CFD with OpenSource Software

A course at Chalmers University of Technology
Taught by Håkan Nilsson

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interPhasChangeFoam Tutorial

and

PANS Turbulence Model

Developed for OpenFOAM-2.2.x

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Disclaimer: This is a student project work, done as part of a course where OpenFOAM and some other OpenSource software are introduced to the students. Any reader should be aware that it might not be free of errors. Still, it might be useful for someone who would like learn some details similar to the ones presented in the report and in the accompanying les. The material has gone through a review process. The role of the reviewer is to go through the tutorial and make sure that it works, that it is possible to follow, and to some extent correct the writing. The reviewer has no responsibility for the contents

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Preface

Current report contains descriptions of interPhaseChangeFoam solver and also detailed explanation of adding a new turbulence model to OpenFoam code as the project report of "MSc/PhD course in CFD with OpenSource software". The OF2.2.x version has been used as the default version for both of the cases.

In the first section of this report, interPhaseChangeFoam solver which has been used for simulation of phase change between two incompressible-impressible flows has been described. For phase change and as a default, different caviation phase change models have been considered in this solver. Therefore, this solver has been used mostly for simulation of cavitation.

Previous students of this course have provided tutorial for this solver. Therefore, the emphasis of this report would be on the sections which either need more explanation comparing to previous tutorial or have been added/modified recently into the solver. Furthermore, in order to introduce the way of modifying the solver, Singhal phase change model has been added to the solver, and undertaken steps have been described.

It should be mentioned that it is assumed that the readers has gone through the lectures and documents of the course, and therefore have some background on CFD/OpenFoam.

Finally, to show performance of the solver and its applicability, flows around two cases have been simulated. The first case is the flow around a flat plate, and the second case is the flow around a hydrofoil (NACA0009). At the end, few limitations and drawbacks of using this solver have been discussed.

In the second section of the report, PANS turbulence model (Partially Averaged Navier Stokes) has been presented. Numerical investigations of PANS turbulence models have shown their merits and possible applicability to achieve high and precise results with lower computational cost comparing to LES and DES approaches. Although there are still few unresolved problems regarding stability of dynamic version of PANS models, promising results of these models have caused its development especially in the cases that very fine mesh resolution is not possible due to the lack of resources. For this tutorial, static version of PANS model based on the k-Epsilon RANS model has been developed and implemented into the OpenFoam code. The implementation is straightforward and can be easily extended to kOmega or other URANS models. To verify the model and its superiority over original URANS model (here kEpsilon), turbulent flow around a square cylinder has been simulated. To give a wider view, K-Epsilon,

OEEVM, and PANS k-Epsilon models have been compared and merits of the implemented model over other models are verified.

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1. First Section: interPhaseChangeFoam

1.1 Introduction

To simulate cavitating flows with OpenFoam code, there are few solvers available which have been designed for simulating this type of fluids. One of these solvers is interPhaseChangeFoam which has been especially written for incompressible/immiscible two phase flows. This solver in the version of 2.2.x is located in OpenFoam/applications/solvers/multiphase. In the recently released version of the code (OF2.2.2), interDyPhaseChangeFoam has been added to simulate cavitation around moving objects like propellers.

In the following parts of the first section, first of all governing equations of two phase incompressible flows are represented. Then all of the members of the solver are listed and for those which we have more concerns all of the code parts have been described and explained.

The case folder for this solver like most of the solvers consists of three folders: time (zero), constant, and system.

In the system folder, you have to define solution parameters (fvSolution file), schemes (fvSchemes) and also time parameters (controlDict). In the constant folder, you have to define the solver parameters like phase change model and its characteristics through transportProperties file.

There is a tutorial for this solver where you can find a template and example of how to set these parameters which is located at

"$WM_PROJECT_DIR/tutorials/multiphase/interPhaseChangeFoam"

In the following, governing equations, solver members list, solver members descriptions, results for a test case, and some issues regarding the drawbacks of simulation of cavitation have been presented.

1.2 Governing equations

Governing equations are conservation of mass, Navier-Stokes, and transport equation of volume fraction:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial (\rho_m u_i)}{\partial x_i} = 0 \qquad (1\text{-}1)$$

$$\frac{\partial(\rho_m u_i)}{\partial t}+\frac{\partial(\rho_m u_i u_j)}{\partial x_j}=-\frac{\partial(P)}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu_{eff}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\right)+\rho_m g \tag{1-2}$$

$$\frac{\partial \alpha_v}{\partial t}+\frac{\partial(\alpha_v u_i)}{\partial x_i}=S_\alpha \tag{1-3}$$

which S stands for phase change rate between vapor and liquid. In interPhaseChangeFoam solver, volume transport equation of liquid is solved. However, because for this tutorial SchnerrSauer cavitation model has been described, let for now, consider transport of vapor volume fraction. Later, we can easily transform this equation to transport equation of liquid.

In transport equation approach used in interPhaseChangeFoam solver, the location of interface is specified using the volume fraction function. For example in vapor-liquid two phase flow, $\alpha_v = 1$ denotes inside vapor and $\alpha_v = 0$ in the liquid. Cells which lie between 0 and 1 contain interface regions. This concept can be written as:

$$\alpha_v(x,t)=\begin{cases}0 & \text{Liquid phase}\\ 0<\alpha_v<1 & \text{liquid-vapor region}\\ 1 & \text{Vapor phase}\end{cases} \tag{1-4}$$

By determination of the volume of fraction, the local mixture properties of fluid can be computed based on the single state of each phase as follows:

$$\begin{aligned}\rho_m &= \alpha_v\rho_v+(1-\alpha_v)\rho_l\\ \mu_m &= \alpha_v\mu_v+(1-\alpha_v)\mu_l\end{aligned} \tag{1-5}$$

As you can see because of variation of density, the divergence of velocity will be generally non-zero. The relation between the velocity divergence and phase change rate would be:

$$\begin{aligned}&\frac{\partial \alpha_v}{\partial t}+\frac{\partial(\alpha_v u_i)}{\partial x_i}=S_\alpha\\ &\frac{\partial(u_i)}{\partial x_i}=\frac{-1}{\rho_m}\frac{D\rho_m}{Dt}=S_m\end{aligned} \tag{1-6}$$

$$Where:\quad S_m=\frac{\rho_l-\rho_v}{\rho_l}S_\alpha$$

1.3 Solver members

This solver consists of the following files/folders.

