How to implement an application

Example: Electric conduction in a rod surrounded by air

Governing equations

Maxwell's equation:

$$\nabla \times E = 0 \tag{1}$$

where E is the electric field strength.

$$\nabla \cdot B = 0 \tag{2}$$

where B is the magnetic flux density.

$$\nabla \times H = J \tag{3}$$

where H is the magnetic field strength and J is current density.

Charge continuity:

$$\nabla \cdot J = 0 \tag{4}$$

Ohm's law:

$$J = \sigma E \tag{5}$$

where σ is the electric conductivity.
Constitutive law:

$$B = \mu_0 H \tag{6}$$

where μ_0 is the magnetic permeability of vacuum.

Combining Equations (1)-(6) and assuming Coulomb gauge condition ($\nabla \cdot A = 0$) leads to a Poisson equation for the magnetic potential and a Laplace equation for the electric potential...

Governing equations in OpenFoam

Magnetic potential:

$$\nabla^2 A = \mu_0 \sigma (\nabla \phi) \tag{7}$$

OpenFOAM representation:

```
solve
    (
    fvm::laplacian(A) ==
    sigma*muMag*(fvc::grad(ElPot))
    );
```

Electric potential:

$$\nabla \cdot [\sigma(\nabla \phi)] = 0 \tag{8}$$

OpenFOAM representation:

```
solve
    (
    fvm::laplacian(sigma,ElPot)
    );
```

We see that A depends on ϕ, but not vice-versa.

Implementing the rodFoam solver

Create the basic files in your user directory:

```
cd $WM_PROJECT_USER_DIR
mkdir -p applications/solvers/electromagnetics/rodFoam
cd applications/solvers/electromagnetics/rodFoam
foamNewSource App rodFoam
tree
```

We see:

```
.
|-- Make
|   |-- files
|   `-- options
`-- rodFoam.C
```

Make sure that the binary file ends up in your user directory:

```
sed -i s/FOAM_APPBIN/FOAM_USER_APPBIN/g Make/files
```

Add a few lines to rodFoam.C

We need a mesh to discretize our equations on, and we need to initialize properties and fields.
After `#include "createTime.H"`, add:

```
#include "createMesh.H"    #In the OpenFOAM installation
#include "createFields.H"  #Must be implemented - see next slides
```

Continue adding (after the above), our equations:

```
    solve ( fvm::laplacian(sigma, ElPot) );
    solve ( fvm::laplacian(A)==sigma*muMag*(fvc::grad(ElPot)) );
```

Add some additional things that can be computed when we know `A` and `ElPot`:

```
    B = fvc::curl(A);
    Je = -sigma*(fvc::grad(ElPot));
```

We also want to write out the results to a new time directory.
Continue adding:

```
    runTime++;
    sigma.write();
    ElPot.write();
    A.write();
    B.write();
    Je.write();
```

The createFields.H file (1/6)

We need to construct and initialize `muMag`, `sigma`, `Elpot`, `A`, `B`, and `Je`.
Edit the `createFields.H` file.

Read `muMag` from a dictionary:

```
Info<< "Reading physicalProperties\n" << endl;
IOdictionary physicalProperties
(
    IOobject
    (
        "physicalProperties",
        runTime.constant(),
        mesh,
        IOobject::MUST_READ,
        IOobject::NO_WRITE
    )
);
dimensionedScalar muMag
(
    physicalProperties.lookup("muMag")
);
```

The createFields.H file (2/6)

Construct `volScalarField sigma`:

```
Info<< "Reading field sigma\n" << endl;
volScalarField sigma
(
    IOobject
    (
        "sigma",
        runTime.timeName(),
        mesh,
        IOobject::MUST_READ,
        IOobject::AUTO_WRITE
    ),
    mesh
);
```

The createFields.H file (3/6)

Construct `volScalarField` `Elpot`:

```
volScalarField ElPot
(
    IOobject
    (
        "ElPot",
        runTime.timeName(),
        mesh,
        IOobject::MUST_READ,
        IOobject::AUTO_WRITE
    ),
    mesh
);
```

The createFields.H file (4/6)

