Modification of Stochastic Model in Lagrangian Tracking Method for the course CFD with OpenSource Software

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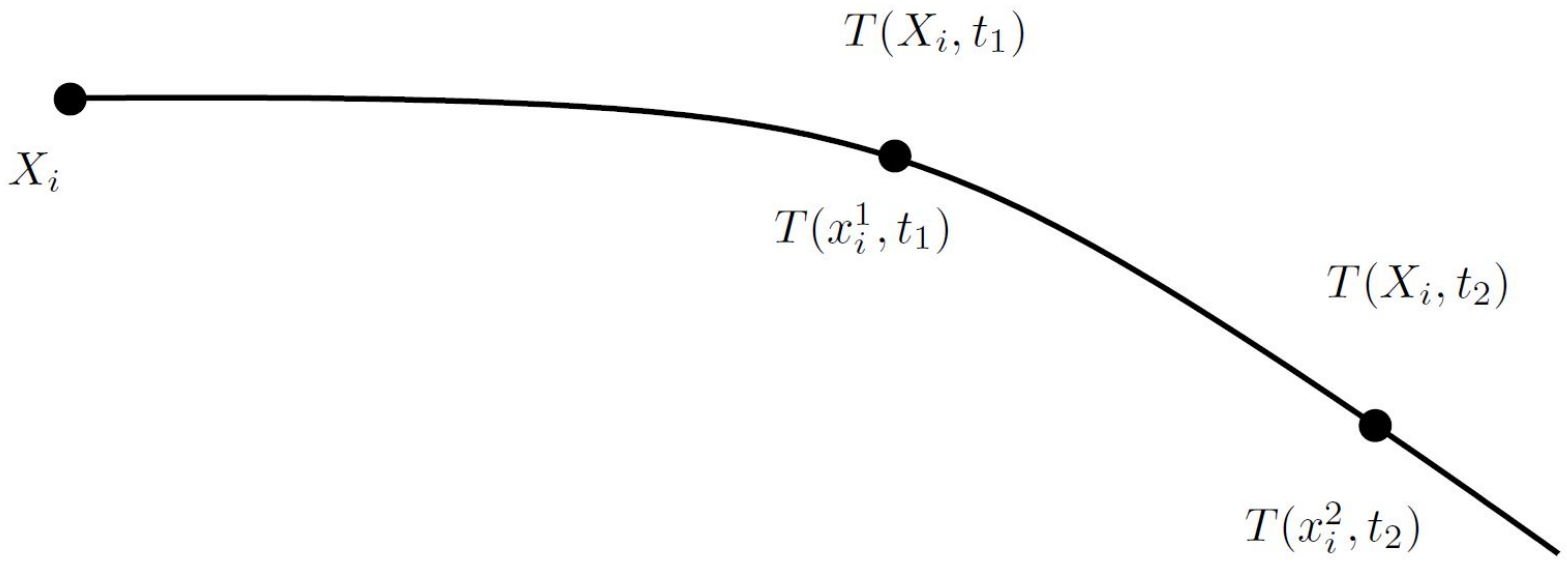
Agenda