- alphaEqn.H
- alphaEqnSubCycle.H
- createFields.H
- interPhaseChangeFoam.C
- pEqn.H
- UEqn.H
- phaseChangeTwoPhaseMixtures Folder
    - Kunz folder
        - Kunz.C
        - Kunz.H
    - Merkle folder
        - Merkle.C
        - Merkle.H
    - phaseChangeTwoPhaseMixture
        - phaseChangeTwoPhaseMixture.C
        - phaseChangeTwoPhaseMixture.H
        - newPhaseChangeTwoPhaseMixture.C
        - newPhaseChangeTwoPhaseMixture.H
    - SchnerrSauer folder
        - SchnerrSauer.C
        - SchnerrSauer.H
- Make
    - files
    - options

Here, we have focused on those files which are more specific for this solver. The solver is located at

"$WM_PROJECT_DIR/applications/solvers/multiphase/interPhaseChangeFoam"

1.3.1 SchnerrSauer.C

In this tutorial SchnerrSauer model will be described in details. Moreover, the emphasis here has put on new concepts comparing to the course lectures. So, description of parameters in header files and other common issues have been considered as previously known.

Code	`// * * * * * * * * Constructors * * * * * * * * * * * * * * * //`
	
	`Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::SchnerrSauer`
	`(`
	`const volVectorField& U,`
	`const surfaceScalarField& phi,`
	`const word& alpha1Name`
	`)`
	`:`
	`phaseChangeTwoPhaseMixture(typeName, U, phi, alpha1Name),`
	
	`n_(phaseChangeTwoPhaseMixtureCoeffs_.lookup("n")),`
	`dNuc_(phaseChangeTwoPhaseMixtureCoeffs_.lookup("dNuc")),`
	`Cc_(phaseChangeTwoPhaseMixtureCoeffs_.lookup("Cc")),`
	`Cv_(phaseChangeTwoPhaseMixtureCoeffs_.lookup("Cv")),`
	
	`p0_("0", pSat().dimensions(), 0.0)`
	`{`
	`correct();`
	`}`

Description	In this section, different parameters which should be read from the input (transportproperties file, in constant folder) have been clarified. These parameters are related to the model and can vary from one phase change model to another. n: number of bubble per volume of liquid, nondimensional dNuc: initial diameter of nuclei, dimension: meter Cc: condensation coefficient Cv: vaporization coefficient

Code	`Foam::tmp<Foam::volScalarField>`
	`Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::rRb`
	`(`
	`const volScalarField& limitedAlpha1`
	`) const`
	`{`
	`return pow`
	`(`
	`((4*constant::mathematical::pi*n_)/3)`
	`*limitedAlpha1/(1.0 + alphaNuc() - limitedAlpha1),`
	`1.0/3.0`
	`);`
	`}`

Description	rRb: reversed Radius bubble $$\alpha_v = \frac{\pi R^3 n_0 4/3}{1+\pi R^3 n_0 4/3} \rightarrow R = \sqrt[3]{\frac{\alpha_v}{1-\alpha_v}\frac{1}{\pi n_0 4/3}}$$ $$\rightarrow \frac{1}{R} = \sqrt[3]{\frac{\alpha_l}{1+\alpha_{Nuc}-\alpha_l}\pi n_0 4/3}$$ In this equation, α_{Nuc} has been added to prevent zero value in denominator.

Code	`Foam::dimensionedScalar`
	`Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::alphaNuc() const`
	`{`
	`  dimensionedScalar Vnuc = n_*constant::mathematical::pi*pow3(dNuc_)/6;`
	`  return Vnuc/(1 + Vnuc);`
	`}`

Description	Calculation of nuclei volume fraction based on the initial radius of vapor bubble

Code	`Foam::tmp<Foam::volScalarField>`
	`Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::pCoeff`
	`(`
	`  const volScalarField& p`
	`) const`
	`{`
	`  volScalarField limitedAlpha1(min(max(alpha1_, scalar(0)), scalar(1)));`
	`  volScalarField rho`
	`  (`
	`  limitedAlpha1*rho1() + (scalar(1) - limitedAlpha1)*rho2()`
	`  );`
	
	`  return`
	`  (3*rho1()*rho2())*sqrt(2/(3*rho1()))`
	`  *rRb(limitedAlpha1)/(rho*sqrt(mag(p - pSat()) + 0.01*pSat()));`
	`}`

Description	pCoeff is just an intermediate coefficient. To prevent unrealistic results, the liquid volume fraction should be bounded between zero and one, here called limitedAlpha1 Rho is the mixture density 0.01*pSat() is small amount to prevent zero in denominator $$pCoeff = \frac{3\rho_l\rho_v}{R}\sqrt{\frac{2}{3\rho_l}}\frac{1}{\rho\sqrt{\lvert p - pSat\rvert + small}}$$

Code	`Foam::Pair<Foam::tmp<Foam::volScalarField> > Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::mDotAlphal() const { const volScalarField& p = alpha1_.db().lookupObject<volScalarField>("p"); volScalarField limitedAlpha1(min(max(alpha1_, scalar(0)), scalar(1))); volScalarField pCoeff(this->pCoeff(p)); return Pair<tmp<volScalarField> > (Cc_*limitedAlpha1*pCoeff*max(p - pSat(), p0_), Cv_*(1.0 + alphaNuc() - limitedAlpha1)*pCoeff*min(p - pSat(), p0_)); }`
Description	mDotAlphal is a pair volScalarField. The first part is related to condensation, and the second is related to evaporation. Pressure is loaded into this section by lookupObject. mDotAlphal will be used in transport equation of liquid volume fraction.

Code	`Foam::Pair<Foam::tmp<Foam::volScalarField> > Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::mDotP() const { const volScalarField& p = alpha1_.db().lookupObject<volScalarField>("p"); volScalarField limitedAlpha1(min(max(alpha1_, scalar(0)), scalar(1))); volScalarField apCoeff(limitedAlpha1*pCoeff(p)); return Pair<tmp<volScalarField> > (Cc_*(1.0 - limitedAlpha1)*pos(p - pSat())*apCoeff, (-Cv_)*(1.0 + alphaNuc() - limitedAlpha1)*neg(p - pSat())*apCoeff); }`
Description	mDotP is a pair volScalarField. The first part is related to condensation, and the second is related to evaporation. Pressure is loaded into this section by lookupObject.