Construct `volVectorField A`:

```
Info<< "Reading field A\n" << endl;
volVectorField A
(
    IOobject
    (
        "A",
        runTime.timeName(),
        mesh,
        IOobject::MUST_READ,
        IOobject::AUTO_WRITE
    ),
    mesh
);
```

The createFields.H file (5/6)

Construct and initialize `volVectorField B`:

```
Info << "Calculating magnetic field B \n" << endl;
volVectorField B
(
    IOobject
    (
        "B",
        runTime.timeName(),
        mesh,
        IOobject::NO_READ,
        IOobject::AUTO_WRITE
    ),
    fvc::curl(A)
);
```

The createFields.H file (6/6)

Construct and initialize `volVectorField Je`:

```
volVectorField  Je
(
    IOobject
    (
        "Je",
        runTime.timeName(),
        mesh,
        IOobject::NO_READ,
        IOobject::AUTO_WRITE
    ),
    -sigma*(fvc::grad(ElPot))
);
```

Compile the solver

We have implemented a solver, which is compiled by:

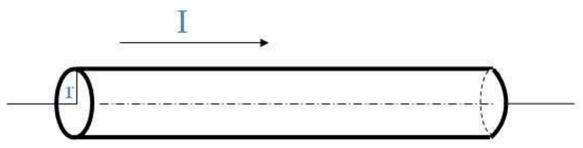
```
wmake
```

If successful, the output should end something like:

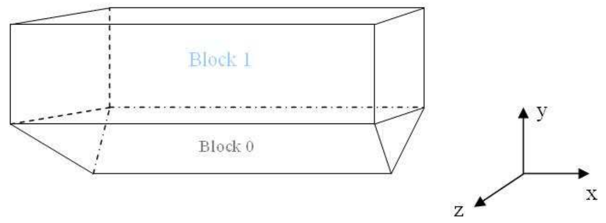
```
-o /chalmers/users/hani/OpenFOAM/hani-2.1.x/platforms/linux64GccDPOpt/bin/rodFoam
```

We now need a case to use the solver on. It is provided to you (`rodFoamCase.tgz`), since it is too much to describe in slides.

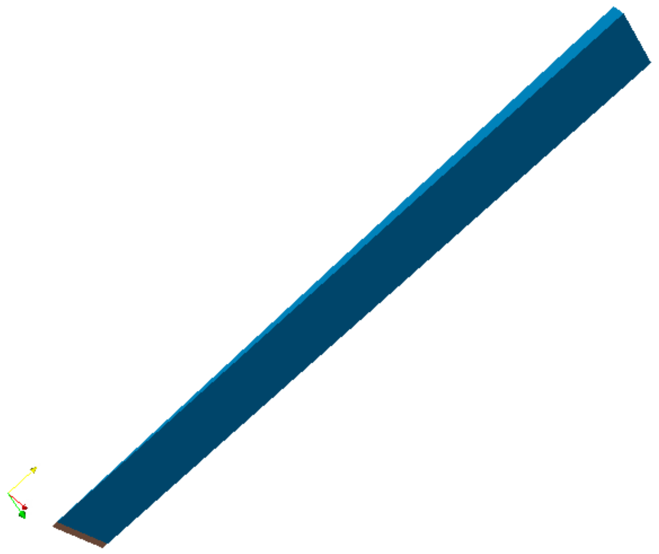
Geometry and mesh, the rodFoamCase case



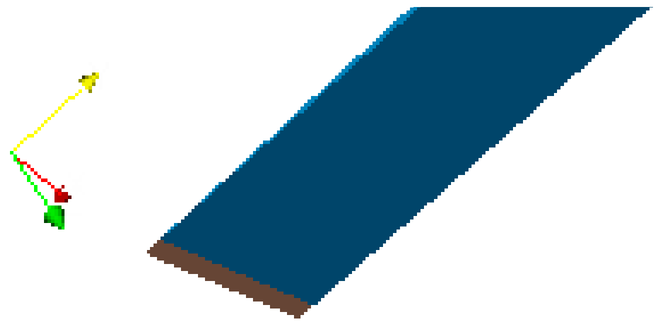
Electric rod.



