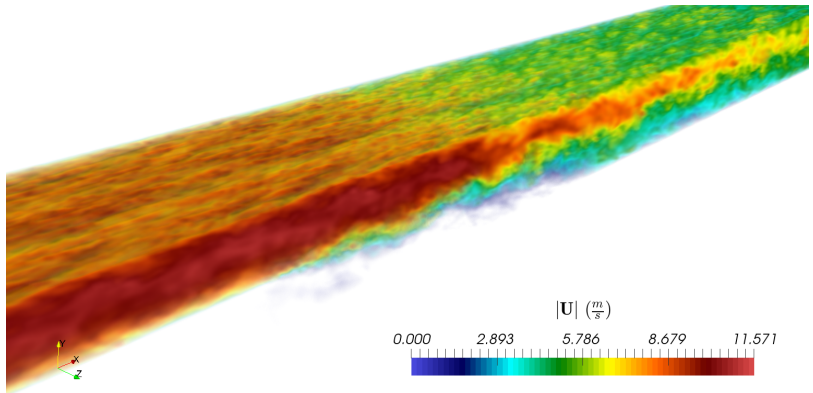


Figure: Snapshot of the instantaneous velocity field $|\mathbf{U}|$ obtained from Large Eddy Simulation (sub-grid scale turbulence model: Dynamic Smagorinsky (DSM)) for $Re_0 = 18.600$

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
```

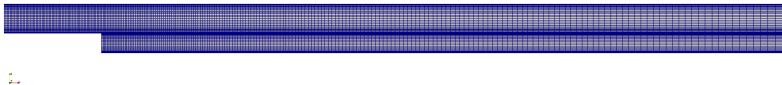


Figure: Two-dimensional block-structured mesh for the particle-laden backward-facing step flow

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];
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
{
    modell
    {
        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

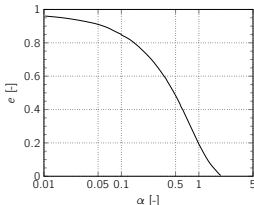


Figure: Relationship between α and the coefficient of restitution e (Tsuji et al., 1992)

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 );
```

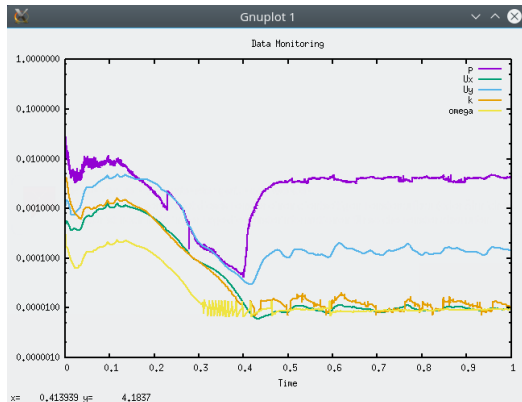
5. Finally, start our solver (and write a log file):

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

How to use your own Eulerian-Lagrangian Solver in OpenFOAM

- Use OpenFOAM's foamMonitor utility to check the convergence:

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

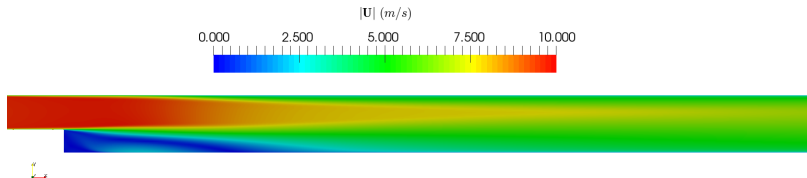


Post-Processing with OpenFOAM/Paraview

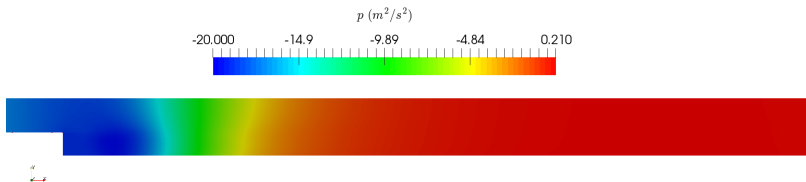
- OpenFOAM provides many utilities (e.g. sampling of data) and functionObjects (e.g. calculation of forces and turbulence fields) for the analysis of simulation results
 - The standard program for the graphical post-processing of OpenFOAM cases is Paraview (see OpenFOAM user guide)
1. Start post-processing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

```
paraFoam
```

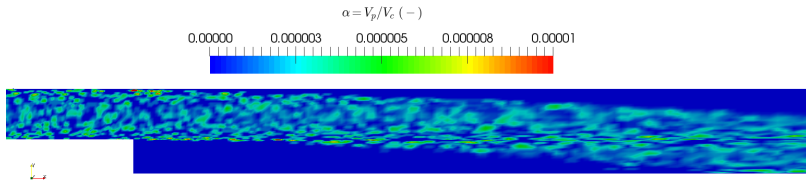
2. Load the last time step and check the velocity and pressure field:



Post-Processing with OpenFOAM/Paraview

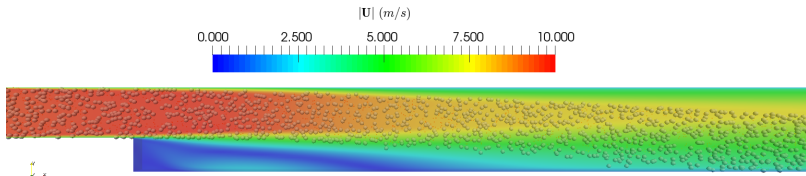


- Let's check how much volume of each grid cell is occupied by particles (void fraction $\alpha = V_p/V_c$):

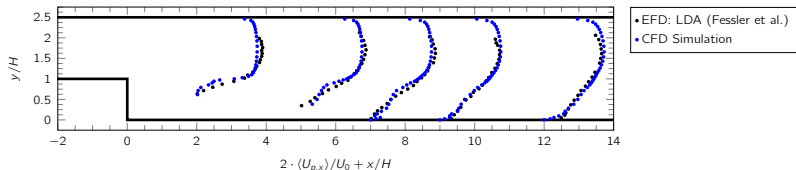


Post-Processing with OpenFOAM/Paraview

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



- 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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