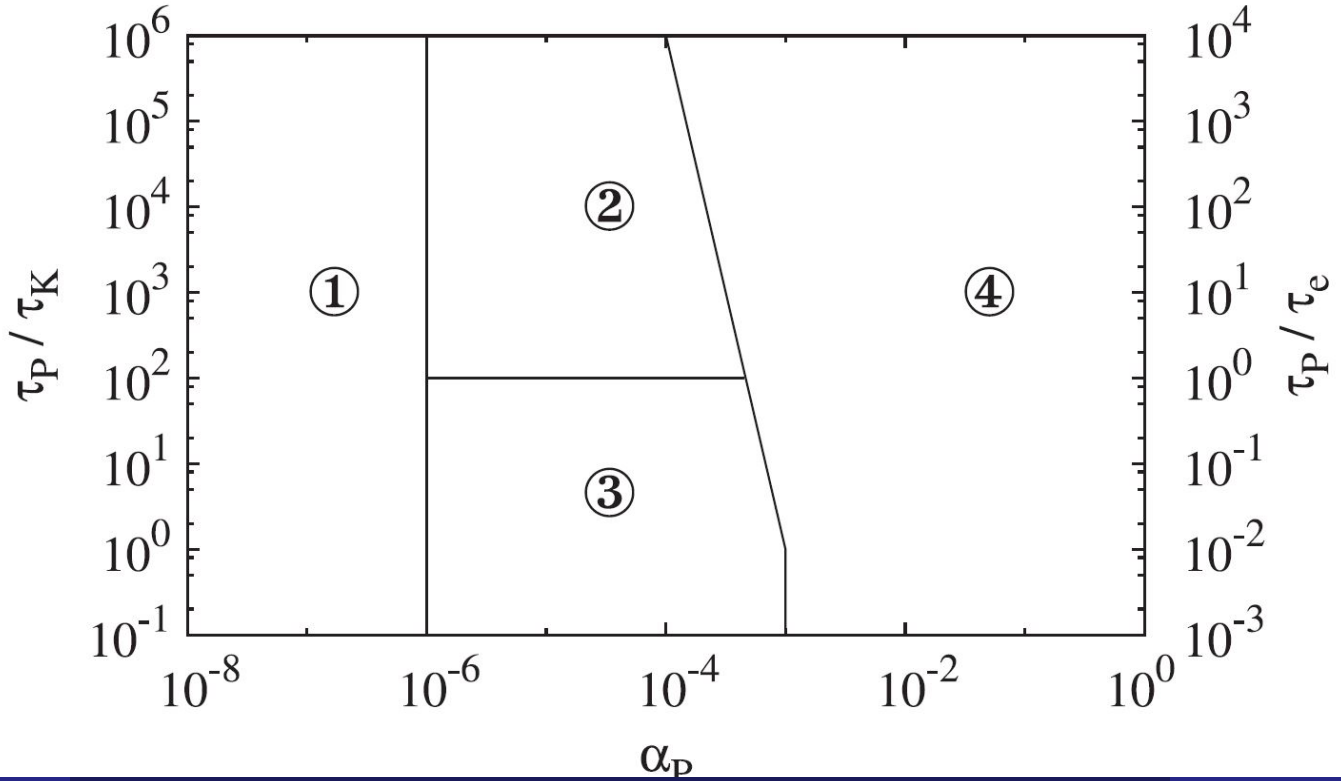
Lagrangian and Eulerian



- *Lagrangian*
- *Eulerian*

Different Phases

1. One-way coupling, highly dilute dispersed flows, $\alpha_p \leq 10^{-6}$,
2. Two-way coupling, dilute dispersed flows, $10^{-3} < \alpha_p < 10^{-6}$
3. Two-way coupling, dilute dispersed flows, $10^{-3} < \alpha_p < 10^{-6}$
4. Four-way coupling, dense dispersed flows, $\alpha_p \geq 10^{-3}$



Governing equation

Fundamental Assumption: For the isothermal, incompressible, turbulent flow of a Newtonian fluid, the continuity and momentum equation of RANS as follows:

$$\nabla \cdot \overline{U_c} = 0$$

$$\frac{\partial \overline{U_c}}{\partial t} + \rho_c(\overline{U_c} \cdot \nabla)\overline{U_c} = -\nabla \overline{p} + \mu \Delta \overline{U_c} - \nabla \cdot \tau^{RS} + \overline{f}_D$$

Forces Acting on Particles: A particle P is defined as: x_P, D_P, U_P ρ_P, and $m_P = \frac{1}{6}\rho_P \pi D_P^3$. The force balance:

$$\frac{dx_P}{dt} = U_P$$

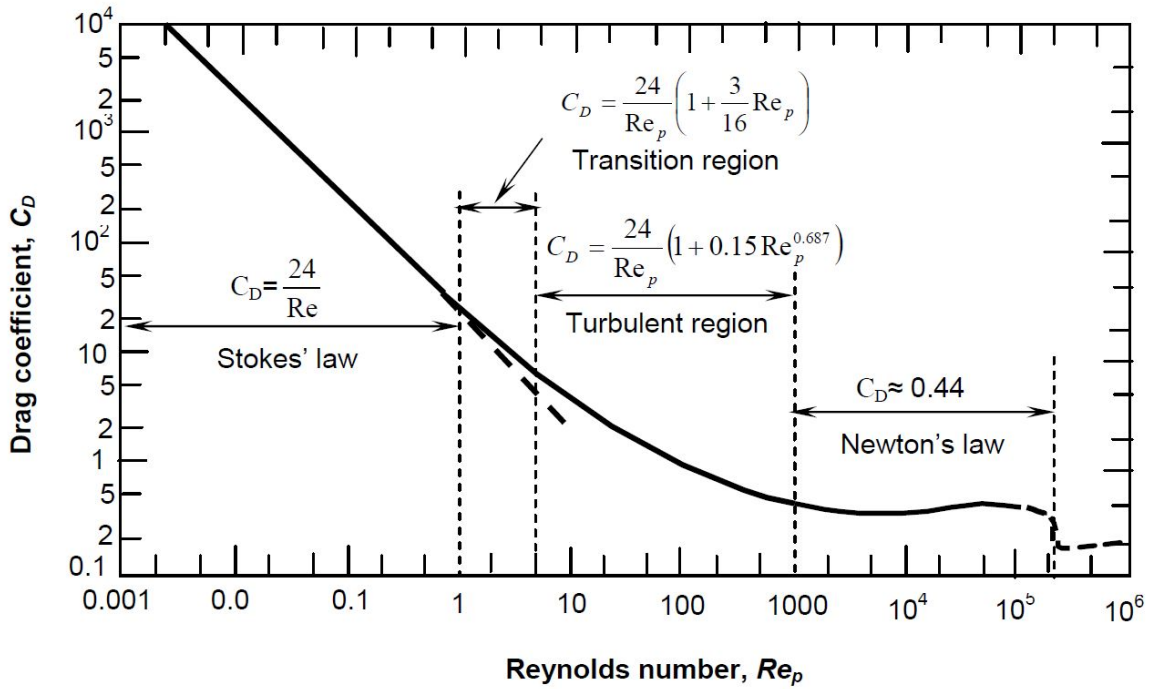
$$m_P \cdot \frac{dU_P}{dt} = \sum F_i$$

$$\sum F_i = F_D + F_G = F_D + m_P g$$

Drag force, Relaxation time τ_P, Drag coefficient C_D:

$$F_D = m_P \frac{U_c - U_P}{\tau_P}$$

$$\tau_P = \frac{3}{4} \frac{\rho_P D_P}{\rho_c C_D U_c - U_P}$$



Lagrangian particle tracking (LPT)

In RANS model, the instantaneous variables of turbulent flow is to be decomposed into a mean value and a fluctuating value, i.e.

$$U_i = \overline{U_i} + U_i'$$
$$p = \overline{p} + p'$$

The fluctuating velocity U' has to be estimated by stochastic model in order to model turbulent dispersion phenomenon. Discrete Random Walk Model(**DRW**) assume that the eddies are isotropic:

$$\overline{U_1'} = \overline{U_2'} = \overline{U_3'}$$

This assumption is not true instantaneously. This equation introduces a large over-prediction for the wall normal component U_2', y-dir, for the boundary layer in turbulence model.