Computational domain



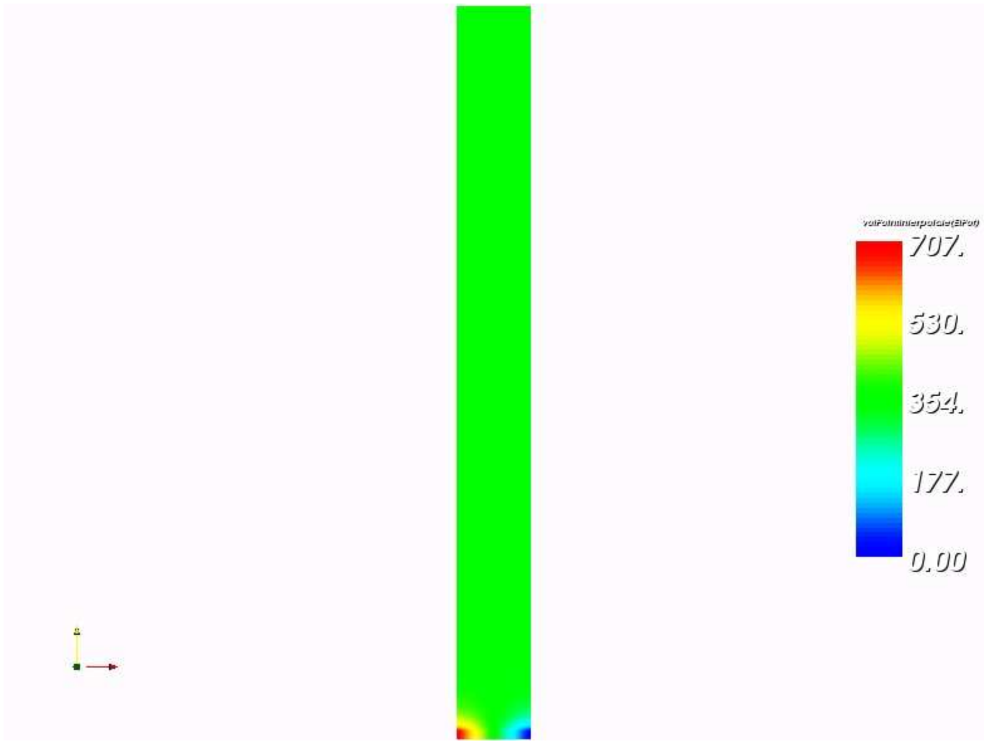
In paraFoam
A 2D axi-symmetric case, with a wedge mesh



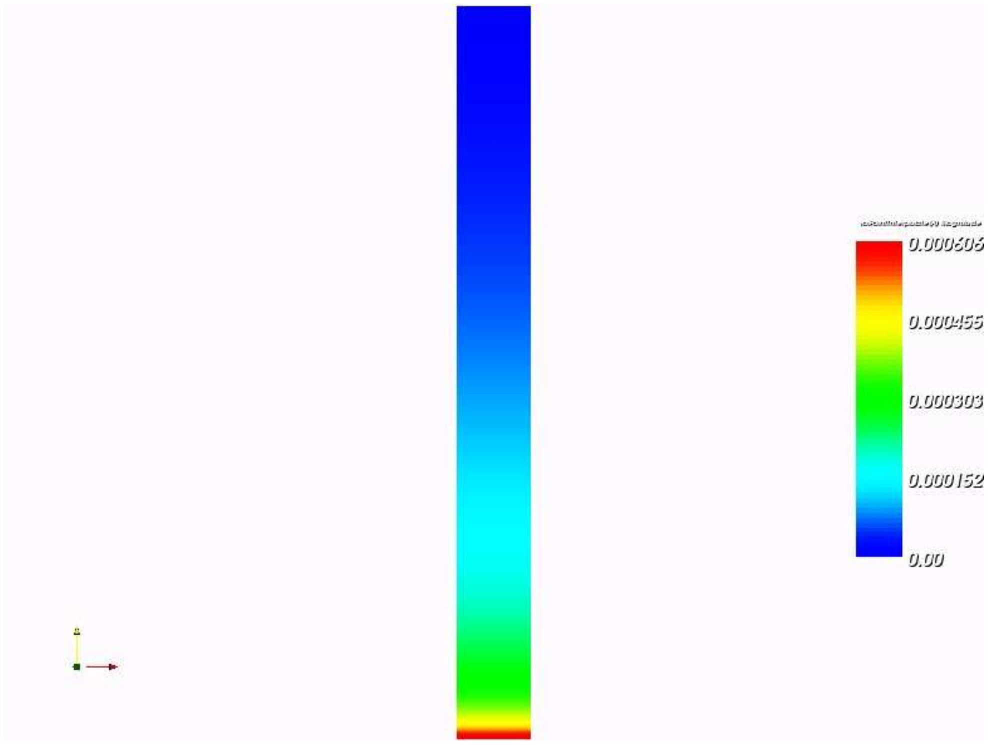
Zoom-up of rod.
For 2D wedge, the symmetry axis must be aligned with the x-axis, the wedge angle should be 5 degrees, with half on each side of the $z = 0$ plane.