Code	`bool Foam::phaseChangeTwoPhaseMixtures::SchnerrSauer::read() { if (phaseChangeTwoPhaseMixture::read()) { phaseChangeTwoPhaseMixtureCoeffs_ = subDict(type() + "Coeffs"); phaseChangeTwoPhaseMixtureCoeffs_.lookup("n") >> n_; phaseChangeTwoPhaseMixtureCoeffs_.lookup("dNuc") >> dNuc_; phaseChangeTwoPhaseMixtureCoeffs_.lookup("Cc") >> Cc_;`

	phaseChangeTwoPhaseMixtureCoeffs_.lookup("Cv") >> Cv_;
	
	return true;
	}
	else
	{
	return false;
	}
	}

Description	Reading model parameters from input (constant/transportProperties)

1.3.2 phaseChangeTwoPhaseMixture.C

Code	Foam::Pair<Foam::tmp<Foam::volScalarField> >
	Foam::phaseChangeTwoPhaseMixture::vDotAlphal() const
	{
	volScalarField alphalCoeff(1.0/rho1() - alpha1_*(1.0/rho1() - 1.0/rho2()));
	Pair<tmp<volScalarField> > mDotAlphal = this->mDotAlphal();
	
	return Pair<tmp<volScalarField> >
	(
	alphalCoeff*mDotAlphal[0],
	alphalCoeff*mDotAlphal[1]
	);
	}

Description	vDotAlphal which consists of two parts defined as follow: $$vDotAlphaL = mDotAlphaL.\left(\frac{1}{\rho_l} - alphaL.\left(\frac{1}{\rho_l} - \frac{1}{\rho v}\right)\right)$$

Code	Foam::Pair<Foam::tmp<Foam::volScalarField> >
	Foam::phaseChangeTwoPhaseMixture::vDotP() const
	{
	dimensionedScalar pCoeff(1.0/rho1() - 1.0/rho2());
	Pair<tmp<volScalarField> > mDotP = this->mDotP();
	
	return Pair<tmp<volScalarField> >(pCoeff*mDotP[0], pCoeff*mDotP[1]);
	}

Description	$$vDotp = mDotp.\left(\frac{1}{\rho_l} - \frac{1}{\rho v}\right)$$

Code	bool Foam::phaseChangeTwoPhaseMixture::read()
	{
	if (incompressibleTwoPhaseMixture::read())
	{
	phaseChangeTwoPhaseMixtureCoeffs_ = subDict(type() + "Coeffs");
	lookup("pSat") >> pSat_;

	return true;
	}
	else
	{
	return false;
	}
	}

Description	Looking up for coefficients and pSat

1.3.3 alphaEqn.H

Code	word alphaScheme("div(phi,alpha)");
	word alpharScheme("div(phirb,alpha)");
	
	surfaceScalarField phir("phir", phic*interface.nHatf());

Description	Reading phi and phirb convection schemes from fvSchemes. Phirb which is related to considering relative velocities between phases. Then by considering phic which is relate to compressibility factor, relative velocity field phir is created.

Code	surfaceScalarField phiAlpha (fvc::flux (phi, alpha1, alphaScheme) + fvc::flux (-fvc::flux(-phir, alpha2, alpharScheme), alpha1, alpharScheme));
Description	Creation of alpha transport equation by considering the relative flux field (second fvc::flux). More Details about the phir and its characteristic can be found in [6].

Code	Pair<tmp<volScalarField> > vDotAlphal =
	twoPhaseProperties->vDotAlphal();
	const volScalarField& vDotcAlphal = vDotAlphal[0]();
	const volScalarField& vDotvAlphal = vDotAlphal[1]();

Description	Creation of vDotcAlphal and vDotvAlphal parameters. Remember that throughout of interPhasechangeFoam, C stands for construction of liquid and V stands for vaporization. These parameters are set equal to vDotAlphal.

Code	volScalarField Sp (IOobject ("Sp", runTime.timeName(), mesh),

	vDotvAlphal - vDotcAlphal
	);
	
	volScalarField Su
	(
	IOobject
	(
	"Su",
	runTime.timeName(),
	mesh
	),
	// Divergence term is handled explicitly to be
	// consistent with the explicit transport solution
	divU*alpha1
	+ vDotcAlphal
	);

Description	Creation of Sp and Su for MULES solver. $Sp = \text{vDotvAlphal - vDotcAlphal}$ $\text{Su} = \text{divU} * \text{alpha1} + \text{vDotcAlphal}$

Code	MULES::implicitSolve (geometricOneField(), alpha1, phi, phiAlpha, Sp, Su, 1, 0);
Description	Solving the alpha equation by using MULES solver. Please take a look at NaiXian Lu report for this course, 2008.

Code	MULES::implicitSolve (geometricOneField(), alpha1, phi, phiAlpha, Sp, Su, 1, 0);
Description	Solving the alpha equation by using MULES solver. Please take a look at NaiXian Lu report for this course [7]. I strongly suggest that you add a bounding for alpha after solving the transport equation to prevent from non-physical values.

1.3.4 alphaEqnSubCycle.H

Code	`surfaceScalarField rhoPhi`
	`(`
	`    IOobject`
	`    (`
	`        "rhoPhi",`
	`        runTime.timeName(),`
	`        mesh`
	`    ),`
	`    mesh,`
	`    dimensionedScalar("0", dimMass/dimTime, 0)`
	`);`

Description	Creation of surface scalar field for rhoPhi: mass flux

Code	`    const dictionary& pimpleDict = pimple.dict();`
	
	`    label nAlphaCorr(readLabel(pimpleDict.lookup("nAlphaCorr")));`
	
	`    label nAlphaSubCycles(readLabel(pimpleDict.lookup("nAlphaSubCycles")));`

Description	Looking up to the pimple dictionary to read values of nAlphaSubCycles, nAlphaCorr

1.3.5 pEqn.H

Code	`    Pair<tmp<volScalarField> > vDotP = twoPhaseProperties->vDotP();`
	`    const volScalarField& vDotcP = vDotP[0]();`
	`    const volScalarField& vDotvP = vDotP[1]();`
	
	`    while (pimple.correctNonOrthogonal())`
	`    {`
	`        fvScalarMatrix p_rghEqn`
	`        (`
	`            fvc::div(phiHbyA) - fvm::laplacian(rAUf, p_rgh)`
	`          - (vDotvP - vDotcP)*(pSat - rho*gh) + fvm::Sp(vDotvP - vDotcP, p_rgh)`
	`        );`
	`    }`
	