Improvement

For inside the boundary layer(y^+ <80): Taking into account anisotropy and using DNS data in channel data results, three functions f_1, f_2 and f_3 introduced for the determination of the local fluctuating velocity:

$$U_1' = f_1 N_1 \sqrt{\frac{2k}{3}}, \quad U_2' = f_2 N_2 \sqrt{\frac{2k}{3}}, U_3' = f_2 N_2 \sqrt{\frac{2k}{3}}$$

where N_1, N_2 and N_3 are random numbers generated from a Gaussian probability density function and the functions are expressed as:

$$f_1 = 1 + 0.285(y^+ + 6)exp[-0.455(y^+ + 6)^{0.53}],$$
$$f_2 = 1 - exp(-0.02y^+),$$
$$f_3 = \sqrt{(3 - f_1^2 - f_2^2)},$$

as y^+:

$$y^+ = \frac{y \cdot \sqrt{\nu \cdot (\partial u/\partial y)_{y=0}}}{\nu}$$

Agenda

Solvers

Target: Find a promising solver which could be modified the stochastic model for one-way coupling without collision.

```
sol
cd lagrangian
```

Methodology: Merge two solvers together for a new one which only for **singlePhaseTransportModel** and **basicKinematicCloud**.

icoUncoupledKinematicParcelFoam.C	uncoupledKinematicParcelFoam.C
#include "fvCFD.H"	#include "fvCFD.H"
#include "singlePhaseTransportModel.H"	#include "psiThermo.H"
#include "turbulentTransportModel.H"	#include "turbulentTransportModel.H"
#include "basicKinematicCollidingCloud.H"	#include "basicKinematicCloud.H"

Comparison (1/4):

basicKinematicCollidingCloud.H and basicKinematicCloud.H

basicKinematicCollidingCloud.H	basicKinematicCloud.H
#include "Cloud.H"	#include "Cloud.H"
#include "KinematicCloud.H"	#include "KinematicCloud.H"
#include "CollidingCloud.H"	
#include "basicKinematicCollidingParcel.H"	#include "basicKinematicParcel.H"

Comparison (2/4):

basicKinematicCollidingCloud.H and basicKinematicCloud.H

basicKinematicCloud.H:

```
namespace Foam
{
   typedef KinematicCloud<Cloud<basicKinematicParcel>> basicKinematicCloud;
}
```

basicKinematicCollidingCloud.H:

```
namespace Foam
{typedef CollidingCloud
      <KinematicCloud<Cloud<basicKinematicCollidingParcel>>>
                                                basicKinematicCollidingCloud;
 }
```

Comparison (3/4):

basicKinematicCollidingParcel.H and basicKinematicParcel.H

basicKinematicCollidingParcel.H	basicKinematicParcel.H
#include "contiguous.H"	#include "contiguous.H"
#include "particle.H"	#include "particle.H"
#include "KinematicParcel.H"	#include "KinematicParcel.H"
#include "CollidingParcel.H"	

Comparison (4/4):

basicKinematicCollidingParcel.H, basicKinematicParcel.H and CollidingParcel.H

basicKinematicCollidingParcel:

```
typedef CollidingParcel<KinematicParcel<particle>>
                                basicKinematicCollidingParcel;
```

basicKinematicParcel.H:

```
typedef KinematicParcel<particle> basicKinematicParcel;
```

CollidingParcel.H:

```
Description
    Wrapper around kinematic parcel types to add collision modelling;
```

Tracking Mechanism (1/3)

icoUncoupledKinematicParcelFoam.C:

```
63      while (runTime.loop())
64      {
65          Info<< "Time = " << runTime.timeName() << nl << endl;
67          Info<< "Evolving " << kinematicCloud.name() << endl;
69          laminarTransport.correct();
71          mu = laminarTransport.nu()*rhoInfValue;
73          kinematicCloud.evolve();
75          runTime.write();
77          Info<< "ExecutionTime = " << runTime.elapsedCpuTime() << " s"
78              << "  ClockTime = " << runTime.elapsedClockTime() << " s"
79              << nl << endl;
80      }
```

The core member function is kinematicCloud<evolve>.

Comparison (1/4):

basicKinematicCollidingCloud.H and basicKinematicCloud.H

basicKinematicCollidingCloud.H	basicKinematicCloud.H
#include "Cloud.H"	#include "Cloud.H"
#include "KinematicCloud.H"	#include "KinematicCloud.H"
#include "CollidingCloud.H"	
#include "basicKinematicCollidingParcel.H"	#include "basicKinematicParcel.H"

Tracking Mechanism (2/3)

kinematicCloud<evolve>:

1. Line 683: `evolve` calls `solve(td)`, `td` is reference of `TrackData`;
2. Line 89-126: `solve(td)` calls `evolveCloud(td)`;
3. Line 174 -215: `evolveCloud(td)` is if-else loop:
   - Line 183-215, when `solution_.transient()` is true, line 202, 204 will be executed, otherwise,
   - Line 213 `CloudType::move` will be performed.
4. `CloudType` is equivalent to `Cloud<basicKinematicParcel>`, investigate the member function `CloudType::move` in `Cloud.C`
   - Line 242-378, "while loop": how the particles transfer through `move` member function;
   - Line 251-295, shows how to move the particle
5. Line 197: `injectors_.inject(td)` injects particles into flow.
6. Line 202: `td.cloud().motion(td)` calls `motion` function in class `KinematicParcel`.
7. Line 204: `stochasticCollision().update(solution_.trackTime())` updates the model under particles collision

Tracking Mechanism (3/4)

KinematicParcel.H:

```
//- Calculate new particle velocity
template<class TrackData>
const vector calcVelocity
(
    TrackData& td,
    const scalar dt,            // timestep
    const label celli,          // owner cell
    const scalar Re,            // Reynolds number
    const scalar mu,            // local carrier viscosity
    const scalar mass,          // mass
    const vector& Su,           // explicit particle momentum source
    vector& dUTrans,            // momentum transfer to carrier
    scalar& Spu                 // linearised drag coefficient
) const;
```