Run and view the results in paraFoam

```
./Allrun 2>&1 | tee log_Allrun
```

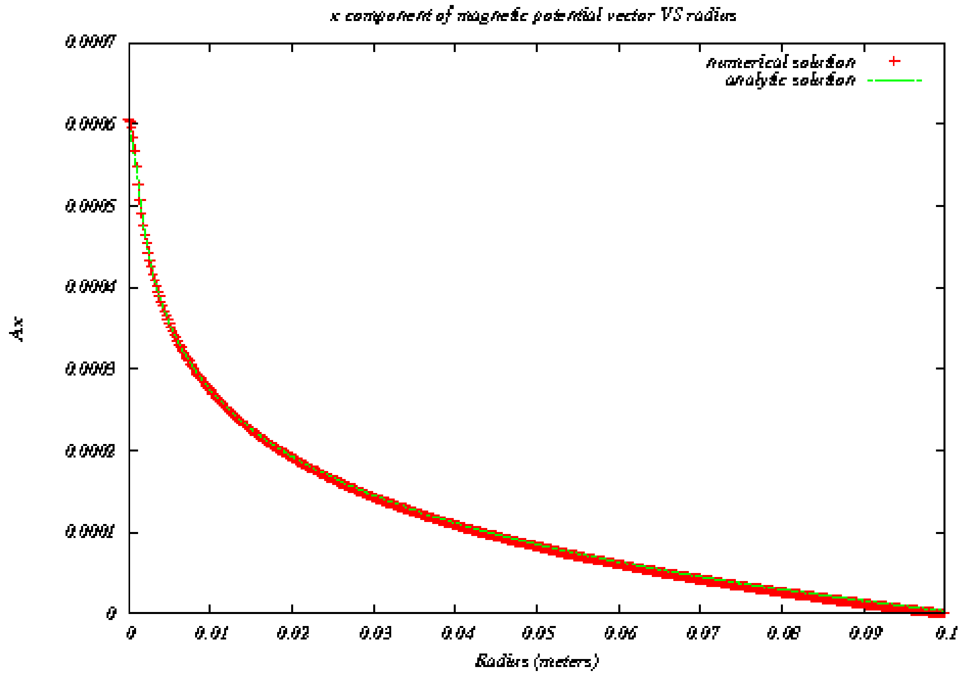


Electric potential (ϕ)