	`}`

Description	Loading vDotP parameters as vDotcP and vDotvP. Since we solve for p_rgh which is equal to p- rho*gh, we have to reduce the hydrostatic pressure from pSat too: pSat - rho*gh

1.4 Modifications

1.4.1 alphaEqn.H

Although the MULES solver was developed to solve the equation of bounded variables; sometimes it fails to keep the variable in its bounds. Therefore, in order to prevent unrealistic values for alpha (i.e. values higher than one or lowers than zero); in alphaEqn.H the following command line has been added after the MULES solver.

```
alpha1 = min(max(alpha1, scalar(0)), scalar(1));
```

14.2 Negative pressure

Depending on the flow conditions, in some cases the minimum pressure value may go below the zero by using default values for number of nuclei, nuclei diameter, and coefficients. To prevent from this unrealistic condition, one option is using a very high value for evaporation coefficient (C_v around 5000). Another approach would be using a high value for number of nuclei (n_0 around 1e14). It should be considered that alphaNuc should always have reasonable value (around 1e-5). Therefore, in the case of using high value for n_0, the diameter of nuclei should be set according the reasonable value of alphaNuc.

Because the pressure values through solution have high importance, it may be necessary to watch the pressure values during solution. Therefore, at the end of "interPhaseChangeFoam.C" file, and inside the time loop add the following simple command.

```
Info << "Max pressure: " << max(p).value() << endl;
Info << "Min pressure: " << min(p).value() << endl;
Info << "Max velocity: " << max(mag(U)).value() << endl << endl;
```

1.5 Test case: flow behind a flat plate

Flow around a 2d flat plate has been simulated using the interPhaseChangeFoam solver. The inlet velocity is 5 m/s, and outlet cavitation number is set equal to one. The height of the plat is 0.1 m and its thickness is 0.01 m. The experimental data for this case have been derived from [8]. In the Figure (1-1), geometry and boundary conditions have been presented. As it can be seen, the inlet condition is velocity constant and outlet condition is pressure constant. H is the height

of the plate. In Figure (1-2), one snap shot of flow around the plate is depicted. This picture shows the interaction between the vapor phases and velocity field.

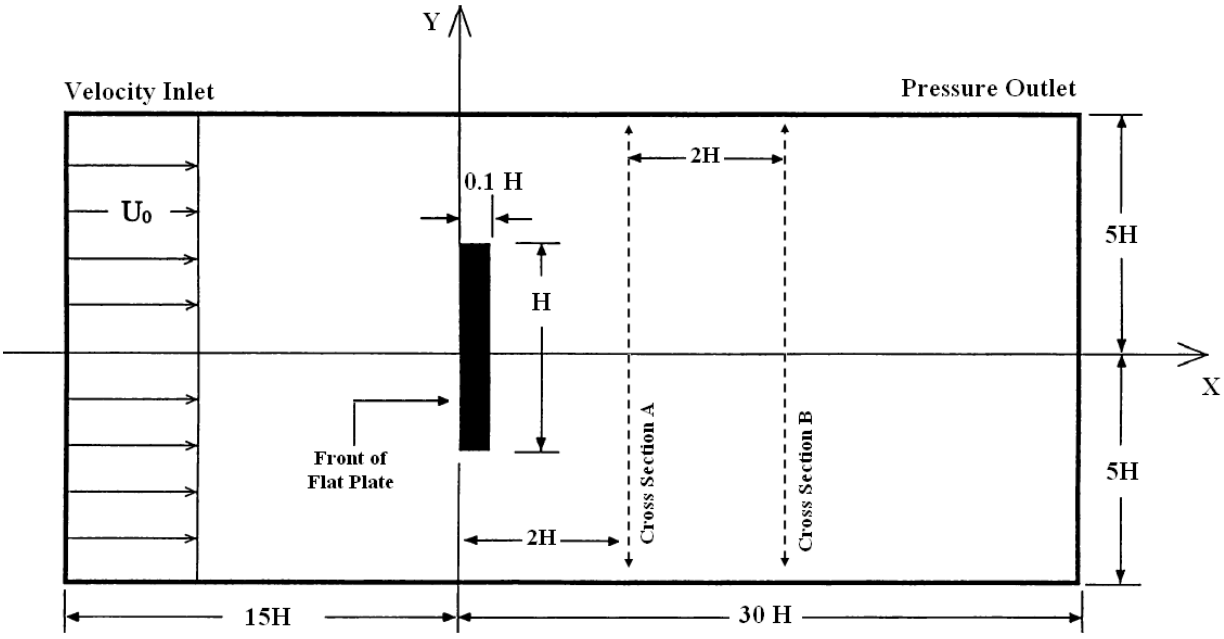


Figure (1-1) – Geometry and boundary conditions for simulation cavitation in 2d flat plate

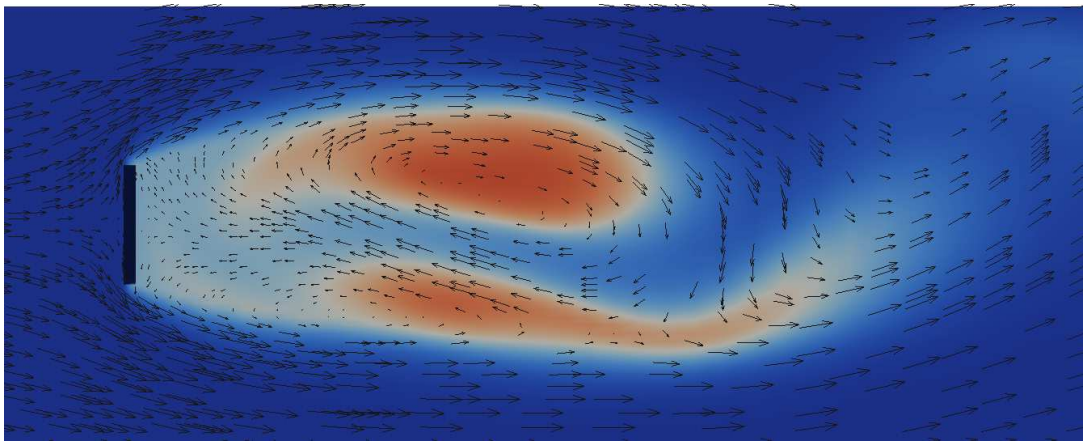


Figure (1-2) – one snapshot of cavitation and velocity vectors around the flat plate

To validate the current simulation with experimental data, in Figure (1-3), variations of drag coefficient by cavitation number is presented. As it can be seen, the comparison shows the accuracy of the performed simulation. To obtain the drag coefficients, openFoam library has been used. More details about post processing and data gathering have been provided in section (2.6) of this report.