Tracking Mechanism (4/4)

`KinematicParcel.C`:
Eventually, `td.cloud().dispersion().update` is called to update:

```
Uc_ = td.cloud().dispersion().update
(
    dt,      // time step
    celli,   // cell number
    U_,      // particle mean velocity
    Uc_,     // flow mean velocity
    UTurb_,  // flow fluctuating velocity in turbulence
    tTurb_   // time fluctuating velocity in turbulence
);
```

Stochastic Model

`stochasticCollision` is called to update the model if the collision happens, but the collision scenarios does not happen in our case; Instead, `StochasticDispersionRAS` model is a promising candidate to update the model, with $UTurb = \zeta \mathbf{d} \sigma$

```
97      const scalar sigma = sqrt(2*k/3.0);
102     const scalar theta = rnd.sample01<scalar>()*twoPi;
103     const scalar u = 2*rnd.sample01<scalar>() - 1;
105     const scalar a = sqrt(1 - sqr(u));
106     const vector dir(a*cos(theta), a*sin(theta), u);
108     UTurb = sigma*mag(rnd.GaussNormal<scalar>())*dir;
```

Line 97: calculate σ with isotropic turbulence assumption, introduce a large over-prediction for the wall normal component v', y-dir,:

$$\sigma = \sqrt{\frac{2k}{3}}, \sigma = \sqrt{\overline{u'^2}} = \sqrt{\overline{v'^2}} = \sqrt{\overline{w'^2}}$$

Agenda

Create New Solver–icoUncoupledKinematicNocollisonFoam

Prototype: `icoUncoupledKinematicParcelFoam.C`;
Header file: `#include "basicKinematicCollidingCloud.H"` replaced by `#include "basicKinematicCloud.H"` (no collision occurs).

```
#include "fvCFD.H"
#include "singlePhaseTransportModel.H"
#include "turbulentTransportModel.H"
#include "basicKinematicCloud.H"
```

Make/files:

```
icoUncoupledKinematicNocollisionFoam.C
EXE = $(FOAM_USER_APPBIN)/icoUncoupledKinematicNocollsionFoam
```

Then compile the new solver.

New Stochastic Model – myStochasticModel (1/8)

Prototype: `StochasticDispersionRAS`;
Renamed as `myStochasticModel`.

Modification as:

- change the class name, from `StochasticDispersionRAS` to `myStochasticModel` using `sed` command in `.H` `.C`
- declare the object `yP_` as class `volScalarField` in `.H`: `volScalarField yP_;`

New Stochastic Model – myStochasticModel (2/8)

- initilize the object yP_ in .C:

```
template<class CloudType>
Foam::myStochasticModel<CloudType>::myStochasticModel
(const dictionary& dict,
 CloudType& owner):
 DispersionRASModel<CloudType>(dict, owner),
    yP_
        (
         IOobject
         (
         "yP",
         this->owner_.mesh().time().timeName(),
         this->owner_.mesh(),
         IOobject::NO_READ,
         IOobject::AUTO_WRITE
         ),
         this->owner_.mesh(),
         dimensionedScalar("yP", dimless, 0.0)
        )
{}
```

New Stochastic Model – myStochasticModel (3/8)

- initilize the object yP_ in .C:

```
template<class CloudType>
Foam::myStochasticModel<CloudType>::myStochasticModel
(
    const myStochasticModel<CloudType>& dm
)
:
    DispersionRASModel<CloudType>(dm),
    yP_(dm.yP_)
{}
```

New Stochastic Model – myStochasticModel (4/8)

- Setup the variables will be used in y^+ calculation:
  - obtain the turbulence model:

```
//setup the patches
const fvPatchList& patches = this->owner().mesh().boundary();
const objectRegistry& obr=this->owner().mesh();
const word turbName=
IOobject::groupName
(
     turbulenceModel::propertiesName,
     this->owner().U().group()
 );
const turbulenceModel& turbModel =
 ↪   obr.lookupObject<turbulenceModel>(turbName);
```

New Stochastic Model – myStochasticModel (5/8)

- Setup the variables will be used in y^+ calculation:
  - use `forAll` loop for the all patches:

```
forAll(patches, patchi)
{
 // the main code for calculation for turbulent fluctuating
 ↪   velocity UTurb
}
```

  - obtain the current Patch

```
// obtain the current Patch
const fvPatch& currPatch = patches[patchi];
```

New Stochastic Model – myStochasticModel (6/8)

- Setup the variables will be used in y^+ calculation:
  - use `if` loop for calculation;
  - setup the varibles for yPlus calculation;

```
// calculation
if (typeid(currPatch) == typeid(wallFvPatch))
{
const scalarField& y_ = turbModel.y()[patchi];
const fvPatchVectorField& Uw =
 ↪   turbModel.U().boundaryField()[patchi];
const tmp<scalarField> tnuw = turbModel.nu(patchi);
const scalarField& nuw = tnuw();
```

New Stochastic Model – myStochasticModel (7/8)

- Setup the variables will be used in y^+ calculation:
  - calculate the y^+ for the current patch;
  - use `const_cast` to release the `const` limitation
- Calculate y^+;

```
// yPlus for the current patch
 fvPatchField<scalar>& yPpatch =
 ↪   const_cast<fvPatchField<scalar>&>(yP_.boundaryField()[patchi]);

yPpatch =(y_*sqrt(nuw*mag(Uw.snGrad()))/nuw);
```

New Stochastic Model – myStochasticModel (8/8)