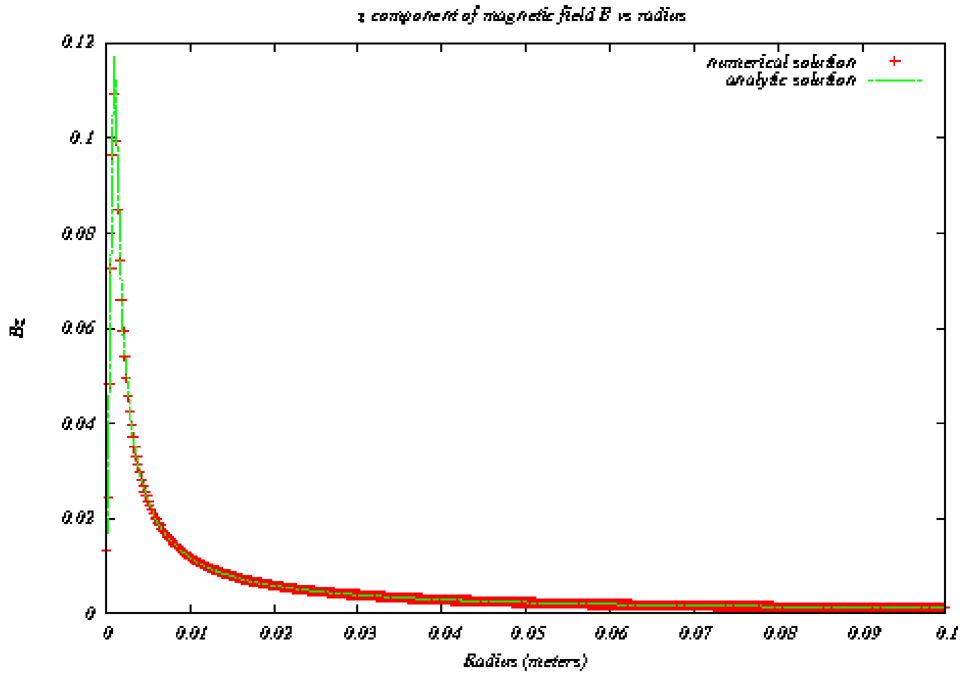


Magnitude of magnetic potential vector (A)

Validation



x-component of magnetic potential vector A vs radius of the domain.



z-component of the magnetic field B vs radius of the domain

Boundary and initial conditions

- We solve for the magnetic potential `A` (A) and the electric potential `ElPot` (ϕ), so we need boundary conditions:

	block 0, sides	block 1, sides	block1, top
A	$\nabla A = 0$	$\nabla A = 0$	$A = 0$
ϕ	$\phi_{left} = 707, \phi_{right} = 0$	$\nabla \phi = 0$	$\nabla \phi = 0$

  and we initialize the fields to zero.

- The internal field of the electric conductivity sigma (σ) is nonuniform:

$$\sigma = \begin{cases} 2700 & \text{if } x < R \text{ where R -radius of the block 1} \\ 1e-5 & \text{otherwise} \end{cases}$$

  so we use a `volScalarField` and `setFields` to set the internal field.

- The magnetic permeability of vacuum (μ_0) is read from the `constant/physicalProperties` dictionary.

Validation of components of A and B using Gnuplot

- Our numerical results should be validated with analytical results
- For this we need to extract the components:

```
foamCalc components A
foamCalc components B
```

- The results are validated with the analytical solution using Gnuplot:

```
gnuplot rodComparisonAxBz.plt
```

- Visualize using:

```
gv rodAxVSy.ps
gv rodBzVSy.ps
```

Analytic solution

- Analytic solution for x component of magnetic potential vector A

$$A_x = \begin{cases} A_x(0) - \frac{\mu_0 J x^2}{4} & \text{if } r < R, \\ A_x(0) - \frac{\mu_0 J R^2}{2}[0.5 + ln(r/R)] & \text{otherwise} \end{cases}$$

  where $A_x(0) = 0.000606129$, $J = 19.086e + 7$ is the current density and R is the radius of the electric rod.

- Analytic solution for z component of magnetic field B

$$B_z = \begin{cases} \frac{\mu_0 J x}{2} & \text{if } r < R, \\ \frac{\mu_0 J R^2}{2r} & \text{otherwise} \end{cases}$$

  where $J = 19.086e+7$ is the current density and R is the radius of the electric rod.

- Have a look in `rodComparisonAxBz.plt` to see how to plot a function in Gnuplot.