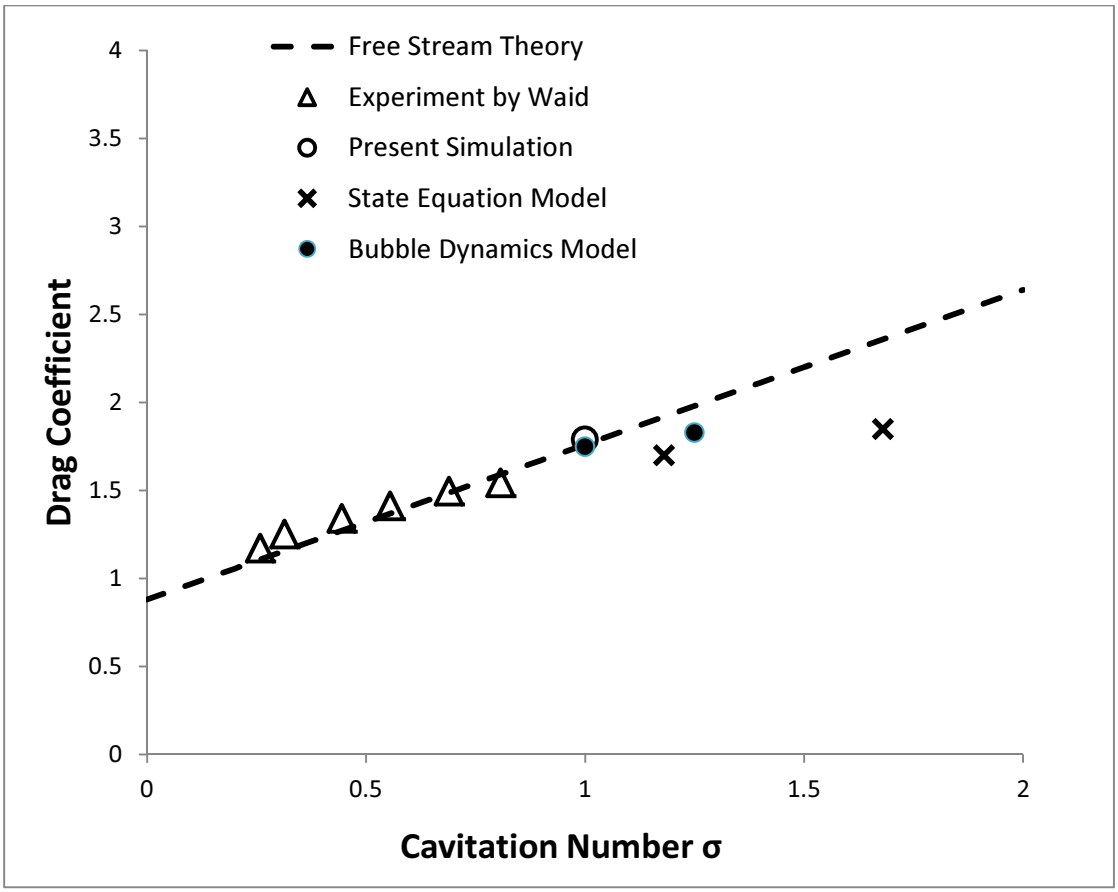


Figure (1-3) – Average drag coefficient of the 2d flat plate for cavitation number equal to one, Experiments [8]

2. Second Section: PANS

2.1 Introduction

Different turbulence models have different levels of accuracy in predicting Reynolds Stress Tensors depending on their time or space turbulence spectrum cut off size. However, there are usually limitations in selecting turbulence models based on the computational utilities, or in simple words affordable computational cost. Among the different turbulence models categories, the following models are more famous and have been used wider both in academic and industrial applications:

- RANS (Reynolds Averaged Navier Stokes)
- LES (Large Eddy Simulation)
- DES (Detached Eddy Simulation)
- DNS (Direct Numerical Simulation) – less used in industry because of huge amount of computational cost
- Hybrid method: combining the above mentioned turbulence models to get more efficient models, e.g. PANS

There are a lot of papers describing these models and their applications which one can easily find more information about these models. Generally speaking, it is hard to say which one of these models is more appropriate than the others for a specified case.

In the following, PANS turbulence model has been described, and then added to OpenFoam Turbulence Library. Finally, for well-known benchmark (flow over a square cylinder) numerical results of this model has been compared with other available turbulence models in OpenFoam.

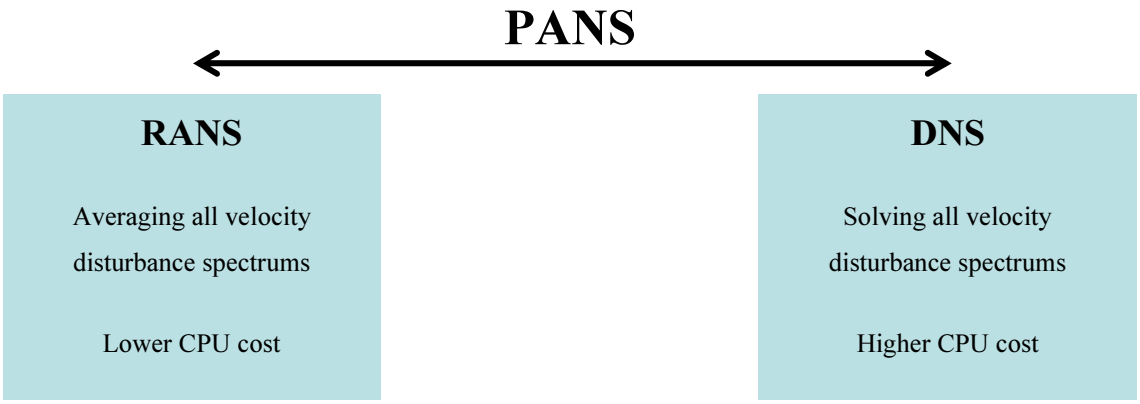
2.2 Background

RANS turbulence models use averaged velocity as the velocity appears in Navier-Stokes equations. This averaged velocity is calculated by averaging over all velocity disturbance spectrums in cut-off size (grid size). Although this approach will lead to an increase in speed of calculation, because of averaging all velocity disturbance (which some of them can have important energy content) it will cause in a lack of accuracy.