- update the turbulence fluctuating velocity for particle when y^+ <80:

```
const scalar sigma = sqrt(2*k/3.0);
const scalar theta = rnd.sample01<scalar>()*twoPi;
const scalar u = 2*rnd.sample01<scalar>() - 1;
const scalar a = sqrt(1 - sqr(u));

f_x=1+0.285*(yPpatch[patchi]+6)*exp(-0.455*pow(yPpatch[patchi]+6,
 ↪   0.53));
f_y=1-exp(-0.02*yPpatch[patchi]);
f_z=sqrt(3-sqr(f_x)-sqr(f_y));

// update the turbulence fluctuating velocity for particle

dir_x=f_x*a*cos(theta);
dir_y=f_y*a*sin(theta);
dir_z=f_z*u;
const vector dir(dir_x, dir_y, dir_z);
UTurb=sigma*dir;
```

Compile New Class myStochasticModel (1/3)

Make/files:

```
PARCELS=parcels
DERIVEDPARCELS=$(PARCELS)/derived

KINEMATICPARCEL=$(DERIVEDPARCELS)/basicKinematicParcel
$(KINEMATICPARCEL)/makeBasicKinematicParcelSubmodels.C

LIB = $(FOAM_USER_LIBBIN)/liblagrangianTurbulence
```

The compile file `makeBasicKinematicParcelSubmodels.C`:

```
26 #include "basicKinematicCloud.H"
27 #include "makeParcelTurbulenceDispersionModels.H"

31 namespace Foam
32 {
33     makeParcelTurbulenceDispersionModels(basicKinematicCloud);
34 }
```

Compile New Class myStochasticModel (2/3)

makeParcelTurbulenceDispersionModels.H includes the options under sub-models for DispersionModel;

```
#include "GradientDispersionRAS.H"
#include "StochasticDispersionRAS.H"
#include "myStochasticModel.H"
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
#define makeParcelTurbulenceDispersionModels(CloudType)                    \
                                                                           \
    typedef Foam::CloudType::kinematicCloudType kinematicCloudType;        \
    defineNamedTemplateTypeNameAndDebug                                    \
    (                                                                      \
        Foam::DispersionRASModel<kinematicCloudType>,                      \
        0                                                                  \
    );                                                                     \
    makeDispersionModelType(GradientDispersionRAS, CloudType);             \
    makeDispersionModelType(StochasticDispersionRAS, CloudType);           \
    makeDispersionModelType(myStochasticModel, CloudType);                 \
```

Compile New Class myStochasticModel (3/3)

Until now, the modification of class `myStochasticModel` is done. Go to compile to add the new model as a submodel of `DispersionModel`:

```
wclean
wmake
```

Agenda

Primitive preparation

Before implement the new solver with the new model, a steady flow with k and ε value should be obtained previously. Therefore, k-ε model will be implemented using `simpleFoam` in a pipe.

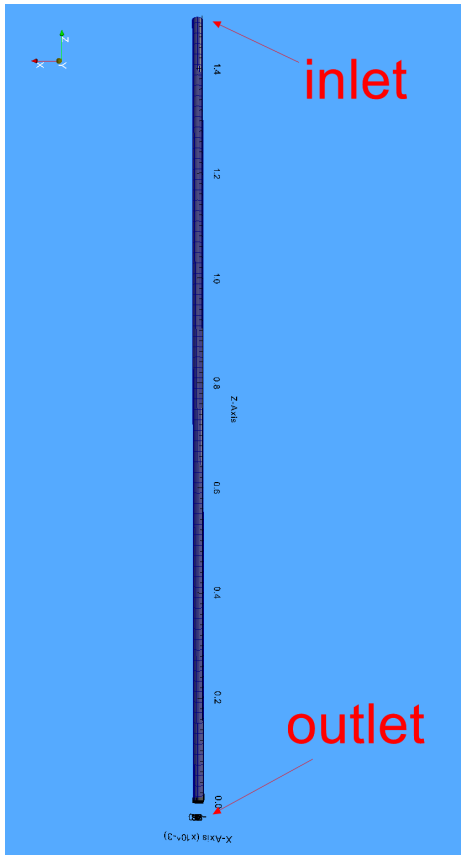
- One tutorial case under `ras` directory will be used as a base case for the modification;
- Create a pipe;
- Modification of the setting;
- Obtain a steady flow

Create a Pipe

The pipe model is created by Star-CCM+, then use `ccm26ToFoam` to convert into OpenFOAM, the profile of the pipe:

```
Radius:                 0.01m
Length:                 1.5m
Mesh stats
    points:             7469
    faces:              20760
    internal faces:     18456
    cells:              6688
    faces per cell:     5.86364
    boundary patches:   3
    point zones:        0
    face zones:         0
    cell zones:         0
    Patch       Faces     Points
    shroud      2128      2156
    outlet      88        97
    inlet       88        97
```

The configuration of the pipe:



Modification in the 0 directory (1/2)

0/p:

```
dimensions      [0 2 -2 0 0 0 0];
internalField   uniform 0;
boundaryField
{
    inlet
    {
        type    zeroGradient;
    }
    outlet
    {
        type   fixedValue;
        value  uniform 0;
    }
    shroud
    {
        type    zeroGradient;
    }
}
```

0/U:

```
dimensions      [0 1 -1 0 0 0 0];
internalField   uniform (0 0 0);
boundaryField
{
    inlet
    {
        type   fixedValue;
        value  uniform (0 0 -12);
    }
    outlet
    {
        type   zeroGradient;
    }
    shroud
    {
        type   fixedValue;
        value  uniform (0 0 0);
    }
```

Modification in the 0 directory (2/2)

0/k:

```
dimensions      [0 2 -2 0 0 0 0];
internalField   uniform 0.0006;
boundaryField
{
    inlet
    {
        type    fixedValue;
        value   uniform 0.0006;
    }
    outlet
    {
        type    zeroGradient;
    }
    shroud
    {
        type    kqRWallFunction;
        value   uniform 0.00375;
    }
}
```

0/epsilon:

```
dimensions      [0 2 -3 0 0 0 0];
internalField   uniform 0.00754;
boundaryField
{
    inlet
    {
        type  zeroGradient;
    }
    outlet
    {
        type  zeroGradient;
    }
    shroud
    {
        type  epsilonWallFunction;
        value uniform 0.00754;
    }
}
```

Modification in the constant directory

To set similar conditions at those used by A.Dehbi, the `transportProperties` should be changed for the same Re number.