How to modify an existing application

- The applications are located in the `$WM_PROJECT_DIR/applications` directory (equivalent to `$FOAM_APP`. Go there using alias `app`).
- Copy an application that is similar to what you would like to do and modify it for your purposes. In this case we will make our own copy of the `icoFoam` solver and put it in our `$WM_PROJECT_USER_DIR` with the same file structure as in the OpenFOAM installation:

```
foam
cp -r --parents applications/solvers/incompressible/icoFoam $WM_PROJECT_USER_DIR
cd $WM_PROJECT_USER_DIR/applications/solvers/incompressible
mv icoFoam passiveScalarFoam
cd passiveScalarFoam
wclean
mv icoFoam.C passiveScalarFoam.C
```

- Modify `Make/files` to:

```
passiveScalarFoam.C
EXE = $(FOAM_USER_APPBIN)/passiveScalarFoam
```

- Compile with `wmake` in the `passiveScalarFoam` directory. `rehash` if necessary.
- Test that it works on the `cavity` case...

Test on cavity case

We will quickly visit the run directory to test...

```
pushd $FOAM_RUN #so that we can easily go back to the current directory
rm -r cavity
cp -r $FOAM_TUTORIALS/incompressible/icoFoam/cavity .
blockMesh -case cavity
passiveScalarFoam -case cavity
```

After checking that it worked, go back to the `passiveScalarFoam` directory:

```
popd #brings you back to the directory where you typed the pushd command
```

You can also do everything 'remotely':

```
rm -r $FOAM_RUN/cavity
cp -r $FOAM_TUTORIALS/incompressible/icoFoam/cavity $FOAM_RUN
blockMesh -case $FOAM_RUN/cavity
passiveScalarFoam -case $FOAM_RUN/cavity
```

Add a passive scalar transport equation (1/3)

- Let's add, to `passiveScalarFoam`, the passive scalar transport equation

$$\frac{\partial s}{\partial t} + \nabla \cdot (\mathbf{u}\, s) = 0$$

- We must modify the solver:
  - Create `volumeScalarField s` (do the same as for `p` in `createFields.H`, since both are scalar fields)
  - Add the equation `solve(fvm::ddt(s) + fvm::div(phi, s));` before `runTime.write();` in `passiveScalarFoam.C`.
  - Compile `passiveScalarFoam` using `wmake`
- We must modify the case - next slide ...

Add a passive scalar transport equation (2/3)

- We must modify the case:
  - Use the `icoFoam/cavity` case as a base:
    ```
    run
    cp -r $FOAM_TUTORIALS/incompressible/icoFoam/cavity passiveCavity
    cd passiveCavity
    ```
  - Copy the `0/p` file to `0/s` and modify `p` to `s` in that file. Choose appropriate dimensions for the scalar field (not important now).
  - In `fvSchemes`, add (if you don't, it will complain):
    ```
        div(phi,s)        Gauss linearUpwind Gauss;
    ```
  - In `fvSolution`, copy the solution settings from `U` (since the equations for velocity and `s` are similar), and just change `U` to `s`. (if you use `PCG`, as for `p`, it will complain - try it yourself!)
- We must initialize and run the case - next slide ...

Add a passive scalar transport equation (3/3)

- We must initialize `s`:
  - `cp $FOAM_TUTORIALS/multiphase/interFoam/laminar/damBreak/system/setFieldsDict system`
  - Set `defaultFieldValues`:
    `volScalarFieldValue s 0`
  - Modify the bounding box to:
    `box (0.03 0.03 -1) (0.06 0.06 1);`
  - Set `fieldValues`:
    `volScalarFieldValue s 1`
- Run the case:
  ```
  blockMesh
  setFields
  passiveScalarFoam >& log
  ```
  `paraFoam` - mark `s` in Volume Fields, color by `s` (cell value) and run an animation.
- You can see that although there is no diffusion term in the equation, there is massive diffusion in the results. This is due to mesh resolution, numerical scheme etc. The `interfoam` solver has a special treatment to reduce this kind of diffusion.

Add particles to the interFoam/damBreak case

Add the solidParticleCloud class to the interFoam/damBreak tutorial by doing the following, and you will have some nice animation to view.