Another option would be to use DNS. This approach considers all of the velocity disturbance spectrums during calculation of turbulence stress tensor. Therefore, this model will guarantee a higher precision in solution. The main disadvantage of DNS is its CPU cost. Because in solving

procedure, all of the velocity disturbance spectrums have been considered (which some of them may be not so important) the computational cost of this approach is very high, and is the major barrier (currently!) in its development.

PANS stands for 'Partially Averaged Navier Stockes", and the idea of this method is to average some portion of velocity disturbance spectrums. Therefore, it would be placed between RANS and DNS.



It should be mentioned that the part of velocity disturbance spectrums that is averaged is called unresolved part because we do not solve it directly. Effects of unresolved part are considered by modeling, i.e. the turbulence model will handle that!

So, Partially Averaged Navier-Stokes (PANS) turbulence method provides a closure model for any degree of velocity filtering - ranging from completely resolved Direct Numerical Simulation (DNS) to completely averaged Reynolds Averaged Navier-Stokes (RANS) method. Preliminary investigations of PANS show promising results but there still exist computational and physical issues that must be addressed.

2.3 Theory

The PANS bridging method [2] provides a smooth transition from DNS to RANS based upon a user specified filter parameter. The flow field is decomposed into resolved and residual terms (unresolved) as opposed to the mean and fluctuating terms of RANS methodology. It is expected that a PANS simulation can be more accurate as key fluctuations are considered in its resolved part of the flow. The difference between PANS and LES methodologies is that PANS is

purposed for resolving significantly lesser number of scales. The control parameters of the PANS model are resolved-to-unresolved kinetic energy and resolved-to-unresolved dissipation. The closure equations are developed in a manner similar to the RANS model equations for an arbitrary filter. Therefore, the PANS model is derived systematically from corresponding parent RANS models. In this study, the parent RANS models used for simulations are kEpsilon. So, let start from standard version of kEpsilon model [3]:

For turbulent kinetic energy K

$$\frac{\partial(\rho_m k)}{\partial t}+\frac{\partial(\rho_m u_i k)}{\partial x_i}=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right]+P_k-\rho\varepsilon \tag{2-1}$$

For dissipation ε

$$\frac{\partial(\rho_m \varepsilon)}{\partial t}+\frac{\partial(\rho_m u_i \varepsilon)}{\partial x_i}=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\left(P_k+C_{3\varepsilon}P_b\right)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon \tag{2-2}$$

Turbulent viscosity is modeled as:

$$\mu_t=\rho C_\mu\frac{k^2}{\varepsilon} \tag{2-3}$$

Production of k:

$$p=\mu_t S^2 \tag{2-4}$$

Model Constants:

$$C_{1\varepsilon}=1.44, C_{2\varepsilon}=1.92, C_{3\varepsilon}=-0.33, C_\mu=0.09, \sigma_k=1.0, \sigma_\varepsilon=1.3 \tag{2-5}$$

By decomposing the velocity field into the resolved and unresolved parts, and also by introducing fK, and fEpsilon as the ratio of unresolved to resolved values, these equations can be mapped into the PANS model. Few assumptions should be considered in order to simplify these equations which have been discussed in literatures [4, 5].

The final equations governing PANS turbulence model are as follows (remember for parent RANS kEpsilon):

$$\frac{\partial(\rho_m k_u)}{\partial t}+\frac{\partial(\rho_m u_i k_u)}{\partial x_i}=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_u}{\sigma_{ku}}\right)\frac{\partial k_u}{\partial x_i}\right]+P_u-\rho\varepsilon_u \tag{2-6}$$

$$\frac{\partial(\rho_m \varepsilon_u)}{\partial t} + \frac{\partial(\rho_m u_i \varepsilon_u)}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_u}{\sigma_{\varepsilon u}}\right)\frac{\partial \varepsilon_u}{\partial x_i}\right] + f_k\left(C_{1\varepsilon}\frac{P_u \varepsilon_u}{k_u} - C^*_{\varepsilon 2}\rho\frac{\varepsilon_u^{\,2}}{k_u}\right) + S_\varepsilon \qquad (2\text{-}7)$$

$$\mu_{ut} = \rho C_\mu \frac{k_u^{\,2}}{\varepsilon_u} \qquad (2\text{-}8)$$

$$f_k = \frac{K_u}{K}, f_\varepsilon = \frac{\varepsilon_u}{\varepsilon} \qquad (2\text{-}9)$$

$$C^*_{\varepsilon 2} = C_{\varepsilon 1} + \frac{f_k}{f_\varepsilon}(C_{\varepsilon 2} - C_{\varepsilon 1}), \quad \sigma_u = \sigma\frac{f_k^2}{f_\varepsilon} \qquad (2\text{-}10)$$

As you can see, the shape of the equations are the same, and therefore relatively easy modification would be required to create this new turbulence model from the already exist kEpsilon model in OpenFoam.

2.4 Implementation into OpenFoam2.2x

Here is the procedure to create PANS turbulence model from original kEpsilon model in OF22x:

1- Open a new terminal
2- Load openfoam
3- Copy kEpsilon turbulence model to your directory
4- Rename the folder and its files (kEpsilon.C and kEpsilon.H) to kEpsilonPANS
5- Replace kEpsilon with kEpsilonPANS in .C and .H files
6- Go to Make folder, and then into the files
7- Replace kEpsilon with kEpsilonPANS, and also libkEpsilon with libkEpsilonPANS
8- Complete description of these procedures are presented in the course, and at the section related to adding a new turbulence model. From now, PANS related modifications have been presented in more details:

2.4.1 kEpsilonPANS.C

- It is necessary to read some information from the input regarding the PANS coefficients (RASproperties file, and in the kEpsilonPANS dictionary). So, in the Constructors part of kEpsilonPANS.C, and between definitions of sigmaEps_ and k_, define the following parameters: fEpsilon, and fK

```
fEpsilon_
(
    dimensioned<scalar>::lookupOrAddToDict
```

```
        (
            "fEpsilon",
            coeffDict_,
            1.0
        )
    ),
    fK_
    (
        dimensioned<scalar>::lookupOrAddToDict
        (
            "fK",
            coeffDict_,
            0.2
        )
    ),
```

As you may say in these definitions, default values (1.0, 0.2) have been considered. So, if the user does not define these parameters, these values would be considered.