For flow in a pipe or tube, the Reynolds number is generally defined as:

$$Re = \frac{QD_H}{\nu A} = \frac{vD}{\nu} \simeq 12000$$

```
rhoInf          [1 -3 0 0 0 0 0] 1.2;

transportModel  Newtonian;

nu              [0 2 -1 0 0 0 0] 1e-05;
```

Modification in the system directory (1/2)

system/controlDict

```
application     simpleFoam;
startFrom       startTime;
startTime       0;
stopAt          endTime;
endTime         600;
deltaT          1;
writeControl    timeStep;
writeInterval   50;
purgeWrite      0;
writeFormat     ascii;
writePrecision  6;
writeCompression off;
timeFormat      general;
timePrecision   6;
runTimeModifiable true;
```

Modification in the system directory (2/2)

system/fvScheme:

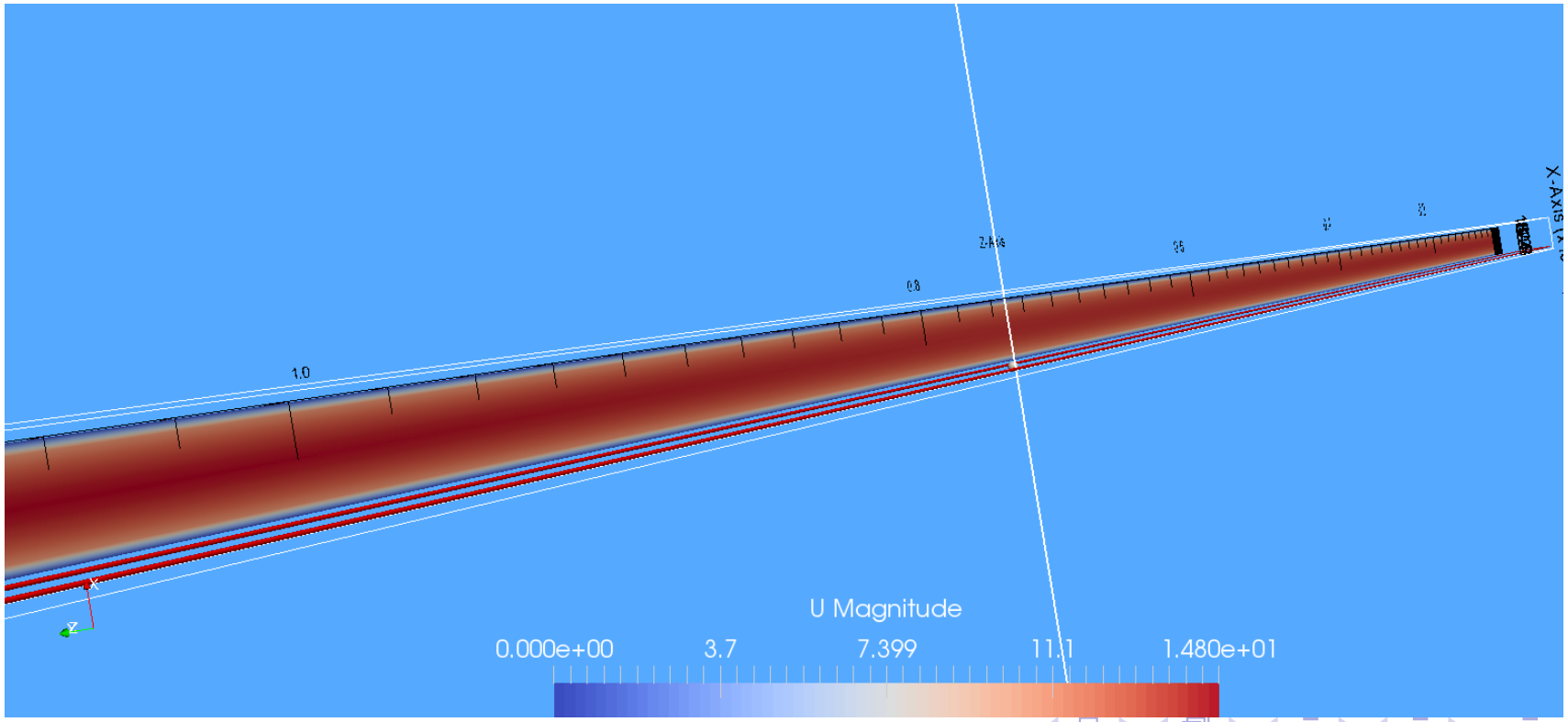
```
ddtSchemes
{
    default                     steadyState;
}
gradSchemes
{
    default                     Gauss linear;
}
divSchemes
{
    default                     none;
    div(phi,U)                  bounded Gauss linearUpwind grad(U);
    div(phi,k)                  bounded Gauss upwind;
    div(phi,epsilon)            bounded Gauss upwind;
    div(phi,nuTilda)            Gauss limitedLinear 1;
    div((nuEff*dev2(T(grad(U))))) Gauss linear;
}
```

Run the simulation

Obtain the steady flow:

```
ccm26ToFoam mesh.ccm
simpleFoam
```

Remain the last time directory, 600, deleted the rest;