Copy the interFoam solver, clean up, re-name and compile:

```
cd $WM_PROJECT_DIR
cp -r --parents applications/solvers/multiphase/interFoam $WM_PROJECT_USER_DIR
cd $WM_PROJECT_USER_DIR/applications/solvers/multiphase
mv interFoam solidParticleInterFoam
cd solidParticleInterFoam
rm -r Allw* interDyMFoam LTSInterFoam MRFInterFoam porousInterFoam
wclean
rm -rf Make/linux*
mv interFoam.C solidParticleInterFoam.C
sed -i.orig s/interFoam/solidParticleInterFoam/g Make/files
sed -i s/FOAM_APPBIN/FOAM_USER_APPBIN/g Make/files
wmake
```

At this point you can check that the code still works for the damBreak tutorial.

Add particles to the interFoam/damBreak case

Now we will add functionality from the `solidParticleCloud` class.
Modify `solidParticleInterFoam.C`:

Include the class declarations of `solidParticleCloud.H`.
At the header, add:

```
#include "solidParticleCloud.H"
```

Create a solidParticleCloud object.
After `#include "setInitialDeltaT.H"`, add:

```
solidParticleCloud particles(mesh);
```

Move the particles.
Before `runTime.write();`, add:

```
particles.move(g);
```

Add particles to the interFoam/damBreak case

We need to add some libraries when we compile.
Make sure that `Make/options` has the following lines (where '. . .' is the original lines):

```
EXE_INC = \
    ... \
    -I$(LIB_SRC)/lagrangian/basic/lnInclude \
    -I$(LIB_SRC)/lagrangian/solidParticle/lnInclude

EXE_LIBS = \
    ... \
    -llagrangian \
    -lsolidParticle
```

Compile:

```
wmake
```

Add particles to the interFoam/damBreak case

We need to set up a case, based on the original `damBreak` case:

```
run
cp -r $FOAM_TUTORIALS/multiphase/interFoam/ras/damBreak solidParticleDamBreak
cd solidParticleDamBreak
```

Initialize the particles:

```
mkdir -p 0/lagrangian/defaultCloud
```

add files for diameter (`d`), positions (`positions`) and velocity (`U`)...

...and set the particle properties in `constant/particleProperties`...

Add particles to the interFoam/damBreak case

Diameter file (`0/lagrangian/defaultCloud/d`):

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.2.x                                 |
|   \\  /    A nd           | Web:      http://www.OpenFOAM.org               |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       scalarField;
    location    "0";
    object      d;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //


2
(
2.0e-3
2.0e-3
)

// ************************************************************************* //
```

Add particles to the interFoam/damBreak case

Positions file (`0/lagrangian/defaultCloud/positions`):

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.2.x                                 |
|   \\  /    A nd           | Web:      http://www.OpenFOAM.org               |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       Cloud<solidParticle>;
    location    "0";
    object      positions;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

2
(
(1e-2 0.58 0.005) 0
(2e-2 0.58 0.005) 0
)


// ************************************************************************* //
```

Add particles to the interFoam/damBreak case

Velocity file (`0/lagrangian/defaultCloud/U`):

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.2.x                                 |
|   \\  /    A nd           | Web:      http://www.OpenFOAM.org               |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       vectorField;
    location    "0";
    object      U;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //


2
(
(1.7e-1 0 0)
(1.7 0 0)
)


// ************************************************************************* //
```

Add particles to the interFoam/damBreak case

Particle properties file (`constant/particleProperties`):

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.2.x                                 |
|   \\  /    A nd           | Web:      http://www.OpenFOAM.org               |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      particleProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

rhop rhop [ 1 -3  0  0  0  0  0] 1000;
e    e    [ 0  0  0  0  0  0  0] 0.8;
mu   mu   [ 0  0  0  0  0  0  0] 0.2;

// ************************************************************************* //
```

Add particles to the interFoam/damBreak case

Run and animate using `foamToVTK` and `paraview`:

```
blockMesh
setFields
solidParticleInterFoam 2>&1 | tee log_solidParticleInterFoam
foamToVTK
paraview
```

- File/open: VTK/solidParticeDamBreak_..vtk
- File/open: VTK/lagrangian/defaultCloud/defaultCloud_..vtk
- For the solidParticleDamBreak object: Display: Opacity 0,3. Color By: alpha1 (cell values)
- For the defaultCloud object: Create box glyphs (length: 10/10/10, Scale Mode off) to visualize the particles.
- Run the animation and enjoy...