- Then between definitions of epsilon_ and nut_, define the fields of kU_ and epsilonU_

```
    kU_
    (
        IOobject
        (
            "kU",
            runTime_.timeName(),
            mesh_,
            IOobject::NO_READ,
            IOobject::AUTO_WRITE
        ),
        autoCreateK("kU", mesh_)
    ),
    epsilonU_
    (
        IOobject
        (
            "epsilonU",
            runTime_.timeName(),
            mesh_,
            IOobject::NO_READ,
            IOobject::AUTO_WRITE
        ),
        autoCreateEpsilon("epsilonU", mesh_)
    ),
```

These types of definitions will bring the necessity of having related files in time folder.

- After printCoeffs() add the following command. So you can be sure during simulation that an appropriate turbulence model has been called.

```
Info << "Defining kEpsilonPANS model" << endl;
```

- In the kEpsilonPANS::read () section add the following commands. They will define where and in which dictionary OF should look for values of fEpsilon_ and fK_ parameters.

```
fEpsilon_.readIfPresent(coeffDict());
fK_.readIfPresent(coeffDict());
```

- In the kEpsilonPANS::correct section, do the following:
  - Add definitions of C2U parameters:

```
const dimensionedScalar C2U   = C1_ + (fK_/fEpsilon_) * (C2_ - C1_);
```

  - Because we are going to solve epsilonU and kU, replace epsilon and k with epsilonU and kU in the section related to creating equations.

```
    // Update unresolved epsilon and G at the wall
    epsilonU_.boundaryField().updateCoeffs();

    // Unresolved Dissipation equation
    tmp<fvScalarMatrix> epsUEqn
    (
        fvm::ddt(epsilonU_)
      + fvm::div(phi_, epsilonU_)
      - fvm::laplacian(DepsilonUEff(), epsilonU_)
     ==
        C1_*G*(epsilonU_)/(kU_)
      + fvm::Sp(C1_*(1-fK_)*(epsilonU_)/(kU_),
epsilonU_)
      - fvm::Sp(C2U*(epsilonU_)/(kU_), epsilonU_)
    );

    epsUEqn().relax();
    epsUEqn().boundaryManipulate(epsilonU_.boundaryFiel
d());
    solve(epsUEqn);
    bound(epsilonU_, fEpsilon_ * epsilonMin_);
```

```
 // Unresolved Turbulent kinetic energy equation
    tmp<fvScalarMatrix> kUEqn
    (
        fvm::ddt(kU_)
      + fvm::div(phi_, kU_)
      - fvm::laplacian(DkUEff(), kU_)
     ==
        G
```

```
    - fvm::Sp(epsilonU_*fK_/kU_, kU_)
);

kUEqn().relax();
solve(kUEqn);
bound(kU_, fK_ * kMin_);
```

- Calculate k, and epsilon based on the kU, and epsilon

```
// Calculation of Turbulent kinetic energy and Dissipation rate
 k_ = kU_/fK_;
 epsilon_ = (epsilonU_)/(fEpsilon_);

 // Re-calculate viscosity
 nut_ = Cmu_*sqr(kU_)/epsilonU_;
```

2.4.2 kEpsilonPANS.H

- Add definition of fEpsilon, and fK to protected data:model coefficients

```
        dimensionedScalar fEpsilon_;
        dimensionedScalar fK_;
```

- Add definition of kU, and epsilonU to protected data:Fields

```
        volScalarField kU_;
        volScalarField epsilonU_;
```

- In the Member Function, add definition of kU and epsilonU fields

```
    //- Return the unresolved turbulence kinetic energy
    virtual tmp<volScalarField> kU() const
    {
        return kU_;
    }
    //- Return the unresolved turbulence kinetic energy dissipation rate
    virtual tmp<volScalarField> epsilonU() const
    {
        return epsilonU_;
    }
```

- Define DkUEff, and DepsilonUEff fields

```
    //- Return the effective diffusivity for unresolved k
    tmp<volScalarField> DkUEff() const
    {
```

```
        return tmp<volScalarField>
        (
            new volScalarField("DkUEff", nut_/(fK_*fK_/fEpsilon_) + nu())
        );
    }
    //- Return the effective diffusivity for unresolved epsilon
    tmp<volScalarField> DepsilonUEff() const
    {
        return tmp<volScalarField>
        (
            new volScalarField("DepsilonUEff", nut_/(fK_*fK_*sigmaEps_/fEpsilon_) + nu())
        );
    }
```

2.5 Results

To investigate PANS turbulence model merits comparing to other turbulence models, flow around a square cylinder has been simulated, Figure (2-1). The boundary conditions and geometry of this case are as follow [5]:

- Inlet velocity is 0.54 m/s with 2% turbulence fluctuation
- Reynolds number Re = 22 000
- Size of the square cylinder is 0.04 m wide and 0.392 m high
- The cylinder is located in a tunnel with a width of 14D = 0.56 m