Test icoUncoupledKinematicNocollisionFoam with myStochasticModel

Copy the default setting from another test case:

```
tut
cp -r lagrangian/icoUncoupledKinematicParcelFoam/hopper/hopperInotialState
↪  $FOAM_RUN/caseStudy
cd $FOAM_RUN/myPipe
cp ../caseStudy/constant/kinematicCloudPositions constant
cp ../caseStudy/constant/kinematicCloudProperties constant
cp ../caseStudy/constant/g constant
cp ../caseStudy/system/controlDict system
cp ../caseStudy/system/fvSchemes system
cp ../caseStudy/system/fvSolution system
```

Modification under 0 directory

Change the directory name: 600 to be 0 including the files;

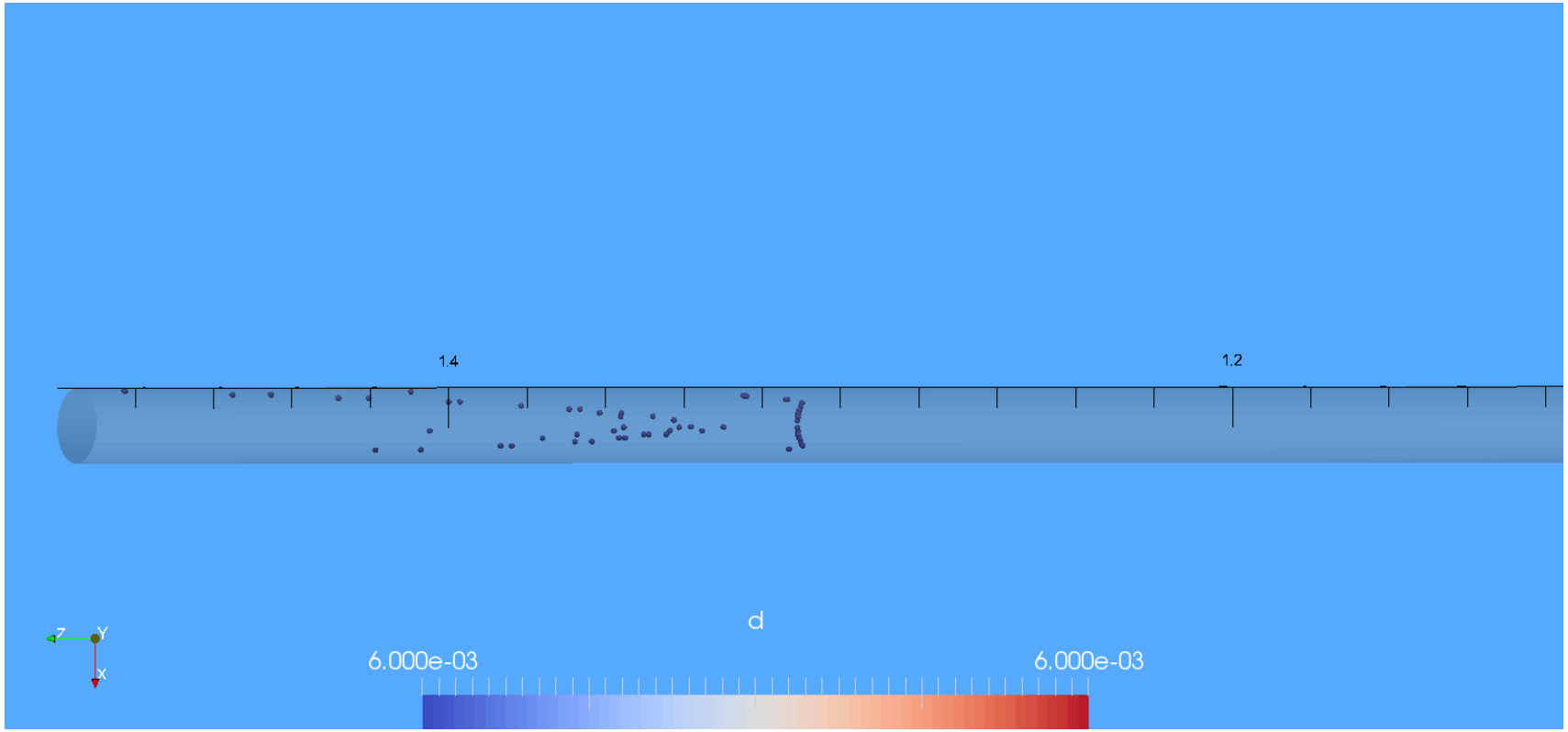
```
cd 0
sed -i s/"600"/"0"/g epsilon
sed -i s/"600"/"0"/g k
sed -i s/"600"/"0"/g nut
sed -i s/"600"/"0"/g p
sed -i s/"600"/"0"/g phi
sed -i s/"600"/"0"/g U
```

Modification under constant directory

Create some random particle positions in `kinematicCloudPositions`;
Change the simulation setting in `kinematicCloudProperties` as:

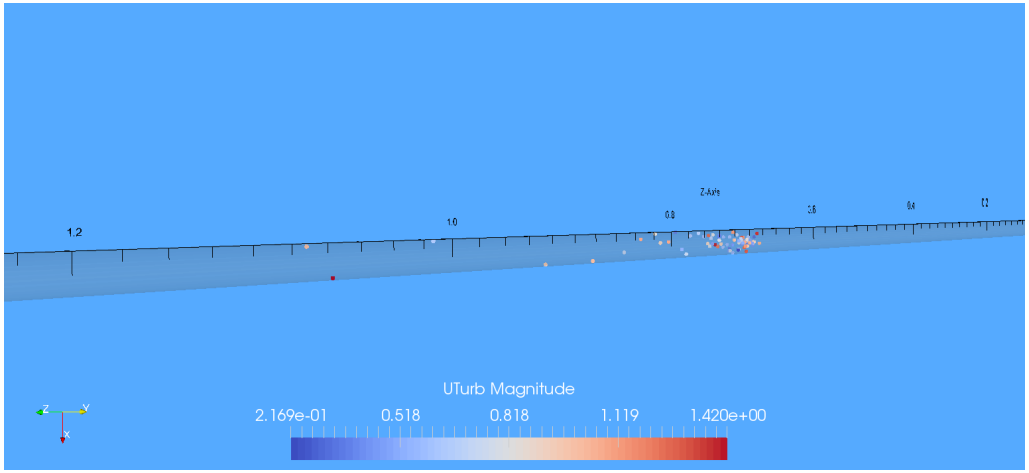
```
dispersionModel myStochasticModel;
patchInteractionModel none;
surfaceFilmModel none;
stochasticCollisionModel none;
collisionModel none;

        inlet
        {
        ...
        }
        outlet
        ...
        shroud
        ...
```