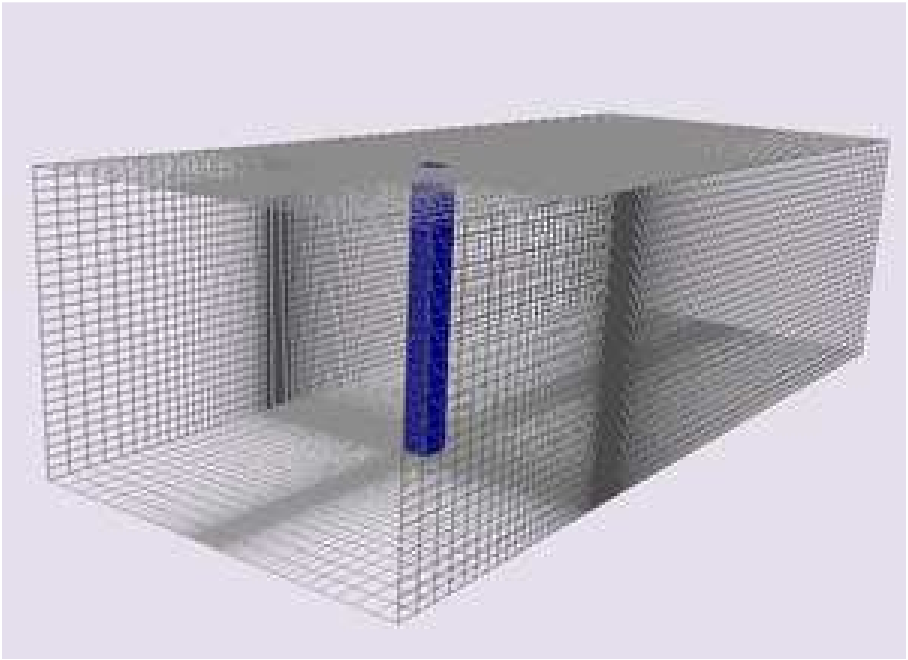


Figure (2-1) –Square cylinder mesh structure

To compare PANS turbulence model with other turbulence models, OEEVM has been selected from LES turbulence family, and from RANS turbulence family, kEpsilon has been selected. Drag coefficients and Strouhal number for these three different turbulence models have been compared with experimental data, Table (2-1). Results show that PANS results are very promising and are in very good agreement with experimental data. Comparing PANS, and its RANS parent turbulence model kEpsilon shows that by small code developing, it would be possible to increase the accuracy of results significantly. However, more efforts especially in the area of CPU cost should be performed to provide appropriate comparison tools.

Next possible steps to improve this work would be:

- Use two-stage PANS model or dynamic version of PANS
- Compare the performance of PANS in higher Reynolds number
- Try to implement PANS in other RANS turbulence models, e. kOmega

Table (2-1) – Comparing different turbulence models results for flow around the square cylinder, Re=22e3, inlet velocity 0.54 m/s with 2% turbulence fluctuation

Turbulence model	Cd	Cd Error (%)	Strouhal number	St. Error (%)
kEpsilon	1.67	-20.5	0.1348	2.12
OEEVM (LES)	2.05	-2.4	0.1333	1
PANS (fK=0.2, fEpsilon=1.0)	2.11	0.5	0.134	1.5
Reference Value (Exp.)	2.1	-----	0.132	-----

2.6 Post processing

Analyzing the obtained numerical simulation and comparing them with experimental data could be very time consuming task. To reduce the difficulty of this task, several libraries have been added to the OpenFoam which using them during simulation for data gathering can increase the simplicity of post processing analyses. In the following, one script to collect data at probe

locations, to calculate drag and lift forces, and to calculate mean fields for pressure, velocity, turbulence intensities, and etc. has been described.

```
functions
{
    probes
    {
        type            probes;
        functionObjectLibs ("libsampling.so");
        enabled         true;
        outputControl   timeStep;
        outputInterval  1;
        probeLocations
        (
            ( 0.05   0.0   0.002 )
            ( 0.05   0.01  0.002 )
        );

        fields
        (
            p
        );
    }

    forces
    {
        type        forceCoeffs;
        functionObjectLibs ( "libforces.so" );
        outputControl timeStep;
        outputInterval 1;
        patches
        (
            walls
        );
                    directForceDensity no;
        pName       p;
        UName       U;
        rhoName     rhoInf;
        rhoInf      994.5;
        CofR        ( 0 0 0 );
        liftDir     ( 0 1 0 );
        dragDir     ( 1 0 0 );
        pitchAxis   ( 0 0 1 );
        magUInf     0.54;
        lRef        0.04;
        Aref        0.0157;
        Aref1       0.004;
        rhoRef      994.5;
    }

    fieldAverage1
    {
        type            fieldAverage;
```

```
        functionObjectLibs ("libfieldFunctionObjects.so");
        enabled         true;
        outputControl   outputTime;
        fields
        (
           U
           {
              mean       on;
              prime2Mean  on;
              base       time;
           }

           p
           {
              mean       on;
              prime2Mean  on;
              base       time;
           }
        );
     }
}
```

As it can be seen from the above code commands, this script is called function which here has three sub functions: probes, forces, fieldAverage1

In the "probes", one has to clarify the locations that he or she wants to collect data by "probeLocations" dictionary. Then in the "fields" dictionary, the fields (pressure, velocity, temperature, turbulence,…) that have to be collected should be specified.

```
    probes
    {
        type            probes;                          //defining type of dictionary
        functionObjectLibs ("libsampling.so");           //defining the related library
        enabled         true;                            //
        outputControl   timeStep;                        //
        outputInterval  1;                               //
        probeLocations                                   //
        (                                                //
           ( 0.05   0.0   0.002 )                        //probe locations
           ( 0.05   0.01  0.002 )                        //
        );                                               //
                                                         //
        fields                                           //
        (                                                //
           p                                             //field to be collected
        );                                               //
    }
```

In the "forces" dictionary, it is possible to define calculation of forces (drag & lift) on specific patches.

```
forces
{
    type        forceCoeffs;                    //defining type of dictionary
    functionObjectLibs ( "libforces.so" );      //defining the related library
    outputControl timeStep;                     //
    outputInterval 1;                           //
    patches                                     //
    (                                           //patch that you want to calculate
        walls                                   //forces on them
    );                                          //probe locations
   directForceDensity no;                       //
                                                //
    pName       p;                              //defining the pressure field
    UName       U;                              // defining the velocity field
                                                // remember that "p" and "U" may be
                                                // differ for different solvers
    rhoName     rhoInf;                         // defining the reference density value
    rhoInf      994.5;                          //
    CofR        ( 0 0 0 );                      // defining center of rotation
    liftDir     ( 0 1 0 );                      // lift direction
    dragDir     ( 1 0 0 );                      //drag direction
    pitchAxis   ( 0 0 1 );                      // third direction
    magUInf     0.54;                           // reference velocity
    lRef        0.04;                           // reference length
    Aref        0.0157;                         // reference area for drag
    Aref1       0.004;                          // reference area for lift
    rhoRef      994.5;                          // reference density
}                                               //
```

In the "fieldAverage" dictionary, it is possible to define calculation of averaging over specified fields. This averaging is very useful tool since for example in calculation of separation point over a circular cylinder one needs the averaged pressure distribution over circle.

```
fieldAverage1
{
    type            fieldAverage;                           //defining type of dictionary
    functionObjectLibs ("libfieldFunctionObjects.so");      //defining the related library
    enabled         true;                                   //
    outputControl   outputTime;                             //
    fields                                                  //defining fields to be averaged
    (                                                       //
        U                                                   //
        {                                                   //
            mean        on;                                 // activating which type of
            prime2Mean  on;                                 // averaging should be done
            base        time;                               //
        }                                                   //
                                                            //
        p                                                   //
        {
            mean        on;
```

```
            prime2Mean  on;
            base        time;
        }
    );
}
```

3. References

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