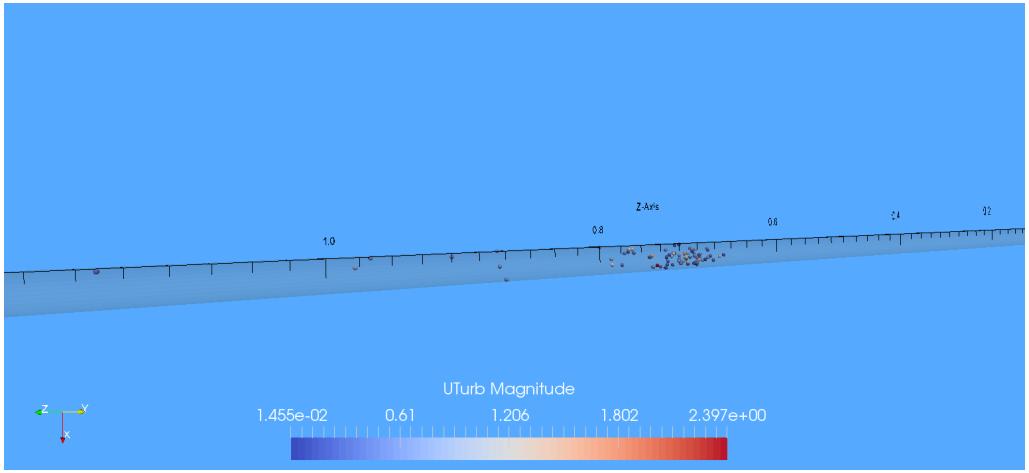
Result: In Transition



Comparison: myStochastisModel vs StochasticDispersionRAS

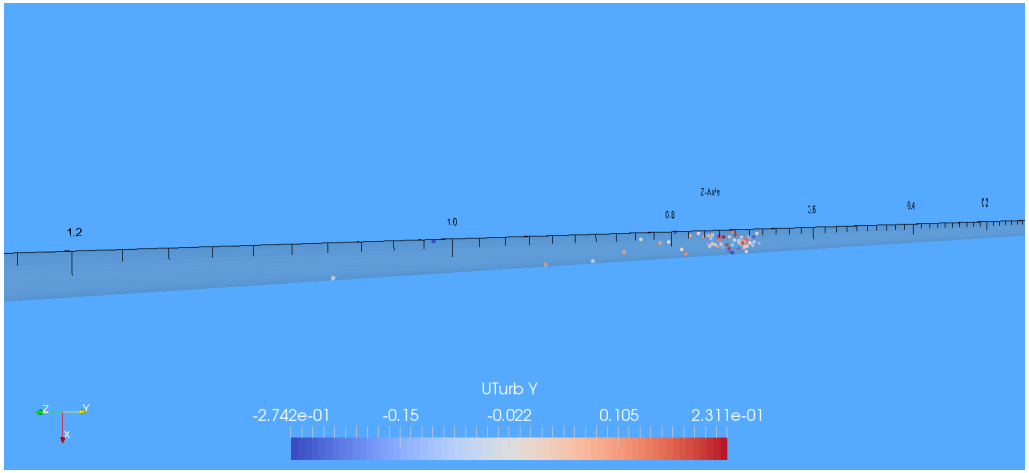
UTurb (magnitude):

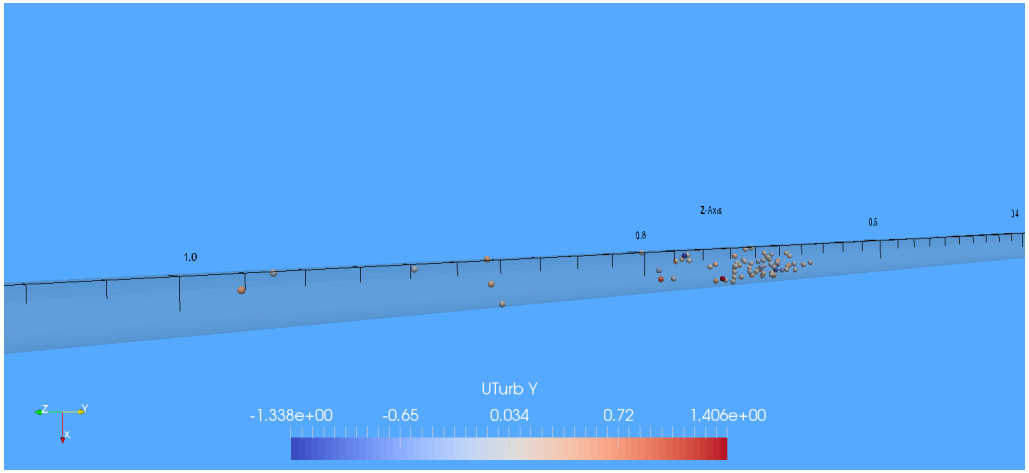




Comparison: myStochastisModel vs StochasticDispersionRAS

UTurb-Y (magnitude):





Thank you!
Questions ?